A tropical interpretation of m-dissimilarity maps Cristiano Bocci * and Filip Cools [†]

Abstract. Let T be a weighted tree with n numbered leaves and let $D = (D(i, j))_{i,j}$ be its distance matrix, so D(i, j) is the distance between the leaves i and j. If m is an integer satisfying $2 \le m \le n$, we prove a tropical formula to compute the m-dissimilarity map of T (i.e. the weights of the subtrees of T with m leaves), given D. For m = 3, we present a tropical description of the set of m-dissimilarity maps of trees. For m = 4, a partial result is given.

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1 Introduction

Let D be a matrix whose rows and columns are indexed by a set X. We assume that D is symmetric and has zero entries on the main diagonal. In phylogenetics, these kind of matrices are called *dissimilarity matrices*. Usually, we take $X = [n] := \{1, 2, ..., n\}$. Hence a dissimilarity matrix D can also be seen as a map $D : [n]^2 \to \mathbb{R}$, with D(i, j) = D(j, i) and D(i, i) = 0 for each $i, j \in [n]$.

A metric is a non-negative dissimilarity matrix which satisfies the triangle inequality $D(i, j) \leq D(i, k) + D(k, j)$ for all $i, j, k \in X$.

We say that D has a graph realization if there is a weighted graph (so a nonnegative weight is assigned to each edge) whose node set contains X and such that the distance (i.e. the length of the shortest path) between nodes $i, j \in X$ is exactly D(i, j). A distance matrix is a non-negative dissimilarity matrix that has a graph realization. In [3, 4], one can find some results on these kind of matrices.

In the case the graph is a tree and X corresponds to the set of leaves, D is called a *tree metric*. This case has been studied intensively and is well understood. The main result is the following (see [2] or [6, Theorem 2.36]).

Theorem 1.1 (Tree Metric Theorem). Let D be a non-negative dissimilarity matrix on [n]. Then D is a tree metric on [n] if and only if, for every four (not necessarily distinct) elements $i, j, k, l \in [n]$, the maximum of the three numbers

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D(i, j) + D(k, l), D(i, k) + D(j, l) and D(i, l) + D(j, k) is attained at least twice. Moreover, the tree T with leaves [n] that realizes D is unique.

The condition of the theorem is called the *four-point condition*. It is a necessary and sufficient condition on a matrix to be realized by a tree.

Tree metrics on n leaves are parameterized by the space of trees $\mathcal{T}_n \subset \mathbb{R}^{\binom{n}{2}}$. The following result gives us a description of \mathcal{T}_n (see [1]).

Theorem 1.2. The space of trees \mathcal{T}_n is the union of (2n-5)!! = 1.3.5...(2n-5) orthants isomorphic to $\mathbb{R}^{2n-3}_{\geq 0}$. More precisely, \mathcal{T}_n is a simplicial fan of pure dimension 2n-3 in $\mathbb{R}^{\binom{n}{2}}$.

We can consider a generalisation of the concept of dissimilarity matrix. Let $m \leq n$ be an integer. A map $D: [n]^m \to \mathbb{R}$ is called an *m*-dissimilarity map if

$$D(i_1,\ldots,i_m)=D(i_{\pi(1)},\ldots,i_{\pi(m)})$$

for all permutations $\pi \in S_m$ and $D(i_1, i_2, \ldots, i_m) = 0$ if the numbers i_1, \ldots, i_m are not pairwise distinct.

We say that D is realized by a tree T if the leaf set of T is [n] and if for each m-subset $V = \{i_1, \ldots, i_m\} \subset [n]$, the weight of the smallest subtree of Tcontaining V is equal to $D(i_1, \ldots, i_m)$. An important result on m-dissimilarity maps of trees is given in [5].

Theorem 1.3. Let T be a tree with n leaves and no vertices of degree 2. Let $m \ge 3$ be an integer. If $n \ge 2m - 1$, then T is uniquely determined by its m-dissimilarity map D. If n = 2m - 2, this is not true.

In this paper, we give a description of a map $\phi^{(m)} : \mathbb{R}^{\binom{n}{2}} \to \mathbb{R}^{\binom{n}{3}}$, sending the distance matrix of a tree T to its corresponding m-dissimilarity map (see Theorem 3.2 in Section 3). In Section 4, we investigate the case m = 3. In particular, we show that $\phi^{(3)}(\mathcal{T}_n)$ is equal to the intersection of the tropical Grassmannian $\mathcal{G}_{3,n}$ with a linear space (see Theorem 4.6). In Section 5, we give a partial result on the case m = 4. An introduction to tropical gemetry is given in Section 2.

