

# Lipschitz polytopes of tree metrics <sup>\*</sup>

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## Abstract

For a finite metric space on  $X$ , its Lipschitz polytope is the intersection of a hyperplane in  $\mathbb{R}^X$  and the set of 1-Lipschitz functions on itself. We show that the Lipschitz polytope of a metric space is a zonotope if and only if the metric is a tree metric and we characterize the pairs of  $X$ -trees from which we generate combinatorially equivalent Lipschitz polytopes. For every tree metric, we give an explicit anti-isomorphism between the face poset of its Lipschitz polytope and the flow poset of its underlying  $X$ -tree. We find a relation between flow posets of graphs and corresponding Albanese tori and provide an explicit realization of all flow posets of graphs through orthogonal projection of Lipschitz polytopes of tree metrics up to anti-isomorphism. For each tree metric  $D$ , we find a natural weight assignment to the edges of the 1-skeleton graph of the Lipschitz polytope of  $D$  so that there is a natural isometric embedding from  $D$  to the weighted 1-skeleton graph. For Lipschitz polytopes of tree metrics, we obtain sharp upper and lower bound on their face numbers and characterize all their simple vertices. We compute the Ehrhart polynomials and volumes of skew Lipschitz polytopes of tree metrics. Finally, inspired by the definition from Loeb, Nešetřil and Reed of integral Lipschitz height and based on the concept of Lipschitz polytope, we suggest a study of Lipschitz height and scale-invariant Lipschitz height.

**Keywords:** combinatorial flow, face poset, isometric embedding, Lipschitz height, phylogenetic tree, zonotope.

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## 1 Introduction

We write  $\mathbb{Z}$  for the set of all integers,  $\mathbb{R}$  for the set of all reals,  $\mathbb{R}_{\geq 0}$  for the set of all nonnegative reals and  $\mathbb{R}_{> 0}$  the set of all positive reals. A *metric space* is a pair  $(X, D)$ , where  $X$  is a set and  $D$  is a map from  $X \times X$  to  $\mathbb{R}_{\geq 0}$  such that

$$\begin{cases} D(x, x) = 0, \\ D(x, y) + D(z, y) \geq D(x, z), \end{cases} \quad (1)$$

for all  $x, y, z \in X$ , in which case  $D$  is called a *metric* on  $X$  [DL97]. Note that a metric  $D$  is necessarily symmetric, that is,  $D(x, z) = D(z, x)$  holds for all  $x, z \in X$ , as putting  $y := x$  in (1) yields that  $D(z, x) = D(x, x) + D(z, x) \geq D(x, z)$  holds for all  $x, z \in X$  [DHK<sup>+</sup>12, p. 14]. The metric  $D$  is *proper* provided  $D(x, y) > 0$  whenever  $x \neq y$ . Both  $\mathbb{Z}$  and  $\mathbb{R}$  are often assigned the metric space structure with the metric  $D$  such that  $D(x, y) = |x - y|$ . For any  $c \in \mathbb{R}_{\geq 0}$ , a map  $f$  from a metric space  $(X, D)$  to another metric space  $(X', D')$  is *c-Lipschitz* provided  $D'(f(x), f(y)) \leq cD(x, y)$  for all  $x, y \in X$ . For any metric space  $(X, D)$ , a *Lipschitz function* on it is a Lipschitz map from  $(X, D)$  to the set of reals.

In the active research field of Lipschitz functions on graphs and metric spaces [Ost13, Wea99], an interesting problem is to characterize the graphs with extremal average range of their Lipschitz functions [LNR03, WXZ16]. The idea is that the shape of the graph or metric space should be reflected in the set of Lipschitz functions on it. To push this idea further, for any set  $X$  and any

matrix  $D \in \mathbb{R}_{\geq 0}^{X \times X}$ , where  $D(a, a) = 0$  for all  $a \in X$ , we define the *Lipschitz polytope with respect to  $(X, D)$*  to be

$$L_D = \{f \in \mathbb{R}^X : \sum_{x \in X} f(x) = 0, f(x) - f(y) \leq D(x, y), \forall x, y \in X\}$$

and, for any  $x \in X$ , we define the *skew Lipschitz polytope of  $(X, D)$  with respect to  $x$*  to be

$$L_D^x = \{f \in \mathbb{R}^X : f(x) = 0, f(y) - f(z) \leq D(y, z) \text{ for all } y, z \in X\}. \quad (2)$$

Let  $p_x^X$  be the linear map from  $\mathbb{R}^X$  to itself such that for every  $f \in \mathbb{R}^X$  and  $y \in X$ ,

$$p_x^X(f)(y) = f(y) - f(x). \quad (3)$$

**Remark 1.1.** Note that the kernel of the linear map  $p_x^X$  is the 1-dimension subspace of  $\mathbb{R}^X$  consisting of constant functions and this subspace is the orthogonal complement of the subspace  $\{f \in \mathbb{R}^X : \sum_{y \in X} f(y) = 0\}$  which the Lipschitz polytope  $L_D$  lies in. It is then easy to check that the linear map  $p_x^X$  induces a volume-preserving bijection from  $L_D$  to  $L_D^x$ , meaning that  $L_D$  and  $L_D^x$  are affinely equivalent for all  $x \in X$  and  $\text{Vol}(L_D) = \text{Vol}(L_D^x)$ .

Let  $(X, D)$  be a metric space. For any  $f \in L_D$ , we define the *tight digraph* for  $f$ , denoted  $\mathcal{T}_D(f)$ , to be the digraph with vertex set  $X$  and arc set

$$A_D(f) = \{(a, b) \in X \times X : f(a) - f(b) = D(a, b), a \neq b\}. \quad (4)$$

For any face  $F$  of  $L_D$ , both  $\mathcal{T}_D(f)$  and  $A_D(f)$  take constant values when  $f$  runs through the relative interior of  $F$ , and we will thus denote these two constant values by  $\mathcal{T}_D(F)$  and  $A_D(F)$ . Especially, we call  $\mathcal{T}_D(F)$  the *tight digraph* for  $F$ . We mention that the role of tight digraph for the study of Lipschitz polytope is similar to the role of the so-called tight-equality graph in the study of tight span [DHK<sup>+</sup>12, §5.3], and their generalization called tight configuration is a fundamental concept for the study of general point configurations [WX17].

