From Modular Decomposition Trees to Rooted Median Graphs

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Abstract

The modular decomposition of a symmetric map \(\delta : X \times X \to Y\) (or, equivalently, a set of symmetric binary relations, a 2-structure, or an edge-colored undirected graph) is a natural construction to capture key features of \(\delta\) in labeled trees. A map \(\delta\) is explained by a vertex-labeled rooted tree \((T,t)\) if the label \(\delta(x,y)\) coincides with the label of the last common ancestor of \(x\) and \(y\) in \(T\), i.e., if \(\delta(x,y) = t(\text{lca}(x,y))\). Only maps whose modular decomposition does not contain prime nodes, i.e., the symbolic ultrametrics, can be explained in this manner. Here we consider rooted median graphs as a generalization to (modular decomposition) trees to explain symmetric maps. We first show that every symmetric map can be explained by “extended” hypercubes and half-grids. We then derive a linear-time algorithm that stepwisely resolves prime vertices in the modular decomposition tree to obtain a rooted and labeled median graph that explains a given symmetric map \(\delta\). We argue that the resulting “tree-like” median graphs may be of use in phylogenetics as a model of evolutionary relationships.

Keywords: 2-structures; symbolic ultrametrics; modular decomposition; prime module; prime vertex replacement; median graph; algorithm; half-grid; hypercube

1 Introduction

The decomposition of an object comprising a finite point set \(X\) into its modules has been a topic of intense research for decades, starting with Tibor Gallai’s seminal work [22]. A module is a subset \(M \subseteq X\) such that the points within \(M\) cannot be distinguished from each other in terms of their relationships with points in \(X \setminus M\). Modular decompositions have been studied for graphs \([10, 11, 19, 26, 31, 47]\), labeling maps or equivalently sets of binary relations and 2-structures \([4, 14–21, 34, 35, 37]\) or sets of \(n\)-ary relations and, equivalently, hypergraphs \([5–7, 25]\). They share fundamental properties irrespective of the type of the objects that determines the nature of the pertinent relationships. In particular, the strong modules, i.e., the modules that do not with overlap with other modules, form a hierarchy and thus can be identified with the vertices of a rooted tree \(T\). This modular decomposition tree, whose leaves correspond to the point set \(X\), captures a wealth of information on the object under consideration.

Models of evolutionary relationships often start from a rooted tree \(T\) endowed with labels of vertices or edges that designate evolutionary events. A broad class of inverse problems thus arises in mathematical phylogenetics that can be phrased as follows: Given a (rooted) tree \(T\) with labels on vertices and edges and a rule to derive a map \(\delta\) on pairs (or \(k\)-tuples) of leaves, one asks (i) which maps \(\delta\) can be explained by such a labeled tree, (ii) how an explaining labeled tree \(T\) can be constructed, and (iii) to characterize the set of labeled trees \(T\) that explain a given map \(\delta\). Not surprisingly, there is a close connection to the modular decomposition.

An “event labeling” \(t\) at the inner vertices of \(T\), naturally defines \(\delta(x,y) := t(\text{lca}(x,y))\) as the label of the last common ancestor of two leaves \(x\) and \(y\). An event-labeled tree \((T,t)\) explaining \(\delta\) in this manner exists if and only if
δ is a symbolic ultrametric [4], which shares the description of a cograph [10]. The corresponding co-tree or symbolic discriminating representation, i.e., the modular decomposition tree of δ, is obtained by contracting edges in (T, t) whose endpoints share the same label [32]. In phylogenetic applications, symbolic ultrametrics describe the key concepts of orthology and paralogy, i.e., the question whether a pair of related genes descends from a speciation or a gene duplication event [32, 36, 38]. Edge weights may model distances or specific types of evolutionary events. In a pairwise compatibility graph (PCG) an edge is drawn whenever the sum of edge weights between two leaves lies within a specified interval [9, 44]. In phylogenetics, they model e.g. rare events [33]. Horizontal gene transfer is captured by Fitch graphs [23, 28–30], a subclass of directed cographs corresponding to pairs (x, y) such that an edge with non-zero weight appears along the path in T connecting lca(x, y) with the leaf y. Interpreting edge-weights as distances, and thus δ(x, y) as distance between leaves, leads to the key theorem of mathematical phylogenetics: There is a unique edge-weighted tree T if and only if δ satisfies the so-called 4-point condition [8, 50].

Phylogenetics also motivates the investigation of generalizations. While trees are an excellent model of many evolutionary systems, they are approximations and sometimes networks are a better model of reality [42]. In the case of distance-based phylogenetics, this naturally connects with theory of split-decomposable metrics [1] and their natural representations, the Buneman graphs [13, 39]. The latter form a subclass of Median graphs. Median networks, furthermore, play an important role as representations of phylogenies within populations [2, 3]. This suggests to consider median graphs, or subclasses of median graphs such as the Buneman graphs, as a natural generalization of trees in the context of phylogenetic questions.

In this contribution, we consider rooted median graphs, i.e., median graphs with a vertex designated as the root. We note in passing that rooted median graphs recently have attracted in the context of the Daisy graph construction [12, 51]. It is natural then to replace the last common ancestor lca(x, y) by the median med(x, y, p) of two vertices x and y and the root p and to ask which maps can be explained as δ(x, y) = t(med(x, y, p)), where t is now a vertex labeling on the median graph. In Sect. 3 we show that every symmetric map δ can be explained by a sufficiently large median graph and provide explicit constructions for extended hypercubes and extended half-grids. Thm. 3.10 shows that O(2^|X|^2) vertices are sufficient. In the second part of this contribution, Sect. 4, we show that for every symmetric map δ a rooted labeled median graph can be obtained by expanding the map’s modular decomposition tree by replacing its vertices with explicitly constructed graphs (Thm. 4.11). This yields a practical algorithm to construct a rooted median graph that explains δ with a running time linear in the size of the input. It reduces to a labeling of the modular decomposition tree exactly for symbolic ultrametrics (Thm. 4.3).

2 Preliminaries

Sets and Maps Let X be a finite set. We write \( X^2_\text{set} := X \times X \setminus \{(x, x) \mid x \in X\} \) for the Cartesian set product without reflexive elements. \( \binom{X}{k} \) for the set of all k-element subsets of X, and \( 2^X \) for the powerset of X. Denoting by |X| the cardinality of X we have |X^2_\text{set}| = |X|(|X| − 1).

A hierarchy on X is a subset \( \mathcal{H} \subseteq 2^X \) such that (i) X \( \in \mathcal{H} \), (ii) \( \{x\} \in \mathcal{H} \) for all x \( \in X \), and (iii) \( \mathcal{H} \cap q \in \{p, q, \emptyset\} \) for all p, q \( \in \mathcal{H} \). Condition (iii) states that no two members of \( \mathcal{H} \) overlap. Let X and Y be non-empty sets. We consider maps \( \delta : X^2_\text{set} \to Y \) that assign to each pair \((x, y) \in X^2_\text{set}\) the unique label \( \delta(x, y) \in Y \). A map \( \delta \) is symmetric if \( \delta(x, y) = \delta(y, x) \) for all distinct x, y \( \in X \). For a subset \( L \subseteq X \) we denote with \( \delta_L : L^2_\text{set} \to Y \) the map obtained from \( \delta \) by putting \( \delta_L(x, y) = \delta(x, y) \) for all distinct x, y \( \in L \).

Graphs All graphs G = (V, E) considered here are undirected and simple. For a subset \( W \subseteq V \), we write \( G - W \) for the graph obtained from G by deleting all vertices in \( W \) and their incident edges.

All paths in G are considered to be simple, that is, no vertex is traversed twice. In particular, the graph \( P_n \) denotes the path on n vertices with vertex set \( V(P_n) = \{1, \ldots, n\} \) and edge set \( E(P_n) = \{\{i, i + 1\} \mid 1 \leq i < n\} \). We also write \( P_G(a, b) \) for a path connecting two vertices a and b in G. A cycle is a graph for which the removal of any edge results in a path. A cycle of length four is called a square.

The distance \( d_G(u, v) \) between vertices u and v in a graph G is the length \( |E(P)| \) of a shortest path P connecting u and v. The interval between u and v is the set \( I_G(x, y) \) of vertices that lie on shortest paths \( P_G(x, y) \) between x and y.

Let \( G = (V, E) \) be a graph and W \( \subseteq V \). A (partial vertex) labeling is a map \( \tau : V \to Y \) that assigns to every vertex \( v \in W \) one label \( \tau(v) \in \Gamma \). We write \( (G, \tau) \) for a given graph G together with labeling \( \tau \) and call \((G, \tau)\) labeled graph.

Rooted Graphs and Trees We consider here rooted graphs, that is, graphs for which there is a particular distinguished vertex \( r_G \in V \), called the root of G. Given a rooted graph G, we can equip the vertex set V with a partial order \( \leq_G \) by putting \( u \leq_G v \) whenever \( v \) lies on some path \( P_G(u, v) \) connecting \( r_G \) and u. If \( u \leq_G v \) and \( u \neq v \), then we write \( u <_G v \). Furthermore, if we have an edge \( \{u, v\} \in E(G) \) such that \( u <_G v \), then \( u \) is a child of \( v \) and \( \text{child}_G(v) \) denotes the set of all children of \( v \) in G. If \( u \leq_G v \) or \( v \leq_G u \), the vertices \( u \) and \( v \) are comparable (in G) and incomparable, otherwise.

