HALFSPACE REPRESENTATIONS OF PATH POLYTOPES OF TREES

FIND THE MOST UPDATED DRAFT AT HTTPS://TINYURL.COM/45UB4UWD

AMER GOEL, AIDA MARAJ, AND ÁLVARO RIBOT

ABSTRACT. Path polytopes are defined by indicator vectors that represent the paths between different leaves of a tree. They arise in polyhedral geometry and many applications, including phylogenetics, tropical geometry, and algebraic statistics. In this paper, we present a halfspace representation of these polytopes. We use the toric fiber product as an inductive tool to build polytopes, compute a characterization of their facets, and obtain their corresponding halfspaces.

1. INTRODUCTION

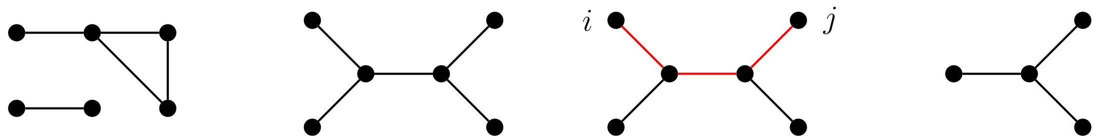
A polytope can be given by its vertex representation ($\mathcal{V}$-representation) or halfspace representation ($\mathcal{H}$-representation). The $\mathcal{V}$-representation describes a polytope as the convex hull of its vertices and the $\mathcal{H}$-representation defines a polytope as the intersection of halfspaces. Therefore, a $\mathcal{V}$-representation is a parametric description of the polytope, and an $\mathcal{H}$-representation is an implicit description of the polytope. We study *path polytopes* of trees, which are defined by their $\mathcal{V}$-representation as follows: given two distinct leaves i, j in a tree $T = (V, E)$, let $i \leftrightarrow j$ be the set of edges in the path between i and j, and let $\mathbf{c}^{i\leftrightarrow j} \in \{0, 1\}^{|E|}$ be the indicator vector for the edges used in $i \leftrightarrow j$. The path polytope of the tree T, denoted P_T, is the convex hull of the vectors $\mathbf{c}^{i\leftrightarrow j}$ for any two distinct leaves i, j in T. Our goal is to find its $\mathcal{H}$-representation.

Path polytopes arrive naturally in graph theory and combinatorics, but they also have diverse applications. In tropical geometry, the space of phylogenetic trees is parametrized by the path map [10], which coincides with the tropical Grassmanian of lines $\mathcal{G}_{2,n}$ [13]. A key motivation of this work is the growing recognition that many statistical models defined on trees or graphs are parametrized by paths between their nodes. Examples include Brownian motion tree models, where the parametrization is given by paths among leaves in a phylogenetic tree [1]; staged tree models, parametrized by the paths from the root to a leaf on a rooted tree [5]; and colored and standard Gaussian graphical models, parametrized by paths between any two nodes on a block graph [12, 2], among others.

Explicit descriptions of the halfspaces for P_T in terms of the tree structure provide a better understanding of the polytope and its applications. In general, polytopes arising from a monomial parametrization of log-linear models, such as our polytope induced by the path parametrization, have shown to be useful in Maximum Likelihood Estimation (MLE) problems [6, 7]. For example, given a normalized vector of counts for a log-linear model, the MLE exists if and only if this vector belongs to the relative interior of the corresponding polytope, and the halfspace description gives a membership test for the interior of the polytope. In fact, the path parametrization has already shown essential for all the progress related to the MLE of Brownian motion tree models [1, 3]. In [8], the authors use halfspace representations to learn causal polytree structures from a combination of observational and interventional data. Therefore, we anticipate that the halfspace representation of our path polytope will be valuable for statistical applications in the models discussed earlier.

The conversion from $\mathcal{V}$-representation to $\mathcal{H}$-representation, or the facet enumeration problem, is computationally expensive. The Fourier-Motzkin elimination algorithm [9] outputs the $\mathcal{H}$-representation given the vertices of the polytope, but its time complexity grows exponentially with the dimension of the polytope. Therefore, computing the $\mathcal{H}$-representation of path polytopes with this algorithm is infeasible for large trees.

Before presenting our main result, let us introduce the necessary notation. A *graph* is a tuple $G = (V, E)$ where V is a set of nodes and E is a set of unordered pairs of nodes, which are called edges. We assume $1 < |V| < \infty$. A *path* in a graph is a sequence of edges that connects a sequence of distinct nodes. A *tree* is a graph in which any pair of nodes is connected by exactly one path. A *star tree* on $n > 1$ leaves is $S_n = (\{v_0, v_1, \dots, v_n\}, \{\{v_0, v_i\} \mid 1 \leq i \leq n\})$. See Figure 1.



(A) Graph G. (B) Tree T. (C) Path $i \leftrightarrow j$ in T. (D) Star tree S_3.

FIGURE 1. Example of a graph, a tree, a path (highlighted in red), and a star tree.

Let T be a tree. Given a node v in T, let $N(v) = \{u \in V \mid \{u, v\} \in E\}$ be the neighborhood of v. The degree of a node v in T is $\deg(v) = |N(v)|$. A node is called a *leaf* if it has degree one. Let $\mathrm{Lv}(T) \subset V$ denote the set of leaves of T, and $\mathrm{Int}(T) = V \setminus \mathrm{Lv}(T)$ denote the set of internal nodes of T. Note that a tree T is a star tree if and only if $|\mathrm{Int}(T)| = 1$. Let $E_{\mathrm{leaf}}(T) = \{\{u, v\} \in E \mid u \in \mathrm{Lv}(T) \text{ or } v \in \mathrm{Lv}(T)\}$ be the set of edges that have a leaf as an endpoint. Let $\mathbb{R}^E$ be the vector space with basis elements indexed by the set E, so $P_T \subset \mathbb{R}^E$. Our main result is the following.

Theorem 1.1. *Given a tree $T = (V, E)$, an $\mathcal{H}$-representation of its path polytope P_T is given by*

$$\begin{cases} x_e & \geq 0 \quad \text{for all } e \in E \\ -x_{\{v,u\}} + \sum\limits_{w \in N(v) \setminus \{u\}} x_{\{v,w\}} & \geq 0 \quad \text{for all } v \in \mathrm{Int}(T) \text{ with } \deg(v) \geq 3 \text{ and all } u \in N(v) \\ -x_{\{v,u\}} + x_{\{v,w\}} & = 0 \quad \text{for all } v \in \mathrm{Int}(T) \text{ such that } N(v) = \{u, w\} \\ \sum\limits_{e \in E_{\mathrm{leaf}}(T)} x_e & = 2. \end{cases}$$

In particular, $\dim(P_T) = |E| - 1 - |\{v \in V \mid \deg(v) = 2\}|$.

Remark 1.2. Some of the inequalities $x_{\{v,u\}} \geq 0$ are redundant for nodes of degree 2. For example, let $v \in V$ with $N(v) = \{u, w\}$. Then $-x_{\{v,u\}} + x_{\{v,w\}} = 0$ and $x_{\{v,u\}} \geq 0$ imply $x_{\{v,w\}} \geq 0$. All other halfspaces are not redundant. The inequality $x_{\{v,u\}} \geq 0$ when $\deg(v) = 3$ is also satisfied by the polytope, but it is redundant. Internal nodes of degree 2 and 3 are special for the following reason. The polytope P_T is closely related to the second hypersimplex $\Delta_{n,2}$. We have $\dim(\Delta_{n,2}) = n - 1$ for all $n > 2$ while $\Delta_{2,2} = \{(1, 1)\}$ is 0-dimensional. Moreover, $\Delta_{n,2}$ has $2n$ facets for $n > 3$ while $\Delta_{3,2}$ has only 3 facets.