To finish this section, we describe the relation with Phylogenetics. A classical problem in computational biology is to construct a phylogenetic tree from a sequence alignment of n species

Species 1	ACAAT	GTCAT	TAGCO	ATACO	GTAGG	TACGA	TGC	•
Species 2	ACGTT	GTCAA	TAGAG	ATTT	FGGAT	GAACG	ATA	
Species 3	ACGTA	GTCAT	TACAC	CATTC	FGGAT	FAACG	TTA	
Species 4	GCACA	GTCAG	TAGAA	GCTAT	FGGTA	CATCG	ATC	•
:	÷	:	:	:	:	:	:	
Species n	GAACT	GTCAG	TAGAA	GCGA	GTGTA	CATTC	GTT	

The main technique to select a tree model is computing the maximum likelihood estimate (MLE) for each of the (2n-5)!! trees. Unluckily, all the MLE computations are very difficult, even for a single tree, and this approach requires examining all exponentially many trees.

A popular way to avoid this problem is the so-called *distance based approach*, where one collapses the data to a dissimilarity matrix and obtains a tree via a projection onto tree space \mathcal{T}_n (by using the neighbor-joining algorithm). In fact, for such sequence data, computational biologists infer the distance between any two taxa. Thus, an interesting problem of phylogenetics concerns the construction of a weighted tree which represents this distance matrix, provided such a tree exists.

More general, we may think of an *m*-dissimilarity map as a measure of how dissimilar each subset of *m* species is. As a generalization of the previous problem, we can search for a weighted tree such that the *m*-subtree weights represent the entries of the *m*-dissimilarity map. This problem has some natural relevance in Phylogenetics. Indeed, for example, it can be more reliable statistically to estimate the triple weights D(i, j, k) rather than the pairwise distances D(i, j) ([5], [6]).

2 Tropical geometry

The tropical semiring $(\mathbb{R} \cup \{-\infty\}, \oplus, \otimes)$ is the set of real numbers completed with $-\infty$, equiped with two binary operations: the tropical sum is the maximum of two numbers and the tropical multiplication is the ordinary sum.

Tropical monomials $x_1^{a_1} \cdots x_k^{a_k}$ represent ordinary linear forms $\sum_{i=1}^k a_i x_i$ and tropical polynomials

$$\bigoplus_{a \in A} \lambda_a \otimes x_1^{a_1} \otimes \dots \otimes x_k^{a_k}, \tag{1}$$

with $A \subset \mathbb{N}^k$ finite and $\lambda_a \in \mathbb{R}$, represent piecewise-linear convex functions

$$F: \mathbb{R}^k \to \mathbb{R}: (x_1, \dots, x_k) \mapsto \max_{a \in A} \{\lambda_a + \sum_{i=1}^k a_i x_i\}.$$
 (2)

Now let K be the field of Puiseux series, i.e. the field of formal power series $a = \sum_{q \in \mathbb{Q}} a_q t^q$ in the variable t such that the set $Q_a = \{q \in \mathbb{Q} \mid a_q \neq 0\}$ is bounded below and has a finite set of denominators. For such an a, the infimum of Q_a is equal to the minimum and we call it the valuation val(a) of a.

A polynomial

$$f(x_1, \cdots, x_k) = \sum_{a \in A} g_a(t) x_1^{a_1} \cdots x_k^{a_k} \in K[X]$$

gives rise to the tropical polynomial in (1), where $\lambda_a = -\operatorname{val}(g_a(t))$. We denote this tropical polynomial by $\operatorname{trop}(f)$.

We define the tropical hypersurface $\mathcal{T}(F) = \mathcal{T}(\operatorname{trop}(f))$ as the corner locus of the function F in (2), i.e. the set of $x = (x_1, \ldots, x_k) \in \mathbb{R}^k$ such that the maximum of the collection of numbers

$$\left\{\sum_{i=1}^{k} a_i x_i + \lambda_a\right\}_{a \in \mathcal{A}}$$

is attained at least twice.

Theorem 2.1. If $I \subset K[x_1, \ldots, x_n]$ is an ideal, the following two subsets of \mathbb{R}^k coincide:

- 1. the intersection of all tropical hypersurfaces $\mathcal{T}(trop(f))$ with $f \in I$;
- 2. the closure in \mathbb{R}^k of the set

$$\{(-val(y_1),\ldots,-val(y_k)) \mid (y_1,\ldots,y_k) \in V(I)\} \subset \mathbb{Q}^k$$

Proof. See [7, Theorem 2.1].

For an ideal $I \subset K[x_1, \ldots, x_k]$, we denote by $\mathcal{T}(I) \subset \mathbb{R}^k$ the set mentioned in Theorem 2.1. It is called the *tropical variety* of the ideal I.