A vertex \( v \neq r_G \) in a graph G is called leaf if its degree \( \text{deg}_G(v) = 1 \). The inner vertices in a graph G are vertices that are not leaves and \( V(G) \) denotes the set of all inner vertices of G. Let G = (V, E) be a graph and assume that
we have added the vertex \( x \notin V \) to \( G \) such that \( x \) is adjacent to exactly one vertex \( v \in V \). Then, we say that \( x \) is leaf-appended to \( v \) (in \( G \)).

A tree is a connected acyclic graph. Given a rooted tree \( T \), the last common ancestor \( \text{lca}_T(x, y) \) of two vertices \( x, y \in V(T) \) is the unique \( \preceq_T \)-minimal vertex that satisfies \( x, y \preceq_T \text{lca}_T(x, y) \), that is, there is no further vertex \( v \) with \( x, y \preceq_T v \). For rooted trees \( T \) with leaf set \( L \), we denote with \( L(v) \) the subset of leaves \( x \in L \) with \( x \preceq_T v \). We also write \( L_T(v) \) instead of \( L(v) \), if there is a risk of confusion. Two labeled trees \((T, t)\) and \((T', t')\) with labeling \( t : V^0(T) \to \Upsilon \) and \( t' : V^0(T') \to \Upsilon \) are isomorphic if \( T \) and \( T' \) are isomorphic via a map \( \psi : V(T) \to V(T') \) such that \( t'(\psi(v)) = t(v) \) holds for all \( v \in V^0(T) \). There is a well-known bijection between hierarchies and rooted trees [49]:

**Proposition 2.1.** Let \( \mathcal{H} \) be a set of non-empty subsets of \( L \). Then, there is a rooted tree \( T = (W, E) \) with leaf set \( L \) and with \( \mathcal{H} = \{ L(v) \mid v \in W \} \) if and only if \( \mathcal{H} \) is a hierarchy on \( L \). Moreover, if there is such a rooted tree, then, up to isomorphism, \( T \) is unique.

**Remark 2.2.** Instead of graphs with leaves we could consider a straightforward generalization of the notion of \( \mathcal{X} \)-trees frequently employed in mathematical phylogenetics. There a set of taxa \( X \) is mapped (not necessarily injectively) to the vertex set \( V(T) \) of a rooted or unrooted tree \( T \), see e.g. [49]. We prefer to instead identify the taxa with the leaf set \( L \) and insist that distinct taxa are represented by distinct vertices in the graphs that describe the phylogenetic relationships. In an \( \mathcal{X} \)-tree like setting we could identify the taxa with the corresponding leaf’s (uniquely defined) “parent”.

**Cartesian Graph Product** The Cartesian product \( G \square H \) of two graphs \( G = (V, E) \) and \( H = (W, F) \) has vertex set \( V(G \square H) = V \times W \) and edge set \( E(G \square H) = \{ (g, h, (g', h')) \mid g = g' \text{ and } (h, h') \in F, \text{ or } h = h' \text{ and } (g, g') \in E \} \). The Cartesian product is known to be commutative and associative and thus, \( G \square \square \square \cdots \square G = G \square \square \square \cdots \square G \) is well-defined [27, 43]. For a vertex \( v = (g_1, \ldots, g_n) \in V(G \square \square \square \cdots \square G) \) we refer to \((g_1, \ldots, g_n)\) as the coordinate vector of \( v \) and to \( g_i \) as the \( i \)-th coordinate of \( v \). The Hamming distance between two vertices \( v, w \) with coordinate vectors \((g_1, \ldots, g_n)\) and \((g'_1, \ldots, g'_n)\), respectively, is the number of coordinates \( i \) for which \( g_i \neq g'_i \).

A complete grid is the Cartesian product \( P_n \square P_m \) of two paths and a grid graph is a subgraph of a complete grid. A hypercube \( Q_n \) is the \( n \)-fold Cartesian product of edges, i.e., \( Q_n = \square_{i=1}^n K_2 \). Equivalently, hypercubes can be defined as graphs having vertex set \( V = \{0, 1\}^n \) and having edges precisely between the vertices that have Hamming distance 1.

Based on the distance formula [27, Cor. 5.2], we obtain the following simple result for complete grid graphs and hypercubes that we shall need for later reference.

**Lemma 2.3.** Let \( P_n \) be a path with \( V(P_n) = \{1, \ldots, n\} \) and edge set \( E(P_n) = \{(i, j) \mid j = i + 1, 1 \leq i < n\} \) and \( G = P_n \square P_n \). Then, for all vertices \((i, j), (i', j') \in V(G)\) it holds that \( d_G((i, j), (i', j')) = |i - i'| + |j - j'| \).

For a hypercube \( Q_n \), the distance \( d_{Q_n}(x, y) \) of vertices \( x, y \in V(Q_n) \) is the Hamming distance of \( x \) and \( y \).

Following [45], we will consider grid graphs as plane graphs, that is, we will assume that they are embedded in the plane in the natural way – as a subgraph of a complete grid.

**Median Graphs** A vertex \( x \) is a median of a triple of vertices \( u, v \) and \( w \) if \( d(u, x) + d(x, v) = d(u, v), d(v, x) + d(x, w) = d(v, w) \) and \( d(u, x) + d(x, w) = d(u, w) \). A connected graph \( G \) is a median graph if every triple of its vertices has a unique median. In other words, \( G \) is a median graph if, for all distinct \( u, v, w \in V(G) \), there is a unique vertex that belongs to shortest paths between each pair of \( u, v \) and \( w \). Equivalently, \( G \) is a median graph if \( |I_G(u, v) \cap I_G(u, w) \cap I_G(v, w)| = 1 \) for every triple \( u, v \) and \( w \) of its vertices [46, 48]. We denote the unique median of three vertices \( u, v \) and \( w \) in a median graph \( G \) by \( \text{med}_G(u, v, w) \). A well-known example of median graphs are trees. In particular, if we consider rooted trees \( T \), then \( \text{lca}_T(x, y) \) lies on all three paths between \( x \) and \( y \), between \( \rho_T \) and \( x \) as well as between \( \rho_T \) and \( y \). Taking the latter two arguments together, we obtain the following

**Observation 2.4.** If \( T \) is a rooted tree, then \( \text{lca}_T(x, y) = \text{med}_T(x, y, \rho_T) \) for every \( x, y \in V(T) \).

A further example of median graphs are particular grid graphs for which a planar drawing is provided. As a direct consequence of Lemma 6 together with Theorem 7 in [45], we obtain

**Theorem 2.5** ([45]). A connected grid graph \( G \) is a median graph if and only if all inner faces of \( G \) are squares.

If \( e \) is an edge in a connected grid graph \( G \) whose removal makes \( G \) disconnected, then \( G \) is a median graph if and only if both components of \( G - e \) (the graph obtained from \( G \) by removing the edge \( e \)) are median graphs [45]. Therefore, we obtain the following simple result that we need for later reference.

**Lemma 2.6.** Let \( G_1 = (V_1, E_1) \) and \( G_2 = (V_2, E_2) \) be two vertex-disjoint graphs and let \( v \in V_1 \) and \( w \in V_2 \). Then, \( G = (V_1 \cup V_2, E_1 \cup E_2 \cup \{(v, w)\}) \) is a median graph if and only if \( G_1 \) and \( G_2 \) are median graphs. In particular, if \( L \) is the set of leaves in \( G \), then \( G \) is median graph if and only if \( G - L \) is median graph.

**Definition 2.7.** Let \( G = (V, E) \) be a rooted median graph with root \( \rho \) and a specified set \( L \subseteq V \) of vertices. Then,

\[
V_{\text{med}_L} := \{ \text{med}_L(\rho, x, y) \mid x, y \in L \text{ and } x, y, \rho \text{ pairwise distinct} \}
\]

denotes the set of all (unique) medians \( \text{med}_L(\rho, x, y) \) for all distinct pairs of vertices \( x, y \in L \).
Definition 2.8. Let $\delta : X^2_{\text{irr}} \to Y$ be a symmetric map. A rooted median graph $G = (V, E)$ with root $r$ and specified set $L = X \subseteq V$ explains $\delta$ if there is a labeling $t : V_{\text{medr}}, L \to Y$ such that $\delta(x, y) = t(\text{med}_G^r(x, y))$ for all distinct $x, y \in X$.

In the following the set $L$ in Def. 2.7 and 2.8 will coincide the leaf set of the median graphs under consideration.

3 Every map $\delta$ can be explained by a labeled median graph

We are interested in rooted median graphs that can explain a given map $\delta$. As noted in the introduction, only a very restricted subclass of maps, namely the symbolic ultrametrics [4], can be explained by rooted trees. This is not surprising since $O(|X|^2)$ values of $\delta(x, y)$ must be explained by only $O(|X|)$ labels at the internal vertices of a tree. This suggests that rooted median graphs with a large enough number of inner vertices should be able to explain any given map. Here we show that this is indeed the case.