**Example 1.2.** Let  $(X, D)$  be a metric space, let  $x \in X$  and set  $s_x := \sum_{z \in X} D(x, z)$ . For any  $y \in X$ , let

$$x^-(y) := D(x, y) - \frac{s_x}{|X|} \text{ and } x^+(y) := \frac{s_x}{|X|} - D(x, y).$$

It is easy to see that the functions  $x^+$  and  $x^-$  are elements of  $L_D$ . If  $s_x > 0$ , we have two measures  $\mu_0$  and  $\mu_1$  on  $X$  where  $\mu_0(z) = \frac{D(x, z)}{s_x}$  and  $\mu_1(z) = \frac{1}{|X|}$  for all  $z \in X$ . It turns out that the total variation distance [LPW09, Chapter 4] between  $\mu_0$  and  $\mu_1$  is given by

$$\max_{A \subseteq X} \left| \sum_{z \in A} \mu_0(z) - \sum_{z \in A} \mu_1(z) \right| = \frac{\sum_{z \in X} |\mu_0(z) - \mu_1(z)|}{2} = \frac{2}{4} \sum_{z \in X} \left| \frac{D(x, z)}{s_x} - \frac{1}{|X|} \right| = \left| \frac{x^+ - x^-}{4s_x} \right|_1,$$

that is, it is equal to the  $L_1$ -norm of  $\frac{x^+ - x^-}{4s_x}$ . Moreover, when  $D$  is a proper metric, the tight digraph  $\mathcal{T}_D(x^-)$  is the digraph on vertex set  $X$  with arc set  $A_D(x^-) = \{\vec{yx} : y \in X \setminus \{x\}\}$ , and the tight digraph  $\mathcal{T}_D(x^+)$  is the digraph on vertex set  $X$  with arc set  $A_D(x^+) = \{\vec{xy} : y \in X \setminus \{x\}\}$ .

For a finite metric space  $(X, D)$  and any  $f \in L_D$ , we have  $-f \in L_D$  and

$$\max_{x \in X} |f(x)| \leq \max_{x, y \in X} D(x, y).$$

This means that both  $L_D$  and  $L_D^x$  are centrally symmetric polytopes, namely bounded polyhedra which contain a point that bisects every maximal line segment passing through it. In the rich theory of polytopes [Zie95], even centrally symmetric polytopes are far from well understood. Will the desire to understand Lipschitz polytopes launch us into any adventure?

After our previous work on Lipschitz functions in [WXZ16], we learn some more background of Lipschitz polytopes. Let  $(X, D)$  be a metric space. To better understand this metric space, it is useful to consider its canonical embeddings into some natural Banach spaces [Zat08]. For each  $x \in X$ , the *Lipschitz space*  $Lip_x(X, D)$  of  $(X, D)$  with respect to  $x \in X$  is the space of Lipschitz functions on  $X$  which vanish at  $x$  equipped with the Lipschitz norm [Wea99]. We let  $Lip^0(X, D)$  be the space of Lipschitz functions on  $X$  which sum to 0 equipped with the Lipschitz norm. The dual normed space of  $Lip_x(X, D)$  is called the *Lipschitz-free space* of  $(X, D)$  with respect to  $x \in X$  [GK03] while the dual normed space of  $Lip^0(X, D)$  is called the *Kantorovich-Rubinstein (KR) normed space* of  $(X, D)$  [Kat88, MPV08], which is related with the *Monge-Kantorovich transportation problem* [Ver13]. Note that  $L_D^x$  is the unit ball of  $Lip_x(X, D)$  and  $L_D$  is the unit ball of  $Lip^0(X, D)$ . Vershik [Ver15] called the unit ball of the KR normed space of  $(X, D)$  the *fundamental polytope* of  $(X, D)$  and advocated a further study of many problems about fundamental polytopes, say the combinatorial structure of fundamental polytopes and a classification of finite metric spaces via the combinatorics of the fundamental polytopes, beyond some existing researches [MPV08, Zat08]. The Lipschitz polytope and fundamental polytope of the same metric space are polar dual to each other while the Lipschitz polytope allows a more direct description. See Example 8.7 and Figure 6 for a small example of these two polytopes. Should this connection to Lipschitz space, Lipschitz-free space and KR normed space promise some nice mathematics structures to be discovered behind the Lipschitz polytopes?

Some progresses have been obtained after the paper of Vershik [Ver15]. In [GP17], Gordon and Petrov gave an upper and lower bound on the total number of combinatorial equivalent classes of Lipschitz polytopes of metric spaces of any fixed size; they also determined the face vectors of Lipschitz polytopes for generic metrics (see the beginning of § 10). In [DH16], Delucchi and Hoessly studied the fundamental polytopes of tree metrics and derived the face vectors of them in some concrete cases. More recently, Jevtić, Jelić and Živaljević [JJv17] found out a close relationship between the cyclohedron (Bott-Taubes polytope) and the fundamental polytope of any generic metric. We will provide a systematic

study on Lipschitz polytopes of tree metrics in this paper and report our study on the stratification of (directed) metric spaces through Lipschitz polytopes in another paper [WX17].

Besides Lipschitz polytope and fundamental polytope, an important geometrical construction associated with a finite metric space is a polytopal complex called the tight span [CL94, Dre84, Isb64]. There exists a natural injective projection from the tight span to the Lipschitz polytope of the same finite metric space which maps vertices to vertices; see § 8. Moreover, it turns out that the study of tight span and Lipschitz polytope do have some close connections [WX17]. Tight span is an important tool in the study of phylogenetic combinatorics [DHK<sup>+</sup>12, SS03, Ste16], a research direction for recovering evolutionary trees and evolutionary networks. Especially, when the metric space is a tree metric, its tight span is really THE tree [Dre84]! The distinguished role of tree structure in phylogenetic combinatorics suggests us to start from tree metrics in our course of studying Lipschitz polytopes. Indeed, in the study of Lipschitz-free spaces, some special interests have already been centered around tree metrics [DKP16, God10].

The main object of this essay is the Lipschitz polytopes of tree metrics and we organize the rest of the paper as follows. In § 2 we recall some basic concepts and definitions that will be needed in the paper. In § 3 we reveal the close relationship between tree metrics and zonotopes; see Theorem 3.4 and Remark 3.5. Furthermore, making use of the connections between zonotopes and realizable oriented matroids, we determine in § 4 the situations when two tree metrics have combinatorially equivalent Lipschitz polytopes; see Theorem 4.8. In § 5.1, we report that one can determine a phylogenetic tree by “watching” the shape of flood tides on it (Remark 5.6); in § 5.2 we find out a connection between tight digraphs of faces of Lipschitz polytopes and tight digraphs of combinatorial flows (Lemma 5.7) and then are able to provide an explicit anti-isomorphism between the flow poset and the face poset of the Lipschitz polytope of an  $X$ -tree (Theorem 5.9). We relate flow posets to Albanese tori in § 6, which enables us to show that, roughly speaking, two tree metrics have combinatorially equivalent Lipschitz polytopes if and only if they have the same Albanese tori; see Theorem 4.8 and Corollary 6.3. The main result of § 7 is that the face poset of orthogonal projections of Lipschitz polytopes of tree metrics can realize all possible flow posets of graphs; see Theorem 7.2. In § 8, we display a natural projection from the tight span into the corresponding Lipschitz polytope and show that there is an isometric embedding of a tree metric  $(X, D)$  into a weighted network constructed from the 1-skeleton of the Lipschitz polytope of  $(X, D)$ . We present in § 9 sharp upper and lower bounds on the face numbers of Lipschitz polytopes of tree metrics; see Theorem 9.9. Our § 10 is devoted to a characterization of those simple vertices of Lipschitz polytopes of tree metrics; see Theorem 10.2. In § 11 we calculate the Ehrhart polynomials and volumes of skew Lipschitz polytopes of tree metrics. Finally, in § 12, we return to the concept of Lipschitz height of a graph, which is a parameter of some interest in the study of graph-indexed random walk [LNR03] and also the topic on which we start our journey on Lipschitz functions [WXZ16]. We define variants of

Lipschitz height there for general metric spaces to capture their combinatorial shadow. We prove Theorem 12.3, an analogue of the main result from [WXZ16] for tree metrics, and then end the paper with a conjecture, Conjecture 12.5.