The intuition behind the $\mathcal{H}$-representation given in Theorem 1.1 is the following. First, in any path, an edge e must be used at least zero times. Second, any path that goes through an internal node v using the edge $\{v, u\}$ must leave that internal node using a different edge $\{v, w\}$, because we only consider paths between leaves. Third, we have a particular case of the second case for nodes v of degree 2: a path that goes through v uses either both edges that contain v or none of them. Finally, every path between two leaves uses exactly one edge per leaf, so exactly two of those edges must be used.

In view of the above, it is easy to check that every vertex in P_T satisfies the conditions implied by the $\mathcal{H}$-representation given in Theorem 1.1, so P_T is included in the polytope defined by that $\mathcal{H}$-representation. Our contribution is proving that these halfspaces are sufficient to define P_T. To do so, we explicitly compute a sufficient characterization facets of P_T using toric fiber products, and then prove that those facets, along with some hyperplanes that contain our entire polytope, produce our halfspace description, which makes it sufficient.

Structure of the paper. In Section 2 we review the literature on trees, polytopes and toric fiber products that is relevant for this paper. In Section 3 we show how to construct path polytopes inductively via toric fiber products. Finally, in Section 4, we describe the facets and their respective halfspaces of path polytopes of trees, which is our main result. We finish with a discussion of the extension of this work to block graphs.

2. Preliminaries

We begin with some useful results on trees, which are the kind of graph we study in this paper. We then show how to induce a polytope from a tree, and finally we introduce the toric fiber product, which is a convenient operation on polytopes. The main strategy we employ throughout the paper is induction, because trees, which are the base of our subsequent objects, can be constructed using induction.

2.1. Gluing of trees.

Here, we show how to construct trees using star trees. A star tree S_n is a tree with one internal node and n leaves, which are all connected to the internal node (see Figure 1d). We present a method to combine trees, called gluing. Then we use gluing to inductively deconstruct any tree into star trees, as follows.

Definition 2.1. Given two trees $T_1 = (V_1, E_1)$, $T_2 = (V_2, E_2)$, and two edges $e_1 \in E_{\text{leaf}}(T_1)$ and $e_2 \in E_{\text{leaf}}(T_2)$. The *gluing* of T_1 and T_2 along e_1, e_2 is the new tree $T = T_1 *_{e_1,e_2} T_2$ obtained as the disjoint union of T_1 and T_2 while identifying $e_1 \sim e_2$. That is, if $e_i = \{v_i, k_i\}$ with $k_i \in \mathrm{Lv}(T_i)$ for $i = 1, 2$, then $V(T) = (V_1 \sqcup V_2) \setminus \{k_1, k_2\}$ and $E(T) = (E_1 \cup E_2 \cup \{v_1, v_2\}) \setminus \{e_1, e_2\}$.

Example 2.2. The tree in Figure 1b can be obtained by gluing two star trees S_3 (Figure 1d).

Proposition 2.3. *Given a tree T with $k \geq 1$ internal nodes, $T = S_{n_1} *_{e'_1,e_2} S_{n_2} *_{e'_2,e_3} \cdots *_{e'_{k-1},e_k} S_{n_k}$, where each S_{n_j} is a star tree with $n_j \geq 2$ leaves.*

Proof. First, note that gluing any tree with S_1 leaves the tree unchanged, so we can assume $n_j \geq 2$ for all j. Each star tree appearing in the decomposition corresponds to an internal node of T. We prove this proposition by induction on $k = |\mathrm{Int}(T)|$. For the base case, let T have one internal node. Then T is a star tree by definition, so the base case holds. Now assume that for a tree T with k internal nodes, T can be decomposed as $T = S_{n_1} *_{e'_1,e_2} \ldots *_{e'_{k-1},e_k} S_{n_k}$, where $S_{n_1}, \ldots, S_{n_k}$ are star trees. Consider a tree T with $k+1$ internal nodes. Pick an internal node $v \in T$ such that all but one of its adjacent nodes are leaves. Such a node v always exists since $k + 1 \geq 2$. Let u be the non-leaf node adjacent to v. Define S as the subtree formed by v and all nodes adjacent to v (including the leaves and u), along with the edges connecting them. By construction, $S \cong S_{\deg(v)}$ is a star tree. Define T' as the tree obtained from T by removing the leaves adjacent to v. This leaves us with a tree T' with k internal nodes. By the inductive hypothesis, T' can be decomposed into star trees as $T' = S_{n_1} *_{e'_1,e_2} \dots *_{e'_{k-1},e_k} S_{n_k}$. Let $e'_k = \{u,v\} \in E(T')$ and let e_{k+1} be any edge from S. Then, T can be expressed by gluing T' and S along the edges e'_k, e_{k+1}, i.e. $T = T' *_{e'_k,e_{k+1}} S = S_{n_1} *_{e'_1,e_2} \dots *_{e'_{k-1},e_k} S_{n_k} *_{e'_k,e_{k+1}} S$. Therefore, T is a gluing of $k+1$ star trees. □

2.2. **Path polytopes on trees.** The primary objects of study in this paper are polytopes, which are geometric objects that can be described in two equivalent ways: the $\mathcal{V}$-representation and the $\mathcal{H}$-representation. The equivalence of these two descriptions is fundamental in polytope theory [15, Theorem 1.1]. We follow the notation from [15].

Definition 2.4. A set $P \subset \mathbb{R}^d$ is a *polytope* if there exist points $\mathbf{v}_1, \dots, \mathbf{v}_k \in \mathbb{R}^d$ such that

$$P = \operatorname{conv}(\{\mathbf{v}_1, \dots, \mathbf{v}_k\}) = \left\{ \sum_{i=1}^{k} \lambda_i \mathbf{v}_i \mid \lambda_i \geq 0, \sum_{i=1}^{k} \lambda_i = 1 \right\}$$

The set $\mathcal{V}(P) = \{\mathbf{v}_1, \dots, \mathbf{v}_k\}$ is called a $\mathcal{V}$- representation of P. Given a vector $\mathbf{a} \in \mathbb{R}^d$ and a scalar $b \in \mathbb{R}$, a linear inequality $\mathbf{a}^\top \mathbf{x} \leq b$ is *valid* for P if it is satisfied for all points $\mathbf{x} \in P$. A *face* of P is any set of the form

$$F = P \cap \{\mathbf{x} \in \mathbb{R}^d : \mathbf{a}^\top \mathbf{x} = b\}$$

where $\mathbf{a}^\top \mathbf{x} \leq b$ is a valid inequality for P. The *dimension* of a face F is the dimension of its affine hull $\operatorname{aff}(F)$, i.e. the smallest affine space containing F. We denote $\dim(F) = \dim(\operatorname{aff}(F))$. Similarly, the dimension of a polytope P is $\dim(\operatorname{aff}(P))$. A d-dimensional polytope is called a d-polytope. Given a face $F = P \cap \{x \in \mathbb{R}^d : \mathbf{a}^\top \mathbf{x} = b\}$, the equation $\mathbf{a}^\top \mathbf{x} = b$ is called the *supporting affine space* of F. A face F of dimension $d-1$ is called a *facet* of P, and a corresponding valid inequality $\mathbf{a}^\top \mathbf{x} \leq b$ is a *halfspace* of P. The set of affine spaces that contain P together with a set of halfspaces which describe the facets of P is called an $\mathcal{H}$-representation of P.