Definition 2.2. If $\mathcal{T}(I) \subset \mathbb{R}^k$ is a tropical variety, we say that $\{f_1, \ldots, f_r\}$ is a tropical basis of $\mathcal{T}(I)$ if and only if $I = \langle f_1, \ldots, f_r \rangle$ and

$$\mathcal{T}(I) = \mathcal{T}(trop(f_1)) \cap \cdots \cap \mathcal{T}(trop(f_r)).$$

Remark 2.3. In general, a set of generators of an ideal I is not a tropical basis for $\mathcal{T}(I)$. Of course, the singleton $\{f\}$ is a tropical basis for the tropical hypersurface $\mathcal{T}(\operatorname{trop}(f))$.

We are mainly interested in the tropical variety $\mathcal{T}(I_{m,n})$, where $I_{m,n}$ is the ideal of the *Grassmannian* $G(m,n) \subset \mathbb{R}^{\binom{n}{m}}$. To be more precise, we fix a polynomial ring

$$\mathbb{Z}[x] = \mathbb{Z}[x_{i_1 i_2 \cdots i_d} \mid 1 \le i_1 < i_2 < \cdots < i_m \le n]$$

in $\binom{n}{m}$ variables with integer coefficients. The Plücker ideal $I_{m,n}$ is the prime ideal in $\mathbb{Z}[x]$, consisting of the algebraic relations among the determinants of the $(m \times m)$ -minors of any $(m \times n)$ -matrix with entries in a commutative ring. It is well-known that $I_{m,n}$ is generated by quadrics (see for example [8]).

The affine variety defined by $I_{m,n}$ is the Grassmannian $G(m,n) \subset \mathbb{R}^{\binom{n}{m}}$, which parameterizes all *m*-dimensional linear subspaces of an *n*-dimensional vector space. It has dimension (n-m)m+1.

Definition 2.4. The tropical variety $\mathcal{T}(I_{m,n})$ is called a tropical Grassmannian and is denoted by $\mathcal{G}_{m,n}$.

Theorem 2.5. The tropical Grassmannian $\mathcal{G}_{m,n}$ is a polyhedral fan in $\mathbb{R}^{\binom{n}{m}}$. Each of its maximal cones has the same dimension, namely (n-m)m+1. Proof. See [7, Corollary 3.1.].

Now we are going to fix our attention on the case m = 2.

Example 2.6 (m = 2 and n = 4). The smallest non-zero Plücker ideal is the principal ideal $I_{2,4} = (x_{12}x_{34} - x_{13}x_{24} + x_{14}x_{23})$. Thus $\mathcal{G}_{2,4}$ is a fan with three five-dimensional cones $\mathbb{R}^4 \times \mathbb{R}_{<0}$ glued along \mathbb{R}^4 .

Theorem 2.7. The ideal $I_{2,n}$ is generated by the quadratic polynomials

$$p_{ijkl} := x_{ik} x_{jl} - x_{ij} x_{kl} - x_{il} x_{jk} \qquad (1 \le i < j < k < l \le n).$$
(3)

These polynomials form the reduced Gröbner basis if the underlined terms are leading.

Proof. See [8, Theorem 3.1.7 and Proposition 3.7.4].

For each quadruple $\{i, j, k, l\} \subset \{1, 2, ..., n\}$, we consider the tropical polynomial

$$\operatorname{trop}(p_{ijkl}) = (x_{ij} \otimes x_{kl}) \oplus (x_{ik} \otimes x_{jl}) \oplus (x_{il} \otimes x_{jk}).$$

This polynomial defines a tropical hypersurface $\mathcal{T}(\operatorname{trop}(p_{ijkl}))$. It turns out that the tropical Grassmannian $\mathcal{G}_{2,n}$ is the intersection of these $\binom{n}{4}$ hypersurfaces, so the quadrics p_{ijkl} forms a tropical basis for $I_{2,n}$ (see [7]).

Let D be an dissimilarity matrix on [n] and $\{i, j, k, l\} \subset [n]$. The maximum of the three numbers D(i, j) + D(k, l), D(i, k) + D(j, l) and D(i, l) + D(j, k) is attained at least twice if and only if $D \in \mathcal{T}(\operatorname{trop}(p_{ijkl}))$. Thus Theorem 1.1 implies that a metric D on [n] is a tree metric if and only if D belongs to \mathcal{T}_n . In particular, one has the following result.

Theorem 2.8. The space of trees \mathcal{T}_n is the tropical Grassmannian $\mathcal{G}_{2,n}$.

Proof. See [7, Theorem 4.2] or the arguments above.

Now we come back to the general case (so the case where $m \leq n$ is arbitrary). The ideal $I_{m,n}$ is generated by quadratic polynomials, known as the Plücker relations. Among these are the three-term Plücker relations

$$p_{R,ijkl} := x_{Rik} x_{Rjl} - x_{Rij} x_{Rkl} - x_{Ril} x_{Rjk},$$

which are closely related to (3). Hereby R is any (m-2)-subset of [n] and $i, j, k, l \in [n] \setminus R$.