## 2 Preliminaries

**2.1 Vector configurations and oriented matroids** Let  $E$  be a set. A *signed subset of  $E$*  is a pair  $\Sigma = (\Sigma^+, \Sigma^-)$  satisfying  $\Sigma^+ \cup \Sigma^- \subseteq E$  and  $\Sigma^+ \cap \Sigma^- = \emptyset$ . We call  $\Sigma^+$  and  $\Sigma^-$  the *positive part* and the *negative part* of  $\Sigma = (\Sigma^+, \Sigma^-)$ , respectively. The *underlying set* of a signed subset  $\Sigma$  of  $E$ , denoted by  $\underline{\Sigma}$ , is  $\Sigma^+ \cup \Sigma^-$ . For any  $F \subseteq E$ , the *reorientation of  $\Sigma$  on  $F$* , denoted by  ${}_{-F}\Sigma$ , is the signed subset of  $E$  whose positive part is  $(\Sigma^+ \setminus F) \cup (\Sigma^- \cap F)$  and whose negative part is  $(\Sigma^- \setminus F) \cup (\Sigma^+ \cap F)$ . If  $S$  is a set of signed subsets of  $E$ , we call  $S' = \{{}_{-F}\Sigma : \Sigma \in S\}$  a set obtained from  $S$  by the reorientation on  $F$  and call  $S$  and  $S'$  *reorientation equivalent*. The set of all signed subsets of  $E$  has a natural partial order structure  $\leq$  such that, for each two signed subsets  $\Sigma$  and  $\Delta$  of  $E$ ,  $\Sigma \leq \Delta$  if and only if  $\Sigma^+ \subseteq \Delta^+$  and  $\Sigma^- \subseteq \Delta^-$  hold. For any  $f \in \mathbb{R}^E$ , its *signed support*, denoted by  $\underline{f}$ , is the signed subset of  $E$  whose positive part is  $\{e \in E : f(e) > 0\}$  and whose negative part is  $\{e \in E : f(e) < 0\}$ .

Let  $X$  be a finite set. We always view  $\mathbb{R}^X$  as the Hilbert space endowed with the inner product  $\langle \cdot, \cdot \rangle$  that  $\langle f, g \rangle = \sum_{x \in X} f(x)g(x)$  for  $f, g \in \mathbb{R}^X$ . For each subspace  $W$  of  $\mathbb{R}^X$ , denote by  $W^\perp$  the *orthogonal complement* of  $W$  in  $\mathbb{R}^X$ . For any finite index set  $E$ , any map from  $E$  to  $\mathbb{R}^X$  is called an  *$E$ -indexed vector configuration in  $\mathbb{R}^X$* . Let  $\mathfrak{A}$  be an  $E$ -indexed vector configuration in  $\mathbb{R}^X$ . Note that this map  $\mathfrak{A}$  naturally corresponds to a map from  $X \times E$  to  $\mathbb{R}$  that sends  $(x, e) \in X \times E$  to  $\mathfrak{A}(e)(x)$ . This suggests to define the *conjugate* of  $\mathfrak{A}$  to be the  $X$ -indexed vector configuration in  $\mathbb{R}^E$ , denoted by  $\mathfrak{A}^\top$ , such that  $\mathfrak{A}^\top(x)(e) = \mathfrak{A}(e)(x)$  for all  $(x, e) \in X \times E$ . Considering a linear extension of the map  $\mathfrak{A}$ , we can send  $f \in \mathbb{R}^E$  to  $\mathfrak{A}f \in \mathbb{R}^X$ , where

$$\mathfrak{A}f = \sum_{e \in E} f(e) \mathfrak{A}(e).$$

We write  $\ker \mathfrak{A}$  for  $\{f \in \mathbb{R}^E : \mathfrak{A}f = 0 \in \mathbb{R}^X\}$  and we write  $\text{im } \mathfrak{A}$  for  $\{\mathfrak{A}f : f \in \mathbb{R}^E\}$ . Note that  $\ker \mathfrak{A}$  is a subspace of  $\mathbb{R}^E$ ,  $\text{im } \mathfrak{A}$  is a subspace of  $\mathbb{R}^X$ , and  $\dim \ker \mathfrak{A} + \dim \text{im } \mathfrak{A} = |E|$ . Let  $\mathcal{V}_{\mathfrak{A}} = \{\underline{f} : f \in \ker \mathfrak{A}\}$ . We call the pair  $\mathcal{M}_{\mathfrak{A}} = (E, \mathcal{V}_{\mathfrak{A}})$  the *oriented matroid* of  $\mathfrak{A}$  [BLVS<sup>+</sup>99], which forms an interesting combinatorial abstraction of the linear dependence relationship and the chirality in the vector configuration  $\mathfrak{A}$ . For the oriented matroid  $\mathcal{M} = (E, \mathcal{V})$ , its *underlying matroid*, denoted by  $\underline{\mathcal{M}}$ , is the pair  $(E, \underline{\mathcal{V}})$ , where  $\underline{\mathcal{V}} = \{\underline{\Sigma} : \Sigma \in \mathcal{V}\}$ , which characterizes only linear dependence relationship. The set  $\mathcal{V}_{\mathfrak{A}}$  is known as the set of *vectors* of  $\mathcal{M}_{\mathfrak{A}}$ . It has a natural partial order structure  $\leq$  inherited from that on the set of all signed subsets of  $E$  and has  $(\emptyset, \emptyset)$  as the unique minimum element. Every *atom* of  $\mathcal{V}_{\mathfrak{A}}$ , namely an element which covers  $(\emptyset, \emptyset)$  in  $\mathcal{V}_{\mathfrak{A}}$ , is called a *circuit* of  $\mathcal{M}_{\mathfrak{A}}$ . The set of all circuits of  $\mathcal{M}_{\mathfrak{A}}$  are characterized by the so-called *circuit axioms of oriented matroids*