The class of polytopes we consider for this paper are *path polytopes*, which are geometric objects that encode the structure of a tree into a geometric object. Every tree induces a path polytope. These polytopes are defined parametrically, as the convex hull of vertices which are encodings of paths over a tree T. These vertices provide a $\mathcal{V}$-representation of the polytope. The goal of this paper is to find a $\mathcal{H}$-representation for path polytopes. The vertices of path polytopes are called *indicator vectors*, and they uniquely encode paths on the graph as binary-valued vectors that denote which edges are used in that path.

Definition 2.5. Consider a tree $T = (V,E)$. For two vertices $u, v \in V$, denote by $E(u \leftrightarrow v) \subseteq E$ the set of edges in the path connecting u and v. We define an *indicator vector* $\mathbf{c}^{T,u\leftrightarrow v} = (c_e)_{e \in E} \in \mathbb{R}^E$ such that $c_e = 1$ if $e \in E(u \leftrightarrow v)$ and $c_e = 0$ otherwise.

For simplicity, we will use $\mathbf{c}^{u\leftrightarrow v}$ instead of $\mathbf{c}^{T,u\leftrightarrow v}$ if there is no risk of ambiguity.

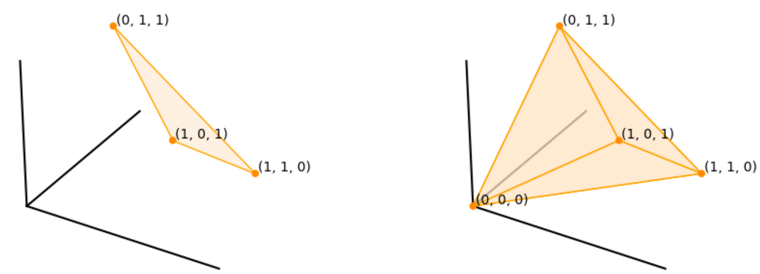
Definition 2.6. The *path polytope* of a tree $T = (V,E)$ is

$$P_T = \operatorname{conv}(\{\mathbf{c}^{i\leftrightarrow j} \mid i,j \in \operatorname{Lv}(T)\}) \subset \mathbb{R}^E.$$

It will become important for us to use the *free join* of two polytopes, which is a special kind of union that can be performed when the polytopes are in *skew* affine spaces. That is, when the two polytopes are in affine subspaces which do not intersect and are not parallel. When we take the union of two polytopes in skew affine subspaces, the result must increase in dimension.

Definition 2.7 (see [11])**.** If P, Q are two polytopes such that $\dim(\mathrm{conv}(P \cup Q)) = \dim(P) + \dim(Q) + 1$, we call $\mathrm{conv}(P \cup Q)$ the *free join* of P and Q, and denote it by $P \circledvee Q$.

Example 2.8. If Q is a point (0-polytope) not contained in a polytope P, then the free join $P \circledvee Q$ is a pyramid with basis P. See Figure 2.



(A) Polytope P_{S_3}. (B) Polytope $P_{S_3} \circledvee \{\mathbf{0}\}$.

FIGURE 2. Path polytope for the star tree S_3 (left), and free join of P_{S_3} and $\{\mathbf{0}\}$ (right). The coordinates correspond to ordering the edges lexicographically, i.e. points are of the form $\mathbf{x} = (x_{\{0,1\}}, x_{\{0,2\}}, x_{\{0,3\}}) \in \mathbb{R}^{|E|}$.

The following result describes the faces of the free join of two polytopes, which will become essential to construct path polytopes inductively.

Lemma 2.9 ([11, Proposition 2.1])**.** *The faces of $P \circledvee Q$ are precisely the sets of the form $F \circledvee G$, where F is a face of P and G is a face of Q (including $F = \emptyset$ or P, and $G = \emptyset$ or Q).*

There results are useful because our path polytope is *always* contained in an affine space which does not contain the origin. Because of that, it is *skew* with the origin, and a union with the origin is resultingly a *free join*.

Proposition 2.10. *Given a tree T with at least two edges, the polytope P_T lives in the hyperplane defined by $\sum_{e \in E_{\mathrm{leaf}}(T)} x_e = 2$. In particular,* $\mathrm{conv}(P_T \cup \{\mathbf{0}\}) = P_T \circledvee \{\mathbf{0}\}$.

Proof. By definition, $P_T = \mathrm{conv}(\{\mathbf{c}^{i \leftrightarrow j} \mid i \neq j \in \mathrm{Lv}(T)\})$. Every vertex $\mathbf{c}^{i \leftrightarrow j}$ satisfies the equation $\sum_{e \in E_{\mathrm{leaf}}(T)} x_e = 2$. Every point in the polytope is a convex combination of its vertices, so it also satisfies this equation. Hence, P_T lives in a hyperplane that does not contain the origin, so we have $\mathrm{conv}(P_T \cup \{\mathbf{0}\}) = P_T \circledvee \{\mathbf{0}\}$. □

2.3. **Toric Fiber Products on Polytopes.** Recall that path polytopes encode the combinatorial structure of paths in their corresponding trees, and thus capture the same underlying structural information. Consequently, operations on trees should have analogous counterparts for their induced polytopes. We note that we can build larger trees T from smaller ones $S_{n_1}, \ldots, S_{n_k}$ inductively using *gluing*. Then we will build P_T from the polytopes of the$P_{S_{n_1}}, \ldots, P_{S_{n_k}}$ inductively using an operation analogous to gluing. This ensures that the polytopes we produce through the operation are the correct polytope for T, because we will build P_T in an analogous way we built T, from analogous building blocks. We construct these polytopes inductively, instead of forming them explicitly from T so we can track their facets as we build them. At the end of our construction, this tracking will lead us to a complete, closed-form description of the facets of P_T, which we would not able to derive directly from T.

To start, we need an operation on polytopes which is analogous to gluing. For this we use the *toric fiber product* as it appears in [8], along with some adjustments, which gives us a $\mathcal{V}$-representation of the polytope resulting from a certain product of two polytopes. Note that this definition was first used by Dinu and Vodicka in [4], who expand on the facets of the product polytope and that toric fiber products were first constructed by Sullivant in [14]. Just as a tree T can be formed using gluing on stars $S_{n_1}, \ldots, S_{n_k}$, we will note that P_T will be retrieved from some adjustments of the toric fiber products on $P_{S_{n_1}}, \ldots, P_{S_{n_k}}$.

To define the toric fiber product, note that an *integral* polytope is a polytope whose vertices all have integer coordinates. Given an integral polytope $P \subset \mathbb{R}^n$, a projection $\pi : P \to \mathbb{R}^m$ is called integral if $\pi(P)$ is an integral polytope.

Definition 2.11. Given integral polytopes P_1 and P_2 and integral projections $\pi_1 : P_1 \to Q$ and $\pi_2 : P_2 \to Q$, the *toric fiber product* of P_1 and P_2 is

$$P_1 \times_Q P_2 = \operatorname{conv}(\{(\mathbf{x}, \mathbf{y}) \in \mathcal{V}(P_1) \times \mathcal{V}(P_2) \mid \pi_1(\mathbf{x}) = \pi_2(\mathbf{y})\}).$$

Definition 2.11 gives the toric fiber product product polytope $P_1 \times_Q P_2$ as a $\mathcal{V}$-representation. We will use this toric fiber product to construct path polytopes, for which we need a $\mathcal{H}$-representation. To achieve this, we first retrieve the facets, which is made possible by the following lemma using an integral projection onto a simplex.