Definition 2.9. The three-term tropical Grassmannian $\mathcal{T}_{m,n}$ is the intersection

$$\mathcal{T}_{m,n} := \bigcap_{R,i,j,k,l} \mathcal{T}(trop(p_{R,ijkl})) \quad \subset \mathbb{R}^{\binom{n}{m}}.$$

In general, the three-term Plücker relations do not generate $I_{m,n}$. If m = 2, then $S = \emptyset$ and $\mathcal{T}_{2,n} = \mathcal{G}_{2,n}$. For $m \geq 3$, the tropical Grassmannian $\mathcal{G}_{m,n}$ is contained in $\mathcal{T}_{m,n}$. This containment is proper for $n \geq m + 4$.

3 A description on the *m*-subtree weight map

In this section, we are going to give an explicit description of a map

$$\phi^{(m)}: \mathbb{R}^{\binom{n}{2}} \to \mathbb{R}^{\binom{n}{m}}.$$

sending the dissimilarity matrix D of a tree T to its m-dissimilarity map.

Let \prec be the order relation on \mathbb{N}^∞ defined as follows. We have

$$(a_1, a_2, a_3, \ldots) \prec (b_1, b_2, b_3, \ldots)$$

if and only if there exists an $n \in \mathbb{N}$ such that $a_i = b_i$ for all i < n and $a_n < b_n$.

Let T be a tree with n leaves. Let r be an inner node of T and consider T as a rooted tree (with root r). Let \mathcal{N} be the set of nodes of T. In particular, the set of leaves $[n] = \{1, \ldots, n\}$ is contained in \mathcal{N} .

Lemma 3.1. There exists a map $\alpha : \mathcal{N} \to \mathbb{N}^{\infty}$ such that the following properties hold:

- 1. α is injective.
- 2. If $n \in \mathcal{N}$ is an ancestor of $m \in \mathcal{N}$, we have $\alpha(m) \succ \alpha(n)$. So the root r of T gives rise to the minimum of $\{\alpha(n) | n \in \mathcal{N}\}$.
- 3. If $n_1, n_2 \in \mathcal{N}$ with n_2 not a descendant nor an ancestor of $n_1, m_1 \in \mathcal{N}$ a descendant of n_1 and $m_2 \in \mathcal{N}$ a descendant of n_2 , we have $\alpha(m_1) \prec \alpha(m_2)$ if and only if $\alpha(n_1) \prec \alpha(n_2)$.

Proof. We will define α inductively. Take $\alpha(r) = (0, 0, 0, \ldots)$. For the induction step, if $\alpha(n) = (a_1, \ldots, a_s, 0, 0, \ldots)$ is defined for some $n \in \mathcal{N}$ with $a_s \neq 0$ and if m_1, \ldots, m_t are the children of n, take $\alpha(n_i) = (a_1, \ldots, a_s, i, 0, \ldots)$. Note that all the properties hold and that the depth of $n \in \mathcal{N}$ in T is equal to the number of non-zero entries in $\alpha(n)$.

We say that the leaves of T are *well-numbered* if and only if $\alpha(i) \prec \alpha(j)$ for all i < j.

A permutation $\sigma \in S_m$ of $\{1, \ldots, m\}$ is called *cyclic* if and only if the decomposition of σ into a product of disjoint cycles consists of only one cycle of order m. Denote the set of cyclic permutations in S_m by C_m . Note that $\sigma^m = Id$ if $\sigma \in C_m$.

Theorem 3.2. Let n and m be integers such that $n > m \ge 2$. Let

$$\phi^{(m)}: \mathbb{R}^{\binom{n}{2}} \to \mathbb{R}^{\binom{n}{m}}: X = (X_{i,j}) \mapsto (X_{i_1,\dots,i_m})$$

be the map with

$$X_{i_1,\dots,i_m} = \frac{1}{2} \cdot \min_{\sigma \in \mathcal{C}_m} \{ X_{i_1,i_{\sigma(1)}} + X_{i_{\sigma(1)},i_{\sigma^2(1)}} + \dots + X_{i_{\sigma^{m-1}(1)},i_{\sigma^m(1)}} \}.$$

If $D \in \mathcal{G}_{2,n} \subset \mathbb{R}^{\binom{n}{2}}$ is the dissimilarity matrix of an n-tree T, then the mdissimilarity map of T is equal to $\phi^{(m)}(D)$. So the set of m-dissimilarity maps of n-trees is equal to $\phi^{(m)}(\mathcal{G}_{2,n})$. Proof. Write

$$f(X;\sigma;i_1,\ldots,i_m) = X_{i_1,i_{\sigma(1)}} + X_{i_{\sigma(1)},i_{\sigma^2(1)}} + \ldots + X_{i_{\sigma^{m-1}(1)},i_{\sigma^m(1)}}.$$

