

L-INFINITY OPTIMIZATION IN TROPICAL GEOMETRY AND PHYLOGENETICS

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ABSTRACT. We investigate uniqueness issues that arise in l^∞ -optimization to linear spaces and Bergman fans of matroids. For linear spaces, we give a polyhedral decomposition of \mathbb{R}^n based on the dimension of the set of l^∞ -nearest neighbors. This implies that the l^∞ -nearest neighbor in a linear space is unique if and only if the underlying matroid is uniform. For Bergman fans of matroids, we show that the set of l^∞ -nearest points is a tropical polytope and give an algorithm to compute its tropical vertices. A key ingredient here is a notion of topology that generalizes tree topology.

These results have practical implications for distance-based phylogenetic reconstruction using the l^∞ -metric. We analyze the possible dimensions of the set of l^∞ -nearest equidistant tree metrics to an arbitrary dissimilarity map and the number of tree topologies represented in this set. For both 3 and 4-leaf trees, we decompose the space of dissimilarity maps relative to the tree topologies represented.

1. INTRODUCTION

One approach to phylogenetic reconstruction is to use *distance-based* methods. Given a distance matrix consisting of the pairwise distances between n species, a distance-based method returns a tree metric or equidistant tree metric (ultrametric) that best fits the data. Typically, the distance matrix is constructed from biological data. It has been shown that both the set of equidistant tree metrics and the set of tree metrics have close connections to tropical geometry [4, 16]. Because addition in the tropical semiring is defined as taking the maximum of two elements, the l^∞ -metric offers an appealing choice as a measure of best fit for phylogenetic reconstruction. A connection between tropical convexity and l^∞ -optimization for equidistant tree metrics was demonstrated in [3].

Computing a nearest tree metric to a given distance matrix using the l^∞ -norm is NP-hard [1]. However, there exists a polynomial-time algorithm for computing an l^∞ -nearest *equidistant* tree metric [5]. Although the algorithm gives us a means to compute a nearest equidistant tree metric to an arbitrary point in $\mathbb{R}^{\binom{n}{2}}$ quickly, the set of nearest equidistant metrics is not in general a singleton. Indeed, it may be of high dimension or contain points corresponding to trees with entirely different topologies. Thus, for phylogenetic reconstruction, there may be several different trees that explain the data equally well from the perspective of the l^∞ -norm. Recent work has studied the properties of equidistant tree space with the l^∞ -norm [3, 12, 13] but to our knowledge the dimensions and topologies of the set of l^∞ -closest equidistant tree metrics have not been examined. Similarly, one might ask all of the same questions for tree metrics. Thus, we are motivated by the following problem.

Problem 1.1. Given a dissimilarity map $x \in \mathbb{R}^{\binom{n}{2}}$, describe the set of (equidistant) tree metrics that are nearest to x in the l^∞ -metric.

For both equidistant tree metrics and tree metrics, we obtain results concerning the dimensions of these sets as well as the tree topologies involved. Since the set of tree metrics and the set of equidistant tree metrics on n species are both polyhedral complexes, we begin by addressing the following problem as a stepping stone.

Problem 1.2. Given a point $x \in \mathbb{R}^n$ and a linear space $L \subseteq \mathbb{R}^n$, describe the subset of L consisting of points that are nearest to x in the l^∞ -metric.

Just as with tree metrics, the l^∞ -infinity nearest point in a linear space is not unique in general. We give a polyhedral decomposition of \mathbb{R}^n based on the dimension of the set of points in L that are l^∞ -nearest to x . One particularly nice implication of this decomposition is the following.

Theorem 2.9. *Let $L \subseteq \mathbb{R}^n$ be a linear space. Then the l^∞ -nearest point to x in L is unique for all $x \in \mathbb{R}^n$ if and only if the matroid underlying L is uniform.*

The set of all equidistant tree metrics on n leaves is the Bergman fan of the matroid underlying the complete graph on n vertices [4]. Therefore, in the course of addressing Problem 1.1 for equidistant tree metrics, we will also consider the following more general problem.

Problem 1.3. Given a matroid \mathcal{M} on ground set E and a point $x \in \mathbb{R}^E$, describe the subset of the Bergman fan $\tilde{\mathcal{B}}(\mathcal{M})$ consisting of points that are l^∞ -nearest to x .

The Bergman fan of a matroid is a subfan of the corresponding matroid polytope [7] that plays an important role in tropical geometry. For example, tropical varieties defined by linear equations with constant coefficients, as well as recession cones of arbitrary tropical linear spaces, are Bergman fans of their underlying matroids [17, 10]. We show that the set of closest points to a Bergman fan of a matroid is a tropical polytope and we give an algorithm for determining its tropical vertices. A key ingredient here is a notion of topology that helps visualize the structure of a particular element of the Bergman fan of a matroid. This notion generalizes the topology of a rooted tree metric and induces a polyhedral subdivision of the Bergman fan that coincides with what is known as the “coarse subdivision” in the literature [4, 9].

We use our results to construct explicit examples that demonstrate some of the pathologies of using the l^∞ -metric for phylogenetic reconstruction. For example, we show that there is a full dimensional set of dissimilarity maps in $\mathbb{R}^{\binom{n}{2}}$ for which the set of l^∞ -closest equidistant tree metrics has dimension $n - 2$. In the case of 4-leaf trees, we also provide a decomposition of $\mathbb{R}^{\binom{4}{2}}$ according to the topologies of the set of closest tree metrics.

We begin in Section 2 with our results on l^∞ -optimization to linear spaces. In particular, we give a natural way to assign a combinatorial type to each $x \in \mathbb{R}^n$ with respect to some linear subspace $L \subseteq \mathbb{R}^n$. We show that this combinatorial type gives a polyhedral decomposition of \mathbb{R}^n based on the dimension of the set of l^∞ -nearest neighbors in L from which Theorem 2.9 follows. Section 3 sketches the necessary background from tropical

geometry and contains our results on l^∞ -optimization to Bergman fans of matroids. We show that the set of l^∞ -nearest neighbors in a Bergman fan to a given x is a tropical polytope and we give an algorithm to find its tropical vertices. Section 4 applies the results and ideas from earlier sections to phylogenetics. We investigate questions that would be of practical interest for phylogenetic reconstruction such as dimension and tree topologies contained in the set of closest rooted tree metrics. We conclude by exploring using the l^∞ -norm as a distance-based method for reconstructing tree metrics.

2. l^∞ -OPTIMIZATION TO LINEAR SPACES

Given a linear space $L \subseteq \mathbb{R}^n$, there is a natural way to assign a sign vector in $\{+, -, 0\}^n$ to each $x \in \mathbb{R}^n$. The sign vectors that appear in this way are precisely the elements of the oriented matroid associated to L . For each $x \in \mathbb{R}^n$, the associated sign vector encodes information about the dimension of the set of l^∞ -nearest points to x in L .

We begin this section by reviewing the necessary background from oriented matroid theory. More details can be found in [18, Ch. 6 and 7].

2.1. Background on Oriented Matroids. For any real number $r \in \mathbb{R}$, $\text{sign}(r) \in \{+, -, 0\}$ is the *sign of* r . For a linear functional $c \in (\mathbb{R}^n)^*$, $\text{sign}(c) \in \{+, -, 0\}^n$ is defined by $\text{sign}(c)_i = \text{sign}(c_i)$. Given a sign vector $\sigma \in \{+, -, 0\}^n$, we define $|\sigma| := \#\{i : \sigma_i \neq 0\}$. For a linear space $L \subseteq \mathbb{R}^n$ the *oriented matroid associated to* L , denoted \mathcal{O}_L , is the set of all sign vectors in $\{+, -, 0\}^n$ such that $s = \text{sign}(c)$ for some linear functional $c \in (\mathbb{R}^n)^*$ that vanishes on L .

The elements of an oriented matroid \mathcal{O} are the *signed vectors* of \mathcal{O} . Let \prec^* be the partial order on $\{+, -, 0\}$ given by $0 \prec +$ and $0 \prec -$ with $+$ and $-$ incomparable. Then \prec is the partial order on $\{+, -, 0\}^n$ that is the cartesian product of \prec^* n times. The *signed circuits* of an oriented matroid \mathcal{O} are the signed vectors of \mathcal{O} that are minimal with respect to \prec .

An oriented matroid can also be derived from a *zonotope*, the image of a cube under an affine map. Let $C_\delta(x) \subseteq \mathbb{R}^n$ denote the cube of side length δ centered at x . That is,

$$C_\delta(x) = \{y \in \mathbb{R}^n : |y_i - x_i| \leq \delta, i = 1 \dots, n\}.$$

To each face F of $C_\delta(x)$, associate a sign vector $\text{sign}(F) \in \{+, -, 0\}^n$ as follows

$$\text{sign}(F)_i = \begin{cases} + & \text{if } y_i = x_i + \delta \text{ for all } y \in F \\ - & \text{if } y_i = x_i - \delta \text{ for all } y \in F \\ 0 & \text{otherwise.} \end{cases}$$

Figure 1 gives an illustration of the sign vectors associated to a square.

Let $V \in \mathbb{R}^{(n-d) \times n}$ be a matrix of full row rank and $\pi : \mathbb{R}^n \rightarrow \mathbb{R}^{n-d}$ an affine map, $\pi(x) = Vx - z$. Fix $x \in \mathbb{R}^n$ and $\delta > 0$, then $\pi(C_\delta(x)) \subset \mathbb{R}^{n-d}$ is a polytope, called a *zonotope associated to* V . The inverse image of each face of the zonotope is a face of $C_\delta(x)$. Thus, for each face G of $\pi(C_\delta(x))$, we define $\text{sign}(G) := \text{sign}(\pi^{-1}(G))$. The collection of all such sign vectors is an oriented matroid which only depends on the matrix V and so we denote it \mathcal{O}_V . The following proposition relates oriented matroids from zonotopes to oriented matroids from linear spaces.

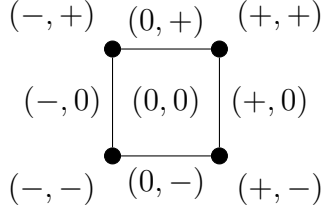


FIGURE 1. Sign vectors corresponding to faces of a square

Proposition 2.1 ([18], Corollary 7.17). *Let $V \in \mathbb{R}^{(n-d) \times n}$ be a matrix of full row rank. Then $\mathcal{O}_V = \mathcal{O}_{\ker V}$.*

Given an oriented matroid $\mathcal{O} \subseteq \{+, -, 0\}^n$ and $\sigma \in \mathcal{O}$, we define the *support* of σ , denoted $\text{supp}(\sigma)$ to be the set of indices of σ that are nonzero. That is, $\text{supp}(\sigma) := \{i \in \{1, \dots, n\} : \sigma_i \neq 0\}$. Then the collection of subsets of $\{1, \dots, n\}$ that are supports of elements of \mathcal{O} forms a matroid, denoted $\mathcal{M}_{\mathcal{O}}$, which we call the *matroid underlying \mathcal{O}* . When \mathcal{O} is associated to a linear space L , that is $\mathcal{O} = \mathcal{O}_L$, we simplify notation and write \mathcal{M}_L instead of $\mathcal{M}_{\mathcal{O}_L}$. For more background on matroids, see [14].

2.2. l^∞ -Optimization to Linear Spaces. In the rest of this section, we will use the language of matroids to state our main results for linear spaces. Before we begin, we establish some notation that will be used throughout the entire paper.

Definition 2.2. Let $S \subseteq \mathbb{R}^n$ be an arbitrary set, and let $x, z \in \mathbb{R}^n$. We denote the l^∞ -distance from x to z by $d(x, z)$, the l^∞ -distance from x to S by $d(x, S)$ and the set of all points in S closest to x by $C(x, S)$. That is

$$d(x, z) := \sup_i |x_i - z_i| \quad d(x, S) := \inf_{y \in S} d(x, y) \quad C(x, S) := \{y \in S : d(x, y) = d(x, S)\}.$$

Note that $C(x, S) = C_{d(x, S)}(x) \cap S$. Furthermore, when S is a linear space, there exists a unique minimal face F of $C_{d(x, S)}(x)$ that contains $C(x, S)$. We use the sign vector $\text{sign}(F)$ to give each $x \in \mathbb{R}^n$ a combinatorial type as in the following definition.

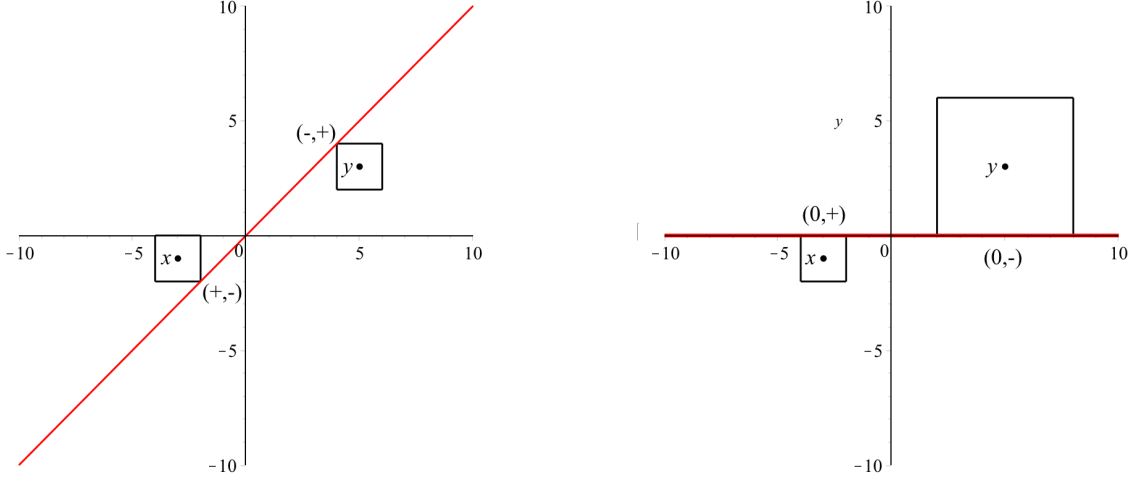
Definition 2.3. Let L be a linear space and F the minimal face of $C_{d(x, L)}(x)$ containing L . The *type of x with respect to L* is $\text{type}_L(x) := \text{sign}(F)$.