[BLVS<sup>+</sup>99, Definition 3.2.1]. If  $\mathcal{C}$  is the set of all circuits of an oriented matroid  $\mathcal{M}$ , we call  $\underline{\mathcal{C}} = \{\underline{\Sigma} : \Sigma \in \mathcal{C}\}$  the set of circuits of the matroid  $\underline{\mathcal{M}}$ . If  $\mathfrak{B}$  is an  $E$ -indexed vector configuration in  $\mathbb{R}^Y$  such that  $\ker \mathfrak{A}$  and  $\ker \mathfrak{B}$  are the orthogonal complements to each other in  $\mathbb{R}^E$ , namely

$$\text{im } \mathfrak{A}^\top = (\ker \mathfrak{A})^\perp = \ker \mathfrak{B} \quad (5)$$

in  $\mathbb{R}^E$ , then  $\mathcal{M}_{\mathfrak{B}}$  is called the *dual oriented matroid of  $\mathcal{M}_{\mathfrak{A}}$*  and is often directly denoted by  $\mathcal{M}_{\mathfrak{A}}^*$  to signify the fact that it is independent with the choice of  $\mathfrak{B}$  but totally determined by (5) [BK92, Example 5.9]. A vector of  $\mathcal{M}_{\mathfrak{A}}^*$  is called a *covector* of  $\mathcal{M}_{\mathfrak{A}}$  and we denote by  $\mathcal{V}^*(\mathcal{M}_{\mathfrak{A}})$  the set of covectors of  $\mathcal{M}_{\mathfrak{A}}$ , namely  $\mathcal{V}^*(\mathcal{M}_{\mathfrak{A}}) = \mathcal{V}(\mathcal{M}_{\mathfrak{A}}^*)$ . Equipped with the natural partial order structure on it,  $\mathcal{V}^*(\mathcal{M}_{\mathfrak{A}}) = \mathcal{V}(\mathcal{M}_{\mathfrak{A}}^*)$  is known as the *face poset* of the oriented matroid  $\mathcal{M}_{\mathfrak{A}}$ . Note that, as suggested by (5), for any vector configuration  $\mathfrak{A}$  in  $\mathbb{R}^X$ , the set

$$\{\underline{f} : f \in \text{im } \mathfrak{A}\}$$

corresponds to the set of vectors of an oriented matroid on  $X$ . For an  $E$ -indexed vector configuration  $\mathfrak{A}$  in  $\mathbb{R}^X$  and an  $F$ -indexed vector configuration  $\mathfrak{B}$  in  $\mathbb{R}^Y$ , we call the two oriented matroids  $\mathcal{M}_{\mathfrak{A}}$  and  $\mathcal{M}_{\mathfrak{B}}$  *isomorphic* provided there is a bijection  $f$  from  $E$  to  $F$  and a subset  $F'$  of  $F$  such that  $(\Sigma^+, \Sigma^-) \in \mathcal{V}_{\mathfrak{A}}$  if and only if  ${}_{-F'}(f(\Sigma^+), f(\Sigma^-)) \in \mathcal{V}_{\mathfrak{B}}$ , where  $f(S)$  is a shorthand for  $\{f(e) : e \in S\}$ . Up to isomorphism, an oriented matroid uniquely determines its dual oriented matroid, namely  $\mathcal{M}_{\mathfrak{A}} = \mathcal{M}_{\mathfrak{B}}$  implies  $\mathcal{M}_{\mathfrak{A}}^* = \mathcal{M}_{\mathfrak{B}}^*$  [BLVS<sup>+</sup>99, Proposition 3.4.1]. The oriented matroids of real vector configurations as introduced above are called *realizable oriented matroids*; the readers should go to [BK92, BLVS<sup>+</sup>99, Bok06] for the theory of general oriented matroids.

We call  $\mathfrak{A} = (v_1, \dots, v_m)$  a *multiplicity-free* vector configuration provided we cannot find any  $\{i, j\} \in \binom{\{1, \dots, m\}}{2}$  such that  $v_i$  and  $v_j$  are parallel, namely are linearly dependent. We call two vector configurations  $\mathfrak{B}$  in  $\mathbb{R}^X$  and  $\mathfrak{B}'$  in  $\mathbb{R}^{X'}$  *\*-equivalent* if there exists an invertible linear map  $g$  from  $\mathbb{R}^X$  to  $\mathbb{R}^{X'}$  such that for any nonzero vector  $\mathfrak{B}(i)$  in  $\mathfrak{B}$  we can find a nonzero vector  $\mathfrak{B}'(i')$  in  $\mathfrak{B}'$  such that  $g(\mathfrak{B}(i))$  is parallel to  $\mathfrak{B}'(i')$  and for any nonzero vector  $\mathfrak{B}'(j')$  in  $\mathfrak{B}'$  we can find a nonzero vector  $\mathfrak{B}(j)$  in  $\mathfrak{B}$  such that  $g^{-1}(\mathfrak{B}'(j'))$  is parallel to  $\mathfrak{B}(j)$ . Surely, every vector configuration is \*-equivalent with a multiplicity-free vector configuration.

**Lemma 2.1.** [BEZ90, Theorem 6.14] [BLVS<sup>+</sup>99, Theorem 4.2.14] *Let  $\mathfrak{A}$  and  $\mathfrak{B}$  be multiplicity-free vector configurations. Then  $\mathcal{M}_{\mathfrak{A}}$  and  $\mathcal{M}_{\mathfrak{B}}$  are isomorphic oriented matroids if and only if  $\mathcal{V}^*(\mathcal{M}_{\mathfrak{A}})$  and  $\mathcal{V}^*(\mathcal{M}_{\mathfrak{B}})$  are isomorphic posets.*

**2.2 Polytopes, face posets and 1-skeleton graphs** Every hyperplane  $H$  in  $\mathbb{R}^X$  divides it into three parts,  $H$  itself and the two connected components of  $\mathbb{R}^X \setminus H$ . We call the two components the *open half spaces for  $H$*  and the complement of any open half space for  $H$  a *closed half space for  $H$* . Let  $P$  be a polyhedron in  $\mathbb{R}^X$ . We call the hyperplane  $H$  a *dividing hyperplane* of  $P$

if  $P$  is contained in a closed half space for  $H$ . A *face* of  $P$  is the nonempty intersection of  $P$  with a closed half space for one of its dividing hyperplanes. The definition here for faces of polyhedra indeed corresponds to that of exposed faces of general convex sets [Lau13, p. 33]. But polyhedra only have exposed faces [Lau13, Lemma 4.2, Proposition 4.3] and so we do not bother to give the general definition. The *face poset* of  $P$  is the set  $\mathcal{F}(P)$  ordered under the inclusion relationship, namely,  $F_1 \leq F_2$  if and only if  $F_1 \subseteq F_2$ . We say that two points  $x$  and  $y$  in  $P$  are *equivalent* provided every dividing hyperplane for  $P$  either contains both of them or contains none of them. We thus partition  $P$  into its equivalent classes, which we call *cells*. Note that a face of  $P$  is the closed closure of a cell of  $P$  in the Euclidean topology for  $\mathbb{R}^X$ . If  $F$  is a face of  $P$ , then  $P$  is the closed closure of a unique cell  $C$  and we call the set of points in  $C$  the relative interior of  $F$ . For any  $f \in P$ , let us write  $[f]_P$  for the minimum face of  $P$  that contains  $f$ . Note that  $[f]_P = F$  if and only if  $f$  is in the relative interior of  $F$ . Every point of  $P$  which form a 0-dimensional face of  $P$  is called a *vertex* of  $P$ . If  $P$  is a polytope, i.e., a bounded polyhedron, then the minimal elements of  $\mathcal{F}(P)$  must be singleton sets consisting of vertices of  $P$ . Two polyhedra with isomorphic face posets are called *combinatorially equivalent* or having the same *combinatorial type*. For any polytope  $P$ , its 1-skeleton graph, denoted by  $\text{SG}_P$ , is the graph which has the 0-dimensional faces of  $P$  as vertices, has 1-dimensional faces of  $P$  as edges and the endpoints of each 1-dimensional face in the graph are the two 0-dimensional faces contained in it. A vertex of a  $d$ -dimensional polytope  $P$  is *simple* if it has degree  $d$  in  $\text{SG}_P$ .