Definition 2.12. Given two positive integers k, n, the (n, k)-*hypersimplex* is

$$\Delta_{n,k} = \left\{ (x_1, \ldots, x_n) \in \mathbb{R}^n \mid \sum_{i=1}^{n} x_i = k,\ 0 \le x_i \le 1 \text{ for all } i \right\}.$$

When $k = 1$, $\Delta_{n,1}$ is called the *standard simplex*.

Lemma 2.13 ([4, lemma 3.2])**.** *Let P_1 and P_2 be two polytopes. Let $\pi_i : P_i \to \mathbb{R}^n$, $(i = 1, 2)$ be integral projections such that $\pi_1(P_1) = \pi_2(P_2) = \Delta_{n,1}$. Then all facets of the toric fiber product $P_1 \times_{\Delta_{n,1}} P_2$ are of the form $F_1 \times_{\Delta_{n,1}} P_2$ or $P_1 \times_{\Delta_{n,1}} F_2$, where F_i is a facet of P_i.*

3. Path Polytopes of Trees via Toric Fiber Products

In this section, we use toric fiber products to combine path polytopes of smaller trees into the path polytope of a bigger tree. Specifically, if we take two trees T_1 and T_2 and glue them along an edge to form T, we can use the toric fiber product to input P_{T_1} and P_{T_2} and retrieve P_T. For our purposes, we need to specify the integral projections π_1 and π_2 to achieve our intended combination. Specifically, we define edges along which two trees T_1 and T_2 will be glued. These edges act as the "connections" between T_1 and T_2 in the resultant glued tree. The mappings π_1 and π_2 are constructed to ensure that any indicator vector $\mathbf{c}^{T_1, i \leftrightarrow j}$ that "connects" to T_2 through the specified edge is aligned with the corresponding vectors $\mathbf{c}^{T_2, i' \leftrightarrow j'}$ that "connects" back to T_1. These matched vectors form new indicator vectors $\mathbf{c}^{T, i \leftrightarrow j'}$ which describe connected paths in T that result from the gluing. Effectively, this matches the indicator vectors of paths that are glued together, forming a larger indicator vector of the glued path.

This is the desired result, because it matches vertices of P_{T_1} and P_{T_2}, which are indicator vectors over T_1 and T_2, to form vertices of a new polytope, according to the gluing of the tree. The resulting polytope's vertices will be the indicator vectors of all paths in T, which is by definition the $\mathcal{V}$-representation of P_T. Due to some concerns with dimensionality, this polytope is actually *isomorphic* to P_T, but this makes P_T easily retrievable. First we define our integral projections, which we call *gluing integral projections* because of how they mimic tree gluing on polytopes.

Definition 3.1. Consider two trees T_1 and T_2, and two edges $e_1 \in E_{\text{leaf}}(T_1)$ and $e_2 \in E_{\text{leaf}}(T_2)$. We call *gluing integral projections for* (T_1, T_2, e_1, e_2) to a pair of integral projections $\pi_i : P_{T_i} \circledvee \{\mathbf{0}\} \to \Delta_{3,1}$ $(i = 1, 2)$ such that $\pi_1(\mathbf{0}) = (0, 0, 1)$, $\pi_2(\mathbf{0}) = (1, 0, 0)$,

$$\pi_1(\mathbf{c}^{T_1,i\leftrightarrow j}) = \begin{cases} (1,0,0) & \text{if } e_1 \notin E(i \leftrightarrow j) \\ (0,1,0) & \text{if } e_1 \in E(i \leftrightarrow j), \end{cases} \qquad \pi_2(\mathbf{c}^{T_2,i\leftrightarrow j}) = \begin{cases} (0,1,0) & \text{if } e_2 \in E(i \leftrightarrow j) \\ (0,0,1) & \text{if } e_2 \notin E(i \leftrightarrow j). \end{cases}$$

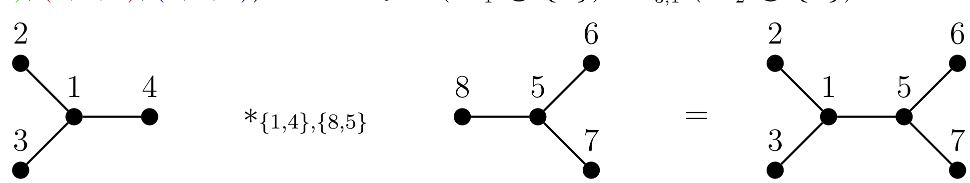
Example 3.2 (Gluing integral projection)**.** Let $\{\mathbf{b}_e^{(i)} \mid e \in E(T_i)\}$ denote the standard basis of $\mathbb{R}^{E(T_i)}$ for $i = 1, 2$. Let $\pi_i : \mathbb{R}^{E(T_i)} \to \mathbb{R}^3$ for $i = 1, 2$ be defined by

$$\pi_1(\mathbf{b}_e^{(1)}) = \begin{pmatrix} \frac{1}{2}\mathbb{1}[e \in E_{\text{leaf}}(T_1)] - \mathbb{1}[e = e_1] \\ \mathbb{1}[e = e_1] \\ -\frac{1}{2}\mathbb{1}[e \in E_{\text{leaf}}(T_1)] + 1 \end{pmatrix}, \quad \pi_2(\mathbf{b}_e^{(2)}) = \begin{pmatrix} -\frac{1}{2}\mathbb{1}[e \in E_{\text{leaf}}(T_2)] + 1 \\ \mathbb{1}[e = e_2] \\ \frac{1}{2}\mathbb{1}[e \in E_{\text{leaf}}(T_2)] - \mathbb{1}[e = e_2] \end{pmatrix}.$$

Here we will use the toric fiber product on modified polytopes $P_{T_1} \circledvee \{\mathbf{0}\}$ and $P_{T_2} \circledvee \{\mathbf{0}\}$. This is because using our toric fiber product without $\mathbf{0}$, paths in T_1 and T_2 which do not "connect" to the other tree are left unmatched. When we attempt use this toric fiber product matching to combine P_{T_1} and P_{T_2}, we see that those "non-connecting" paths are not included as indicator vectors in the resulting product polytope, which is supposed to be P_T. However, these leaf paths remain leaf paths in the glued tree T, and therefore must be included in P_T as indicator vectors. To remedy this, we include a null $\mathbf{0}$ vector in our polytopes that we can match with those non-gluing leaf paths of T_1 and T_2 so we can preserve them in P_T as we construct it using the toric fiber product.

Example 3.3. Here we show an example of how to use this toric fiber product to derive the $\mathcal{V}$-representation of the path polytope of a small tree T. The colors in the matrices correspond to vectors matched together by gluing integral projections π_1 and π_2.

Consider $T_1 = S_3$, with center 1 and leaves $2, 3, 4$. Consider $T_2 = S_3$, with center 5 and leaves $6, 7, 8$. We let $T = T_1 *_{\{1,4\},\{8,5\}} T_2$ (see Figure 3). We use the affine linear $\pi_1 : \mathbb{R}^3 \to \mathbb{R}^3$ and $\pi_2 : \mathbb{R}^3 \to \mathbb{R}^3$ defined above such that $\pi_1(P_{T_1} \circledvee \{\mathbf{0}\}) = \pi_2(P_{T_2} \circledvee \{\mathbf{0}\}) = \Delta_{3,1} = \text{conv}((1, 0, 0), (0, 1, 0), (0, 0, 1))$. We let $Q = (P_{T_1} \circledvee \{\mathbf{0}\}) \times_{\Delta_{3,1}} (P_{T_2} \circledvee \{\mathbf{0}\})$.