Example 2.4. Consider linear spaces $L_1 = \{(t, t) \in \mathbb{R}^2 : t \in \mathbb{R}\}$ and $L_2 = \{(t, 0) \in \mathbb{R}^2 : t \in \mathbb{R}\}$ and let $x = (5, 3)$ and $y = (-3, -1)$. Then $\text{type}_{L_1}(x) = (+, -)$, $\text{type}_{L_1}(y) = (-, +)$, $\text{type}_{L_2}(x) = (0, +)$, and $\text{type}_{L_2}(y) = (0, -)$. See Figure 2 for an illustration.

We will see that the sign vectors arising as types of a linear space are precisely the vectors in its oriented matroid. To aid in the proof we introduce the following convention for generating a vector with a given sign signature.

Definition 2.5. For $\sigma \in \{0, -, +\}^n$, $u(\sigma)$ is the vector in \mathbb{R}^n with

$$u(\sigma)_i := \begin{cases} 1 & \text{if } \sigma_i = + \\ -1 & \text{if } \sigma_i = - \\ 0 & \text{if } \sigma_i = 0 \end{cases}.$$

FIGURE 2. Types of x and y with respect to L_1 and L_2

Lemma 2.6. *Let $L \subseteq \mathbb{R}^n$ be a linear space. Then the sign vectors that can arise as the type of a point with respect to L are precisely the elements of the oriented matroid associated to L . That is,*

$$\mathcal{O}_L = \{\text{type}_L(x) : x \in \mathbb{R}^n\}.$$

Proof. Let $\sigma \in \mathcal{O}_L$ and let $c \in L^\perp$ with $\text{sign}(c) = \sigma$. First we claim that $d(-u(\sigma), L) = 1$ with $\mathbf{0} \in C(-u(\sigma), L)$. To see that $d(-u(\sigma), L) \leq 1$, note that $d(-u(\sigma), \mathbf{0}) = 1$. If $x \in \mathbb{R}^n$ and $d(-u(\sigma), x) < 1$, then for each index i , $\text{sign}(x_i) = -\sigma_i$. Therefore, $cx > 0$ which implies $x \notin L$. Thus, $d(x, L) = 1$.

We claim that $\text{type}_L(-u(\sigma)) = \sigma$. Observe that

$$F = \{x \in C_1(-u(\sigma)) : x_i = 0 \text{ whenever } \sigma_i \neq 0\}$$

is a face of $C_1(-u(\sigma))$ with $\text{sign}(F) = \sigma$. If $x \in C(-u(\sigma), L)$ then $x \in L$ so $cx = 0$ and $d(-u(\sigma), x) = 1$. These two conditions imply that $x \in F$, so $C(-u(\sigma), L) \subseteq F$. Note that $\mathbf{0} \in C(-u(\sigma), L)$ and since $\mathbf{0} = -u(\sigma) + u(\sigma)$, F is the minimal face of $C(-u(\sigma), L)$ containing $\mathbf{0}$. Hence, $\text{type}_L(-u(\sigma)) = \sigma$.

Now let $x \in \mathbb{R}^n$, we will show that $\text{type}_L(x) \in \mathcal{O}_L$. Assume L has dimension d and let $V \in \mathbb{R}^{(n-d) \times n}$ be a matrix whose rows form a basis for L^\perp . Let $\pi : \mathbb{R}^n \rightarrow \mathbb{R}^{n-d}$ be the map $x \mapsto Vx$. Let F be the minimal face of $C_{d(x,L)}(x)$ that contains $C(x, L)$ so that $\text{type}(x) = \text{sign}(F)$. Then there exists some $c \in (\mathbb{R}^n)^*$ in the row-span of V such that the hyperplane $\{y \in \mathbb{R}^n : cy = 0\}$ is a face-defining hyperplane for F . So we may write $c = bV$ for some $b \in (\mathbb{R}^{n-d})^*$.

Let π be the linear map defined by $y \mapsto Vy$. Then $\pi(F)$ is a face of the zonotope $\pi(C_{d(x,L)})$ with face-defining hyperplane b . Furthermore, we claim that $\pi^{-1}(\pi(F)) = F$. If $y \in \pi^{-1}(\pi(F))$ then $Vy \in \pi(F)$ so $b(Vy) = cy = 0$ and so $y \in F$. Therefore $\text{sign}(\pi^{-1}(\pi(F))) = \text{sign}(F)$, so Proposition 2.1 implies that $\text{type}(x) = \text{sign}(F) \in \mathcal{O}_L$. \square

As we show in the following theorem, the dimension of $C(x, L)$ depends entirely on $\text{type}_L(x)$. For any $\sigma \in \mathcal{O}_L$, the *rank* of σ in \mathcal{O}_L , denoted $\text{rank}(\sigma)$, is the rank of the

support of σ in the matroid underlying \mathcal{O}_L . So $\text{rank}(\sigma)$ is the smallest number k such that there exists indices i_1, \dots, i_k with $\sigma_{i_j} \neq 0$ and for all $y \in L$, if $y_{i_1} = \dots = y_{i_k} = 0$, then $y_j = 0$ for $\sigma_j \neq 0$.

Theorem 2.7. *Let $L \subset \mathbb{R}^n$ be a linear space of dimension d and let $\sigma \in \mathcal{O}_L$ be a sign vector in the oriented matroid associated to L . If $x \in \mathbb{R}^n$ has $\text{type}_L(x) = \sigma$, then the collection of l^∞ -nearest points to x in L has dimension $d - \text{rank}(\sigma)$.*

Proof. Let $L(\sigma)$ denote the linear space obtained by intersecting L and the $|\sigma|$ hyperplanes $\{x \in \mathbb{R}^n : x_i = 0\}$ for $\sigma_i \neq 0$. We claim that if $x \in \mathbb{R}^n$ with $\text{type}_L(x) = \sigma$, then $\dim C(x, L) = \dim L(\sigma)$.

Suppose $\text{type}(x) = \sigma$, and let F be the minimal face of $C_{d(x,L)}(x)$ containing $C(x, L)$. Let y be a point in $C(x, L)$ that is also in the interior of F . Then given any point $z \in L(\sigma)$, it is possible to choose ε so that $y + \varepsilon z \in F$ and hence in $C(x, L)$. Therefore, $\dim C(x, L) \geq \dim L(\sigma)$. Moreover, given any two points in $C(x, L)$, both are contained in F and L and so they differ only by an element of $L(\sigma)$. Therefore, $\dim C(x, L) \leq \dim L(\sigma)$.

We now show that $\dim(L(\sigma)) = d - \text{rank}(\sigma)$. Let $k := \text{rank}(\sigma)$ and let i_1, \dots, i_k be indices such that for all $y \in L$, $y_{i_1} = \dots = y_{i_k} = 0$ implies $y_j = 0$ when $\sigma_j \neq 0$. So $L(\sigma)$ is the intersection of L with the hyperplanes $\{x \in \mathbb{R}^n : x_{i_j} = 0\}$, and by minimality of rank, no subset of these hyperplanes has this property. So $\dim(L(\sigma)) = d - \text{rank}(\sigma)$. \square

Example 2.8. Let $L := \{(t, t, 0) \in \mathbb{R}^3 : t \in \mathbb{R}\}$. Consider the points $x = (0, 0, -1)$ and $y = (6, 4, 0)$. Then $\text{type}_L(x) = (0, 0, +)$ and $\text{type}_L(y) = (-, +, 0)$. Since $\text{rank}(0, 0, -) = 0$ and $d = 1$, Theorem 2.7 tells us that $\dim(C(x, L)) = 1$. Since $\text{rank}(+, -, 0) = 1$, Theorem 2.7 tells us that $\dim(C(y, L)) = 0$. Figure 3 shows x and y each surrounded by a cube of side length 1 (colored red and light blue, respectively). The intersections with L are $C(x, L)$ and $C(y, L)$.

We can use the structure of the matroid \mathcal{M}_L to glean information about possible values of $\dim(C(x, L))$. Let $U_{d,n}$ denote the uniform matroid of rank d on ground set $\{1, \dots, n\}$; that is, the circuits of $U_{d,n}$ are all $d + 1$ -element subsets of $\{1, \dots, n\}$.

Theorem 2.9. *Let $L \subseteq \mathbb{R}^n$ be a linear space. Then the l^∞ -nearest point to x in L is unique for all $x \in \mathbb{R}^n$ if and only if the matroid underlying L is uniform.*

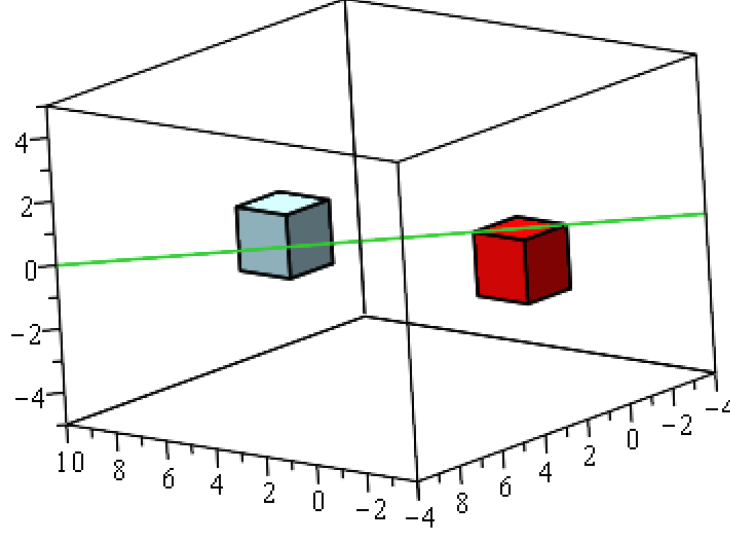
Proof. Let d be the dimension of L . If \mathcal{M}_L is not uniform, then \mathcal{O}_L has a circuit σ with $|\sigma| \leq d$, so $\text{rank}(\sigma) \leq d - 1$. Then Lemma 2.6 and Theorem 2.7 imply that there exists a point $x \in \mathbb{R}^n$ such that $\dim C(x, L) = d - \text{rank}(\sigma) \geq 1$.

If $\mathcal{M}_L = U_{d,n}$ then $\text{rank}(\sigma) = d$ for all $\sigma \in \mathcal{O}_L$. Theorem 2.7 implies that $\dim(C(x, L)) = 0$ for all $x \in \mathbb{R}^n$. \square

Lemma 2.6 enables us to give a partition of \mathbb{R}^n by type with respect to L .

Proposition 2.10. *Let $L \subseteq \mathbb{R}^n$ be a linear space and let $\sigma \in \mathcal{O}_L$ be a sign vector in the oriented matroid associated to L . Then the set of all points in \mathbb{R}^n with type σ with respect to L is $L + \text{int}(\text{cone}(\{-u(\tau) : \sigma \preceq \tau\}))$.*

Proof. Let $\sigma \in \mathcal{O}_L$. Define $\mathcal{V}_\sigma := \{-u(\tau) : \sigma \preceq \tau\}$. First, we will show that everything in $L + \text{Int}(\text{cone}(\mathcal{V}_\sigma))$ has type σ . Since adding an element of L to an element does not

FIGURE 3. L and cubes around $(0, 0, -1)$ and $(6, 4, 0)$

change its type with respect to L , it will suffice to show everything in $\text{Int}(\text{cone}(\mathcal{V}_\sigma))$ has type σ .

Let $x \in \text{Int}(\text{cone}(\mathcal{V}_\sigma))$. Then there exists $\alpha > 0$ such that if $\sigma_i = +$ or $\sigma_i = -$, then $|x_i| = \alpha$ and $|x_i| < \alpha$ otherwise. By Lemma 2.6, there exists $c \in (\mathbb{R}^n)^*$ such that $\text{sign}(c) = \sigma$ and $cy = 0$ for all $y \in L$. Let $\mathcal{H}_c := \{y \in \mathbb{R}^n : cy = 0\}$ be the hyperplane defined by c . It is clear that $d(x, \mathcal{H}_c) = \alpha$, and any $y \in C(x, \mathcal{H}_c)$ must have $y_i = 0$ if $|x_i| = \alpha$. Since $L \subseteq \mathcal{H}_c$, the same is true for each $y \in C(x, L)$. Therefore, if $\sigma_i = +$ or $\sigma_i = -$, then $\sigma_i = \text{type}(x)_i$.

Since $d(x, \mathcal{H}_c) = \alpha$ and $L \subseteq \mathcal{H}_c$, $d(x, L) \geq \alpha$. Since $d(x, \mathbf{0}) = \alpha$ and $\mathbf{0} \in L$, this implies $d(x, L) = \alpha$ and $\mathbf{0} \in C(x, L)$. If $\sigma_i = 0$ then $|x_i - 0| = |x_i| < \alpha$, which implies that if $\sigma_i = 0$, $\text{type}(x)_i = 0$. Thus, $\text{type}(x) = \sigma$.