Let  $P$  be a polytope in  $\mathbb{R}^X$ . For any  $f \in \mathbb{R}^X$ , the *face of  $P$  determined by  $f$*  is

$$\{g \in P : \langle g, f \rangle \geq \langle g', f \rangle, \forall g' \in P\},$$

which we denote by  $\mathcal{F}_{\max}(P, f)$ . We call  $f \in \mathbb{R}^X$  a *normal* to  $F \in \mathcal{F}(P)$  provided  $F = \mathcal{F}_{\max}(P, f)$ . For each  $F \in \mathcal{F}(P)$ , let

$$\text{N}_P(F) := \{f \in \mathbb{R}^X : F \subseteq \mathcal{F}_{\max}(P, f)\},$$

and call it the *outer normal cone of  $P$  with respect to  $F$* . We remark that the set of normals to every face  $F \in \mathcal{F}(P)$  is nonempty, which is the relative interior of  $\text{N}_P(F)$  [DCP11, §1.2.4]. The *outer normal fan* of  $P$  in  $\mathbb{R}^X$ , denoted by  $\mathcal{N}_P$  [DLRS10, Definition 2.1.8] [LR08] [Zie95, Example 7.3], consists of all those  $\text{N}_P(F)$  for  $F \in \mathcal{F}(P)$ . The *normal poset of  $P$* , denoted by  $\mathcal{N}(P)$ , has  $\mathcal{N}_P$  as its elements where  $N_1 \leq N_2$  in  $\mathcal{N}(P)$  if and only if  $N_1$  is a subset of  $N_2$ . Because the map from  $\mathcal{F}(P)$  to  $\mathcal{N}(P)$  that sends  $F$  to  $\text{N}_P(F)$  is a bijection which reverses the inclusion relationship, the normal poset of  $P$  is anti-isomorphic with the face poset of  $P$ , and so isomorphic with the face poset of the polar of  $P$  [Bar02, Chapter VI, Theorem (1.3)]. Note that two polytopes sharing the same outer normal fan surely have the same normal poset and hence are combinatorially equivalent. The next remark tells us that the face poset, the normal poset and the poset of tight digraphs are basically the same thing for Lipschitz polytopes.



**Remark 2.2.** Let  $(X, D)$  be a metric space, let  $P = L_D \subseteq \mathbb{R}^X$ , and let  $f \in P$ . Let

$$g = \sum_{(a,b) \in A_D(f)} c_{a,b}(\chi_a - \chi_b)$$

where  $c_{a,b} > 0$  for all  $(a, b) \in A_D(f)$ . Then

$$[f]_P = \mathcal{F}_{\max}(P, g). \quad (6)$$

For any  $x \in X$  and the two elements  $x^-, x^+$  defined in Example 1.2, (6) allows us to check that  $[x^-]_P = \{x^-\}$  and  $[x^+]_P = \{x^+\}$ , namely both  $x^-$  and  $x^+$  are vertices of  $P$ .

A zonotope is the image of a hypercube under an affine transformation; that is, it is the vector sum, also known as the Minkowski sum [Agn13], of a sequence of line segments in an Euclidean space. Zonotopes have many equivalent definitions/characterizations, say the supports of box splines and others [BLVS+99, Bol69, DCP11, DL97]. Zonotopes have played a central role in the recently established theory of arithmetic matroids and arithmetic Tutte polynomials [ACH15, DM12]. Here is one of many interesting properties of zonotopes.

**Lemma 2.3.** [BEZ90, Theorem 6.14] Let  $P$  and  $P'$  be two zonotopes. If  $\text{SG}_P$  and  $\text{SG}_{P'}$  are isomorphic as graphs, then  $\mathcal{F}(P)$  and  $\mathcal{F}(P')$  are isomorphic as posets.

For  $v_1, \dots, v_m \in \mathbb{R}^X$ , we often write  $\mathfrak{A} = (v_1, \dots, v_m)$  to mean that  $\mathfrak{A}$  is a vector configuration in  $\mathbb{R}^X$  indexed by  $E = \{1, \dots, m\}$  which sends  $i$  to  $v_i$  for all  $i \in E$ . We use  $\mathcal{Z}(\mathfrak{A})$  or  $\mathcal{Z}(v_1, \dots, v_m)$  for the zonotope

$$\{t_1 v_1 + \dots + t_m v_m : 0 \leq t_i \leq 1, i = 1, \dots, m\}$$

and we use  $\mathcal{Z}(\pm \mathfrak{A})$  or  $\mathcal{Z}(\pm v_1, \dots, \pm v_m)$  for

$$\mathcal{Z}(v_1, -v_1, \dots, v_m, -v_m) = \{t_1 v_1 + \dots + t_m v_m : -1 \leq t_i \leq 1, i = 1, \dots, m\}.$$

We call  $\mathcal{Z}(\mathfrak{A})$  the *zonotope generated by  $\mathfrak{A}$* .

**Remark 2.4.** Note that  $\mathcal{Z}(\pm \mathfrak{A}) = 2 \mathcal{Z}(\mathfrak{A}) - \sum_{i=1}^m v_i$  and so  $\mathcal{Z}(\mathfrak{A})$  and  $\mathcal{Z}(\pm \mathfrak{A})$  have the same combinatorial type.

Real hyperplane arrangements, zonotopes and vector configurations are different guises of the structure of realizable oriented matroids [BLVS+99]. Associated with the zonotope  $\mathcal{Z}(\mathfrak{A}) = \mathcal{Z}(v_1, \dots, v_m)$  is the central hyperplane arrangement  $H_{\mathfrak{A}}$  given by the hyperplanes orthogonal to one of the nonzero vectors from  $\{v_1, \dots, v_m\}$ . The regions of  $H_{\mathfrak{A}}$  are naturally identified with the elements of  $\text{im } \mathfrak{A}^\top$ . The normal fan of a zonotope is equal to the fan of the corresponding hyperplane arrangement [DCP11, Theorem 2.41][McM71, p. 94] [Zie95, Theorem 7.16]. These simple considerations then suggest the following useful fact.