3.1 Extended Hypercubes

One of the best known median graphs is possibly the hypercube. In particular, every median graph is a distance-preserving subgraph of some hypercube [45].

Definition 3.1. Let $Q_n = (V, E)$ be a hypercube. An extended hypercube $Q^\text{ext}_n$ with leaf set $L = \{x_1, \ldots, x_n\}$ is obtained from $Q_n$ as follows: every $x_i \in L$ is leaf-appended to the vertex for which only the $i$-th coordinate is a 1. The root $r$ of $Q^\text{ext}_n$ will always be the vertex with coordinate vector $(1, \ldots, 1)$.

Lemma 3.2. $Q^\text{ext}_n$ is a median graph and $\text{med}_{Q^\text{ext}_n}(r, x_i, x_j) \neq \text{med}_{Q^\text{ext}_n}(r, x_k, x_l)$ whenever $x_i$ and $x_j$, resp. $x_k$ and $x_l$ are distinct vertices and $|\{i, j\} \cap \{k, l\}| \leq 1$.

Proof. Since $Q_n$ as well all single vertex graphs $G_j = (\{x_j\}, \emptyset), 1 \leq j \leq n$ are median graphs, Lemma 2.6 implies that $Q^\text{ext}_n$ is a median graph.

Now, let $L$ be the set of leaves in $Q^\text{ext}_n$ and let $x_i, x_j \in L$ and $x_k, x_l \in L$ be two distinct vertices, respectively, such that $\{i, j\} \neq \{k, l\}$. Since $Q^\text{ext}_n$ is a median graph, the medians in $Q^\text{ext}_n$ are unique for all three vertices in $Q^\text{ext}_n$ and it is easy to verify that $\text{med}_{Q^\text{ext}_n}(r, v_i, v_j) = \text{med}_{Q^\text{ext}_n}(r, v_k, v_l)$ for every distinct $v_i, v_j \in V(Q_n)$ with $v_i, v_j \neq r$. By construction, $x_i \in L$ is leaf-appended to the unique vertex $v_i$ with all coordinates being 0 except the $i$-th coordinate which is a 1 and every shortest path from $x_i$ to any other vertex must contain $v_i$. The latter two arguments imply that it suffices to show that $\text{med}_{Q^\text{ext}_n}(r, v_i, v_j) \neq \text{med}_{Q^\text{ext}_n}(r, v_k, v_l)$ in order to show that $\text{med}_{Q^\text{ext}_n}(r, x_i, x_j) \neq \text{med}_{Q^\text{ext}_n}(r, x_k, x_l)$.

Assume for contradiction that $w := \text{med}_{Q^\text{ext}_n}(r, v_i, v_j) = \text{med}_{Q^\text{ext}_n}(r, v_k, v_l)$. Based on Lemma 2.3 and the respective Hamming distances we easily obtain,

$$d_{Q^\text{ext}_n}(v_i, w) + d_{Q^\text{ext}_n}(w, v_j) = d_{Q^\text{ext}_n}(v_i, v_j) = d_{Q^\text{ext}_n}(v_k, w) + d_{Q^\text{ext}_n}(w, v_l).$$

There are two possibilities for $w$ to satisfy $d_{Q^\text{ext}_n}(v_i, w) + d_{Q^\text{ext}_n}(w, v_j) = d_{Q^\text{ext}_n}(v_k, w) + d_{Q^\text{ext}_n}(w, v_l) = 2$, that is, $w$ either the vertex with coordinate vector $(0, \ldots, 0)$ or the vertex for which the coordinate vectors have precisely two 1s, namely the $i$-th and $j$-th coordinate. Analogously, for $d_{Q^\text{ext}_n}(v_i, v_j) = d_{Q^\text{ext}_n}(v_k, v_l) = 2$, the median $w$ is either the vertex $(0, \ldots, 0)$ or the vertex for which the coordinate vectors have precisely two 1s, namely the $k$-th and $l$-th coordinate. This together with $\{i, j\} \neq \{k, l\}$ implies that $w$ must be the vertex $(0, \ldots, 0)$. Since $w = \text{med}_{Q^\text{ext}_n}(r, v_i, v_j)$ it must also hold that $d_{Q^\text{ext}_n}(v_i, v_j) + d_{Q^\text{ext}_n}(w, r) = d_{Q^\text{ext}_n}(v_i, v_j) = n - 1$. However, since $d_{Q^\text{ext}_n}(v_i, w) = 1$ and $d_{Q^\text{ext}_n}(w, r) = n$, we obtain $d_{Q^\text{ext}_n}(v_i, v_j) + d_{Q^\text{ext}_n}(w, r) = n + 1$; a contradiction.

Corollary 3.3. Every symmetric map $\delta : X^2_{\text{irr}} \to Y$ can be explained by a labeled extended hypercube $(Q^\text{ext}_{|X|}, t)$.

Proof. Let $X$ be the set of leaves in $Q^\text{ext}_{|X|}$. Put $t(\text{med}_{Q^\text{ext}_{|X|}}(r, x, y)) = \delta(x, y)$ for all distinct $x, y \in X$. By Lemma 3.2, we have $\text{med}_{Q^\text{ext}_{|X|}}(r, x_i, x_j) \neq \text{med}_{Q^\text{ext}_{|X|}}(r, x_k, x_l)$ given that $\{i, j\} \neq \{k, l\}$ and $i \neq j$ and $k \neq l$. Hence, $t(\text{med}_{Q^\text{ext}_{|X|}}(r, x, y))$ is well-defined and $(Q^\text{ext}_{|X|}, t)$ explains $\delta$.

An illustrative example for Cor. 3.3 is provided in Fig. 2. Of course, $Q^\text{ext}_n$ has $O(2^n)$ vertices and many vertices are not part of $V_{\text{medr}}(X)$ which makes this construction intractable in practice. Hence, we focus now on graphs that have significantly less vertices and still explain a symmetric map $\delta$.

3.2 Extended Halfgrids

We next consider a class of much smaller median graphs.

Definition 3.4. A half-grid $H_n$ with $n \geq 2$ is defined as $H_2 = P_2 \square P_2$ or, if $n \geq 3$, then $H_n$ is obtained from the Cartesian product $P_2 \square P_2$ by removing all vertices with coordinate vectors $(i, j)$ with $1 \leq j \leq n - 2$ and $j + 2 \leq i \leq n$. and its incident edges; see also Fig. 1.
**Proof.** For simplicity we put $\text{med}_{H_n^{ext}}(\ldots) = \text{med}_{H_n^{ext}}(\ldots)$. Since $H_n$ as well as all single vertex graphs $G_j = (\{x_j\}, \emptyset)$, $1 \leq j \leq n + 1$ are median graphs, we can apply Lemma 3.6 together with Lemma 2.6 to conclude that $H_n^{ext}$ is a median graph.

We continue by showing that each inner face is a square. Let $H_n^{ext}$ be an extended half-grid with leaf set $L = \{x_1, \ldots, x_{n+1}\}$. Then, $H_n^{ext}$ is a median graph and for all leaves $x_i$ and $x_j$, $i < j$ we have $\text{med}_{H_n^{ext}}(\rho, x_i, x_j) = (i, j - 1)$.

**Proposition 3.8.** Let $H_n^{ext}$ be an extended half-grid with leaf set $L = \{x_1, \ldots, x_{n+1}\}$. Then, $H_n^{ext}$ is a median graph and for all leaves $x_i$ and $x_j$, $i < j$ we have $\text{med}_{H_n^{ext}}(\rho, x_i, x_j) = (i, j - 1)$.

**Proof.** For simplicity we put $\text{med}(\ldots) = \text{med}_{H_n^{ext}}(\ldots)$. Since $H_n$ as well as all single vertex graphs $G_j = (\{x_j\}, \emptyset)$, $1 \leq j \leq n + 1$ are median graphs, we can apply Lemma 3.6 together with Lemma 2.6 to conclude that $H_n^{ext}$ is a median graph.

We continue by showing that each inner face is a square. Let $H_n^{ext}$ be an extended half-grid with leaf set $L = \{x_1, \ldots, x_{n+1}\}$. Then, $H_n^{ext}$ is a median graph and for all leaves $x_i$ and $x_j$, $i < j$ we have $\text{med}_{H_n^{ext}}(\rho, x_i, x_j) = (i, j - 1)$.
There is a shortest path $P$.

Claim 3.8.1. There is a shortest path $P$ in $H$ connecting $v_i$ and $v_j$, $i < j$ that contains the vertex $w_{i,j} = (i, j - 1)$.

Proof of Claim. Let us start with the special case $v_1 = (1, 1)$ and $v_{n+1} = (n, n)$. By construction of $H_k$, all vertices $(1, k)$ with $1 \leq k \leq n$ and all vertices $(k, n)$ with $1 \leq k \leq n$ are contained in $H_k$. Thus, there is a path $P_{n+1}$ induced by the vertices $(1,1),\ldots,(1,n),\ldots,(n,n)$ that has length $2(n-1) = 2n - 2$. By Lemma 2.3, $d_G(v_1, v_{n+1}) = (n - 1) + (n - 1) + 2n - 2$, which implies that $P_{n+1}$ is a shortest path in $H$ that, in particular, includes $w_{1,n+1} = (1, n)$.