To see that everything of type σ is contained in $L + \text{Int}(\text{cone}(\mathcal{V}_\sigma))$, let x be such that $\text{type}_L(x) = \sigma$. By definition of type, this means that σ is the unique sign vector such that if F is the face of the unit cube $C_1(\mathbf{0})$ with type σ , then there exists some $y \in \text{Int}(F)$ such that $x + \lambda y \in L$ for some $\lambda > 0$. So there exists some $l \in L$ such that $x = l + \lambda(-y)$ thus showing that $x \in L + \text{Int}(\text{cone}(\mathcal{V}_\sigma))$. \square

There is a natural way to think about the type of $x \in \mathbb{R}^n$ in terms of the zonotope obtained by projecting the cube $C_{d(x,L)}(x)$ onto L^\perp . Namely, if V is a matrix whose rows span L^\perp , then Vx lies in the relative interior of a unique cone in the face fan of $Z(V)$. Then $\text{type}_L(x)$ is equal to the sign of the corresponding face of $Z(V)$.

The signs of the facets of $Z(V)$ correspond to circuits of \mathcal{O}_L [18, Corollary 7.17]. This implies that the full dimensional cones of the partition correspond to circuits. Hence $\text{type}_L(x)$ is generically a circuit of \mathcal{O}_L .

3. l^∞ -OPTIMIZATION TO BERGMAN FANS OF MATROIDS

Ardila and Klivans show in [4] that the set of rooted tree metrics on n leaves is the Bergman fan of the matroid underlying the complete graphs on n vertices. Thus, before we study the problem of l^∞ -optimization to the set of rooted tree metrics, we will consider the more general problem of optimizing to a Bergman fan. Section 3.1 offers a brief review of the basics of tropical geometry, including tropical convexity, and Section 3.2 gives our results.

We begin Section 3.2 by reviewing the basics of Bergman fans of matroids. We then show that the set of points in a Bergman fan closest to a given point in the l^∞ -norm is a tropical polytope. We introduce a notion of topology for points in an arbitrary Bergman fan which helps us visualize the structure of such points. This generalizes the notion of tree topology for equidistant tree metrics. We then lay the groundwork for Algorithm 1, which takes an arbitrary point and a Bergman fan and computes a tropical V -description of this polytope. We close by showing that the polyhedral subdivision of a Bergman fan induced by topology is coarsest possible.

3.1. Tropical Geometry. The *tropical semiring*, also known as the max-plus algebra, is the set $\mathbb{R} \cup \{-\infty\}$ together with the operations $a \oplus b := \max\{a, b\}$ and $a \odot b := a + b$. We denote this semiring by \mathbb{R}_{\max} . The additive identity of \mathbb{R}_{\max} is $-\infty$ and the multiplicative identity is 0. The set \mathbb{R}_{\max}^n is a semimodule where for $x, y \in \mathbb{R}_{\max}^n$ and $\alpha \in \mathbb{R}_{\max}$, $(x \oplus y)_i := x_i \oplus y_i$ and $(\alpha \odot x)_i := \alpha + x_i$. If $A \in \mathbb{R}_{\max}^{m \times n}$ is a matrix and $x \in \mathbb{R}_{\max}^n$, then the product $A \odot x$ is the usual matrix product, but with multiplication and addition interpreted tropically. That is, if A has columns a_1, \dots, a_n , then

$$A \odot x := \bigoplus_{j=1}^n x_j \odot a_j.$$

Several notions from ordinary convexity theory have tropical analogs. We say that $P \subseteq \mathbb{R}_{\max}$ is a *tropical cone* if whenever $x, y \in P$ and $\lambda, \mu \in \mathbb{R}_{\max}$, $\lambda \odot x \oplus \mu \odot y \in P$. If this only holds with the restriction that $\lambda \oplus \mu = 0$, then we say that P is *tropically convex*.

A *tropical polyhedron* is a set of the form

$$\{x \in \mathbb{R}_{\max}^n : A \odot x \oplus b \geq C \odot x \oplus d\}$$

where $A, C \in \mathbb{R}_{\max}^{m \times n}$ and $b, d \in \mathbb{R}_{\max}^m$. We denote this set $P(A, b, C, d)$. Note that $P(A, b, C, d)$ is always tropically convex. When $b = d = (-\infty, \dots, -\infty)^T$ then $P(A, b, C, d)$ is a tropical cone and we call it a *tropical polyhedral cone*. Bounded tropical polyhedra are called *tropical polytopes*. Given $V \subseteq \mathbb{R}_{\max}$, $\text{tconv}(V)$ is the *tropical convex hull* of V . That is,

$$\text{tconv}(V) := \{\lambda \odot x + \mu \odot y : x, y \in V, \lambda + \mu = 0\}.$$

We define the *tropical conic hull* $\text{tcone}(V)$ similarly. Gaubert and Katz showed in [8] that any tropical polytope (cone) P can be expressed as the tropical convex (conic) hull of a finite set V . Conversely, Joswig showed in [11] that if $V \subseteq \mathbb{R}^n$ is a finite set and $P = \text{tcone}(V)$, then P is a tropical polyhedral cone. The analogous result for

$P = \text{tconv}(V)$ follows from results in [8]. We call V the *tropical vertices* (extreme rays) of P .

3.2. Bergman fans of matroids. Familiarity with the fundamental definitions of matroid theory are essential for this section. For this, we refer the reader to [14].

Let \mathcal{M} be a matroid of rank r with ground set E . Each $w \in \mathbb{R}^E$ defines a weight vector on E . Given any basis B of \mathcal{M} , the *weight of B* is $\sum_{b \in B} w_b$. If the weight of some basis B is minimal with respect to w , then B is a *w -minimal basis*.

Definition 3.1. Let \mathcal{M} be a matroid on ground set E . If each $e \in E$ appears in some w -minimum basis of \mathcal{M} then w is an \mathcal{M} -ultrametric. The collection of \mathcal{M} -ultrametrics, denoted $\tilde{\mathcal{B}}(\mathcal{M})$, is the *Bergman fan of \mathcal{M}* .

Example 3.2. Our recurring example matroid will be $\mathcal{M}(K_4)$, the graphic matroid of the complete graph on four vertices. The ground set E is the collection of edges. Each $x \in \mathbb{R}^E$ is an \mathbb{R} -labeling of the edges in $\mathcal{M}(K_4)$. Figure 4 gives two examples of $\mathcal{M}(K_4)$ -ultrametrics.

For any $w \in \tilde{\mathcal{B}}(\mathcal{M})$, there is a unique flag of flats of \mathcal{M}

$$\emptyset = F_0 \subsetneq F_1 \subsetneq \cdots \subsetneq F_k = E$$

such that w has constant value c_i on each $F_i \setminus F_{i-1}$, and $c_1 < \cdots < c_r$.

Example 3.3. Let u be the $\mathcal{M}(K_4)$ -ultrametric depicted on the left in Figure 4. Then the flag of flats

$$\emptyset \subsetneq \{AB\} \subsetneq \{AB, BC, AC\} \subsetneq E$$

satisfies the above conditions with $c_1 = 5$, $c_2 = 7$ and $c_3 = 9$.

Proposition 3.4 ([3]). *The Bergman fan $\tilde{\mathcal{B}}(\mathcal{M})$ is a tropical polyhedral cone.*

Proposition 3.5. *If \mathcal{M} is a matroid on ground set E and $x \in \mathbb{R}^E$, then the set of l^∞ -nearest \mathcal{M} -ultrametrics to x , $C(x, \tilde{\mathcal{B}}(\mathcal{M}))$, is a tropical polytope.*

Proof. Note that $C(x, \tilde{\mathcal{B}}(\mathcal{M})) = \tilde{\mathcal{B}}(\mathcal{M}) \cap C_d(x)$ where $d = d(x, \tilde{\mathcal{B}}(\mathcal{M}))$. Proposition 3.4 tells us that $\tilde{\mathcal{B}}(\mathcal{M})$ is a tropical polyhedron and it is clear that $C_d(x)$, the cube of side-length d centered at x is a tropical polytope. Their intersection is again a tropical polyhedron. Since it is bounded it is by definition a tropical polytope. \square

Much of the remainder of this section is devoted to describing the set of tropical vertices of $C(x, \tilde{\mathcal{B}}(\mathcal{M}))$. We begin by defining a notion of topology for an \mathcal{M} -ultrametric. When $\mathcal{M} = \mathcal{M}(K_n)$, the $\mathcal{M}(K_n)$ -ultrametrics are rooted tree metrics [4]. In this case, two ultrametrics will have the same topology if and only if they have the same underlying rooted tree topology. Our notion of \mathcal{M} -ultrametric topology is meant to generalize this notion to arbitrary matroids.

We quickly recall the direct sum operation on matroids and matroid connectivity. For more details, see [14, Ch. 4]. Let \mathcal{M}_1 and \mathcal{M}_2 be matroids on disjoint ground sets E_1 and E_2 . We define their direct sum, denoted $\mathcal{M}_1 \oplus \mathcal{M}_2$, to be the matroid on ground set $E_1 \cup E_2$ such that $I \subseteq E_1 \cup E_2$ is independent in $\mathcal{M}_1 \oplus \mathcal{M}_2$ if and only if $I \cap E_i$ is

independent in \mathcal{M}_i for each i . A key property is that $F \subseteq E_1 \oplus E_2$ is a flat of $\mathcal{M}_1 \oplus \mathcal{M}_2$ if and only if F_i is a flat of \mathcal{M}_i for each i . It is unfortunate that direct sum and tropical addition are denoted by the same symbol. However, the context will always makes the proper interpretation clear.

We say that \mathcal{M} is *connected* if $\mathcal{M} = \mathcal{M}_1 \oplus \mathcal{M}_2$ implies that either $\mathcal{M}_1 = \mathcal{M}$ and $\mathcal{M}_2 = \emptyset$ or $\mathcal{M}_2 = \mathcal{M}$ and $\mathcal{M}_1 = \emptyset$. Up to relabeling of indices, each matroid \mathcal{M} can be uniquely written as $\mathcal{M} = \mathcal{M}_1 \oplus \cdots \oplus \mathcal{M}_k$ where each \mathcal{M}_i is connected. Each \mathcal{M}_i is called a *connected component* of \mathcal{M} .

Definition 3.6. Let \mathcal{M} be a matroid on ground set E . Let \mathcal{F} be a collection of connected flats of \mathcal{M} partially ordered by inclusion. We call \mathcal{F} a *hierarchy of connected flats* if

- (1) $\emptyset \in \mathcal{F}$, and
- (2) for all $F, G \in \mathcal{F}$, either $F \subseteq G$, $G \subseteq F$, or $F \cap G = \emptyset$.

Cover relations will be denoted $F <_{\mathcal{F}} G$, or simply $F < G$ when \mathcal{F} is clear from context.

As we will see, there is a well-defined way to associate a hierarchy of connected flats to each \mathcal{M} -ultrametric. Before proving this, we recall some notation from matroid theory and prove an intermediate lemma. If \mathcal{M} is a matroid on ground set E and $S \subseteq E$, then the *restriction of \mathcal{M} to S* , denoted $\mathcal{M}|_S$, is the matroid on ground set S such that $I \subseteq S$ is independent in $\mathcal{M}|_S$ if and only if I is independent in \mathcal{M} . The *contraction of S in \mathcal{M}* , denoted \mathcal{M}/S , is the matroid on ground set $E \setminus S$ such that $I \subseteq E \setminus S$ is independent in \mathcal{M}/S if and only if there exists a basis B of $\mathcal{M}|_S$ such that $I \cup B$ is independent in \mathcal{M} . When $T \subseteq S \subseteq E$, we will abuse notation and write S/T to mean $\mathcal{M}|_S/T$.

Lemma 3.7. *Let \mathcal{M} be a matroid on ground set E . If $w \in \mathbb{R}^E$ is an \mathcal{M} -ultrametric and F is a flat of \mathcal{M} , then $w|_F$ is an $\mathcal{M}|_F$ -ultrametric.*

Proof. Since w is an \mathcal{M} -ultrametric, there is a flag of flats

$$\emptyset = F_0 \subsetneq F_1 \subsetneq \cdots \subsetneq F_k = E$$

such that w has constant value c_i on each $F_i \setminus F_{i-1}$, and $c_1 < \cdots < c_r$. Intersecting all the F_i 's with F gives a flag of flats of $\mathcal{M}|_F$ after removing redundant entries. Denote this new flag $\emptyset = G_0 \subsetneq G_1 \subsetneq \cdots \subsetneq G_{k'} = F$. Let $e \in F$, we are going to show that e is contained in some w -minimum basis of $\mathcal{M}|_F$. Let j be the smallest index such that $e \in G_j$. Every $w|_F$ -minimum basis of $\mathcal{M}|_F$ can be constructed by choosing a basis of each G_i/G_{i-1} and taking their union. Since G_j is a flat, e is not a loop in G_j/G_{j-1} . Therefore, we can choose a basis for G_j/G_{j-1} containing e and complete it to a $w|_F$ -minimum basis of $\mathcal{M}|_F$. \square

Proposition 3.8. *Let \mathcal{M} be a matroid on ground set E . Let $w \in \mathbb{R}^E$ be an \mathcal{M} -ultrametric. Then there exists a unique hierarchy of connected flats \mathcal{F} such that for each $F \in \mathcal{F}$,*

- (1) w is constant on $F \setminus (\bigcup_{G < F} G)$, and
- (2) if $G < F$, $g \in G$, and $f \in F$, then $w_g < w_f$.

Proof. We proceed by induction on the number of connected components of \mathcal{M} and the number of distinct values of w . If w has only one distinct value then the connected

components of \mathcal{M} form the unique hierarchy of connected flats satisfying the desired properties.