**Proposition 2.5.** [BLVS<sup>+</sup>99, Proposition 2.2.2, Corollary 2.2.3] Let  $\mathfrak{A}$  be a vector configuration in  $\mathbb{R}^X$ . Then the face poset  $\mathcal{V}^*(\mathcal{M}_{\mathfrak{A}})$  of the oriented matroid  $\mathcal{M}_{\mathfrak{A}}$  and the face poset of the zonotope  $\mathcal{Z}(\mathfrak{A})$  are anti-isomorphic.

**Remark 2.6.** Checking (5) and the definition of covectors, it follows from Proposition 2.5 that the zonotopes of two  $*$ -equivalent vector configurations have the same combinatorial type [McM71, p. 92]. This gives a better understanding of Remark 2.4.

We say that two subsets  $S_1$  and  $S_2$  of  $\mathbb{R}^X$  are *sign equivalent* if there exists a bijection  $f$  from  $S_1$  to  $S_2$  such that  $f(v) \in \{\pm v\}$  for all  $v \in S_1$ .

**Lemma 2.7.** [Zie95, p. 206] Let  $P$  be a nonempty zonotope in  $\mathbb{R}^X$ . Then there is a unique vector  $v \in P$  and, up to sign equivalence, a unique multiplicity-free vector configurations  $\{v_1, \dots, v_m\} \subseteq \mathbb{R}^X$  such that  $P = v + \mathcal{Z}(\pm v_1, \dots, \pm v_m)$ .

*Proof.* Let  $u_1, \dots, u_n$  be the set of all vertices of  $P$  and let  $[A_1, B_1], \dots, [A_m, B_m]$  be a maximal nonparallel set of edges of  $P$ . It is easy to check that we should take  $v = \sum_{i=1}^n \frac{u_i}{n}$  and  $v_i \in \{\frac{A_i - B_i}{2}, \frac{B_i - A_i}{2}\}$  for  $i = 1, \dots, m$ .  $\square$

For any zonotope  $P$ , we call the vector  $v$  claimed in Lemma 2.7 the *center* of  $P$ , call the set of vectors  $\{v_1, \dots, v_m\}$  claimed in Lemma 2.7 the *generators* of  $P$  and define the *oriented matroid* of  $P$ , denoted by  $\mathcal{M}_P$ , to be  $\mathcal{M}_{(v_1, \dots, v_m)}$ .

**Remark 2.8.** For any vector configuration  $\mathfrak{A}$  and polytope  $P = \mathcal{Z}(\mathfrak{A})$ , it holds  $\mathcal{M}_P = \mathcal{M}_{\mathfrak{A}}$  if and only if  $\mathfrak{A}$  is a multiplicity-free. The zonotopes generated by two  $*$ -equivalent vector configurations share the same oriented matroid up to isomorphism.

**2.3 Graphs, weighted  $X$ -networks and flow posets** A digraph  $G$  consists of a set  $V(G)$  of its vertices, a set  $A(G)$  of its arcs, and two maps from  $A(G)$  to  $V(G)$ ,  $\text{o}_G$  and  $\text{t}_G$ . For each  $\alpha \in A(G)$ , we call  $\text{o}_G(\alpha)$  the *origin* of  $\alpha$  and  $\text{t}_G(\alpha)$  the *terminus* of  $\alpha$ . A *subgraph of a digraph  $G$  induced by  $W \subseteq V(G)$* , denoted by  $G[W]$ , is the digraph with vertex set  $W$ , arc set  $\text{t}_G^{-1}(W) \cap \text{o}_G^{-1}(W)$  and the origin and terminus maps obtained by restricting those maps of  $G$  on  $\text{t}_G^{-1}(W) \cap \text{o}_G^{-1}(W)$ . If the map  $(\text{o}_G, \text{t}_G)$  from  $A(G)$  to  $V(G) \times V(G)$  is injective, we will naturally identify every arc  $\alpha$  with the pair  $(\text{o}_G(\alpha), \text{t}_G(\alpha))$ . A sequence of  $\ell$  arcs in  $G$ , say  $P = (\alpha_1, \dots, \alpha_\ell)$ , is a *path of length  $\ell$  in  $G$* , provided  $\text{o}_G(\alpha_1), \dots, \text{o}_G(\alpha_\ell)$  are all different vertices, and  $\text{o}_G(\alpha_{i+1}) = \text{t}_G(\alpha_i)$  for all  $i$  satisfying  $1 \leq i \leq \ell - 1$ . We call  $\text{o}_G(\alpha_1)$  the *origin* of  $P$ ,  $\text{t}_G(\alpha_\ell)$  the *terminus* of  $P$ ,  $\text{o}_G(\alpha_2), \dots, \text{o}_G(\alpha_\ell)$  the *interior vertices* of  $P$ , and say that  $P$  runs from  $\text{o}_G(\alpha_1)$  to  $\text{t}_G(\alpha_\ell)$ ; for easy of reference, we will write  $\text{o}_G(P)$  for  $\text{o}_G(\alpha_1)$  and  $\text{t}_G(P)$  for  $\text{t}_G(\alpha_\ell)$ . If  $\text{o}_G(P) = \text{t}_G(P)$ , we say that the path  $P$  is a *cycle*.

A *graph* is a digraph  $G$  together with an involution of  $A(G)$  which sends  $\alpha \in A(G)$  to  $\bar{\alpha} \in A(G)$  such that  $\text{o}_G(\bar{\alpha}) = \text{t}_G(\alpha)$  and  $\text{t}_G(\bar{\alpha}) = \text{o}_G(\alpha)$ . For each  $\alpha \in A(G)$ , let  $[\alpha]$  stand for the orbit  $\{\alpha, \bar{\alpha}\}$  of the involution. Denote by  $E(G)$  the set of orbits of the involution. For each edge  $e \in E(G)$ , say  $e = \{\alpha, \bar{\alpha}\}$ , we

call  $o_G(\alpha)$  and  $t_G(\alpha)$ , which may not be different, the *endpoints* of  $e$ , and we write  $\text{bd}_G(e)$  for the set  $\{o_G(\alpha), t_G(\alpha)\}$  of its endpoints and call it the *boundary* of  $e$ . Therefore, a graph  $G$  consists of its vertex set  $V(G)$ , edge set  $E(G)$ , and a map  $\text{bd}_G$  from  $E(G)$  to  $\binom{V(G)}{1} \cup \binom{V(G)}{2}$  that sends an edge to its endpoints. A graph  $G$  is *simple* provided  $\text{bd}_G$  is an injective map from  $E(G)$  to  $\binom{V(G)}{2}$ . For a simple graph  $G$ , we also adopt the convention of writing an edge  $e$  as  $uv$  when  $\text{bd}_G(e) = \{u, v\}$ . The *degree* of  $v \in V(G)$  in a graph  $G$ , denoted by  $\deg_G(v)$ , is the number of edges of  $G$  which has  $v$  as one of its endpoints, i.e.,  $\deg_G(v) = |\{e \in E(G) : v \in \text{bd}_G(e)\}|$ . A *partial orientation* of  $G$  is a set  $\sigma \subseteq A(G)$  such that  $|\sigma \cap \{\alpha, \bar{\alpha}\}| \leq 1$  for all  $\alpha \in A(G)$ . We sometimes identify a partial orientation  $\sigma$  with the digraph  $(V(G), \sigma)$ . If the partial orientation  $\sigma$  attains its maximum possible size, namely,  $|\sigma| = |E(G)|$ , we call it an *orientation* of  $G$ . The pair  $(G, \sigma)$  consisting of a graph  $G$  and an orientation  $\sigma$  of it is called an *oriented graph*. A *partial orientation* of  $G$  also gives rise to a graph, that is, the subgraph of  $G$  with vertex set  $V(G)$  and edge set  $\{[\alpha] : \alpha \in \sigma\}$ , which we will denote by  $G^\sigma$ . If  $T$  is a tree and  $x$  is a vertex of  $T$ , we write