Now consider $v_1 = (1,1)$ and $v_j = (j, j - 2), 2 \leq j \leq n$. Note, by construction of $H_k$, all vertices $(1,k)$ with $1 \leq k \leq j - 1 < n$ and all vertices $(k,j-1)$ with $1 \leq k \leq j$ are contained in $H_k$. Thus, there is a path $P_{j}$ induced by vertices $(1,1),\ldots,(1,j-1),\ldots,(j,j-1),\ldots,(j-1,j-1),\ldots,(1,1)$ of length $(j - 2) + (j - 1), 2 \leq j \leq n$. By Lemma 2.3, $d_G(v_1, v_j) = (j - 1) + (j - 2)$, which implies that $P_j$ is a shortest path in $H$ that, in particular, includes $w_{1,j} = (j, 1) - 1$.

By similar arguments, there is a path $P_{i+1}$ from $v_i = (i, i - 1)$ and $v_{n+1} = (n, n), 2 \leq i \leq n$ along the vertices $(i,i-1),\ldots,(i,n),\ldots,(n,n)$ of length $(n-i+1) + (n-i)$. By Lemma 2.3, $d_G(v_i, v_{n+1}) = (n - i) + (n - i + 1)$, which implies that $P_{i+1}$ is a shortest path in $H$ that, in particular, includes $w_{i,n+1} = (i, n)$.

Now consider $v_i = (i, i - 1)$ and $v_j = (j, j - 2), 2 \leq i < j \leq n$. By Remark 3.5, all vertices $(i,k)$ with $i \leq k \leq n$ and all vertices $(k,j-1)$ with $i - 1 \leq k \leq j - 1$ are contained in $H_k$. Thus, there is a path $P_{i,j}$ induced by vertices $(i,i-1),(i,i),(i,j-1),(i,1),(1,1),\ldots,(j,j-1),\ldots,(1,1)$ of length $(j - 1 - (i - 1)) + (j - i) = 2j - 2i$. By Lemma 2.3, $d_G(v_i, v_j) = (j - 1) + (j - (i - 1)) = 2j - 2i$, which implies that $P_{i,j}$ is a shortest path in $H$ that, in particular, includes $w_{i,j} = (i,j)$.

Claim 3.8.2. There are shortest paths $P_{i,j}(v_i, v_j)$ and $P_{j,i}(v_j, v_i)$ that both contain vertex $w_{i,j} = (i, j - 1)$ for all $1 \leq i < j \leq n + 1$.

Proof of Claim. For simplicity, we put $P_{i,i} := P_i(v_i, v_i)$ and $P_{i,j} := P_i(v_j, v_j)$.

Let us start again with $v_1 = (1,1)$. In this case, there is a path $P_{n+1}$ from $v_1$ along the vertices $\rho = (1,n),\ldots,(1,1)$ of length $n - 1$ which is, by Lemma 2.3, the same as $d_G(v_1, v_{n+1})$. Hence, $P_{n+1}$ is a shortest path in $G$. In particular, $w_{1,n+1} = (1, j - 1)$ is contained in $P_{i,j}$ for all $1 \leq j \leq n + 1$.

By similar arguments and using the path $P_{n+1}$ along the vertices $\rho = (1,n),\ldots,(n,n)$, the path $P_{i,j}$ contains all vertices $w_{i,n+1} = (i, n)$ with $1 \leq i < j \leq n + 1$.

Now assume that $v_i$ and $v_j$ are chosen such that $1 < i < j < n + 1$. By similar arguments as in the proof of Claim 3.8.1, there is a path $P_{j,i}$ along the vertices $\rho = (1,n),\ldots,(i,n),\ldots,(i,j),\ldots,(i,1)$ of length $\rho = (1,n),\ldots,(i,n),\ldots,(i,j),\ldots,(i,1) = w_{i,j}$. This path $P_{j,i}$ has length $(j - 1) + (n - (i - 1)) = n$. Moreover, there is a path $P_{i,j}$ along the vertices $\rho = (1,n),\ldots,(1,j-1),\ldots,(i,j-1),\ldots,(j,j-1)$ of length $\rho = (1,n),\ldots,(1,j-1),\ldots,(i,1)$ of length $n - (j - 1) - (i - 1) + (i,1)$. By Lemma 2.3, the same as $d_G(v_i, v_j)$. For both cases, Lemma 2.3 implies that $P_{i,j}$ and $P_{j,i}$ are shortest paths. In particular, both paths contain $w_{i,j} = (i,j)$.

We are now in the position to prove the final statement $\delta(x,y) = (i,j)$ where $x_i, x_j = X, i < j$. Since each $x_i$ is leaf-attached to $v_i$ every shortest path from $x_i$ to every other vertex must contain $v_i$. In other words, every shortest path from $x_i$ to some vertex $z$ consists of the edge $\{x_i, v_i\}$ and a shortest path from $v_i$ to $z$. Thus, Claims 3.8.1 and 3.8.2 imply that $w_{i} = (i, j - 1)$ is contained in a shortest path from $x_i$ to $x_j$ as well as in a shortest path from

Figure 2: Left: the graph-representation of a map $\delta : X_{\text{med}} \rightarrow Y$ with $X = \{a,b,c,d\}$ and $\delta(a,b) = \delta(a,c) = \delta(b,d) = \text{blue (solid line)}, \delta(b,c) = \text{red (dashed line)}, \delta(c,d) = \text{purple (dashed-dotted line)}, \delta(a,d) = \text{green (dotted line). For the two graphs $(Q_{\text{ext}}^Y, t)$ (middle) and $(H_{\text{ext}}^Y, t)$ (right) all non-black vertices belong to $V_{\text{med}} \times X$, and $V_{\text{med}} \times X$. Respectively. Both labeled graphs $(Q_{\text{ext}}^Y, t)$ and $(H_{\text{ext}}^Y, t)$ explain $\delta$.
ρ = (1, n) to x_i and x_j, respectively. Finally, since H is a median graph it must hold that med(ρ, x_i, x_j) = (i, j − 1), 1 ≤ i < j ≤ n + 1.

\[\text{Corollary 3.9. Let } H_{str}^{\mathcal{X}_1} \text{ be an extended half-grid with leaf set } L = \{x_1, \ldots, x_{n+1}\}. \text{ Then, for each } w \in V_{med_{str}} L \text{ there is a unique pair } (x_i, x_j) \text{ such that } w = med_{str}(\rho, x_i, x_j).\]

\[\text{Theorem 3.10. For every symmetric map } \delta : X^2 \rightarrow Y \text{, there is a labeled median graph } (G, t) \text{ with } O(|X^2|) \text{ vertices and leaf-set } X \text{ that explains } \delta \text{ and such that its root } \rho_G \text{ is in } V_{med_{str}} X.\]

\[\text{Proof. If } |X| = 2, \text{ then one can easily verify that this can explained by a rooted tree with one inner vertex and two leaves. Consider } H_{str}^{\mathcal{X}_1} \text{ with leaf set } X = \{x_1, \ldots, x_{n+1}\}, |X| \geq 3 \text{ and root } \rho. \text{ By construction, } H_{str}^{\mathcal{X}_1} \text{ has } O(|X^2|) \text{ vertices. Put } t(med_{str}(\rho, x, y)) = \delta(x, y) \text{ for all distinct } x, y \in X. \text{ By Cor. 3.9, } med_{str}(\rho, x, y) \text{ is uniquely determined for all distinct } x, y \in X. \text{ Hence, } t(med_{str}(\rho, x, y)) \text{ is well-defined and } (G = H_{str}^{\mathcal{X}_1}, t) \text{ explains } \delta. \text{ Moreover, by Prop. 3.8, } med_{str}(\rho, x_1, x_{n+1}) = (1, n) = \rho. \text{ Therefore, } \rho \in V_{med_{str}} X.\]

An example for the construction as in the proof of Thm. 3.10 is provided in Fig. 2.

While \(G_{str}^{\mathcal{X}_1}\) has \(|X| + |X|\) vertices, the graph \(H_{str}^{\mathcal{X}_1}\) has only \(\Theta(|X|^2)\) vertices, and thus, is more space-efficient. There are maps for which we cannot avoid that the graph that explains it has \(\Theta(|X|^2)\) vertices. In particular, if \(\delta : X^2 \rightarrow Y\) is a surjective map with \(|Y| = |\frac{X}{2}|\), then \(\delta(x, y) \neq \delta(x', y')\) for all pairs \((x, y), (x', y') \in X^2\) with \((x, y) \neq (x', y')\). In this case, all the labels of the respective medians must be distinct and thus, \(\Theta(|X|^2)\) medians must exist. In other words, halfgrids are in some sense optimal if all \(\delta(x, y)\) are distinct. In general, however, we want to explain maps \(\delta\) by median graphs that are closer to trees. This leads us directly to the concept of the modular decomposition of a map which is explained in the next section.