Now assume \mathcal{M} is connected and that w takes multiple values on E . Let $e \in E$ such that $w_e = \max_{f \in E} w_f$. Then $F := \{f \in E : w_f < w_e\}$ is a flat of \mathcal{M} since w is an \mathcal{M} -ultrametric. So $w|_F$ is an $\mathcal{M}|_F$ -ultrametric by Lemma 3.7. By induction on the number of distinct values that w takes, $\mathcal{M}|_F$ has a unique hierarchy of connected flats, \mathcal{F} , such that the two desired properties are satisfied on F . Then $\mathcal{F} \cup \{E\}$ is the unique hierarchy of connected flats satisfying the desired properties for \mathcal{M} .

Now assume \mathcal{M} is disconnected with $\mathcal{M} = \mathcal{M}_1 \oplus \mathcal{M}_2$ and each \mathcal{M}_i nonempty. Let E_i denote the ground set of \mathcal{M}_i . Then E_i is a flat of \mathcal{M} so $w|_{E_i}$ is a \mathcal{M}_i -ultrametric by Lemma 3.7. By induction on the number of connected components, \mathcal{M}_i has a unique hierarchy of connected flats \mathcal{F}_i that satisfies the desired properties. Therefore $\mathcal{F}_1 \cup \mathcal{F}_2$ satisfies the desired properties for \mathcal{M} and is also unique. \square

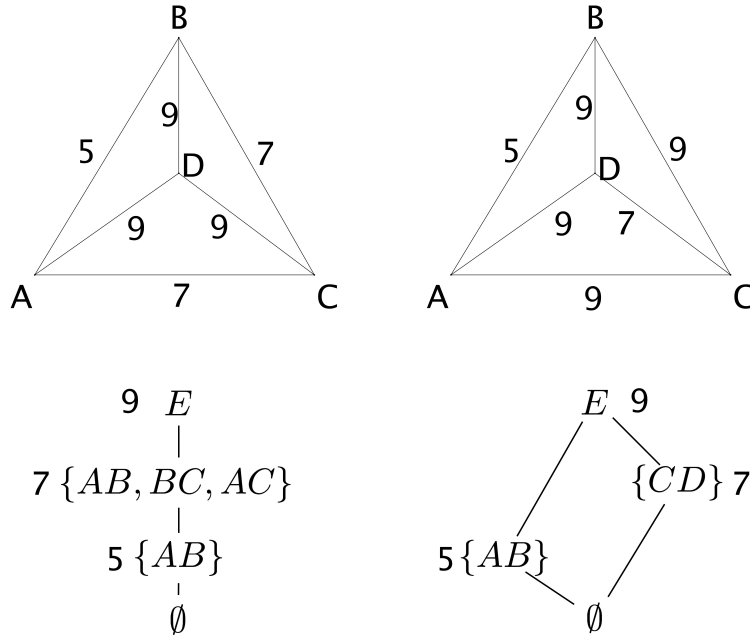


FIGURE 4. $\mathcal{M}(K_4)$ -ultrametrics with different topologies

Definition 3.9. Let \mathcal{M} be a matroid on ground set E and let $w \in \mathbb{R}^E$ be an \mathcal{M} -ultrametric. The unique hierarchy of connected flats from Proposition 3.8 is called the *topology of w* , denoted $\mathcal{T}(w)$.

Given $F \in \mathcal{T}(w)$, we abuse notation and let w_F denote the constant value taken by w_e when $e \in F \setminus (\bigcup_{G \triangleleft F} G)$. We can express an \mathcal{M} -ultrametric w by drawing the Hasse diagram for $\mathcal{T}(w)$ and labeling each flat F by w_F .

Example 3.10. Figure 4 shows two $\mathcal{M}(K_4)$ -ultrametrics and their topologies. Each flat F is labeled by the constant value taken by elements of $F \setminus (\bigcup_{G \triangleleft F} G)$.

The terminology above comes from the fact that the topology of an \mathcal{M} -ultrametric generalizes the notion of a topology of a rooted-tree metric, as we will see. The notion of a polytomy also generalizes in this context.

Definition 3.11. Let \mathcal{M} be a matroid on ground set E and let \mathcal{F} be a hierarchy of connected flats of \mathcal{M} . If $F \in \mathcal{F}$ such that $\text{rank}(F/\bigcup_{G \triangleleft F} G) > 1$, then we say that F is a *polytomy*.

We can resolve a polytomy of an \mathcal{M} -ultrametric just as we resolve polytomies in the phylogenetic tree associated to an equidistant tree metric.

Definition 3.12. The *resolutions* of \mathcal{F} , denoted $R(\mathcal{F})$, is the collection of all polytomy-free hierarchies of connected flats of \mathcal{M} that contain \mathcal{F} as an induced sub-poset. We let $E(\mathcal{F})$ denote the collection of flats of \mathcal{M} that appear in some resolution of \mathcal{F} - that is $E(\mathcal{F}) := \{F : F \in \mathcal{G} \text{ for some } \mathcal{G} \in R(\mathcal{F})\}$.

Example 3.13. The posets in Figure 5 are hierarchies of connected flats of $\mathcal{M}(K_4)$. The hierarchy on the left has a polytomy since $\text{rank}(E/\{AB\}) = 2$. To its right are the three possible resolutions.

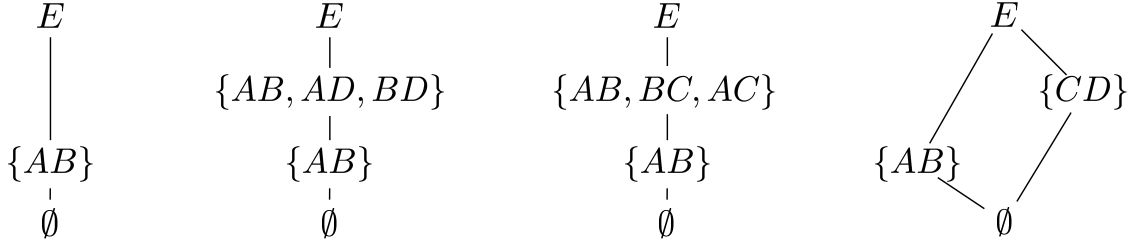


FIGURE 5. A polytomy and its resolutions

We will use this concept of topology to describe the tropical vertices of $C(x, \tilde{\mathcal{B}}(\mathcal{M}))$. First we must recall the concept of a subdominant \mathcal{M} -ultrametric, the existence of which was proven by Ardila in [3].

Definition 3.14. Let \mathcal{M} be a matroid on ground set E and let $x \in \mathbb{R}^E$. Let $x^{\mathcal{M}}$ denote the unique coordinate-wise maximum \mathcal{M} -ultrametric which is coordinate-wise at most x . We call $x^{\mathcal{M}}$ the *subdominant \mathcal{M} -ultrametric of x* .

The subdominant ultrametric can easily be shifted to obtain an l^∞ -nearest ultrametric. The following lemma shows that there exists some $e \in E$ such that u_e is constant across all $u \in C(x, \tilde{\mathcal{B}}(\mathcal{M}))$. For what follows, $\mathbf{1}$ denotes the all-1s vector in \mathbb{R}^E .

Lemma 3.15. Let \mathcal{M} be a matroid on ground set E , $x \in \mathbb{R}^E$, and $\delta = \frac{1}{2}d(x, x^{\mathcal{M}})$. Define $S := \{e \in E : x_e - x_e^{\mathcal{M}} = 2\delta\}$. Then

- (1) The l^∞ -distance from x to $\tilde{\mathcal{B}}(\mathcal{M})$ is δ
- (2) $x^{\mathcal{M}} + \delta \cdot \mathbf{1}$ is an l^∞ -nearest \mathcal{M} -ultrametric to x
- (3) If y is an l^∞ -nearest \mathcal{M} -ultrametric, then for all $e \in S$, $y_e = x_e^{\mathcal{M}} + \delta$.

Proof. The existence of $x^{\mathcal{M}} + \delta \cdot \mathbf{1}$ shows that $d(x, \tilde{\mathcal{B}}(\mathcal{M})) \leq \delta$. Suppose there exists $w \in \tilde{\mathcal{B}}(\mathcal{M})$ such that $d(x, w) < \delta$, then $w - d(x, w) \cdot \mathbf{1}$ is coordinate-wise less than x . Then there exists $e \in E$ such that $x_e - w_e = 2\delta$ and so $x_e^{\mathcal{M}} < w_e - d(x, w) \leq x_e$. Thus, $w - d(x, w) \cdot \mathbf{1}$ is an ultrametric coordinate-wise less than x but not coordinate-wise less than $x^{\mathcal{M}}$, contradicting that $x^{\mathcal{M}}$ is the subdominant \mathcal{M} -ultrametric. So (1) is proven and (2) immediately follows.

Now we prove (3). Let $y \in C(x, \tilde{\mathcal{B}}(\mathcal{M}))$. If $y_e < x_e^{\mathcal{M}} + \delta$ for some $e \in S$, then $d(y, x) \geq x_e - y_e = 2\delta - y_e + x_e^{\mathcal{M}} > \delta$ contradicting (1). If $y_e > x_e^{\mathcal{M}} + \delta$ for some $e \in S$, then $y - \delta \cdot \mathbf{1}$ is an \mathcal{M} -ultrametric that is coordinate-wise at most x , but $(y - \delta \cdot \mathbf{1})_e > x_e^{\mathcal{M}}$ contradicting that $x^{\mathcal{M}}$ is the subdominant \mathcal{M} -ultrametric. \square

Example 3.16. Letting E denote the edge set of K_4 , Figure 6 shows an element of \mathbb{R}^E along with $x^{\mathcal{M}}$ and $x^{\mathcal{M}} + d(x, \tilde{\mathcal{B}}(\mathcal{M})) \cdot \mathbf{1}$, an l^∞ -nearest $\mathcal{M}(K_4)$ -ultrametric.

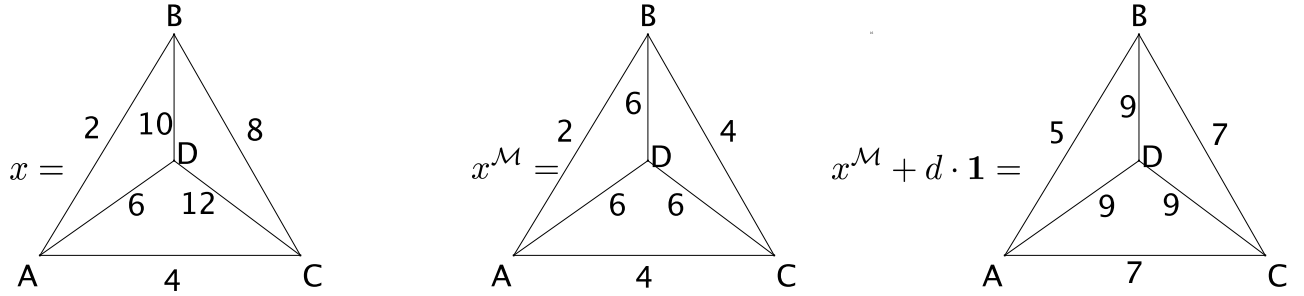


FIGURE 6. A point in \mathbb{R}^E that is not an $\mathcal{M}(K_4)$ -ultrametric, its subdominant ultrametric, and an l^∞ -nearest $\mathcal{M}(K_4)$ ultrametric

Definition 3.17. Let $u \in C(x, \tilde{\mathcal{B}}(\mathcal{M}))$. We define the *slack* of u to be the following nonnegative vector

$$s(u, x) := u - x + d(x, \tilde{\mathcal{B}}(\mathcal{M})) \cdot \mathbf{1}.$$

In other words, $s(u, x)_e$ gives the maximum amount u_e can be decreased before being further away than $d(x, \tilde{\mathcal{B}}(\mathcal{M}))$ from x .

Definition 3.18. Fix a resolution $\mathcal{F} \in R(\mathcal{T}(u))$ of $\mathcal{T}(u)$. We define the slack of any $F \in \mathcal{F}$ to be

$$s(u, x, \mathcal{F})_F := \min\{s(u, x)_e : e \in F \text{ and } e \notin G \text{ for all } G \triangleleft_{\mathcal{F}} F\}.$$

We say that F is *mobile* in \mathcal{F} if $s(u, x, \mathcal{F})_F > 0$ and one of the following holds.

- (1) F lies in $\mathcal{T}(u)$ and is not a polytomy, or
- (2) $F \notin \mathcal{T}(u)$ and if $G \triangleleft_{\mathcal{F}} F$ then $G \in \mathcal{T}(u)$.

Observation 3.19. Let $F \in E(\mathcal{T}(u))$. If F is mobile in some resolution containing F then the collection of flats $\{G : G \triangleleft_{\mathcal{F}} F\}$ is independent of the choice of resolution. In particular, if F is mobile in some resolution of $\mathcal{T}(u)$ then F is mobile in all resolutions.

In light of Observation 3.19, it makes sense to say that some $F \in E(\mathcal{T}(u))$ is mobile without reference to any particular resolution. Moreover, when F is mobile, we can write $G \leq F$ to mean $G \leq_{\mathcal{F}} F$ for some resolution $\mathcal{F} \in R(\mathcal{T}(u))$. Because of this, $s(u, x, \mathcal{F})_F$ does not depend on \mathcal{F} for mobile F , and so in this case we simply write $s(u, x)_F$. When F is not mobile, we say that F is *immobile*.

Example 3.20. Let E be the edge set of K_4 and let x be as in Figure 6. Then $u = x^{\mathcal{M}} + d(x, \tilde{\mathcal{B}}(\mathcal{M})) \cdot \mathbf{1}$ is l^∞ -nearest to x . Figure 7 shows the slack vector $s(u, x)$ and the topology $\mathcal{T}(u)$ where each flat F is labeled by $s(u, x)_F$. Note that the flat E is immobile, whereas the other two nonempty flats are mobile.