Note that

$$f(X;\sigma;i_{\pi(1)},\ldots,i_{\pi(m)}) = f(X;\pi\sigma\pi^{-1};i_1,\ldots,i_m)$$

for all $\pi \in \mathcal{S}_m$, hence

$$\min_{\sigma \in \mathcal{C}_m} \{ f(X; \sigma; i_{\pi(1)}, \dots, i_{\pi(m)}) \} = \min_{\sigma \in \mathcal{C}_m} \{ f(X; \sigma; i_1, \dots, i_m) \}.$$
(4)

We have to prove that the weight $D(i_1, \ldots, i_m)$ of the smallest subtree T' of T containing the leaves i_1, \ldots, i_m is equal to $\frac{1}{2} \cdot \min_{\sigma \in \mathcal{C}_m} \{f(D; \sigma; i_1, \ldots, i_m)\}$. It is enough to prove this for $i_1 = 1, \ldots, i_m = m$ (the general case is proved completely analogously). By equation (4), we may also assume the leaves of T' are well-numbered.

Let e = (x, y) be an edge of T' with y a child of x. We claim that for all $\sigma \in \mathcal{C}_m$, the weight w(e) of e is taken into account in at least two of the m terms of

$$f(D;\sigma;1,\ldots,m) = D(1,\sigma(1)) + D(\sigma(1),\sigma^2(1)) + \ldots + D(\sigma^{m-1}(1),1)$$

and in exactly two of the summands of

$$f(D;\tau;1,\ldots,m) = D(1,2) + D(2,3) + \ldots + D(m,1),$$

where

$$\tau = \begin{pmatrix} 1 & 2 & \dots & m-1 & m \\ 2 & 3 & \dots & m & 1 \end{pmatrix} \in \mathcal{C}_m.$$

Using this claim, we immediately see

$$D(i_1, \dots, i_m) = \frac{1}{2} \cdot f(D; \tau; 1, \dots, m) = \frac{1}{2} \cdot \min_{\sigma \in \mathcal{C}_m} \{ f(D; \sigma; 1, \dots, m) \}.$$

To finish this theorem, we only need to prove the claim. Consider the split of T' induced by e and let T'' be the component of the split containing y (hence T'' is the maximal subtree of T' containing y but not x). Denote the set of leaves of T'' by L''. We may assume $1 \in L''$ (the case $1 \notin L''$ is analogous). Note that in this case L'' is of the form $\{1, \ldots, s\}$ for some s < m.

The weight of e is taken into account in the term D(i, j) (i.e. the path between the leaves i and j of T'' passes e) if and only if $i \in L''$ and $j \notin L''$ or vice versa. Thus w(e) is only counted in the two terms D(s, s + 1) and D(m, 1)of $f(D; \tau; 1, \ldots, m)$.

So it is enough to show that there exists a $t \in \{0 \dots, m-1\}$ such that $\sigma^t(1) \in L''$ and $\sigma^{t+1}(1) \notin L''$ (the other case is proved analogously). If we assume this is not the case (so $\sigma^t(1) \in L''$ implies $\sigma^{t+1}(1) \in L''$), we get $L'' = \{1, \dots, m\}$, a contradiction.

Corollary 3.3. If $D \in \mathcal{G}_{2,n} \subset \mathbb{R}^{\binom{n}{2}}$, we have that $D(i_1, \ldots, i_m)$ is equal to

$$\left(\bigoplus_{\sigma\in\mathcal{C}_m} \left(D(i_1,i_{\sigma(1)})\otimes D(i_{\sigma(1)},i_{\sigma^2(1)})\otimes\cdots\otimes D(i_{\sigma^{m-1}(1)},i_{\sigma^m(1)})\right)^{-1}\right)^{-\frac{1}{2}}.$$

Remark 3.4. In each component $D(i_1, \ldots, i_m)$, the minimum is attained at least twice. Indeed, assume the minimum is attained for $\sigma = \tau$. Since

$$f(D;\tau;i_1,\ldots,i_m) = f(D;\tau^{-1};i_1,\ldots,i_m),$$

the minimum is also attained for $\sigma = \tau^{-1}$. Note that this could be useful for computations, since it permits us to consider only $\frac{|\mathcal{C}_m|}{2}$ permutations. Furthermore, if $\{i_j, i_k\}$ is a cherry of T', the minimum is also attained for $\sigma = (jk) \circ \tau \circ (jk)$, whereby (jk) is the transposition in \mathcal{S}_m switching j and k.

Remark 3.5. The map $\phi^{(m)}$ is not injective on the whole domain $\mathbb{R}^{\binom{n}{2}}$. For example, consider $D, D' \in \mathbb{R}^{\binom{n}{2}}$, whereby D(i, j) = 1 for all $1 \leq i < j \leq n$ and D' only differs from D in the last coordinates, with D'(n-1,n) = 2. Clearly, one has $D \in \mathcal{G}_{2,n}, D' \notin \mathcal{G}_{2,n}$ and $\phi^{(m)}(D) = \phi^{(m)}(D')$. However, Theorem 1.3 implies that the restriction of $\phi^{(m)}$ to $\mathcal{G}_{2,n}$ is injective if $n \geq 2m - 1$.