(A) Tree T_1. (B) Tree T_2. (C) Tree T.

FIGURE 3. Gluing T_1 and T_2 along edges $\{1, 4\}$ and $\{8, 5\}$ to form T.

$\mathcal{V}(P_{T_1} \circledvee \{\mathbf{0}\})$	$\mathbf{c}^{2\leftrightarrow 3}$	$\mathbf{c}^{2\leftrightarrow 4}$	$\mathbf{c}^{3\leftrightarrow 4}$	$\mathbf{0}$
{1,2}	1	1	0	0
{1,3}	1	0	1	0
{1,4}	0	1	1	0

$\mathcal{V}(P_{T_2} \circledvee \{\mathbf{0}\})$	$\mathbf{c}^{6\leftrightarrow 7}$	$\mathbf{c}^{8\leftrightarrow 6}$	$\mathbf{c}^{8\leftrightarrow 6}$	$\mathbf{0}$
{8,5}	0	1	1	0
{5,6}	1	1	0	0
{5,7}	1	0	1	0

$\mathcal{V}(Q)$	$\mathbf{c}^{2\leftrightarrow 3}$	$\mathbf{c}^{6\leftrightarrow 7}$	$\mathbf{c}^{2\leftrightarrow 6}$	$\mathbf{c}^{2\leftrightarrow 7}$	$\mathbf{c}^{3\leftrightarrow 6}$	$\mathbf{c}^{3\leftrightarrow 7}$
{1,2}	1	0	1	1	0	0
{1,3}	1	0	0	0	1	1
{1,4}	0	0	1	1	1	1
{8,5}	0	0	1	1	1	1
{5,6}	0	1	1	0	1	0
{5,7}	0	1	0	1	0	1

$\mathcal{V}(P_T)$	$\mathbf{c}^{2\leftrightarrow 3}$	$\mathbf{c}^{6\leftrightarrow 7}$	$\mathbf{c}^{2\leftrightarrow 6}$	$\mathbf{c}^{2\leftrightarrow 7}$	$\mathbf{c}^{3\leftrightarrow 6}$	$\mathbf{c}^{3\leftrightarrow 7}$
{1,2}	1	0	1	1	0	0
{1,3}	1	0	0	0	1	1
{1,5}	0	0	1	1	1	1
{5,6}	0	1	1	0	1	0
{5,7}	0	1	0	1	0	1

Notice from the above example that the toric fiber product polytope $(P_{T_1} \circledvee \{\mathbf{0}\}) \times_{\Delta_{3,1}} (P_{T_2} \circledvee \{\mathbf{0}\})$ is not exactly P_T, since the edge which becomes $\{1,5\}$ in T after gluing is duplicated as separate edges $\{1,4\}$ and $\{8,5\}$ from T_1 and T_2. However, this polytope is isomorphic to P_T, and it is simple to retrieve P_T from the toric fiber product polytope.

Theorem 3.4. *Consider a gluing of two trees $T = T_1 *_{e_1,e_2} T_2$. Let $\pi_i : P_{T_i} \circledvee \{\mathbf{0}\} \to \Delta_{3,1}$ $(i = 1,2)$ be a pair of gluing integral projections for (T_1, T_2, e_1, e_2). Then,*

$$P_T \cong (P_{T_1} \circledvee \{\mathbf{0}\}) \times_{\Delta_{3,1}} (P_{T_2} \circledvee \{\mathbf{0}\}).$$

Proof. Let $Q = (P_{T_1} \circledvee \{\mathbf{0}\}) \times_{\Delta_{3,1}} (P_{T_2} \circledvee \{\mathbf{0}\})$. It suffices to construct an affine transformation ϕ that establishes a bijection between the vertices of Q and the vertices of P_T. Let $e_1 = \{u_1, k_1\}, e_2 = \{u_2, k_2\}$ where $k_i \in \mathrm{Lv}(T_i)$ for $i = 1,2$. Let $\{\mathbf{a}_e \mid e \in E(T_1) \cup E(T_2)\}$ be the standard basis of $\mathbb{R}^{E(T_1)} \times \mathbb{R}^{E(T_2)} \cong \mathbb{R}^{E(T_1)\cup E(T_2)}$, and let $\{\mathbf{b}_e \mid e \in E(T)\}$ be the standard basis of $\mathbb{R}^{E(T)}$. Consider the afiine map given by $\phi(\mathbf{a}_{e_1}) = \phi(\mathbf{a}_{e_2}) = \frac{1}{2}\mathbf{b}_{\{u_1,u_2\}}$ and $\phi(\mathbf{a}_e) = \mathbf{b}_e$ if $e \neq e_1, e_2$.

The vertices of Q can be divided in three classes, one for each vertex of $\Delta_{3,1}$, according to Definition 3.1. First, given two distinct leaves $i, j \in \mathrm{Lv}(T_1) \setminus \{k_1\}$, the vertex $(\mathbf{c}^{T_1,i\leftrightarrow j}, \mathbf{0}) \in \mathcal{V}(Q)$ is mapped to $\mathbf{c}^{T,i\leftrightarrow j} \in \mathcal{V}(P_T)$ under ϕ. Second, given two distinct leaves $i, j \in \mathrm{Lv}(T_2) \setminus \{k_2\}$, the vertex $(\mathbf{0}, \mathbf{c}^{T_1,i\leftrightarrow j}) \in \mathcal{V}(Q)$ is mapped to $\mathbf{c}^{T,i\leftrightarrow j} \in \mathcal{V}(P_T)$ under ϕ. Finally, given $i \in \mathrm{Lv}(T_1) \setminus \{k_1\}$ and $j \in \mathrm{Lv}(T_2) \setminus \{k_2\}$ the vertex $(\mathbf{c}^{T_1,i\leftrightarrow k_1}, \mathbf{c}^{T_2,k_2\leftrightarrow j}) \in \mathcal{V}(Q)$ is mapped to $\mathbf{c}^{T,i\leftrightarrow j} \in \mathcal{V}(P_T)$ under ϕ. We have considered all the vertices of both Q and P_T, so $P_T \cong Q$. □

This gives us our desired result. Now, we can input P_{T_1} and P_{T_2} and retrieve P_T using the toric fiber product, which mimics the operation gluing on trees. We had to append $\mathbf{0}$ to account for unmatched paths, which is why we needed Definition 2.7, because as noted in Proposition 2.10,

P_T is skew with the origin. Now, when we need to add the origin as a null vector, our union is a free join. As noted in Lemma 2.13, this characterization is fortunate, since it will allow us to characterize the facets of these free-join polytopes, which is important in our halfspace representation. We also noted an isomorphism which results from the two edges being identified as one during gluing, allowing us to retrieve P_T from the toric fiber product polytope. We end the section with another result about isomorphism, which is not explicitly related to toric fiber products but will be important for our later characterization of facets.