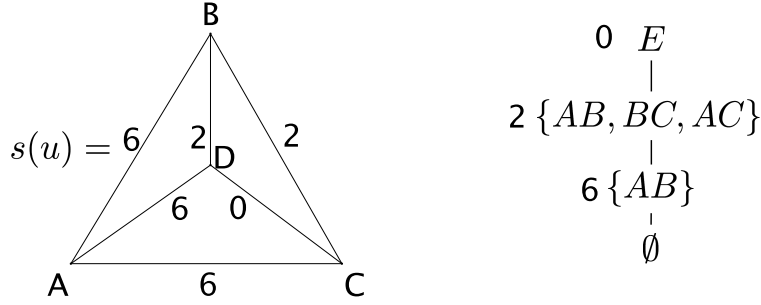


FIGURE 7. Slack vector and topology of u

Lemma 3.23 characterizes the vertices of $C(x, \tilde{\mathcal{B}}(\mathcal{M}))$. However, before we can prove it, we need two technical lemmas about tropical polyhedra. Lemma 3.21 gives us a tropical cone with the same combinatorics as $C(x, \tilde{\mathcal{B}}(\mathcal{M}))$, and Lemma 3.22 characterizes the extreme rays of a tropical cone.

Lemma 3.21. *Let $P \subseteq \mathbb{R}^E$ be a tropical polytope with a fixed coordinate - i.e. there exists some $e \in E$ and a constant k such that $x_e = k$ for all $x \in P$. Then $\text{tcone}(P)$ is a tropical polyhedral cone. If $v \in \text{tcone}(P)$ with $v_e = k$, then $v \in P$. In this case moreover, v lies on an extreme ray of $\text{tcone}(P)$ if and only if v is a vertex of P .*

Proof. Define $C_P := \{(\lambda \odot x, \lambda) : x \in P, \lambda \in \mathbb{R}_{\max}\}$. Then C_P is a tropical polyhedral cone, and v is a vertex of P if and only if $(v, 0)$ lies on an extreme ray of C_P (cf. [8, Corollary 2.15]). Let V denote the set of vertices of P . Note that if $(x, x_0) = \bigoplus_{v \in V} a_v \odot (v, 0)$ is an arbitrary point of C_P , then $x = \bigoplus_{v \in V} a_v \odot v$ lies in $\text{tcone}(P)$. Moreover, we can invert this projection map. Namely, if $x = \bigoplus_{v \in V} a_v \odot v$ is an arbitrary point in $\text{tcone}(P)$, then $x_e = k + \max_{v \in V} a_v$ and so $(x, x_e - k) \in C_P$. Therefore if $x \in \text{tcone}(P)$ with $x_e = k$, then $x \in P$. Moreover x is a vertex of P if and only if $(x, 0)$ lies on an extreme ray of C_P which is true if and only if x lies on an extreme ray of $\text{tcone}(P)$. \square

Lemma 3.22 ([2], Proposition 3.1). *Let $P \subseteq \mathbb{R}^E$ be a tropical cone. Then $g \in P$ lies on an extreme ray if and only if there exists some $e \in E$ such that for each $x \in P$, if $x_e = g_e$ and $x \leq g$, then $x = g$.*

Now we are ready to describe the tropical vertices of $C(x, \tilde{\mathcal{B}}(\mathcal{M}))$.

Lemma 3.23. *Let \mathcal{M} be a matroid on ground set E and let $u \in C(x, \tilde{\mathcal{B}}(\mathcal{M}))$. Then u is a tropical vertex of $C(x, \tilde{\mathcal{B}}(\mathcal{M}))$ if and only if one of the following holds*

- (1) *Each $F \in E(\mathcal{T}(u))$ is immobile, or*
- (2) *Exactly one $F \in E(\mathcal{T}(u))$ is mobile and one of the following holds*
 - (a) *$F \in \mathcal{T}(u)$ and some $e \in F \setminus \bigcup_{G \triangleleft F} G$ satisfies $u_e = (x^{\mathcal{M}} + d(x, \tilde{\mathcal{B}}(\mathcal{M})) \cdot \mathbf{1})_e$,
or*
 - (b) *$F \notin \mathcal{T}(u)$ and if H is the minimal polytomy containing F , then whenever $J \subseteq H$ is a flat such that $F \subseteq H \setminus J$, some $e \in H \setminus J$ satisfies $u_e = (x^{\mathcal{M}} + d(x, \tilde{\mathcal{B}}(\mathcal{M})) \cdot \mathbf{1})_e$.*

Proof. Let $u \in C(x, \tilde{\mathcal{B}}(\mathcal{M}))$. We proceed by cases. Cases 1, 2, and 3 handle the ways in which u can satisfy one of the above conditions. Cases 4, 5, and 6 handle the ways in which u fails them all.

Case 1: u satisfies (1). By Lemma 3.15 there exists $e \in E$ such that for all $u \in C(x, \tilde{\mathcal{B}}(\mathcal{M}))$, $u_e = k$ for some fixed k . If $v \in \text{tcone}(C(x, \tilde{\mathcal{B}}(\mathcal{M})))$ satisfies $v_e = u_e$, then $v \in C(x, \tilde{\mathcal{B}}(\mathcal{M}))$ by Lemma 3.21.

Now suppose $v \leq u$. We will show that $v = u$. If not, define $u^t := (t \odot u) \oplus v \in C(x, \tilde{\mathcal{B}}(\mathcal{M}))$ for some $t < 0$ with $|t|$ small. Fix f so that $v_f < u_f$. Then there exists some resolution $\mathcal{F} \in R(\mathcal{T}(u))$ and some $F \in \mathcal{F}$ such that $f \in F$ and $u_F^t = u_F + t < u_F$. But every $F \in E(\mathcal{T}(u))$ is immobile, so this is a contradiction. So $v = u$ and then by Lemma 3.22, u lies on a tropical extreme ray of $\text{tcone}(C(x, \tilde{\mathcal{B}}(\mathcal{M})))$. Since $u_e = k$, Lemma 3.21 implies that u is a tropical vertex of $C(x, \tilde{\mathcal{B}}(\mathcal{M}))$.

Case 2: u satisfies (2) and (a). Let $e \in F \setminus \bigcup_{G \triangleleft F} G$ be such that $u_e = (x^{\mathcal{M}} + d(x, \tilde{\mathcal{B}}(\mathcal{M})) \cdot \mathbf{1})_e$. Assume $v \in \text{tcone}(C(x, \tilde{\mathcal{B}}(\mathcal{M})))$ satisfies $v_e = u_e$ and $v \leq u$. We now show $v = u$. Since $v \leq u$ and $v_e = (x^{\mathcal{M}} + d(x, \tilde{\mathcal{B}}(\mathcal{M})) \cdot \mathbf{1})_e$ is the largest possible e -coordinate among elements of $C(x, \tilde{\mathcal{B}}(\mathcal{M}))$, we must have $v \in C(x, \tilde{\mathcal{B}}(\mathcal{M}))$. Define $v^t := (t \odot u) \oplus v$ for $t < 0$ with $|t|$ small. Now if $v \neq u$, then choosing $f \in E$ such that $v_f < u_f$ gives $v_f^t < u_f$. Since F is the unique mobile flat of $E(\mathcal{T}(u))$ and $v^t \in C(x, \tilde{\mathcal{B}}(\mathcal{M}))$, we have $v_F^t < u_F$ which implies $v_e^t < u_e$ and so $v_e < u_e$. This contradicts $v_e = u_e$ and so we must have $v = u$. As before, Lemmas 3.22 and 3.21 imply that u is a tropical vertex.

Case 3: u satisfies (2) and (b). Arguments of the previous paragraph apply if there exists some $e \in F \setminus \bigcup_{G \triangleleft F} G$ such that $u_e = x^{\mathcal{M}} + d(x, \tilde{\mathcal{B}}(\mathcal{M})) \cdot \mathbf{1}$. So assume that no such e exists. Let $e \in F \setminus \bigcup_{G \triangleleft F} G$. Let $v \in \text{tcone}(C(x, \tilde{\mathcal{B}}(\mathcal{M})))$ such that $v \leq u$ with $v_e = u_e$. So $v = t \odot w$ where $w \in C(x, \tilde{\mathcal{B}}(\mathcal{M}))$. If $t = 0$ then $v = u$ as F is the unique mobile flat. We cannot have $t > 0$ since then if $f \in S$ as in Lemma 3.15, then $v_f = (t \odot w)_f > w_f = u_f$ contradicting $v \leq u$. So assume $t < 0$. Then $w_e > u_e$ and $t = u_e - w_e$. By our assumptions on u , this implies that there exists $K \in \mathcal{T}(u)$ with $K \subsetneq F$ with $f \in K$ and so $u_f < u_e$, but $w_f = w_e$. Then $v_f = w_f + t = u_e > u_f$, contradicting $v \leq u$.

Case 4: Exactly one flat $F \in E(\mathcal{T}(u))$ is mobile, $F \in \mathcal{T}(u)$ but (a) fails. Since F is mobile, there exists $v \in C(x, \tilde{\mathcal{B}}(\mathcal{M}))$ such that $v_e < u_e$ whenever $e \in F \setminus \bigcup_{G \triangleleft F} G$ and $v_e = u_e$ otherwise. Since $u_e < (x^{\mathcal{M}} + d(x, \tilde{\mathcal{B}}(\mathcal{M})) \cdot \mathbf{1})_e$ for all $e \in F \setminus \bigcup_{G \triangleleft F} G$, there exists a $w \in C(x, \tilde{\mathcal{B}}(\mathcal{M}))$ such that $w_e > u_e$ whenever $e \in F \setminus \bigcup_{G \triangleleft F} G$ and $w_e = u_e$ otherwise.

Letting t be the unique non-zero entry of $w - u$ gives $u = (-t \odot v) \oplus w$. As we have just expressed u as a tropical convex combination of two other elements in $C(x, \tilde{\mathcal{B}}(\mathcal{M}))$, u is not a tropical vertex.

Case 5: Exactly one flat $F \in E(\mathcal{T}(u))$ is mobile, $F \notin \mathcal{T}(u)$ where H is the minimal polytomy containing F , and (b) fails with flat $J \subseteq H$ as witness. Since F is mobile, there exists $v \in C(x, \tilde{\mathcal{B}}(\mathcal{M}))$ such that $v_e < u_e$ whenever $e \in F \setminus \bigcup_{G \leq F} G$ and $v_e = u_e$ otherwise. Since $u_e < (x^{\mathcal{M}} + d(x, \tilde{\mathcal{B}}(\mathcal{M})) \cdot \mathbf{1})_e$ for all $e \in H \setminus J$, there exists a $w \in C(x, \tilde{\mathcal{B}}(\mathcal{M}))$ such that $w_e > u_e$ whenever $e \in H \setminus J$ and $w_e = u_e$ otherwise. Just as before, we let t be the unique non-zero entry of $w - u$ gives $u = (-t \odot v) \oplus w$ and then $u = (-t \odot v) \oplus w$ and so u is not a tropical vertex.

Case 6: u has distinct mobile flats $F_1, F_2 \in E(\mathcal{T}(u))$. We show that no choice of $e \in E$ makes u satisfy the conditions of Lemma 3.22 for $\text{tcone}(x, \tilde{\mathcal{B}}(\mathcal{M}))$. Assume $e \in E \setminus F_i$. Let $\chi \in \mathbb{R}^E$ be the characteristic vector of $F_i \setminus \bigcup_{G \leq F_i} G$. Now set $v_\varepsilon := u - \varepsilon \chi$. Note that $v_\varepsilon \leq u$ with $(v_\varepsilon)_e = u_e$. If $\varepsilon > 0$ is small enough, then $v_\varepsilon \in \text{tcone}(C(x, \tilde{\mathcal{B}}(\mathcal{M})))$ but $v_\varepsilon \neq u$. This same argument works in the case where $F_j \subseteq F_i$ and $e \in F_j$.

It remains to consider the case where $F_1, F_2 \neq F_1 \cap F_2$ and $e \in F_1 \cap F_2$. In this case, choose the minimal polytomy $H \in \mathcal{T}(u)$ such that $F_1 \cup F_2 \subseteq H$. We claim that there exists some $G \in \mathcal{T}(u)$ such that $G \leq H$ with $e \in G$. Otherwise, there exists a resolution $\mathcal{F} \in R(\mathcal{T}(u))$ that contains both F_1 , and $\text{cl}(e) \subseteq F_1 \cap F_2 \subsetneq F_1$ where cl is the closure operator in \mathcal{M} (note $\text{cl}(e)$ is a parallel class and therefore connected). But then some $H \in \mathcal{F}$ with $\text{cl}(e) \subseteq H$ has $H \leq_{\mathcal{F}} F_1$ with $H \notin \mathcal{T}(u)$. This contradicts F_1 being mobile thus proving the claim. We can now let $\chi \in \mathbb{R}^E$ be the characteristic vector of $F_i \setminus \bigcup_{G \leq F_i} G$ and proceed as in the previous paragraph. \square

We now give an algorithm for computing the tropical vertices of $C(x, \tilde{\mathcal{B}}(\mathcal{M}))$.

Theorem 3.24. *Given a matroid \mathcal{M} on ground set E and $x \in \mathbb{R}^E$, Algorithm 1 returns the tropical vertices of the set of all \mathcal{M} -ultrametrics that are l^∞ -nearest to x .*

Proof. We first prove termination. Each w produced in the inner for-loop of Algorithm 1 has coordinates that are either $w_e = (x^{\mathcal{M}} + d(x, \tilde{\mathcal{B}}(\mathcal{M})) \cdot \mathbf{1})_f$, or $w_e = (x^{\mathcal{M}} + d(x, \tilde{\mathcal{B}}(\mathcal{M})) \cdot \mathbf{1})_f - s(x^{\mathcal{M}} + d(x, \tilde{\mathcal{B}}(\mathcal{M})) \cdot \mathbf{1}, x)_f$ for some $f \in E$ (note e and f may be different). In particular, there are only finitely many such values. Note that each $w \in S_{i+1}$ is coordinate-wise less than some $w' \in S_i$ with strict inequality at some coordinate. Therefore $S_i = \emptyset$ for some $i > 0$ and so Algorithm 1 terminates.