Proposition 3.6. $\phi^{(m)}(\mathcal{G}_{2,n}) \subseteq \mathcal{T}_{m,n} \cap \phi^{(m)}(\mathbb{R}^{\binom{n}{2}})$

Proof. The inclusion $\phi^{(m)}(\mathcal{G}_{2,n}) \subset \phi^{(m)}(\mathbb{R}^{\binom{n}{2}})$ is obvious, while $\phi^{(m)}(\mathcal{G}_{2,n}) \subset \mathcal{T}_{m,n}$ follows from [5]. For sake of completeness, we include the proof in this paper.

Consider a tree T with leaf set [n] and distance matrix D. Let R be an (m-2)-subset of [n] and $i, j, k, l \in [n] \setminus R$. We have to prove that

$$\phi^{(m)}(D) \in \mathcal{T}(\operatorname{trop}(p_{R,ijkl})).$$

Let [R] be the smallest subtree of T containing the leaves in R and let T' be the tree obtained from T by contracting [R] to a point. Denote by i', j', etc. the images of respectively i, j, etc. in T'. Note that R' is a leaf of T'. We have

$$D(R, i, j) = D'(R', i', j') + D(R),$$

hence $\phi^{(m)}(D) \in \mathcal{T}(\operatorname{trop}(p_{R,ijkl}))$ if and only if $\phi^{(3)}(D') \in \mathcal{T}(\operatorname{trop}(p_{R',i'j'k'l'}))$, where D' is the distance matrix of T'.

Now Remark 4.1 below implies

$$D'(R',i',j') = \frac{1}{2}(D'(i',j') + D'(i',R') + D'(j',R')),$$

so $\phi^{(3)}(D') \in \mathcal{T}(\operatorname{trop}(p_{R',i'j'k'l'}))$ if and only if $D' \in \mathcal{T}(\operatorname{trop}(p_{i'j'k'l'}))$. Hence the statement follows from Theorem 1.1.

4 The 3-dissimilarity maps of trees

Denote the coordinates of $\mathbb{R}^{\binom{n}{2}}$ by X(i, j) (here we index over all integers i, j with $1 \leq i < j \leq n$) and the coordinates of $\mathbb{R}^{\binom{n}{3}}$ by X(i, j, k) (here we index over all integers i, j, k with $1 \leq i < j < k \leq n$). Recall that if $D \in \mathcal{G}_{2,n}$ is a tree, D(i, j) is the distance between leaf i and leaf j.

Remark 4.1. Since $C_3 = \{\sigma_1, \sigma_2\}$ with

$$\sigma_1 = \begin{pmatrix} 1 & 2 & 3 \\ 2 & 3 & 1 \end{pmatrix}$$
 and $\sigma_2 = (\sigma_1)^{-1} = \begin{pmatrix} 1 & 2 & 3 \\ 3 & 1 & 2 \end{pmatrix}$

the map $\phi^{(3)}$ sends $X = (X(i,j))_{i,j}$ to $(X(i,j,k))_{i,j,k}$ with

$$X(i, j, k) = \frac{1}{2} \cdot (X(i, j) + X(i, k) + X(j, k)).$$

So if $D \in \mathcal{G}_{2,n}$, the 3-subtree weights of the tree D are given by $D(i, j, k) = \frac{1}{2} \cdot (D(i, j) + D(i, k) + D(j, k)).$

The following results states that for the case m = 3 the equality holds in Proposition 3.6 if $n \ge 5$.

Proposition 4.2. If $n \geq 5$, we have $\phi^{(3)}(\mathcal{G}_{2,n}) = \mathcal{T}_{3,n} \cap \phi^{(3)}(\mathbb{R}^{\binom{n}{2}})$

Proof. By Proposition 3.6, it is enough to show that for a general point $P \in \phi^{(3)}(\mathbb{R}^{\binom{n}{2}}) \cap \mathcal{T}_{3,n}$, there exists a point $D \in \mathcal{G}_{2,n}$ such that $\phi^{(3)}(D) = P$. Since $P \in \phi^{(3)}(\mathbb{R}^{\binom{n}{2}})$, there exists a point $D \in \mathbb{R}^{\binom{n}{2}}$ such that $\phi^{(3)}(D) = P$. It suffices to prove that $D \in \mathcal{G}_{2,n}$. In order to do this, we show that in each triplet

$$\{D(i,j) + D(k,l), D(i,k) + D(j,l), D(i,k) + D(j,k)\},\$$

the maximum is attained at least twice. Fix $S \in [n] \setminus \{i, j, k, l\}$ $(n \ge 5)$. Since $P \in \mathcal{T}_{3,n}$, in the triplet