4 Median graphs from Modular Decomposition Trees

This section makes extensive use of results established in [34] for so-called 2-structures (cf. [14–20, 20, 21, 47] and (not necessarily symmetric) maps \(\delta\). A (labeled) 2-structure \(g = (X, Y, \delta)\) where \(X\) and \(Y\) are nonempty sets and \(\delta : X^2 \rightarrow Y\) is a map. Since 2-structures are essentially determined by \(\delta : X^2 \rightarrow Y\) we use such maps, instead of 2-structures, which is more suitable for our purposes. The idea underlying this section is to start from the modular decomposition tree of a symmetric map \(\delta\) and to “expand” this tree in a principled manner into a rooted median graph that explains \(\delta\). We thus start with the notion of modules for symmetric maps.

Definition 4.1. A module of a symmetric map \(\delta : X^2 \rightarrow Y\) is a subset \(M \subseteq X\) such that \(\delta(x, z) = \delta(y, z)\) holds for all \(x, y \in M\) and \(z \in X \setminus M\). A module \(M\) of \(\delta\) is strong if \(M\) does not overlap with any other module of \(\delta\), that is, \(M \cap M' \in \{M, M', \emptyset\}\) for all modules \(M'\) of \(\delta\).

We write \(M(\delta)\) for the set of all modules of a symmetric map \(\delta\) and \(M_{str}(\delta) \subseteq M(\delta)\) for the set of all strong modules of \(\delta\). The empty set \(\emptyset\), the complete vertex set \(X\), and the singletons \(\{v\}\) are always modules. They are called the trivial modules of \(\delta\). We will assume from here on, that a module is non-empty unless otherwise indicated.

The set \(M_{str}(\delta)\) of strong modules is uniquely determined [19, 34]. While there may be exponentially many modules, the size of the set of strong modules is in \(O(|X|)\) [19]. In particular, \(X\) and the singletons \(\{v\}, v \in X\) are strong modules. Since strong modules do not overlap this implies that \(M_{str}(\delta)\) forms a hierarchy and, by Prop. 2.1, gives rise to a unique tree representation \(T_G(\delta)\), known as the modular decomposition tree (MDT) of \(\delta\). The vertices of \(T_G(\delta)\) are (identified with) the elements of \(M_{str}(\delta)\). Adjacency in \(T_G(\delta)\) is defined by the maximal proper inclusion relation, that is, there is an edge \([M, M']\) between \(M, M' \in M_{str}(\delta)\) iff \(M \subseteq M'\) and there is no \(M'' \in M_{str}(\delta)\) such that \(M \subseteq M'' \subseteq M'\). The root of \(T_G(\delta)\) is (identified with) \(X\) and every leaf \(v\) corresponds to the singleton \(\{v\}, v \in X\).

Uniqueness and the hierarchical structure of \(M_{str}(\delta)\) implies that there is a unique partition \(M_{max}(\delta) = \{M_1, \ldots, M_k\}\) of \(X\) into maximal (w.r.t. inclusion) strong modules \(M_j \neq X\) of \(\delta\) [17, 18]. Since \(X \notin M_{max}(\delta)\) the set \(M_{max}(\delta)\) consists of \(k \geq 2\) strong modules, whenever \(|X| > 1\).

For later reference, we recall

Lemma 4.2 ([17], Lemma 4.11). Let \(M_1, M_2 \in M(\delta)\) be two disjoint modules of a symmetric map \(\delta\). Then there is a unique label \(i \in Y\) such that \(\delta(x, y) = (y, x) = i\) for all \(x \in M_1\) and \(y \in M_2\).

In order to infer \(\delta\) from \(T_G(\delta)\) we need to determine the label \(\delta(x, y)\) of all pairs of distinct leaves \(x, y\) from \(T_G(\delta)\). Hence, we need to define a labeling function \(l_G\) that assigns this “missing information” to the inner vertices of \(T_G(\delta)\).

The simplest case for the construction of \(l_G\) is given by symmetric maps \(\delta : X^2 \rightarrow Y\) that satisfy the following two axioms:

(U1) there exists no subset \(\{x, y, u, v\} \subseteq X\) such that \(\delta(x, y) = \delta(u, v) \neq \delta(y, v) = \delta(x, v) = \delta(x, u)\).

(U2) \(|\{\delta(x, y), \delta(x, z), \delta(y, z)\}| \leq 2\) for all \(x, y, z \in X\).
A symmetric map that satisfies (U1) and (U2) is called a symbolic ultrametric \([4]\). In this case, there is a unique vertex labeled tree \((T^*,t^*)\), called discriminant symbolic representation of \(\delta\), that satisfies \(t^*(v) \neq t^*(u)\) for all edges \((u,v) \in E(T')\) being inner vertices and for which \(t(lca(x,y)) = \delta(x,y)\) for all distinct \(x,y \in X\) (cf. \([4]\) and \([32, \text{Prop. 1}]\)). Hence, given the discriminant symbolic representation \((T^*,t^*)\) of a symbolic ultrametric \(\delta\) we can uniquely recover \(\delta\) from \((T^*,t^*)\).

Now consider the MDT \(T_8\) of \(\delta\). In case \(\delta\) is a symbolic ultrametric we can also equip \(T_8\) with a labeling \(t_8\), by setting \(t_8(lca_{T_8}(x,y)) = \delta(x,y)\) for all distinct \(x, y \in X\). If \(\delta\) is a symbolic ultrametric then Lemma 7 and Theorem 6 in \([34]\) imply that \(t_8\) is well-defined and satisfies \(t_8(v) \neq t_8(u)\) for all edges \((u,v) \in E(T_8)\) with \(u, v \in V(T_8)\). In particular, we have \(\delta(x,y) = i\) if and only if \(t_8(lca_{T_8}(x,y)) = i\). Since the discriminant symbolic representation \((T^*,t^*)\) and modular decomposition trees \((T_8,t_8)\) are unique (up to isomorphism), we can conclude that the two trees \((T^*,t^*)\) and \((T_8,t_8)\) must be isomorphic. We summarize this discussion in the following

**Theorem 4.3.** Suppose \(\delta: \mathcal{X}^2_{\text{in}} \to Y\) is a symmetric map. Then there is a discriminant symbolic representation \((T^*,t^*)\) of \(\delta\) if and only if \(\delta\) is a symbolic ultrametric. In this case, \((T^*,t^*)\) and the labeled MDT \((T_8,t_8)\) are isomorphic.

Note, for symbolic ultrametrics \(\delta\), we thus obtain a vertex labeled median graph \((T_8,t_8)\) that explains \(\delta\), since \(lca_{T_8}(x,y) = \text{medi}_d(p,x,y)\).

Not all maps \(\delta\) are symbolic ultrametrics. The modular decomposition tree \(T_8\) still exists, but in general there will be no labeling \(t_8\) such that \(t_8(lca_{T_8}(x,y)) = \delta(x,y)\) holds for all \(x \neq y\), see Fig. 4. As a remedy, let us consider the following

**Definition 4.4.** Let \(\delta: \mathcal{X}^2_{\text{in}} \to Y\) be a symmetric map. A quotient map is the map \(\delta/M_{\text{max}}(\delta): M_{\text{max}}(\delta)^2_{\text{in}} \to Y\) obtained from \(\delta\) by putting, for all \(M, M' \in M_{\text{max}}(\delta)\), \(\delta/M_{\text{max}}(\delta)(M,M') = \delta(x,y)\) for some \(x \in M, y \in M'\).

We first note that \(\delta/M_{\text{max}}(\delta)\) is well-defined because \(M_{\text{max}}(\delta)\) is well-defined and for every two distinct and, therefore, disjoint modules \(M, M' \in M_{\text{max}}(\delta)\) there is a label \(i \in Y\) with \(\delta(x,y) = i\) for all \(x \in M\) and \(y \in M'\) (cf. Lemma 4.2).

In addition to symbolic ultrametrics, there are two other important subclasses of symmetric maps \(\delta: \mathcal{X}^2_{\text{in}} \to Y\):

- A map \(\delta\) is prime if \(M(\delta)\) consists of trivial modules only.
- \(\delta\) is complete if for all \((x,y), (x',y') \in \mathcal{X}^2_{\text{in}}, \delta(x,y) = \delta(x',y')\).

Although maps \(\delta\) are not necessarily prime or complete, their quotients \(\delta/M_{\text{max}}(\delta)\) are always either of one or the other type.

**Lemma 4.5 ([18, 21, 34]).** Let \(\delta\) be a symmetric map. Then the quotient \(\delta/M_{\text{max}}(\delta)\) is either complete or prime. If \(\delta\) is a symbolic ultrametric, then \(\delta/M_{\text{max}}(\delta)\) is complete.