Because the set V returned by Algorithm 1 only contains tropical vertices of $C(x, \tilde{\mathcal{B}}(\mathcal{M}))$, it only remains to show that each tropical vertex is reached. Let $v \in C(x, \tilde{\mathcal{B}}(\mathcal{M}))$ be a tropical vertex. We now describe a sequence of points w_0, w_1, \dots such that w_i gets included in S_i in Algorithm 1 and the final w_i is equal to v .

Define $w_0 := x^{\mathcal{M}} + d(x, \tilde{\mathcal{B}}(\mathcal{M})) \cdot \mathbf{1}$. We show how to construct w_{i+1} given that w_i has already been defined and that $w_i \in S_i$. In each case, we will have $w_i \geq w_{i+1} \geq v$.

First assume $\mathcal{T}(w_i) \subseteq \mathcal{T}(v)$. Then $E(\mathcal{T}(w_i)) \supseteq E(\mathcal{T}(v))$. If $w_i \neq v$, let $e \in E$ such that $v_e < (w_i)_e$. Let $H \in \mathcal{T}(v)$ be the minimal flat containing e . If H is a polytomy, let F be the closure of e in \mathcal{M} . Then F is a parallel class and therefore connected so $F \in E(\mathcal{T}(v))$.

Algorithm 1 Algorithm for computing the tropical vertices of $C(x, \tilde{\mathcal{B}}(\mathcal{M}))$

Input: A matroid \mathcal{M} on ground set E and a point $x \in \mathbb{R}^E$
 Set $V := \emptyset$, $S_0 := \{x^{\mathcal{M}} + d(x, \tilde{\mathcal{B}}(\mathcal{M})) \cdot \mathbf{1}\}$, $S_i := \emptyset$ for $i = 1, 2, \dots$
for $i := 1, 2, \dots$ **do**
 if $S_{i-1} = \emptyset$ **then**
 break
 end if
 for $u \in S_{i-1}$ **do**
 for each mobile $F \in E(\mathcal{T}(u))$ **do**
 initialize $w \in \mathbb{R}^E$ such that $w_e = u_e$ for all $e \notin F \setminus \bigcup_{G \triangleleft F} G$
 if $u_F - s(u, x)_F \geq \max\{w_G : G \triangleleft F\}$ **then**
 set $w_e = u_F - s(u, x)_F$ for each $e \in F \setminus \bigcup_{G \triangleleft F} G$.
 else
 set $w_e = \max\{w_G : G \triangleleft F\}$ for each $e \in F \setminus \bigcup_{G \triangleleft F} G$
 end if
 put w in S_i
 if w is a tropical vertex by Lemma 3.23 **then**
 put w in V
 end if
 end for
 end for
end for
return V

Moreover, if $G \in E(\mathcal{T}(w_i))$ satisfies $G \subsetneq F$, then $G = \emptyset$ and so $G \in \mathcal{T}(w_i) \subseteq \mathcal{T}(v)$. If H is not a polytomy, define $F := H$. In either case, we have $(w_i)_F = (w_i)_e > v_e = v_F$ and so F is mobile in w_i . Define w_{i+1} such that $(w_{i+1})_e = v_e$ for $e \in F \setminus \bigcup_{G \triangleleft F} G$ and $(w_{i+1})_e = (w_i)_e$ otherwise (note that $\{G : G \triangleleft F\}$ is the same in $\mathcal{T}(w_i)$ and $\mathcal{T}(v)$). If F is immobile in v , then w_{i+1} gets added to S_{i+1} in the first “if” clause of the innermost for loop of Algorithm 1.

Since v is a vertex, if F is mobile in v then F must satisfy condition (a) or (b) of Lemma 3.23. However, if $e \in F \setminus \bigcup_{G \triangleleft F} G$, then $v_e < (w_i)_e \leq (x^{\mathcal{M}} + d(x, \tilde{\mathcal{B}}(\mathcal{M})) \cdot \mathbf{1})_e$ and so (a) cannot be satisfied. If H is the minimal polytomy in $\mathcal{T}(v)$ containing F , then if $e \in H \setminus \bigcup_{G \triangleleft_{\mathcal{T}(v)} H} G$, then $v_e = v_F < (w_i)_F = (w_i)_e \leq (x^{\mathcal{M}} + d(x, \tilde{\mathcal{B}}(\mathcal{M})) \cdot \mathbf{1})_e$. Moreover if $f \in H$, then $v_f \leq v_e$. So condition (b) cannot be satisfied and so F must be immobile in v .

Now assume $\mathcal{T}(w_i) \not\subseteq \mathcal{T}(v)$. Define $v^t := t \odot w_i \oplus v$ for $t \leq 0$. Note that $v^0 = w_i$, $v^t = v$ for $t \ll 0$, and $v^t \in C(x, \tilde{\mathcal{B}}(\mathcal{M}))$. Therefore, for each flat $G \in \mathcal{T}(w_i) \setminus \mathcal{T}(v)$, there exists some t such that $G \notin \mathcal{T}(v^t)$; let t_G denote the maximal such t . Now, fix G such that t_G is maximal and denote $t := t_G$. Let $H \in \mathcal{T}(w_i) \cap \mathcal{T}(v^t)$ be minimal such that $H \supsetneq G$. Then $(w_i)_H > (w_i)_G \geq v_H^t$. If H is a polytomy, then we can choose a mobile flat $F \subset H$. Otherwise, set $F := H$. Now define w_{i+1} such that $(w_{i+1})_e = (w_i)_G$ for all

$e \in F \setminus \bigcup_{H \leq F} H$ and $(w_{i+1})_e = (w_i)_e$ otherwise. Then w_{i+1} is added to S_{i+1} in the “else” clause in the innermost for loop of Algorithm 1.

Since Algorithm 1 terminates, $S_k = \emptyset$ for large enough k . So if k is smallest such that $S_k = \emptyset$, then $v \oplus t \odot w_{k-1} = v$ for all $t \in [-\infty, 0]$, since otherwise we would be able to construct $w_k \in S_k$. Therefore $w_{k-1} = v$ and so each vertex $v \in C(x, \tilde{\mathcal{B}}(\mathcal{M}))$ that has no mobile flats is reached by Algorithm 1. For $-\infty \leq t \leq 0$, define $v^t := (t \odot w_i) \oplus v$. Let t be the maximum value such that either $\mathcal{T}(w_i)$ is not an induced sub-poset of $\mathcal{T}(v^t)$, or v^t has more coordinates in common with v than with w_i . \square

Example 3.25. Let $\mathcal{M} = \mathcal{M}(K_4)$, let x be as in Figure 6, and let u_1, \dots, u_5 be as in Figure 8. Running Algorithm 1 with input \mathcal{M} and x gives $S_0 = \{u_1\}$, $S_1 = \{u_2, u_3\}$, and $S_2 = \{u_4, u_5\}$. Note that u_5 gets added to S_2 two times - once when $u = u_2$ and $F = \{AB\}$ and once when $u = u_3$ and $F = \{AB, AC, BC\}$. The tropical vertices are u_3, u_4 and u_5 . Note that $\mathcal{T}(u_3) = \mathcal{T}(u_5) \neq \mathcal{T}(u_4)$.

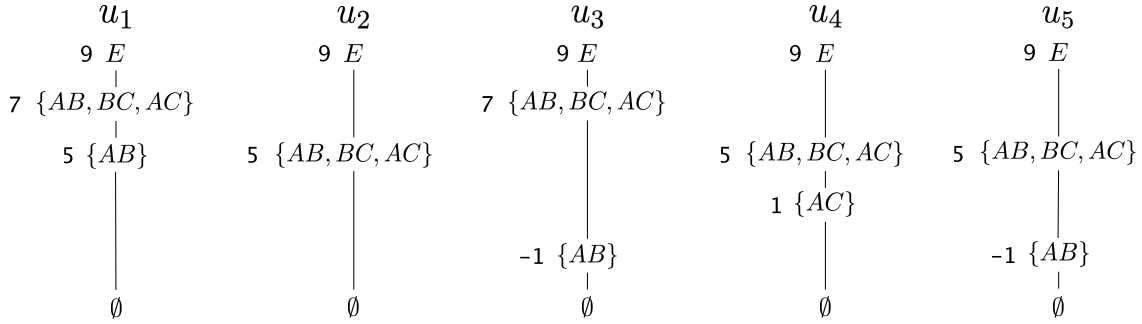


FIGURE 8. $\mathcal{M}(K_4)$ -ultrametrics produced by Algorithm 1

The following proposition gives us a way to use Algorithm 1 to check that all elements of $C(x, \tilde{\mathcal{B}}(\mathcal{M}))$ have the same topology. Namely, it suffices to check that all vertices have the same topology.

Proposition 3.26. *The set of \mathcal{M} -ultrametrics that have a particular topology \mathcal{F} is tropically convex.*

Proof. It is clear that topology of a \mathcal{M} -ultrametric is preserved under tropical scalar multiplication, so it suffices to show that topology is preserved under tropical sums. To this end, let u, v be \mathcal{M} -ultrametrics with topology \mathcal{F} . Note that $(u \oplus v)$ is constant on $F \setminus (\bigcup_{G \leq F} G)$ for each $F \in \mathcal{F}$ and that $(u \oplus v)_F > (u \oplus v)_G$ whenever $G \leq F$. Proposition 3.8 then implies that $\mathcal{T}(u \oplus v) = \mathcal{F}$. \square

Corollary 3.27. *Let \mathcal{M} be a matroid on ground set E and let $x \in \mathbb{R}^E$. Then set of all \mathcal{M} -ultrametrics that are l^∞ -nearest to x have the same topology if and only if all tropical vertices of $C(x, \tilde{\mathcal{B}}(\mathcal{M}))$ have the same topology.*

We end this section by showing that the polyhedral subdivision of $\tilde{\mathcal{B}}(\mathcal{M})$ induced by topology coincides with the coarsest possible subdivision of $\tilde{\mathcal{B}}(\mathcal{M})$.

Definition 3.28. Let \mathcal{M} be a matroid on ground set E and let $w \in \mathbb{R}^E$. Then \mathcal{M}_w denotes the matroid on ground set E whose bases are the w -minimum bases of \mathcal{M} .

The collection of \mathcal{M} -ultrametrics that induce a particular collection of w -minimal bases \mathcal{M}_w forms an open polyhedral cone. Their closures form the coarsest possible subdivision of $\tilde{\mathcal{B}}(\mathcal{M})$ (cf. [9, Section 3]). This coincides with the subdivision given by topology.

Proposition 3.29. For any $w, u \in \tilde{\mathcal{B}}(\mathcal{M})$, $\mathcal{T}(w) = \mathcal{T}(u)$ if and only if $\mathcal{M}_w = \mathcal{M}_u$.

Proof. We proceed by showing that $\mathcal{T}(u)$ uniquely determines \mathcal{M}_u and vice versa. To see that $\mathcal{T}(u)$ determines \mathcal{M}_u , note that each u -minimum basis of \mathcal{M} is obtained by choosing a basis of $F / (\bigcup_{G \leq F} G)$ for each $F \in \mathcal{T}(u)$ and taking their union.

We now show that \mathcal{M}_u determines $\mathcal{T}(u)$. Choose some \mathcal{M} -ultrametric w such that $\mathcal{M}_w = \mathcal{M}_u$. Then w determines a flag of flats

$$\mathcal{F} := F_0 \subsetneq F_1 \subsetneq \cdots \subsetneq F_k$$

such that $F_0 = \emptyset$, $F_k = E$, w is constant on each $F_i \setminus F_{i-1}$, and if $e \in F_i \setminus F_{i-1}$ and $f \in F_{i-1}$, then $w_e > w_f$. If each F_i is connected, then $\mathcal{F} = \mathcal{T}(w)$ by Proposition 3.8. Now assume this is not the case and let i be the largest number such that F_i is disconnected. Express F_i as a direct sum $F_i = C \oplus D$. Then we can express the first $i + 1$ parts of \mathcal{F} as

$$\emptyset \subsetneq C'_1 \oplus D'_1 \subsetneq \cdots \subsetneq C'_{i+1} \oplus D'_{i+1}.$$

Without changing \mathcal{M}_w , we can change the values of w so that $D'_j = \emptyset$ for all $j \leq \text{rank}(C)$. This is true because any \mathcal{M}_w -minimum basis of \mathcal{M} must contain a basis of each C'_j / C'_{j-1} and a basis of each D'_j / D'_{j-1} . Such a change also preserves the ordering of coordinates of w within each connected component, and hence $\mathcal{T}(w)$. Now we can write the first $i + 1$ parts of \mathcal{F} as

$$\emptyset \subsetneq C_1 \subseteq \cdots \subsetneq C \subsetneq C \oplus D_1 \subsetneq \cdots \subsetneq C \oplus D.$$

We can repeat this process recursively on each disconnected C_j and D_j until every direct summand is connected. The resulting collection of connected flats is $\mathcal{T}(w)$ by Proposition 3.8. \square

4. APPLICATIONS TO PHYLOGENETICS

In this section, we will consider how the results above can be applied to phylogenetic reconstruction. First, we will explain the connection between the set of \mathcal{M} -ultrametrics discussed in Section 3.2 and the field of phylogenetics. Next, we will address Question 1.1, concerning the structure of the set of l^∞ -closest points to the set of equidistant tree metrics. We also decompose the space of 3 and 4-leaf dissimilarity maps according to the tree topologies represented in the set of l^∞ -closest equidistant tree metrics. Finally, we investigate optimizing to the set of tree metrics and show how many of the results for equidistant tree metrics carry over.