$$\sigma_{T,x}^+ \tag{7}$$

for the orientation of  $T$  in which there is a path from  $x$  to  $v$  for all  $v \in V(T)$  and we write

$$\sigma_{T,x}^- \tag{8}$$

for the orientation of  $T$  in which there is a path from  $v$  to  $x$  for all  $v \in V(T)$ .

Let  $G$  be a graph and take  $U \subseteq V(G)$ . Let  $u$  be an element disjoint from  $V(G)$  and, for every  $x \in V(G)$ , let

$$m_U(x) = \begin{cases} x & \text{if } x \notin U; \\ u & \text{if } x \in U. \end{cases}$$

We now define  $G/U$  to be the graph with  $V(G/U) = (V(G) \setminus U) \cup \{u\}$ ,  $E(G/U) = E(G)$  and  $\text{bd}_{G/U}(e) = \{m_U(x), m_U(y)\}$  for all  $e \in E(G/U)$  with  $\text{bd}_G(e) = \{x, y\}$ . That is,  $G/U$  is obtained from  $G$  by *contracting* all vertices inside  $U$  into one vertex. When there is no danger of confusion, we will often directly name this new vertex  $u$  of  $G/U$  as  $U$ . We illustrate this vertex-contracting operation in Figure 1.

Let  $G$  be a graph. For any orientation  $\sigma$  of  $G$ , the *incidence matrix* of  $(G, \sigma)$ , denoted by  $\mathfrak{I}_{G,\sigma}$ , is the  $\sigma$ -indexed vector configuration in  $\mathbb{R}^{V(G)}$  such that

$$\mathfrak{I}_{G,\sigma}(\alpha) = \chi_{o_G(\alpha)} - \chi_{t_G(\alpha)} \in \{0, \pm 1\}^{V(G)} \subseteq \mathbb{R}^{V(G)}$$

for all  $\alpha \in \sigma$ . We write  $\partial_{G,\sigma}$  for the conjugate of  $\mathfrak{I}_{G,\sigma}$ , namely  $\partial_{G,\sigma} = \mathfrak{I}_{G,\sigma}^\top$  is the  $V(G)$ -indexed vector configuration in  $\mathbb{R}^\sigma$  such that

$$\partial_{G,\sigma}(v) = \sum_{\alpha \in o_G^{-1}(v) \cap \sigma} \chi_\alpha - \sum_{\alpha \in t_G^{-1}(v) \cap \sigma} \chi_\alpha \subseteq \mathbb{R}^\sigma$$

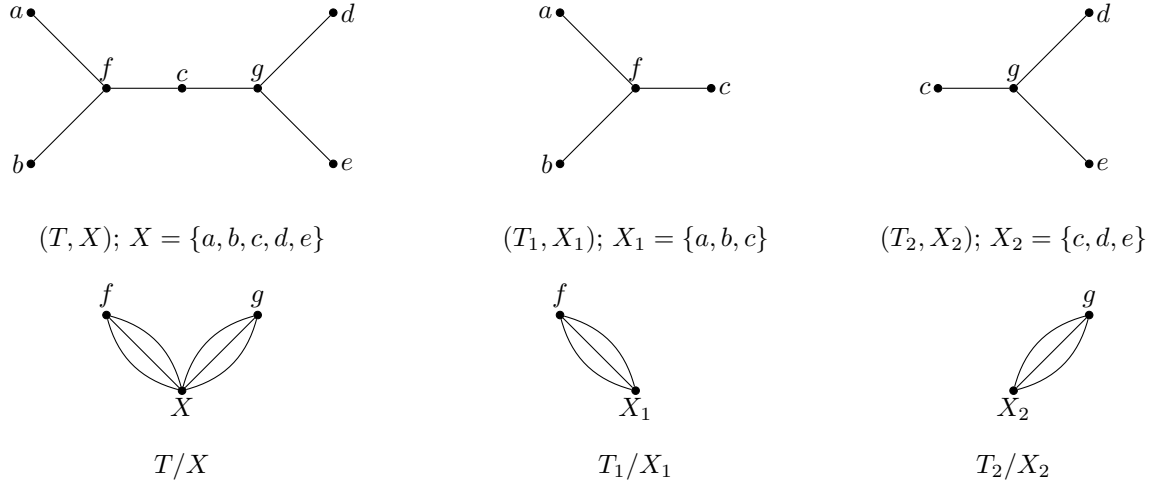


Figure 1: Three trees and the corresponding graphs after vertex-contraction.

for all  $v \in V(G)$ . We call  $\ker \mathfrak{J}_{G,\sigma}$  the *cycle space* of  $(G, \sigma)$  and  $\text{im } \partial_{G,\sigma}$  the *cut space* of  $(G, \sigma)$ , which are surely the orthogonal complements of each other in  $\mathbb{R}^\sigma$ . For any two orientations  $\sigma$  and  $\sigma'$  of  $G$ , we can find a unique bijection  $\pi$  from  $\sigma$  to  $\sigma'$  such that  $\pi(\alpha) = \{\alpha, \bar{\alpha}\} \cap \sigma'$  for all  $\alpha \in \sigma$ . This map  $\pi$  induces a natural linear isomorphism  $L^\pi$  from  $\mathbb{R}^\sigma$  to  $\mathbb{R}^{\sigma'}$  such that

$$(L^\pi f)(\alpha) = \begin{cases} f(\alpha) & \text{if } \alpha = \pi(\alpha), \\ -f(\alpha) & \text{if } \bar{\alpha} = \pi(\alpha), \end{cases}$$