An illustrative example of the notation established above is provided in Fig. 3 and 4. We shall say that an inner vertex \(v\) of \(T_8\) (or, equivalently, the module \(L(v)\) where \(L = L_{T_8}\) is complete or prime if the quotient \(\delta_{L(v)}/M_{\text{max}}(\delta_{L(v)})\) is complete or prime, respectively. We can now adjust the labeling function by setting

\[
t_8(v) = \begin{cases} \text{prime}, & \text{if } v \text{ is prime} \\ i, & \text{else, in which case } v = lca_{T_8}(x,y) \text{ and } \delta(x,y) = i \text{ for some leaves } x, y \in L(v) \end{cases}
\]
Consequently, \( M \) is symmetric, and any two distinct modules \( M, M' \in \text{meds}(\delta(v)) \) must be disjoint. Hence, Lemma 4.2 implies that there is a unique label \( i \in \mathcal{Y} \) such that \( \delta_{(x,y)} = \delta_{(y,x)}' = i \) for all \( x \in M \) and \( y \in M' \). By definition, we thus have \( \delta_{(x,y)}(M,M') = \delta((M',M)) = i \) for some unique label \( i \in \mathcal{Y} \). Consequently, \( \delta_i \) is a symmetric map and well-defined. By Theorem 3.10 there is a labeled median graph \( (G_n,t_i) \) for all inner vertices \( v \in \mathcal{V}(\mathcal{G}) \).

**Theorem 4.6.** [34, Thm. 3 and Prop. 1] For a symmetric map \( \delta : X_{in}^2 \rightarrow \mathcal{Y} \) the following statements are equivalent:

1. \( \delta \) is a symbolic ultrametric.
2. The labeled MDT \((T_\delta,t_\delta)\) of \( \delta \) has no inner vertex \( v \) labeled prime, that is, the quotient \( \delta_{(i,j)} / \max(\delta_{(i,j)}) \) is always complete where \( L = \mathcal{X} \) in the leaf set of \( T_\delta \).

In order to infer \( \delta \) from \( T_\delta \), we need to determine the label \( \delta_{(x,y)} \) of all pairs of distinct leaves \( x,y \) of \( T_\delta \). In the case of prime nodes, however, we must therefore drag the entire information of the quotient maps. An alternative idea is to replace prime vertices by suitable median graphs and extend the labeling function \( t_\delta \) that assigns the “missing information” to the inner vertex of the new graph.

**Definition 4.7** (prime-vertex replacement (pvr) graphs). Let \( \delta : X_{in}^2 \rightarrow \mathcal{Y} \) be a symmetric map with MDT \((T_\delta,t_\delta)\) that has leaf set \( L = \mathcal{X} \). Denote \( \mathcal{P} \) be the set of all prime vertices in \( T_\delta \). A prime-vertex replacement (pvr) graph \((G^*,t^*)\) of \((T_\delta,t_\delta)\) is obtained by the following procedure:

1. For all \( v \in \mathcal{P} \), remove all edges \( \{v,u\} \) with \( u \in \text{child}_{t_\delta}(v) \) from \( T_\delta \) to obtain the forest \((T',t')\). We note that each child \( u \in \text{child}_{t_\delta}(v) \) corresponds to a unique module \( L(u) \in \max(\delta_{(i,j)}) \).
2. For all \( v \in \mathcal{P} \), choose a median graph \( G_v \) with root \( v \) and leaf-set \( L(G_v) = \{u \mid L(u) \in \max(\delta_{(i,j)})\} \) and labeling \( \delta_{(i,j)} : V_{\text{meds},L(G_v)} \rightarrow \mathcal{Y} \) such that \( \delta_{(i,j)}(G_v,t_v) \) explains \( \delta_{(i,j)} / \max(\delta_{(i,j)}) \) and such that \( v \in V_{\text{meds},L(G_v)} \).
3. For all \( v \in \mathcal{P} \), add \( G_v \) to \( T' \) by identifying the root of \( G_v \) with \( v \) in \( T' \) and each leaf \( u \) of \( G_v \) with the corresponding child \( u \in \text{child}_{t_\delta}(v) \), for all \( v \in \mathcal{P} \). This results in a pvr graph \( G^* \).
4. Let \( W(G^*) = \mathcal{V}(T_\delta) \cup \bigcup_{v \in \mathcal{P}} V_{\text{meds},L(G_v)} \) be the set of vertices that either obtained a label in \( T_\delta \) or in one of the chosen median graphs \((G_v,t_v)\). We define a new labeling \( t^* : W(G^*) \rightarrow \mathcal{Y} \) by putting, for all \( v \in W(G^*) \),
   \[
   t^*(v) = \begin{cases} 
   t_\delta(v) & \text{if } v \in \mathcal{V}(T_\delta) \setminus \mathcal{P} \\
   t_v(v) & \text{if } v \in \mathcal{P} \\
   t_v(w) & \text{else, i.e., } v \in W(G^*) \setminus \mathcal{V}(T_\delta) \text{ and thus, } v \text{ is a vertex of } G_w \text{ for some } w \in \mathcal{P} 
   \end{cases}
   \]

We next derive some basic properties for pvr graphs that we need later in order to show that pvr graphs can explain a given map \( \delta \).

**Lemma 4.8.** Let \( \delta : X_{in}^2 \rightarrow \mathcal{Y} \). Then, the pvr graph \((G^*,t^*)\) of the MDT \((T_\delta,t_\delta)\) constructed according to Def. 4.7 is well-defined and unique up to the choice of the median graphs \((G_v,t_v)\) in Def. 4.7(2). Furthermore, we have \( V(T_\delta) \subseteq V(G^*) \).

**Proof.** Let \((T_\delta,t_\delta)\) be the MDT of \( \delta \) and let \( L = \mathcal{X} \) denote the leaf set of \( T_\delta \). Let \( \mathcal{P} \) be the set of all prime vertices in \( T_\delta \). We show first that \((G^*,t^*)\) is well-defined. By construction, \( L \subseteq V(G^*) \). Moreover, if \( v \in \mathcal{V}(T_\delta) \) is a non-prime vertex, then it still exists in \( G^* \) and \( v \in W(G^*) \). Thus, we can put \( t^*(v) = t_\delta(v) \). This part is clearly well-defined.

Now let \( v \in V(T_\delta) \) be a prime vertex. By definition, \( \delta_i := \delta_{(i,j)} / \max(\delta_{(i,j)}) \) consists of trivial modules only. Since \( \max(\delta_{(i,j)}) \) is a subset of strong modules of \( \delta \) and \( \delta \) is a symmetric map, any two distinct modules \( M,M' \in \max(\delta_{(i,j)}) \) must be disjoint. Hence, Lemma 4.2 implies that there is a unique label \( i \in \mathcal{Y} \) such that \( \delta_{(x,y)} = \delta_{(y,x)}' = i \) for all \( x \in M \) and \( y \in M' \). By definition, we thus have \( \delta_i(M,M') = \delta_i(M',M) = i \) for some unique label \( i \in \mathcal{Y} \). Consequently, \( \delta_i \) is a symmetric map and well-defined. By Theorem 3.10 there is a labeled median graph \((G_v,t_v)\)
that explains $\delta$ and such that $v \in V_{\text{med}}(T_G)$. Hence, $(G, \delta)$ is well defined. Note that every $M \in \mathbb{M}(G)$ corresponds to some module $L(u), u \in \text{child}_{P}(v)$ and that $G_v$ has leaf set $L(G_v) = \text{child}_{P}(v)$ where each child $u \in \text{child}_{P}(v)$ is uniquely identified with the module $L(u)$. Since $v$ is prime, the edges between the children of $v$ and vertex $v$ are removed and we add the median graph $G_v$ with leaf-set $L(G_v) = \text{child}_{P}(v)$ by identifying its root with $v$ and every $u \in L(G_v)$ with the unique child $u \in \text{child}_{P}(v)$ in $T'$. As this step is uniquely determined (up to the choice of $G_v$) and applied precisely once to prime vertices $v$, we can conclude that $G^*$ is well-defined.

These arguments in particular imply $V(T_G) \subseteq V(G^*)$.

We continue to show that the labeling $t^*$ is well-defined. As argued above, $t^*(v) = t_q(v)$ is well-defined for non-prime vertices $v$ of $T_q$. Moreover, since $t_q$ is a map from $V(T_G) \to T$ and since $v \in V_{\text{med}}(L(G_v))$, the assignment $t^*(v) = t_q(v)$ is well defined for all $v \in \mathcal{P}$. Note, none of the leaves $u \in L(G_v)$ are contained in $V_{\text{med}}(L(G_v))$ and thus, do not obtain a label $t_q(u)$. By construction, $u \in L(G_v)$ implies that $u \in V(T_q)$. Hence, $u \in L(G_v)$ obtains either the unique label $t^*(u) = t_q(u)$ if $u \notin \mathcal{P}$ or $t^*(u) = t_q(u)$ if $u \in \mathcal{P}$. In summary, for all vertices $V(T_G)$ the labeling $t^*$ is well-defined. Now let $v \in W(G^*) \setminus V(T_q)$. In this case, there is a vertex $v$ distinct from $v$ such that $v \in V(G_{u_n})$ and $G_{u_n}$ is the median graph chosen in Step 2. Now, $G_{u_n}$ has root $w$. Since $v \in W(G^*) \setminus V(T_q)$ we have $w \in V_{\text{med}}(L(G_v))$ by construction, and therefore $v$ is labeled by $t_q(v)$. By construction of $t^*$, we have $t^*(v) = t_q(v)$, which is well-defined.