4.1. Phylogenetics and Bergman fans of matroids. Let $RP(n)$ be the set of all n -leaf rooted trees with leaves labeled by $[n] := \{1, \dots, n\}$. Following the convention of [15, Section 2.2], we call the elements of $RP(n)$ *rooted phylogenetic $[n]$ -trees*. We will also consider the set of *rooted binary phylogenetic $[n]$ -trees* which we will denote $RB(n)$. To represent the topology of $\mathcal{T} \in RB(n)$ we use the notation $(S_1(S_2))$ to indicate that the leaves labeled by the set S_1 and S_2 are on opposite sides of the root in \mathcal{T} . We apply this notation recursively to give the topology of the rooted subtree in \mathcal{T} induced by the labels in S_1 and S_2 . Thus, for example, we can express the topology of the the rooted tree in Figure 9 by $(D(C(AB)))$.

Let $\mathcal{T} \in RP(n)$ and assign a positive weighting to the edges of \mathcal{T} . This naturally induces a metric δ on the leaves of \mathcal{T} where $\delta(i, j)$ is the length of the unique path between i and j . If we further assume that the distance from each leaf vertex to the root is the same then δ is an *ultrametric*.

Definition 4.1. [15, Definition 7.2.1] A dissimilarity map $\delta : X \times X \rightarrow \mathbb{R}$ is called an *ultrametric on X* if for every three distinct elements $i, j, k \in X$,

$$\delta(i, j) \leq \max\{\delta(i, k), \delta(j, k)\}.$$

Using this definition, the set of ultrametrics on $[n]$ is exactly the set of $\mathcal{M}(K_n)$ -ultrametrics [4]. Hence, the \mathcal{M} -ultrametrics introduced in Section 3 generalize this special case. We will think of each dissimilarity map on n elements as a point in $\mathbb{R}^{\binom{n}{2}}$ where $\delta_{ij} = \delta(i, j)$. For simplicity, we will use U_n to denote the set of all ultrametrics on n elements which could be denoted $U_{\mathcal{M}(K_n)}$ using the notation of the previous section.

An equidistant edge weighting of a rooted tree is a weighting of the edges where the distance from each leaf to the root is the same and where the weight of every internal edge is nonnegative. Note that this allows the possibility of negative weights on leaf edges. Given any ultrametric u on $[n]$, there exists a unique $\mathcal{T} \in RP(n)$ and an equidistant weighting such that the ultrametric induced by $(\mathcal{T} : w)$ is equal to u . We call $(\mathcal{T} : w)$ an *equidistant representation of u* and we think of the tree as the *topology of u* .

We can also convert an equidistant weighting of a tree into a *vertex weighting* of that same tree. Namely, given any internal vertex v in an equidistant representation of an ultrametric δ , $\delta(i, j)$ is constant over all pairs of leaves i, j that have v as their most recent common ancestor. We obtain a vertex weighting from an edge weighting by labeling each internal vertex by this constant value. Conversely, if for each pair of internal vertices u, v , the label of v is greater than the label of u if and only if v is an ancestor of u , then we can convert this vertex weighting into an equidistant edge weighting.

The following proposition shows that this notion of topology is consistent with that of Definition 3.9. This is what motivated our choice of terminology there. It also justifies our slight abuse of notation in using $\mathcal{T}(u)$ to refer to the topology of the equidistant representation of u .

Proposition 4.2. *If $\mathcal{M} = \mathcal{M}(K_n)$, then $\mathcal{T}(u) = \mathcal{T}(v)$ if and only if there exist equidistant tree metric representations (\mathcal{T}, w_u) and (\mathcal{T}, w_v) of u and v respectively.*

Proof. This follows from Proposition 3.29 and results in [4]. □

Example 4.3. Figure 9 shows three equivalent ways to represent u , an $\mathcal{M}(K_4)$ -ultrametric.

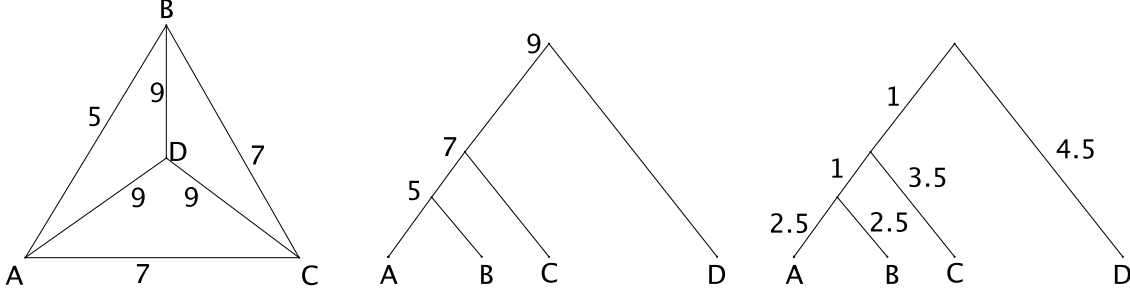


FIGURE 9. Three different representation of an $\mathcal{M}(K_4)$ -ultrametric.

The image on the far left shows u as an edge weighting of K_4 . This same ultrametric was depicted in Figure 9 along with its corresponding flag of flats. The center image depicts a vertex representation of u . The image to the far right is an equidistant representation of u on an element of $RB(4)$. Letting $(x_{12}, x_{13}, x_{14}, x_{23}, x_{24}, x_{34})$ be the coordinates of an arbitrary point in $\mathbb{R}^{\binom{4}{2}}$, we can also write u as the vector $(5, 7, 9, 7, 9, 9) \in \mathbb{R}^6$.

To determine an l^∞ -closest ultrametric to a dissimilarity map δ , we first compute the subdominant ultrametric $\delta^{\mathcal{M}(K_m)}$ and then observe as in Lemma 3.15 that

$$d(\delta, U_n) = \frac{1}{2}d(\delta, \delta_U).$$

We call $\delta_U = \delta_u + \frac{1}{2}d(\delta, \delta_U)$ the *canonical closest ultrametric to δ* .

As noted in the introduction, the set of l^∞ -closest ultrametrics is in general not a single point. Moreover, in many instances, the set of l^∞ -closest ultrametrics to δ , $C(\delta, U_n)$, will contain ultrametrics with different topologies. Thus, there may be several different trees that explain the data equally well from the perspective of the l^∞ -metric. By Corollary 3.27, this happens if and only if the output of Algorithm 1 contains ultrametrics with multiple tree topologies.

Algorithm 1 has a nice interpretation in the context of trees. Let $\delta \in \mathbb{R}^{\binom{n}{2}}$ be a dissimilarity map and let $u \in C(\delta, U_n)$ be an l^∞ -nearest ultrametric with equidistant representation on the tree $\mathcal{S} \in RP(n)$. Since u is an $\mathcal{M}(K_n)$ -ultrametric, by Proposition 3.8 there is a unique hierarchy of connected flats of $\mathcal{M}(K_n)$ associated to u which we denoted $\mathcal{T}(u)$. The nonempty flats of $\mathcal{T}(u)$ not equal to E are in one-to-one correspondence with the internal vertices of \mathcal{S} . Namely, if i_1, \dots, i_k are the leaves that lie below an internal vertex of \mathcal{S} , then the associated flat of K_n is the collection of edges among i_1, \dots, i_k . For the rest of this section, given an ultrametric u we will use the notation $\mathcal{T}(u)$ for the tree topology of the equidistant tree representation.

We can visualize the process of using Algorithm 1 to compute the tropical vertices of $C(\delta, U_n)$. We start with a vertex representation of the canonical closest ultrametric δ_U and slide internal vertices down (i.e., decreasing vertex labels) until either running out of slack or reaching a polytomy. When we reach a polytomy, we resolve it in all possible

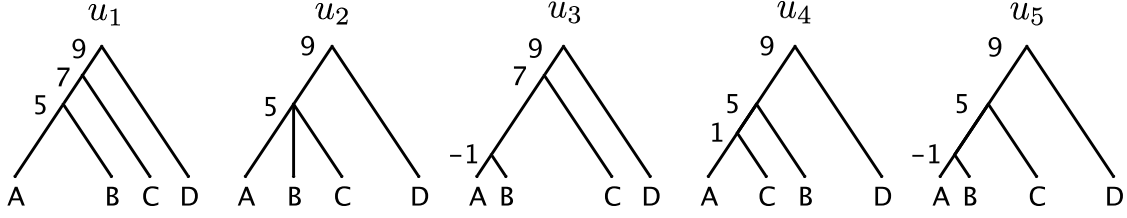


FIGURE 10. Trees produced by Algorithm 1

ways, and then continue. At each step, we use Lemma 3.23 to check if we have a tropical vertex.

Example 4.4. Figure 10 shows the ultrametrics from Example 3.25 expressed as trees. We obtain u_2 from u_1 by sliding the middle internal vertex until it reaches the bottom one. We obtain u_3 from u_1 by sliding the bottom internal vertex down until the slack runs out. Then, we obtain u_4 from u_2 by resolving the tritomy so that A and C form a cherry, and sliding the new internal vertex down until the slack runs out. The ultrametric u_5 is obtained by sliding the middle internal vertex of u_3 down as far as it can go, or by resolving the tritomy in u_2 . The tropical vertices are u_3 , u_4 , and u_5 .

Example 4.4 show that it is possible for the set of l^∞ -nearest ultrametrics to a point to contain different topologies. Below, we consider what sets of topologies are possible in $C(\delta, U_n)$ for an arbitrary point $\delta \in \mathbb{R}^{\binom{n}{2}}$.

Definition 4.5. Let $\delta \in \mathbb{R}^{\binom{n}{2}}$ and $u \in U_n$. Define

$$\text{Top}(\delta) := \{\mathcal{T}(u) : u \in C(\delta, U_n)\}.$$

In [6], the authors study the geometry of the set of dissimilarity maps around a polytomy with respect to the euclidean norm. They showed that locally this space could be partitioned according to the closest tree topology. In contrast to that situation, we have the following result for the l^∞ -metric.

Proposition 4.6. *Let \mathcal{T} be a rooted phylogenetic $[n]$ -tree with a polytomy. Assume that \mathcal{T} is not the star tree. Then there exists $\delta \in \mathbb{R}^{\binom{n}{2}}$ such that $\text{Top}(\delta)$ contains \mathcal{T} and all of its resolutions.*

Proof. Let u be an ultrametric with $\mathcal{T}(u) = \mathcal{T}$. Since \mathcal{T} is not the star tree, there exist three leaves $\{i, j, k\}$ such that $u_{ij} < u_{ik} = u_{jk}$. Define $\delta := u + \varepsilon(e_{ik} - e_{jk})$ for some $0 < \varepsilon < u_{ik} - u_{ij}$. Then u is in $C(\delta, U_n)$ and so are all possible resolutions of the the polytomy (cf. Algorithm 1). \square

Example 4.7. Let $u = (5, 5, 10, 5, 10, 10)$. Choosing $\{1, 2, 4\}$ and $\varepsilon = 1$, we have $\delta = (5, 5, 10, 5, 9, 11)$. The canonical closest ultrametric $\delta_c = (6, 6, 10, 6, 10, 10)$ has an unresolved tritomy. $C(\delta, U_n)$ also contains ultrametrics corresponding to each different resolution of the tritomy, for example, $(4, 6, 10, 6, 10, 10)$, $(6, 4, 10, 6, 10, 10)$, and $(6, 6, 10, 4, 10, 10)$.

We obtain the following corollary by choosing a tree with a single resolved triple in the proof of Proposition 4.6.

Corollary 4.8. *There exists points in $\mathbb{R}^{\binom{n}{2}}$ where $Top(\delta) \cap RB(n)$ contains $(2n-3)!!/3$ different tree topologies.*

We will also see from our decomposition of $\mathbb{R}^{\binom{n}{2}}$ that there are actually 6-dimensional polyhedral cones in which every point in the interior has five l^∞ -closest binary tree topologies.

Even when all l^∞ -nearest ultrametrics to some given $\delta \in \mathbb{R}^{\binom{n}{2}}$ have the same topology, the dimension of the set of l^∞ -nearest ultrametrics can be high. The affine hull of each maximal cone of U_n is a linear space defined by relations of the form $x_{ik} - x_{jk} = 0$ where $(k(ij))$ is a triple compatible with the corresponding tree. Locally, optimizing to U_n is equivalent to optimizing to such a linear space and so our results from Section 2 can be applied.

Proposition 4.9. *Let $\mathcal{T} \in RB(n)$. There exists $\delta \in \mathbb{R}^{\binom{n}{2}}$ such that $\dim(C(\delta, U_n)) = n-2$ and every ultrametric in $C(\delta, U_n)$ has topology \mathcal{T} .*

Proof. Let u be an ultrametric and $(k(ij))$ a triple compatible with $\mathcal{T}(u)$. For $\varepsilon > 0$, let $\delta = u + \varepsilon(e_{ik} - e_{jk})$. If ε is sufficiently small, $C(\delta, U_n) = C(\delta, L)$ where L is the affine hull of the maximal cone corresponding to epsilon. \mathcal{T} . The type of x relative to L is the signed vector σ where $\sigma_{ij} = +$, $\sigma_{ik} = -$, and all other entries are zero. The rank of σ in \mathcal{O}_L is one, and thus by Theorem 2.7, $\dim(C(\delta, U_n)) = (n-1) - 1 = n-2$. \square

Example 4.10. Let $(x_{12}, x_{13}, x_{14}, x_{23}, x_{24}, x_{34})$ be the coordinates of a point in $\mathbb{R}^{\binom{4}{2}}$. Choose $u = (5, 7, 9, 7, 9, 9)$, the ultrametric corresponding to the tree in Figure 9. The triple $(3(12))$ is compatible with $\mathcal{T}(u)$ and so we choose

$$\delta = (5, 7, 9, 7, 9, 9) + (0, 1, 0, -1, 0, 0) = (5, 8, 9, 6, 9, 9).$$

The subdominant ultrametric $\delta^{\mathcal{M}(K_m)} = (5, 6, 9, 6, 9, 9)$ and the canonical ultrametric $\delta_c = (6, 7, 10, 7, 10, 10)$. The interior vertex at height seven of the canonical ultrametric is immobile. We have two remaining degrees of freedom that come from simultaneously adjusting the values of $\{c_{14}, c_{24}, c_{34}\}$ and $\{c_{12}\}$.