$$\{P(S, i, j) + P(S, k, l), P(S, i, k) + P(S, j, l), P(S, i, l) + P(S, j, k)\},\$$

the maximum is attained at least twice. Note that

$$\begin{split} P(S,i,j) + P(S,k,l) &= \frac{1}{2}(C + D(i,j) + D(k,l)),\\ P(S,i,k) + P(S,j,l) &= \frac{1}{2}(C + D(i,k) + D(j,l)),\\ P(S,i,l) + P(S,j,k) &= \frac{1}{2}(C + D(i,k) + D(j,k)), \end{split}$$

where C = D(S,i) + D(S,j) + D(S,k) + D(S,l). Hence the maximum in $\{D(i,j) + D(k,l), D(i,k) + D(j,l), D(i,k) + D(j,k)\}$ is also attained at least twice, thus $D \in \mathcal{G}_{2,n}$ and $P \in \phi^{(3)}(\mathcal{G}_{2,n})$.

For the proof of the proposition below, we need an extra definition.

Definition 4.3. An ultrametric D on [n] is a metric which satisfies the following strengthened version of the triangle inequality:

$$\forall i, j, k \in [n] : D(i, j) \le \max\{D(i, k), D(j, k)\}.$$

Equivalently, at least two of the three terms D(i, j), D(i, k), D(j, k) are the same.

Remark 4.4. In general, the dissimilarity matrix D of a tree T is not an ultrametric. In case $D \in \mathcal{G}_{2,n}$ is an ultrametric, we can realize D by an *equidistant* tree, i.e. a rooted tree such that the distance F between the root and each leaf is equal. In particular, $2F = \max\{D(i, j) \mid i, j \in X \text{ and } i \neq j\}$.

Proposition 4.5. $\phi^{(3)}(\mathcal{G}_{2,n}) \subset \mathcal{G}_{3,n}$

Proof. Let T be a tree with 3-dissimilarity map

$$P = (D(i, j, k))_{i,j,k} = \phi^{(3)}((D(i, j)_{i,j}) \in \phi^{(3)}(\mathcal{G}_{2,n}) \subset \mathbb{R}^{\binom{n}{3}}.$$

If $M \in K^{3 \times n}$, we denote the (3×3) -minor with columns i, j, k by M(i, j, k). By Theorem 2.1, $\mathcal{G}_{3,n}$ is the closure in $\mathbb{R}^{\binom{n}{3}}$ of the set

$$S := \{ (-\operatorname{val}(\det(M(i,j,k))))_{i,j,k} \mid M \in K^{3 \times n} \} \subset \mathbb{Q}^{\binom{n}{3}}.$$

Assume first that all the edges of T have rational weights, a fortiori $P \in \mathbb{Q}^{\binom{n}{3}}$. We are going to show there exists a matrix $M \in K^{3 \times n}$ such that

$$D(i, j, k) = -\operatorname{val}(\det(M(i, j, k)))$$

Fix a rational number E with $E \ge D(i, n)$ for all $i \in \{1, \ldots, n-1\}$ and define a new metric D' by

$$D'(i,j) = 2E + D(i,j) - D(i,n) - D(j,n)$$

for all different $i, j \in [n]$ (in particular, D'(i, n) = 2E for $i \neq n$). Note that $D' \in \mathcal{G}_{2,n}$ and that D' an ultrametric on $\{1, \ldots, n-1\}$, so it can be realized by an equidistant (n-1)-tree T'' with root r. Each edge e of T'' has a well-defined height h(e), which is the distance from the top node of e to each leaf below e. Pick a random rational number a(e) and associate the label $a(e)t^{2h(e)}$ to e. If $i \in \{1, \ldots, n-1\}$ is a leaf of T'', define the polynomial $x_i(t)$ by adding the labels of all edges between r and i. It is easy to see that $D'(i, j) = \deg(x_j(t) - x_i(t))$ for all $i, j \in \{1, \ldots, n-1\}$.

Denote the distance from r to each edge by F. Since

$$2F = \max\{D'(i,j) \mid 1 \le i < j \le n-1\} < 2E,$$

we have F < E. The metric D' on [n] can be realized by a tree T', where T' is the tree obtained from T'' by adding the leave n together with an edge (r, n) of length 2E - F. If we define $x_n(t) = t^{2E}$, we get that $D'(i, j) = \deg(x_j(t) - x_i(t))$ for all $i, j \in [n]$.