In summary, therefore, $t^*$ is well-defined.

\begin{lemma}
\text{Lemma 4.9.} Let $\delta: \mathcal{X}^2_{\text{irr}} \to \mathcal{Y}$ be a map and let $(G^*, t^*)$ be a prv graph of the MDT $(T_q, t_q)$. If $u, v \in V(T_q)$ such that $u \not\leq_G v$ and the vertices on the (unique) shortest path $P_{P}(u, v)$ in $T_q$ are contained in the vertex set of every path $P_{G^*}(u, v)$ in $G^*$.

\text{Proof.} If $u = v$ in $T_q$, then we can apply Lemma 4.9 to conclude that $V(T_q) \subseteq V(G^*)$ and thus, $u = v$ in $G^*$. In this case, the path $P_{P}(u, v)$ in $T_q$ consists of $u$ only and so, $P_{G^*}(u, v)$ does. Hence, we assume in the following that $u, v \in V(T_q)$ are chosen such that $u \prec_G v$.

Assume that $\{u, v\} \in E(T_q)$. If $v$ is not a prime vertex, then this edge $\{u, v\}$ also exists in $G^*$, by construction. Thus $u \prec_{G^*} v$. Otherwise, if $v$ is a prime vertex it is replaced by a median graph $G_v$, with root $v$ and $u \in L(G_v)$. That is, $u \prec_{G_v} v$, and by construction, $u \prec_{G^*} v$.

Assume now that $\{u, v\} \notin E(T_q)$ and consider the unique path $P_{P}(u, v)$. By analogous arguments, $b \prec_{G^*} a$ for every edge $\{a, b\}$ in the path $P_{P}(u, b)$ with $b \prec_{T_q} a$. By induction on the number of edges, we thus conclude that $u \prec_{G^*} v$.

It remains to show that the vertices in the unique shortest $P_{P}(u, v)$ in $T_q$ are contained in the vertex set of every path $P_{G^*}(u, v)$ in $G^*$. By Lemma 4.8, the vertices in $P_{P}(u, v)$ are contained in $V(G^*)$. Let $\{a, b\}$ be an edge in $P_{P}(u, v)$ with $b \prec_{T_q} a$. As argued above, if $a$ is not prime, then $\{a, b\}$ is an edge in $G^*$ and, otherwise, we still have $b \prec_{G^*} a$. Hence, if $a$ is not prime, then $P_{P}(a, b)$ must contain the edge $\{a, b\}$ (since $a$ is the unique last ancestor of $a$ and, if $a$ is prime, then $P_{P}(a, b)$ must contain a subpath of $a$ to $b$ in $G^*$ that starts at the root $a_0$ of $G_a$ and ends in the leaf $b$ of $G_b$). In summary, $P_{P}(a, b)$ either still contains the edge $\{a, b\}$ or a path from $a$ to $b$ in $G^*$. Hence, the vertices $a$ and $b$ are contained in $P_{P}(a, b)$. Since the choice of the edge in $P_{P}(a, b)$ was arbitrary, all vertices of $P_{P}(a, b)$ are contained in $P_{G^*}(a, b)$. Since these arguments apply to all paths $P_{P}(u, v)$, the statement follows.

\begin{lemma}
\text{Lemma 4.10.} Let $\delta: \mathcal{X}^2_{\text{irr}} \to \mathcal{Y}$ be a map and let $(G^*, t^*)$ be a prv graph of the MDT $(T_q, t_q)$. Let $x, y \in X$ be distinct and denote by $v_x$ and $v_y$ the two children of $v := \text{lca}_{P}(x, y)$ with $x \leq_{T_q} v_x$ and $y \leq_{T_q} v_y$, respectively. Then the following two statements are true:

(i) $v_x, v_y \in P_{G^*}(x, y)$.

(ii) $\text{med}_{G^*}(\rho, x, y) = \text{med}_{G}(v_x, v_y, v)$. Moreover, $\text{med}_{G^*}(v_x, v_y, v) = \text{med}_{G}(v_x, v_y, v)$ in case $v$ is prime and $G_v$ is chosen in Step 2 in Def. 4.7.

\text{Proof.} (i) If $v = \text{lca}_{P}(x, y)$ is not a prime vertex, then every path between $v$ and $x$ in $G^*$ contains $v_x$, while every path between $v$ and $y$ in $G^*$ contains $v_y$. Moreover, every path between $x$ and $y$ in $G^*$ must contain vertex $v$. Since every path between $v$ and $x$ in $G^*$ as well as between $v$ and $y$ in $G^*$ is a subpath of some path between $x$ and $y$, the vertices $v_x$ and $v_y$ are contained in $P_{G^*}(x, y)$. If $v$ is a prime vertex, then it is replaced by a median graph $G_v$ and, by construction, $v_x$ and $v_y$ are leaves in $G_v$. Hence, by construction, $v_x$ and $v_y$ are incomparable. Moreover, by Lemma 4.9 we have $x \leq_{G^*} v_x$ and $y \leq_{G^*} v_y$. Note, by construction, there is no vertex that is incomparable to $v$ (resp., $v_x$) that is also an ancestor of $x$ (resp., $y$). Consequently, $v_x$ and $v_y$ are contained in $P_{G^*}(x, y)$.

(ii) Application of Lemma 4.9 implies that $v_x, v_y \in P_{G}(\rho, x) \subseteq P_{G^*}(\rho, x)$ and $v_x, v_y \in P_{G}(\rho, y) \subseteq P_{G^*}(\rho, y)$. Moreover, $P_{G^*}(\rho, x) \subseteq P_{G^*}(x, y)$ and $P_{G^*}(\rho, x) \subseteq P_{G^*}(x, y) \subseteq P_{G^*}(x, y)$, respectively.

Therefore, $\text{med}_{G^*}(v_x, v_y) = \text{med}_{G^*}(v_x, v_y, v) = \text{med}_{G^*}(v_x, v_y, v) = \text{med}_{G^*}(v_x, v_y, v)$ in case $v$ is prime. Hence, by construction, we furthermore obtain $\text{med}_{G^*}(v_x, v_y) = \text{med}_{G^*}(v_x, v_y, v) = \text{med}_{G^*}(v_x, v_y, v)$ in case $v$ is prime.

\begin{theorem}
\text{Theorem 4.11.} Let $\delta$ be a symmetric map with MDT $(T_q, t_q)$ and let $(G^*, t^*)$ be a prv graph for $(T_q, t_q)$. Then, $(G^*, t^*)$ is a median graph that explains $\delta$.

10
Algorithm 1 Construction of a labeled median graph that explains a given symmetric map.

Require: symmetric map $\delta: X^2 \to Y$

Ensure: pvr graph $(G^*, t^*)$ that explains $\delta$

1: Compute MDT $(T_5, t_5)$
2: $(G^*, t^*) = (T_5, t_5)$
3: $\mathcal{P} \leftarrow \text{set of prime vertices in } (T_5, t_5)$
4: for all $v \in \mathcal{P}$ do
5: \hspace{1em} $n_v \leftarrow |\text{child}_T(v)|$
6: \hspace{1em} $(G^*, t^*) \leftarrow \text{graph obtained from } (G^*, t^*)$ by replacing $v$ by $(G_v, t_v)$ where $G_v \simeq H_n^{\text{ext}}$ (cf. Def. 4.7)
7: return $(G^*, t^*)$

Proof. Let $\mathcal{P}$ be the set of all prime vertices in $T_5$. We show first that $G^*$ is a median graph. To this end, consider the graph $G_v - L(G_v)$ obtained from the labeled median graph $(G_v, t_v)$ constructed in Step (2) in Def. 4.7. By Lemma 2.6, $G_v - L(G_v)$ remains a median graph. We denote with $H$ the graph that is the disjoint union of the graphs $G_v - L(G_v)$ (for all prime vertices $v$) and the connected components of the forest $T'$ obtained in Step (1) in Def. 4.7. Note, all connected components of $H$ are median graphs and, in particular, $H$ is a spanning subgraph of $G^*$. It is an easy task to verify that every edge $e \in E(G^*) \setminus E(H)$ connects precisely two connected components of $H$. Moreover, all edges $e \in E(G^*) \setminus E(H)$ that are added to obtain $G^*$ are only edges that are already contained in $T_5$. In other words, stepwise addition of edges $e \in E(G^*) \setminus E(H)$ cannot create new cycles in $G^*$. Hence, whenever we have added a proper subset $F \subseteq E(G^*) \setminus E(H)$ of edges to $H$ and take a further edge $f \in E(G^*) \setminus (E(H) \cup F)$ then it must connect again two connected components of the graph $(V(G^*), E(H) \cup F)$. By induction and Lemma 2.6, the connected components that are joined by a new edge $f$ are again median graphs. As a consequence, $G^*$ is a median graph.