Proposition 3.5. *If $T = T' *_{e_1,e_2} S_2$, then $P_T \cong P_{T'}$.*

Proof. Let $f \in E(T)$ be the edge resulting from identifying e_1 with e_2, and let $g \in E(T)$ be the edge in S_2 distinct from e_2. Let $\{\mathbf{a}_e \mid e \in E(T')\}$ be the standard basis of $\mathbb{R}^{E(T')}$, and let $\{\mathbf{b}_e \mid e \in E(T)\}$ be the standard basis of $\mathbb{R}^{E(T)}$. Consider the affine map $\phi : \mathbb{R}^{E(T')} \to \mathbb{R}^{E(T)}$ given by $\phi(\mathbf{a}_e) = \mathbf{b}_e$ if $e \neq e_1$ and $\phi(\mathbf{a}_{e_1}) = \mathbf{b}_f + \mathbf{b}_g$. The map ϕ is injective and maps the vertices of $P_{T'}$ to the vertices of P_T, so $P_T \cong P_{T'}$. □

4. Proof of our main theorem

In this section, we prove Theorem 1.1. We use the toric fiber product, along with facet-descriptions of our intermediate polytopes from Lemma 2.13 and Lemma 2.9 to create explicit descriptions for the facets of P_T.

Proposition 2.3 implies that all trees can decompose into star trees. The following result shows that Theorem 1.1 is true for star trees, which will serve as a base case of our inductive argument.

Lemma 4.1. *Let $S_n = (V, E)$ be the star tree on $n > 1$ leaves, and let v_0 be the only internal node of S_n, i.e. $N(v_0) = \mathrm{Lv}(S_n)$. Then, $P_{S_n} = \Delta_{n,2}$. In particular, if $n \geq 4$ an $\mathcal{H}$-representation of P_{S_n} is given by*

$$\begin{cases} x_e & \geq 0 \quad \text{for all } e \in E \\ -x_{\{v_0,k\}} + \sum\limits_{j \in N(v_0)\setminus\{k\}} x_{\{v_0,j\}} & \geq 0 \quad \text{for all } k \in N(v_0) \\ \sum_{e \in E} x_e & = 2. \end{cases}$$

The corresponding set of facets is $\mathcal{F} = \{F_e \mid e \in E\} \cup \{G_{(v_0,k)} \mid k \in N(v_0)\}$ where

$$F_e = \operatorname{conv}\left(\{\mathbf{c}^{i\leftrightarrow j} \mid i, j \in \mathrm{Lv}(S_n), e \notin E(i \leftrightarrow j)\}\right)$$
$$G_{(v_0,k)} = \operatorname{conv}\left(\{\mathbf{c}^{i\leftrightarrow k} \mid i \in \mathrm{Lv}(S_n) \setminus \{k\}\}\right).$$

When $n = 2$, P_{S_2} is a point. When $n = 3$, the first class of halfspaces is redundant and the F_e's are not facets, but the rest of the statement holds.

Proof. By construction, we have

$$\Delta_{n,2} = \operatorname{conv}\left(\left\{(x_{\{v_0,v_1\}}, \ldots, x_{\{v_0,v_n\}}) \in \{0,1\}^n \mid \sum_{e \in E} x_e = 2\right\}\right) = P_{S_n}.$$

The cases $n = 2, 3$ are trivial (see Figure 2). Assume that $n \geq 4$. For a star tree, $E_{\text{leaf}}(T) = E$, so $\sum_{e \in E} x_e = 2$, by Proposition 2.10. By definition of $\Delta_{n,2}$ (2.12), the halfspaces of P_{S_n} are $0 \leq x_e \leq 1$ for all $e \in E$. Subtracting $2x_e \leq 2$ from $\sum_{e \in E} x_e = 2$ we get the desired $\mathcal{H}$-representation. Finally, given an edge $e = \{v_0, k\}$ with $k \in \mathrm{Lv}(S_n)$, we have $F_e = P_{S_n} \cap \{x_e = 0\}$ and $G_{(v_0,k)} = P_{S_n} \cap \{x_e = 1\}$, so the statement follows. □

Now, we have all of the parts we need to contruct the facets of a path polytope P_T. We have the facets of the polytope of a star tree from Lemma 4.1, which will serve as the base case and the building blocks for our larger polytope. We have the toric fiber product, along with Definition 2.7 and Theorem 3.4, which we can use to combine these smaller polytopes into the polytope of P_T, and we have Lemma 2.9 and Lemma 2.13, which we can use to track the facets of P_T as we construct it through the process of the toric fiber product. We use these results to inductively construct the facets of any P_T.

Theorem 4.2. *Given a tree T, the facets of P_T are of the form*

$$\begin{aligned} F_e^T &= \operatorname{conv}\big(\{\mathbf{c}^{i\leftrightarrow j} \mid i,j \in \operatorname{Lv}(T), e \notin E(i \leftrightarrow j)\}\big) \\ G_{(v,u)}^T &= \operatorname{conv}\big(\{\mathbf{c}^{i\leftrightarrow j} \mid i,j \in \operatorname{Lv}(T), \{v,u\} \in E(i \leftrightarrow j)\} \\ &\qquad \cup \{\mathbf{c}^{i\leftrightarrow j} \mid i,j \in \operatorname{Lv}(T), \{v,w\} \notin E(i \leftrightarrow j) \text{ for any } w \in N_T(v)\}\big) \end{aligned}$$

for all $e \in E$, $v \in \operatorname{Int}(T)$ and $u \in N_T(v)$.

Proof. We prove it by strong induction on $r = |\operatorname{Int}(T)|$. The case $r = 1$ follows from Lemma 4.1. Suppose the claim holds for r and let T be $r+1$ nodes. By Proposition 2.3, let $T = T_1 *_{e_1,e_2} T_2$, where T_i is a tree with $r_i < r$ internal nodes for $i = 1,2$. Let $e_i = \{v_i, k_i\}$ with $k_i \in \operatorname{Lv}(T_i)$ for $i = 1,2$. For simplicity of notation, let $\tilde{P}_{T_i} = P_{T_i} \circledvee \{\mathbf{0}\}$. Hence, $P_T \cong \tilde{P}_{T_1} \times_{\Delta_{3,1}} \tilde{P}_{T_2}$ by Theorem 3.4. By Lemma 2.13, the facets of P_T are isomorphic to facets of the form $\{F_1 \times_{\Delta_{3,1}} \tilde{P}_{T_2} \mid F_1 \text{ facet of } \tilde{P}_{T_1}\}$ and $\{\tilde{P}_{T_1} \times_{\Delta_{3,1}} F_2 \mid F_2 \text{ facet of } \tilde{P}_{T_2}\}$. We consider the first case ($F_1 \times_{\Delta_{3,1}} \tilde{P}_{T_2}$) and, by symmetry, the same argument holds for the other facets.

By Lemma 2.9 and the induction hypothesis, the facets of $\tilde{P}_{T_1}$ are $F_e^{T_1} \circledvee \{\mathbf{0}\}$ and $G_{(v,u)}^{T_1} \circledvee \{\mathbf{0}\}$ for all $e \in E(T_1)$, $v \in \operatorname{Int}(T_1)$ and $u \in N_{T_1}(v)$, together with P_{T_1}.