Now consider the matrix

$$M' = \begin{bmatrix} 1 & 1 & 1 & \dots & 1 \\ x_1(t) & x_2(t) & x_3(t) & \dots & x_n(t) \\ x_1(t)^2 & x_2(t)^2 & x_3(t)^2 & \dots & x_n(t)^2 \end{bmatrix}.$$

We have $det(M'(i, j, k)) = (x_j(t) - x_i(t))(x_k(t) - x_i(t))(x_k(t) - x_j(t))$, hence

 $D'(i,j) + D'(i,k) + D'(j,k) = \deg(\det(M'(i,j,k))).$

Let M be the matrix obtained from M' by multiplying, for each i, the *i*-th column of M' by $(t^{D(i,n)-E})^2$. Since

$$D(i,j) = D'(i,j) + (D(i,n) - E) + (D(j,n) - E)$$

= deg $\left(t^{D(i,n)-E} \cdot t^{D(j,n)-E} \cdot (x_i(t) - x_j(t)) \right)$,

we get that $D(i, j) + D(i, k) + D(j, k) = \deg(\det(M(i, j, k)))$. If we replace each t in M by $t^{-1/2}$, we get

$$D(i,j,k) = -\mathrm{val}(\det(M(i,j,k))).$$

Now assume T has irrational edge weights. We can approximate T arbitrarily close by a tree \tilde{T} with rational edge weights. From the arguments above, it follows that the 3-dissimilarity map \tilde{D} of \tilde{T} belongs to S, hence $D \in \mathcal{G}_{3,n}$.

Theorem 4.6. If $n \ge 5$, we have $\phi^{(3)}(\mathcal{G}_{2,n}) = \phi^{(3)}(\mathbb{R}^{\binom{n}{3}}) \cap \mathcal{G}_{3,n}$.

Proof. The statement follows from Proposition 4.2, Proposition 4.5 and the fact that $\mathcal{G}_{3,n} \subset \mathcal{T}_{3,n}$.

5 The 4-dissimilarity maps of trees

In this section, we give a geometric description of $\phi^{(4)}(\mathcal{G}_{2,n})$.

Remark 5.1. The set $C_4 = \{\sigma_1, \sigma_1^{-1}, \sigma_2, \sigma_2^{-1}, \sigma_3, \sigma_3^{-1}\}$ with

$$\sigma_1 = \begin{pmatrix} 1 & 2 & 3 & 4 \\ 2 & 3 & 4 & 1 \end{pmatrix}, \sigma_2 = \begin{pmatrix} 1 & 2 & 3 & 4 \\ 2 & 4 & 1 & 3 \end{pmatrix}, \sigma_3 = \begin{pmatrix} 1 & 2 & 3 & 4 \\ 3 & 4 & 2 & 1 \end{pmatrix}.$$

Hence the map $\phi^{(4)}$ sends $(X(i,j))_{i,j}$ to $(X(i,j,k,l))_{i,j,k,l}$ where X(i,j,k,l) is equal to the minimum of the three terms

$$\begin{split} X(1,2) + X(2,3) + X(3,4) + X(4,1), \\ X(1,2) + X(2,4) + X(4,3) + X(3,1), \\ X(1,3) + X(3,2) + X(2,4) + X(4,1), \end{split}$$

divided by two.

Consider $M = \mathbb{R}^{\binom{n}{2} \cdot \binom{n-2}{2}}$ and take X(i, j; k, l), with $\{i, j, k, l\} \subset [n]$ a quadruple, as coordinates on M. For example, X(j, i; l, k) = X(i, j; k, l), but $X(i, k; j, l) \neq X(i, j; k, l)$ and $X(k, l; i, j) \neq X(i, j; k, l)$.

Let $\pi : \mathbb{R}^{\binom{n}{2}} \to M : (X(i,j))_{i,j} \mapsto (X(i,j;k,l))_{i,j,k,l}$ with

$$X(i,j;k,l) = \frac{1}{2} \cdot (X(i,j) + X(k,l) + \min\{X(i,k) + X(j,l), X(i,l) + X(j,k)\}).$$

Let L be the linear subspace of M consisting of points X(i, j; k, l) with

$$X(i, j; k, l) = X(i, k; j, l) = X(i, l; j, k) = X(j, l; i, k) = X(j, k; i, l) = X(k, l; i, j)$$

for all different $i, j, k, l \in [n]$. Points in L can be projected naturally to $\mathbb{R}^{\binom{n}{4}}$ by sending X(i, j; k, l) to X(i, j, k, l). Denote this projection by p.

Proposition 5.2. $\phi^{(4)}(\mathcal{G}_{2,n}) = p(\pi(\mathbb{R}^{\binom{n}{2}}) \cap L).$

Proof. Note that for any real numbers a, b, c, we have

$$a + \min\{b, c\} = b + \min\{a, c\} = c + \min\{a, b\}$$
(5)

if and only if $\max\{a, b, c\}$ is attained at least twice. If the latter holds, the terms in (5) are equal to $\min\{a + b, a + c, b + c\}$.

If we take a = X(i, j) + X(k, l), b = X(i, k) + X(j, l) and c = X(i, l) + X(j, k), the statement follows from the Tree Metric Theorem.

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