Let $p$ be the root of $G^*$. It remains to show that $(G^*, t^*)$ explains $\delta$. Recall that we have $L(G^*) = X$ by construction. In order to verify that $\delta(x, y) = t^*(\text{med}_{G_v}(p, x, y))$ for all distinct $x, y \in X$ we consider the following cases: Either $t_5(\text{lca}_T(x, y)) = i$ for some $i \in \mathcal{P}$ or $t_5(\text{lca}_T(x, y)) = \text{prime}$. Set $v := \text{lca}_T(x, y)$ and denote by $v_x$ and $v_y$ the two children of $v$ with $x \leq_T v_x$ and $y \leq_T v_y$. Note, $v_x$ and $v_y$ are incomparable in $T_5$ since $v = \text{lca}_T(x, y)$. By Lemma 4.9, the vertices $v_x$ and $v_y$ still exist in $G^*$ and are, by construction still incomparable in $G^*$.

Suppose first $t_5(v) = i$ for some $i \in \mathcal{P}$ in which case $\delta(x, y) = i$. In this case, $v$ is not a prime vertex and, by construction, its two children in $G^*$ are still $v_x$ and $v_y$. By Lemma 4.9, $v$ is contained in the shortest paths $P_{G_v}(p, x)$ as well as $P_{G_v}(p, y)$. Moreover, by Lemma 4.10(i), $P_{G_v}(x)$ contains $v_x$ and $v_y$. Since $v_x$ and $v_y$ have only vertex $v$ as common adjacent vertex and since any path connecting $v_x$ and $v_y$ contains $v$, we can conclude that $P_{G_v}(x, y)$ must contain $v$. Since $G^*$ is a median graph this implies that $\text{med}_{G_v}(p, x, y) = v$. Since $v$ is not a prime vertex, we have, by construction, $t^*(\text{med}_{G_v}(p, x, y)) = t_5(v) = \delta(x, y)$.

Now assume that $v$ is prime. In this case, $v$ has been replaced by the median graph $G_v$ according to Def. 4.7(2). In particular, $(G_v, t_v)$ explains $\delta_v := \delta|_{L(v)}/\text{max}(\delta|_{L(v)})$. Note, for each child $u \in \text{child}_T(v)$, the set $L(u)$ is a module in $\text{max}(\delta|_{L(v)})$. Since $v$ is prime, $\delta_v$ consists of trivial modules only, that is, every $L(u) \in \text{max}(\delta|_{L(v)})$ forms a trivial module $M = \{L(u)\}$ in $M(\delta_v)$. This and definition of $\delta_v$ implies that $\delta_v$ maps pairs $(M, M')$ of distinct trivial modules to some label in $Y$. By definition of $L(G_v)$, the leaves $v_x$ and $v_y$ are contained in $L(G_v)$ and represent the trivial modules $L(v_x)$ and $L(v_y)$ of $\delta_v$. Since $L(v_x), L(v_y) \in \text{max}(\delta|_{L(v)})$, they are disjoint and hence, Lemma 4.2 implies that there is a unique label $i \in Y$ such that such that $\delta(a, b) = i$ for all $a \in L(v_x)$ and $b \in L(v_y)$. Therefore we have, by definition, $\delta_v((L(v_x), L(v_y))) = i = \delta(x, y)$. Since $v_x$ and $v_y$ are contained in $L(G_v)$ and represent the trivial modules $L(v_x)$ and $L(v_y)$ of $\delta_v$, and since $(G_v, t_v)$ explains $\delta_v$, we have $t_i(\text{med}_{G_v}(p, x, v_x)) = \delta(x, y)$. By Lemma 4.10(ii), $\text{med}_{G_v}(p, x, v_x) = \text{med}_{G_v}(v_x, v_x, v_y) = \text{med}_{G_v}(v_x, v_y, v_y)$. This and Def. 4.7(4) implies $t^*(\text{med}_{G_v}(p, x, y)) = t_i(\text{med}_{G_v}(v_x, v_y, v_y)) = \delta(x, y)$.

As a direct consequence of Thm. 4.11 we obtain a practical algorithm to compute a pvr graph for a given map $\delta$ that is linear in the size of the input.

Theorem 4.12. Algorithm 1 correctly computes a labeled median graph $(G, t)$ that explains a given symmetric map $\delta: X^2 \to Y$ in $O(m)$ time, where the input size is $m = |X^2|$.

Proof. By Theorem 4.11, every pvr graph as constructed in Def. 4.7 explains $\delta$. Hence, it remains to show that replacing each prime vertex $v$ by $(G_v, t_v) = (H_n^{\text{ext}}, t_v)$ with $n_v = |\text{child}_T(v)|$ yields a valid pvr graph. Observe first that every prime vertex $v$ must have at least three children since otherwise, $\delta|_{L(v)}/\text{max}(\delta|_{L(v)})$ is incomplete. Hence, $H_n^{\text{ext}}$ is well-defined since $n_v \geq 3$ for all $v \in \mathcal{P}$. This and Prop. 3.8 implies that $H_n^{\text{ext}}$ is a well-defined median graph for all $v \in \mathcal{P}$. As outlined in the proof of Thm. 3.10, there is a labeling $t_0$ such that $(H_n^{\text{ext}}, t_0)$ explains any map $\delta|_{L(v)}/\text{max}(\delta|_{L(v)})$. Hence, Algorithm 1 is correct.

To compute the running time, we first note that by [34, Thm. 7] the MDT $(T_5, t_5)$ can be computed in $O(|X|^2)$ time. Computing the initial graph $(G^*, t^*)$ and the set of prime vertices $\mathcal{P}$ can be done in $O(|X|)$ because $T_5$ is a tree and thus has $O(|X|)$ edges and vertices. Set $V := V(T_5)$. By construction, $H_n^{\text{ext}}$ has $O(n_v^2)$ edges and vertices. Each
population-level variations e.g. in [3]. It seems, however, that in the unrooted setting ternary rather than binary relationships. Median networks again appear as a natural generalization of trees. In fact they are used to describe population-level variations e.g. in [3]. It seems, however, that in the unrooted setting ternary rather than binary relationships.

Prime vertex \( v \in \mathcal{P} \) therefore can be replaced by \((G_*, t_*)\) with \( G_* \cong H^{irr}_{n2} \) in \( O(n_2^2) \) time. Repeating the latter for all prime vertices works thus in \( O(\sum_{v \in \mathcal{P}} n_2^2) \) \( \subseteq O(\sum_{v \in V} n_2^2) \) \( \subseteq O(|V| \sum_{v \in V} n_v) \) \( \subseteq O(|V| \sum_{v \in V} \deg(v)) \) \( \subseteq O(|V| |E(T_\delta)|) = O(|V|^2) = O(|X|^2) \) time. The total effort is therefore in \( O(|X|^2) \).

5 Future Directions

In summary, we have shown that labeled extended hypercubes, extended half-grids, and pvr graphs can be used to explain a given symmetric map \( \delta \). Clearly, pvr graphs with leaf set \( X \) have usually fewer vertices than extended half-grids \( H^c_{|X|} \), which in turn are much smaller than extended hypercubes \( G^c_{|X|} \). This begs the question under which conditions it is possible to further simplify a rooted median graph \((G, t)\) that explains a map \( \delta \). More precisely, a given labeled rooted median graph \((G, t)\) with leaf set \( X \) is least-resolved w.r.t. a given map \( \delta \) if it explains \( \delta \) and there is no labeled rooted median graph \((G', t')\) explaining \( \delta \) that can be obtained from \( G \) by edge contraction (and the removal of any multi-edge that may result in the process). Furthermore, let us say that \((G, t)\) is minimally-resolved w.r.t. \( \delta \), if it explains \( \delta \) and has among all labeled rooted median graphs with leaf set \( X \) that explain \( \delta \) the fewest number of vertices.

The graph in Fig. 5(right), for example, is obtained from the halfgrid in Fig. 5(middle) by contraction of two edges and removal of one of the resulting multi-edges connecting the root \( \rho \) and the purple-colored vertex. The resulting graph is still a median graph that explains \( \delta \). Hence, the halfgrid is not least-resolved w.r.t. the given map \( \delta \). The tree \((T_\delta, t_\delta)\) in Fig. 6 is least-resolved w.r.t. \( \delta \). It is not minimally resolved, however, since the median graph \((G, t)\) in Fig. 6 explains the same map \( \delta \) with fewer vertices. These example suggest to characterize least resolved and minimally resolved rooted median graphs that explain a given map \( \delta \). The example in Fig. 6 begs the question which symbolic ultrametrics can be explained by median graph with fewer vertices than the MDT or cotree?

The definition of minimal resolution suggested above above uses \( |V(G)| \) to measure the size of \((G, t)\). It may no be the most natural choice, however. As an alternative, one might want to consider median graphs with a minimal number of edges. Are the discriminating cotrees minimal explanations for symbolic ultrametrics if \( |E(G)| \) is used to quantify size?

A related topic for future work is the use of unrooted instead of rooted graphs as models of evolutionary relationships. Median networks again appear as a natural generalization of trees. In fact they are used to describe population-level variations e.g. in [3]. It seems, however, that in the unrooted setting ternary rather than binary
relations become the natural mathematical objects to encode events and properties. This line of reasoning has led to investigations into symbolic ternary metrics and the characterization of a generalization of symbolic ultrametrics [24, 40]. In [41] such relations are considered in the context of orthology in the setting of level-1 networks as a generalization of trees.

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