First, fix an edge $e \in E(T_1)$. Then

$$\begin{aligned} (F_e^{T_1} \circledvee \{\mathbf{0}\}) \times_{\Delta_{3,1}} \tilde{P}_{T_2} = \operatorname{conv}\big(&\{(\mathbf{c}^{T_1,i\leftrightarrow k_1}, \mathbf{c}^{T_2,k_2\leftrightarrow j}) \mid \mathbf{c}^{T_1,i\leftrightarrow k_1} \in F_e^{T_1}, \mathbf{c}^{T_2,k_2\leftrightarrow j} \in P_{T_2}\} \\ &\cup \{(\mathbf{c}^{T_1,i\leftrightarrow j}, \mathbf{0}) \mid \mathbf{c}^{T_1,i\leftrightarrow j} \in F_e^{T_1}, i,j \neq k_1\} \\ &\cup \{(\mathbf{0}, \mathbf{c}^{T_2,i\leftrightarrow j}) \mid \mathbf{c}^{T_2,i\leftrightarrow j} \in P_{T_2}, i,j \neq k_2\}\big) \end{aligned}$$

which is isomorphic to F_e^T if $e \neq e_1$, and to $F_{\{u_1,u_2\}}^T$ if $e = e_1$. Second, fix $v \in \operatorname{Int}(T_1)$ and $u \in N_{T_1}(v)$. Then

$$\begin{aligned} (G_{(v,u)}^{T_1} \circledvee \{\mathbf{0}\}) \times_{\Delta_{3,1}} \tilde{P}_{T_2} = \operatorname{conv}\big(&\{(\mathbf{c}^{T_1,i\leftrightarrow k_1}, \mathbf{c}^{T_2,k_2\leftrightarrow j}) \mid \mathbf{c}^{T_1,i\leftrightarrow k_1} \in G_{(v,u)}^{T_1}, \mathbf{c}^{T_2,k_2\leftrightarrow j} \in P_{T_2}\} \\ &\cup \{(\mathbf{c}^{T_1,i\leftrightarrow j}, \mathbf{0}) \mid \mathbf{c}^{T_1,i\leftrightarrow j} \in G_{(v,u)}^{T_1}, i,j \neq k_1\} \\ &\cup \{(\mathbf{0}, \mathbf{c}^{T_2,i\leftrightarrow j}) \mid \mathbf{c}^{T_2,i\leftrightarrow j} \in P_{T_2}, i,j \neq k_2\}\big) \end{aligned}$$

which is isomorphic to $G_{(v,u)}^T$ if $(v,u) \neq (v_1,k_1)$, and to $G_{(v_1,v_2)}^T$ if $(v,u) = (v_1,k_1)$. Finally,

$$\begin{aligned} P_{T_1} \times_{\Delta_{3,1}} \tilde{P}_{T_2} = \operatorname{conv}\big(&\{(\mathbf{c}^{T_1,i\leftrightarrow k_1}, \mathbf{c}^{T_2,k_2\leftrightarrow j}) \mid i \in \operatorname{Lv}(T_1) \setminus \{k_1\}, j \in \operatorname{Lv}(T_2) \setminus \{k_2\}\} \\ &\cup \{(\mathbf{c}^{T_1,i\leftrightarrow j}, \mathbf{0}) \mid i,j \in \operatorname{Lv}(T_1) \setminus \{k_1\}\}\big) \end{aligned}$$

is included in $\tilde{P}_{T_1} \times_{\Delta_{3,1}} (G_{(v_2,k_2)}^{T_2} \circledvee \{\mathbf{0}\})$, which is isomorphic to $G_{(v_2,v_1)}^T$. ☐

This should be interpreted similar to 4.1. The facets of the tree path polytope,

$$\begin{aligned} F_e^T &= \operatorname{conv}\big(\{\mathbf{c}^{i\leftrightarrow j} \mid i,j \in \operatorname{Lv}(T), e \notin E(i \leftrightarrow j)\}\big)\\ G_{(v,u)}^T &= \operatorname{conv}\big(\{\mathbf{c}^{i\leftrightarrow j} \mid i,j \in \operatorname{Lv}(T), \{v,u\} \in E(i \leftrightarrow j)\}\\ &\qquad \cup \{\mathbf{c}^{i\leftrightarrow j} \mid i,j \in \operatorname{Lv}(T), \{v,w\} \notin E(i \leftrightarrow j) \text{ for any } w \in N(v)\}\big) \end{aligned}$$

Are analogous to the facets of the star tree path polytope

$$\begin{aligned} F_e &= \operatorname{conv}\left(\{\mathbf{c}^{i\leftrightarrow j} \mid i,j \in \operatorname{Lv}(S_n), e \notin E(i \leftrightarrow j)\}\right)\\ G_{(v_0,k)} &= \operatorname{conv}\left(\{\mathbf{c}^{i\leftrightarrow k} \mid i \in \operatorname{Lv}(S_n) \setminus \{k\}\}\right). \end{aligned}$$

An intuitive way of thinking is that each internal node v of T induces a star structure, with adjacent nodes $u \in N(v)$ starting branches of the star tree centered at v. This is analogous to collapsing all leaves passing through u on the path to v into a single leaf at node u, reducing the tree to a star tree. Instead of considering only the leaf $u \in N(v)$ as in the star tree, we consider any leaf in the branch starting at u, denoted $T_{v\to u}$, reflecting the induced star structure of the tree.

Now we are ready to form a complete $\mathcal{H}$-representation of P_T. Recall that this representation requires us to find two kinds of halfspaces: facet-defining halfspaces, which are inequalities satisfied by the entire polytope and are derived from its facets, and polytope-containing halfspaces, which are hyperplanes (equalities) that contain the polytope in a affine subspace. The intersection of all of these halfspaces defines the polytope.

We have everything we need to verify the facet-defining halfspaces as listed in Theorem 1.1. The points in F_e^T and $G_{(v_0,k)}^T$ will provide us with enough affinely independent points which satisfy each equality to prove those to be facet-defining linear spaces. Then, the fact that every point in the polytope satisfies the inequality proves those to each be halfspaces, which are members of the $\mathcal{H}$-representation. By Lemma 2.13, we know the sets F_e^T and $G_{(v_0,k)}^T$ to contain all facets of P_T, so they produce all facet-defining halfspaces of P_T. We will show their form in the full $\mathcal{H}$-representation in the proof of Theorem 1.1.

Before that, we must see if there are any polytope-containing hyperplanes, which must intersect with the facet-defining halfspaces of F_e^T and $G_{(v_0,k)}^T$ define a to completely define the polytope. We fully describe these hyperplanes in the following theorem. After we find those, we will have all inequalities (facet-defining halfspaces) and equalities (polytope-containing halfspaces) needed for a $\mathcal{H}$-representation.

Theorem 4.3. *Given a tree $T = (V,E)$ with $|V| > 2$, the dimension of the path polytope P_T is $|E(T)| - 1 - |\{v \in V \mid \deg(v) = 2\}|$, and P_T is contained in the linear space defined by*

$$\begin{cases} x_{\{v,u\}} - x_{\{v,w\}} &= 0 \quad \textit{for all } v \in \operatorname{Int}(V) \textit{ such that } N(v) = \{u,w\}\\ \sum_{e\in E_{\text{leaf}}(T)} x_e &= 2. \end{cases}$$

Proof. Let $v \in \operatorname{Int}(V)$ such that $N(v) = \{u,w\}$. Given any pair of distinct leaves $i,j \in \operatorname{Lv}(T)$, $\{v,u\} \in i \leftrightarrow j$ if and only if $\{v,w\} \in i \leftrightarrow j$. So $\mathbf{c}^{i\leftrightarrow j}_{\{v,u\}} - \mathbf{c}^{i\leftrightarrow j}_{\{v,w\}}$. Therefore, every point in the polytope satisfies the first set of equations. The polytope also satisfies the last equation by Proposition 2.10. All these equations are linearly independent, so the dimension of the polytope is at most $|E(T)| - 1 - |\{v \in V \mid \deg(v) = 2\}|$. We show that it is equal to this quantity.