4.2. The Decomposition for 3-Leaf and 4-Leaf Trees. The following definition makes formal the idea of decomposing the points in $\mathbb{R}^{\binom{n}{2}}$ according to their sets of l^∞ -closest trees.

Definition 4.11. Let $\{\mathcal{T}_1, \dots, \mathcal{T}_k\} \subseteq RP(n)$. The *district* of $\{\mathcal{T}_1, \dots, \mathcal{T}_k\}$ is the set

$$D(\{\mathcal{T}_1, \dots, \mathcal{T}_k\}) := \{\delta \in \mathbb{R}^{\binom{n}{2}} : Top(\delta) = \{\mathcal{T}_1, \dots, \mathcal{T}_k\}\}.$$

We can represent a dissimilarity map on three elements as a point $(x_{12}, x_{13}, x_{23}) \in \mathbb{R}^3$. There are three maximal cones of U_3 corresponding to the three elements of $RB(3)$. Modulo the common lineality space of each of these cones, $\text{span}\{(1, 1, 1)\}$, we can fix the first coordinate at zero and represent the space of dissimilarity maps on three elements in the plane.

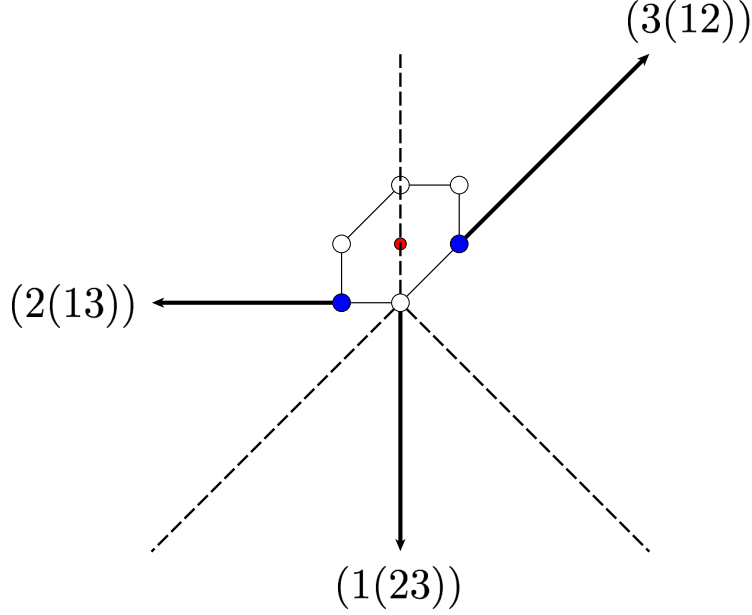


FIGURE 11

Figure 11 depicts a polyhedral subdivision of \mathbb{R}^3 according to districts. There are seven cones in this subdivision. The labels $(1(23))$, $(3(12))$, and $(2(13))$ label the image of the set of ultrametrics for each topology. These labels also label the areas between the dashed lines which are the 2-dimensional images of the three 3-dimensional districts $D\{(1(23))\}$, $D\{(2(13))\}$, and $D\{(3(12))\}$. The dotted lines themselves are the images of the 2-dimensional cones whose interiors form the districts $D\{(123), (1(23)), (2(13))\}$, $D\{(123), (1(23)), (3(12))\}$, and $D\{(123), (2(13)), (3(12))\}$. The origin represents the image of $\text{span}((1, 1, 1))$ which is the district of the 3-leaf claw tree, $D\{(123)\}$.

Example 4.12. The image of the dissimilarity map $\delta = (1, 1, 3)$ after modding out by U_3 's lineality space is pictured in Figure 11. Note that $d(\delta, U_3) = 1$. The hexagon surrounding it is the zonotope that is the image of the cube $C_1(\delta)$. The filled vertices of the zonotope are the tropical vertices corresponding to the l^∞ -closest ultrametrics $(2, 1, 2)$ and $(1, 2, 2)$. The origin corresponds to the l^∞ -closest ultrametric $(2, 2, 2)$ and $\delta \in D\{(123), (2(13)), (3(12))\}$.

The decomposition for 4-leaf trees is much more complicated. The supplemental materials, located on the authors' websites, contain a polyhedral subdivision of $\mathbb{R}^{\binom{4}{2}}$ into a fan consisting of 723 maximal polyhedral cones labeling 43 different districts. Each maximal cone is labeled by a set $\{\mathcal{T}_1, \dots, \mathcal{T}_k\} \subseteq RB(n)$, meaning that each point in the interior of the cone is in $D(\{\mathcal{T}_1, \dots, \mathcal{T}_k\})$.

The fan was obtained by first considering each of the fifteen different trees in $RB(n)$ individually. For each $\mathcal{T} \in RB(n)$, we constructed a fan with support $\mathbb{R}^{\binom{4}{2}}$, where all of the points in the interior of each maximal cone in the fan satisfied either $\mathcal{T} \in \text{Top}(\delta)$ or

$\mathcal{T} \notin \text{Top}(\delta)$. The resulting fan is the common refinement of these fifteen fans. Note that there are even more than 43 districts since our construction only considers 6-dimensional districts.

Based on the 3-leaf case, one might hope that districts are easily described or possess some nice properties. However, the 4-leaf case shows that many of these properties do not hold in general.

Proposition 4.13. *Districts are not necessarily convex nor tropically convex.*

Proof. We offer the following counterexample in $\mathbb{R}^{(4)}_{(2)}$. Let $\delta^1 = (10, 20, 21, 23, 25, 27)$ and $\delta^2 = (10, 23, 21, 20, 25, 27)$. Not only is $\text{Top}(\delta^1) = \text{Top}(\delta^2) = \{(4(3(12)))\}$, but in fact $\delta^1_U = \delta^2_U = (10, 20, 21, 20, 21, 21)$. The point $\delta^3 = \frac{1}{2}\delta^1 + \frac{1}{2}\delta^2$ lies on the line between these two points but $\text{Top}(\delta^3) = \{(3(4(12)))\}$.

Similarly, recalling the notation for tropical addition and multiplication, the point $\delta^4 = (0 \odot \delta^1) \oplus (-\frac{3}{2} \odot \delta^2)$ lies on the tropical line between these two points but $\text{Top}(\delta^4) = \{(3(4(12)))\}$. \square

Two arbitrary points δ^1 and δ^2 have the same subdominant ultrametric topology if they have the same relative ordering of coordinates - that is, $\delta^1_{ij} \leq \delta^1_{kl}$ if and only if $\delta^2_{ij} \leq \delta^2_{kl}$ and $\delta^1_{ij} < \delta^1_{kl}$ if and only if $\delta^2_{ij} < \delta^2_{kl}$. For 3-leaf trees, relative ordering also completely determines district. The example below demonstrates that for trees with more than three leaves this is not the case.

Example 4.14. Let $\delta^1 = (4, 8, 12, 9, 21, 22)$ and $\delta^2 = (4, 8, 12, 9, 13, 14)$. Both dissimilarity maps satisfy $\delta^1_{12} < \delta^1_{13} < \delta^1_{23} < \delta^1_{14} < \delta^1_{24} < \delta^1_{34}$. However, $\text{Top}(\delta^1) = \{(4(3(12)))\}$ and $\text{Top}(\delta^2) = \{(4(3(12))), (4(2(13))), (4(1(23)))\}$.

It does not appear possible to represent these districts with significantly fewer polyhedral cones by combining cones. Consider for example the forty maximal cones that constitute the district $D(\{(4(3(12)))\})$. Any five element subset of these cones contains a pair whose convex hull has full dimensional intersection with the interior of a maximal cone from another district. Therefore, by combining these cones the best we could hope for is to represent this district as the union of ten maximal convex cones. While a few can be patched together the final description does not appear any simpler.

This polyhedral subdivision was constructed by examining each possible 4-leaf subdominant ultrametric topology and determining under what conditions we could slide vertices as in Algorithm 1 to obtain a new topology. It is certainly possible, though likely much more difficult, to do the same thing for trees with any fixed number of leaves. It is unclear how to generalize our approach to an arbitrary number of leaves and so the following problem remains open.

Problem 4.15. Give a polyhedral decomposition of $\mathbb{R}^{(n)}_{(2)}$ according to districts.

4.3. Tree Metrics. We end with a note about l^∞ -optimization to the set of tree metrics. A tree metric δ on $[n]$ is a metric induced by a positive edge weighting of an n -leaf tree (no longer rooted nor equidistant). The pair $(\mathcal{T} : w)$ that realizes this metric is called a

tree metric representation of δ . A metric δ is a tree metric if and only if it satisfies the four-point condition [15, Theorem 7.2.6].

Definition 4.16. [15, Definition 7.2.1] A dissimilarity map $\delta : X \times X \rightarrow \mathbb{R}$ satisfies the four-point condition if for every four (not necessarily distinct) elements $w, x, y, z \in X$,

$$\delta(w, x) + \delta(y, z) \leq \max\{\delta(w, y) + \delta(x, z), \delta(w, z) + \delta(x, y)\}.$$

We use the notation $\mathcal{T}_n \subset \mathbb{R}^{\binom{n}{2}}$ to denote the set of all tree metrics on $[n]$. If we insist that the points in Definition 4.16 are distinct, then the set of metrics satisfying the *distinct* 4-point condition is the tropical Grassmannian [16]. Thus, the problem of finding the closest tree metric is closely related to the problem of l^∞ -optimization to this tropical variety. We find the l^∞ -distance from an arbitrary point to the set of tree metrics by considering each tree topology separately. The set of binary phylogenetic trees with label set $[n]$ is $B(n)$. For each $\mathcal{T} \in B(n)$, the distance to the set of tree metrics corresponding to \mathcal{T} can be found by solving a linear program. Taking the minimum of these $(2n - 5)!!$ distances gives us the distance to the set of tree metrics. As a corollary to Proposition 3.4, we have that $C(\delta, U_n)$ is always connected. However, this is not true for tree metrics.

Proposition 4.17. *There exists $\delta \in \mathbb{R}^{\binom{6}{2}}$ such that $C(\delta, \mathcal{T}_6)$ and $C(\delta, \mathcal{G}_{2,6})$ are not connected.*

Proof. Let

$$\delta = (35, 22, 32, 49, 42, 26, 34, 23, 32, 39, 41, 34, 46, 49, 32)$$

be the metric in $\mathbb{R}^{\binom{6}{2}}$ with coordinates $(\delta_{12}, \delta_{13}, \delta_{14}, \dots, \delta_{45}, \delta_{46}, \delta_{56})$. Then $d(\delta, \mathcal{T}_6) = d(\delta, \mathcal{G}_{2,6}) = 5$. The set $C(\delta, \mathcal{T}_6)$ is the union of two disjoint polyhedra. One is four-dimensional and corresponds to the 6-leaf tree with nontrivial splits $13|2456$, $134|256$ and $25|1346$ and the other is six-dimensional and corresponds to the 6-leaf tree with nontrivial splits $14|2356$, $134|256$ and $56|1234$. In this instance, $C(\delta, \mathcal{T}_6) = C(\delta, \mathcal{G}_{2,6})$ \square

Unfortunately, many of the less than desirable properties exhibited in the ultrametric case hold for tree metrics. Simple modifications to the constructions for ultrametrics give analogous results for tree metrics and unrooted trees to the results in Propositions 4.6 and 4.18, and Corollary 4.8. We conclude with one such example about the possible dimension of the set of l^∞ -closest tree metrics to a point.

Proposition 4.18. *Let $\mathcal{T} \in B(n)$. There exists $\delta \in \mathbb{R}^{\binom{n}{2}}$ such that $\dim(C(\delta, \mathcal{T}_n)) = 2n - 6$ and every tree metric in $C(\delta, \mathcal{T}_n)$ has \mathcal{T} as a tree metric representation.*

Proof. Let z be a tree metric with tree metric representation \mathcal{T} . Let L be the affine hull of the cone of tree metrics corresponding to \mathcal{T} . This is the linear space of dimension $2n - 3$ defined by all of the equalities of the form $x_{ik} + x_{jl} - x_{il} - x_{kj} = 0$ where $ij|kl$ is an induced quartet of \mathcal{T} .

Choose i, j, k and l so that $ij|kl$ is a fully resolved quartet of \mathcal{T} . For $\varepsilon > 0$, let $\delta = z + \varepsilon(e_{ik} + e_{jl} - e_{il} - e_{kj})$. If ε is sufficiently small, $C(\delta, U_n) = C(\delta, L)$. The type of z relative to L is the signed vector σ where $\sigma_{il} = +, \sigma_{kj} = +, \sigma_{ik} = -, \sigma_{jl} = -$, and all other entries are zero. The rank of σ in \mathcal{O}_L is three, and thus by Theorem 2.7, $\dim(C(\delta, U_n)) = (2n - 3) - 3 = 2n - 6$. \square

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