Consider a gluing of two trees $T = T_1 *_{e_1,e_2} T_2$. Let $\pi_i : P_{T_i} \circledvee \{\mathbf{0}\} \to \Delta_{3,1}$ $(i = 1, 2)$ be a pair of gluing integral projections for (T_1, T_2, e_1, e_2). Then

$$\begin{aligned}\dim(P_T) &= \dim((P_{T_1} \circledvee \{\mathbf{0}\}) \times_{\Delta_{3,1}} (P_{T_1} \circledvee \{\mathbf{0}\})) = \\ &= \dim(P_{T_1} \circledvee \{\mathbf{0}\}) + (P_{T_2} \circledvee \{\mathbf{0}\}) - \dim(\Delta_{3,1}) = \\ &= \dim(P_{T_1}) + \dim(P_{T_2}),\end{aligned}$$

because $\dim((P_{T_1} \circledvee \{\mathbf{0}\}) \times_{\Delta_{3,1}} (P_{T_1} \circledvee \{\mathbf{0}\})) = \dim(P_{T_1} \circledvee \{\mathbf{0}\}) + (P_{T_2} \circledvee \{\mathbf{0}\}) - \dim(\Delta_{3,1})$ by [4], $\dim(\Delta_{3,1}) = 2$ and $\dim(P_{T_i} \circledvee \{\mathbf{0}\}) = \dim(P_{T_i}) + 1$ for $i = 1, 2$ by Definition 2.7. Therefore, if $T = S_{n_1} *_{e_1,e_2} \ldots *_{e_{r-1},e_r} S_{n_r}$ where S_{n_i} is a star tree, we have $\dim(P_T) = \sum_{i=1}^r \dim(P_{S_{n_i}})$ and $|E(T)| = 1 + \sum_{i=1}^r (n_i - 1)$. Finally, $\dim(P_{S_2}) = 0$ and $\dim(P_{S_n}) = n - 1$ for $n > 2$ by Lemma 4.1, so the statement follows. □

We are now ready to prove our main theorem, which describes all halfspaces that form a complete $\mathcal{H}$-representation of P_T.

Theorem 1.1. *Given a tree $T = (V, E)$, an $\mathcal{H}$-representation of its path polytope P_T is given by*

$$\begin{cases} x_e & \geq 0 \quad \text{for all } e \in E \\ -x_{\{v,u\}} + \sum\limits_{w \in N(v)\setminus\{u\}} x_{\{v,w\}} & \geq 0 \quad \text{for all } v \in \operatorname{Int}(T) \text{ with } \deg(v) \geq 3 \text{ and all } u \in N(v) \\ -x_{\{v,u\}} + x_{\{v,w\}} & = 0 \quad \text{for all } v \in \operatorname{Int}(T) \text{ such that } N(v) = \{u, w\} \\ \sum\limits_{e \in E_{\text{leaf}}(T)} x_e & = 2. \end{cases}$$

In particular, $\dim(P_T) = |E| - 1 - |\{v \in V \mid \deg(v) = 2\}|$.

Proof. Consider a tree $T = (V, E)$. The last two equalities come from Proposition 2.10 and Theorem 4.3. By Theorem 4.2, all the facets of P_T of the form F_e^T, and $G_{(u,v))}^T$ for all $e \in E$, $u \in \operatorname{Int}(T)$ and $v \in N(u)$. Recall that every vertex in the polytope satisfies the inequalities described above, so it enough to check that the facets satisfy them with equality. Fix an arbitrary edge $e \in E$, then $F_w^T = P_T \cap \{x_e = 0\}$. Fix $u \in \operatorname{Int}(T), v \in N(u)$, then

$$G_{(u,v)}^T = P_T \cap \{-x_{\{v,u\}} + \sum_{w \in N(v)\setminus\{u\}} x_{\{v,w\}} = 0\}.$$

This conclude the proof. □

Acknowledgments

AG and AM were supported by the National Science Foundation under Grant DMS-2306672. AG was supported by an REU at the University of Michigan funded under this grant. AR was supported by a fellowship from "la Caixa" Foundation (ID 100010434), with fellowship code LCF/BQ/EU23/12010097, and by an RCCHU fellowship. Most of the work was done in Pierce Hall (SEAS) at Harvard University. We thank Emma Cardwell for listening and the feedback during the weekly group meetings.

REFERENCES

[1] Tobias Boege, Jane Ivy Coons, Christopher Eur, Aida Maraj, and Frank Roettger. Reciprocal maximum likelihood degrees of brownian motion tree models. *Le Matematiche*, 76(2):383–398, 2021.

[2] Jane I Coons, Aida Maraj, Pratik Misra, and Miruna-Ştefana Sorea. Symmetrically colored gaussian graphical models with toric vanishing ideals. *SIAM Journal on Applied Algebra and Geometry*, 7(1):133–158, 2023.

[3] Jane Ivy Coons, Shelby Cox, Aida Maraj, and Ikenna Nometa. Maximum likelihood degrees of brownian motion tree models: Star trees and root invariance. *arXiv preprint arXiv:2402.10322*, 2024.

[4] Rodica Dinu and Martin Vodička. Gorenstein property for phylogenetic trivalent trees. *Journal of Algebra*, 575:233–255, 2021.

[5] Eliana Duarte and Christiane Görgen. Equations defining probability tree models. *Journal of Symbolic Computation*, 99:127–146, 2020.

[6] Eliana Duarte, Benjamin Hollering, and Maximilian Wiesmann. Toric fiber products in geometric modeling. In *International Conference on Geometric Science of Information*, pages 494–503. Springer, 2023.

[7] Stephen E Fienberg and Alessandro Rinaldo. Maximum likelihood estimation in log-linear models. *The Annals of Statistics*, pages 996–1023, 2012.

[8] Benjamin Hollering, Joseph Johnson, and Liam Solus. Hyperplane representations of interventional characteristic imset polytopes, 2024.

[9] Rui-Juan Jing, Marc Moreno Maza, and Delaram Talaashrafi. Complexity estimates for fourier-motzkin elimination. *arXiv preprint arXiv:1811.01510*, 2019.

[10] Diane Maclagan and Bernd Sturmfels. *Introduction to tropical geometry*, volume 161. American Mathematical Society, 2021.

[11] Peter McMullen. Constructions for projectively unique polytopes. *Discrete Mathematics*, 14:241–266, 1975.

[12] Pratik Misra and Seth Sullivant. Gaussian graphical models with toric vanishing ideals. *Annals of the Institute of Statistical Mathematics*, 73:757–785, 2021.

[13] David Speyer and Bernd Sturmfels. The tropical grassmannian. *Adv. Geom*, 4:389–411, 2004.

[14] Seth Sullivant. Toric fiber products. *arXiv preprint math/0602052*, 2006.

[15] Günter M Ziegler. *Lectures on polytopes*, volume 152. Springer Science & Business Media, 2012.

AMER GOEL, UNIVERSITY OF MICHIGAN

Email address: amergoel@umich.edu

AIDA MARAJ, MAX PLANCK INSTITUTE OF MOLECULAR CELL BIOLOGY AND GENETICS

Email address: maraj@mpi-cbg.de

ÁLVARO RIBOT, HARVARD UNIVERSITY

Email address: aribotbarrado@g.harvard.edu