for all  $f \in \mathbb{R}^\sigma$ . Moreover, it is easy to check that  $L^\pi$  maps  $\ker \mathfrak{J}_{G,\sigma}$  to  $\ker \mathfrak{J}_{G,\sigma'}$  and maps  $\text{im } \partial_{G,\sigma}$  to  $\text{im } \partial_{G,\sigma'}$ . So, different orientations of  $G$  just give us different coordinate systems and we will sometimes just call  $\ker \mathfrak{J}_{G,\sigma}$  and  $\text{im } \partial_{G,\sigma}$  the cycle space and the cut space of  $G$ . Considering this identification  $\pi$  between  $\sigma$  and  $\sigma'$  and using the reorientation on  $F' = \{\pi(\alpha) : \pi(\alpha) \neq \alpha\}$ , we see that  $\mathcal{M}_{\mathfrak{J}_{G,\sigma}}$  and  $\mathcal{M}_{\mathfrak{J}_{G,\sigma'}}$  are isomorphic; surely, this is simply because  $L^\pi$  induces an isomorphism from  $\ker \mathfrak{J}_{G,\sigma}$  to  $\ker \mathfrak{J}_{G,\sigma'}$ . Therefore, we will abbreviate  $\mathcal{M}_{\mathfrak{J}_{G,\sigma}}$  as  $\mathcal{M}_G$  and call it the *oriented matroid of  $G$* . For any  $f \in \ker \mathfrak{J}_{G,\sigma}$ , its support  $\underline{f}$  can be encoded as a partial orientation  $\sigma_f$  of  $G$  such that  $\sigma_f = \{\alpha \in \sigma : f(\alpha) > 0\} \cup \{\bar{\alpha} : \alpha \in \sigma, f(\alpha) < 0\}$ . We call  $\sigma_f$  a *combinatorial flow* of  $G$ , which is also named as a *cyclic partial orientation* of  $G$  [Bol98, p. 372, Ex. 10]. It is obvious that, for any  $f_1, f_2 \in \ker \mathfrak{J}_{G,\sigma}$ ,  $\underline{f_1} \leq \underline{f_2}$  if and only if  $\sigma_{f_1} \subseteq \sigma_{f_2}$ . A partial orientation  $\tau$  of  $G$  is a combinatorial flow if and only if, for every  $\alpha \in \tau$ , we can find a cycle which contains  $\alpha$  and falls into  $\tau$ . Denote by  $\mathcal{CF}(G)$  the poset of all combinatorial flows of  $G$  ordered under the inclusion relationship, and call it the *flow poset* of  $G$ . Clearly,  $\mathcal{CF}(G)$  is just a coordinate-free description of the poset  $\mathcal{V}(\mathcal{M}_G)$ .

**Proposition 2.9.** *Let  $G$  be a graph and  $\sigma$  be any orientation of  $G$ . If  $\mathfrak{A}$  is*

a  $\sigma$ -indexed vector configuration such that  $\ker \mathfrak{A}$  coincides with the cut space  $\text{im } \partial_{G,\sigma} = (\ker \mathfrak{J}_{G,\sigma})^\perp$  of  $G$ , or equivalently,  $\text{im } \mathfrak{A}^\top$  coincides with the cycle space  $\ker \mathfrak{J}_{G,\sigma} = (\text{im } \partial_{G,\sigma})^\perp$  of  $G$ , then the face poset of  $\mathcal{Z}(\mathfrak{A})$  is anti-isomorphic with  $\mathcal{CF}(G)$ .

*Proof.* Note that  $\mathcal{CF}(G) = \mathcal{V}(\mathcal{M}_{\mathfrak{J}_{G,\sigma}}) = \mathcal{V}^*(\mathcal{M}_{\mathfrak{A}})$ . An application of Proposition 2.5 completes the proof.  $\square$

A *network* is a graph  $G$  together with a subset  $X$  of its vertex set which can be reckoned as outlets and inlets. We will refer to  $(G, X)$  as an *X-network* if all those vertices of  $G$  having degree at most two are contained in  $X$ . If  $G$  itself is a tree, the *X-network*  $(G, X)$  is an *X-tree*. An *X-tree*  $(T, X)$  is called a *phylogenetic X-tree* if  $X$  coincides with the set of vertices of degree at most one in  $T$ . Let  $(G, X)$  be an *X-network*. A *flow* on  $(G, X)$  is a map  $f$  from  $A(G)$  to  $\mathbb{R}$  such that

- $f(\alpha) = -f(\bar{\alpha})$  for all  $\alpha \in A(G)$ ; and
- $\sum_{u=t(\alpha)} f(\alpha) = 0$  for all  $u \in V(G) \setminus X$ .

The *support* of the flow  $f$  on  $(G, X)$  is the set  $\{\alpha \in A(G) : f(\alpha) > 0\}$ , which we denote by  $\text{supp}(f)$ . A subset of  $A(G)$  is called a *combinatorial flow* on the *X-network*  $(G, X)$  if it is the support of some flow on it. We write  $\mathcal{CF}(G, X)$  for the poset of all combinatorial flows of  $(G, X)$ . We call an orientation  $\sigma$  of  $G$  which is also in  $\mathcal{CF}(G, X)$  a *full combinatorial flow* on  $(G, X)$  and we use  $\mathcal{CF}^*(G, X)$  to denote the set of all full combinatorial flows on  $(G, X)$ . It is claimed that passing through single spaces to pairs of spaces as objects of study was a great breakthrough in algebraic topology in the past [Sat99, p. 5]. Analogously, we believe that going to combinatorial flows of *X-network*  $(G, X)$  from combinatorial flows of an  $\emptyset$ -network, say the graph  $G/X$ , should provide insight and convenience, which we plan to discuss further elsewhere.

For any connected graph  $G$  and any function  $w \in \mathbb{R}_{>0}^{E(G)}$ , we have the natural shortest path metric  $D_{G,w}$  defined on  $V(G)$  [Geo11, KKN15]. For any connected *X-network*  $(G, X)$  and any  $w \in \mathbb{R}_{>0}^{E(G)}$ , the triple  $(G, X, w)$  is a *weighted X-network* and we let  $D_{G,X,w}$  be the metric on  $X$  which is obtained from  $D_{G,w}$  by restricting its range to  $X \times X$ . We say that  $(G, X, w)$  is a *weighted network representation* of the metric  $D_{G,X,w}$ . If  $w$  takes constant value 1, we use the shorthand  $D_G$  and  $D_{G,X}$  for  $D_{G,w}$  and  $D_{G,X,w}$ , respectively. If  $\mathcal{T} = (T, X)$  is an *X-tree* and  $w$  is a positive weight function on  $E(T)$ , we call  $D_{\mathcal{T},w}$  a *tree metric*. The relation between a metric space and its weighted network representation has been examined seriously in phylogenetic combinatorics [DHK<sup>+</sup>12, SS03, Ste16]. Tree metrics have many local characterizations [DHK<sup>+</sup>12, SS03], including the following four-point condition (4PC) characterization, which have been discovered independently several times by different authors [DHK<sup>+</sup>12, §3.1].

**Lemma 2.10.** [DHK<sup>+</sup>12, Theorem 3.1] *Let  $(X, D)$  be a proper metric space. Then, there exists a weighted X-tree  $(T, X, w)$  such that  $D = D_{T,X,w}$  if and only*

if, for every four (not necessarily distinct) elements  $a, b, c, d \in X$ , the maximum of the three numbers

$$D(a, d) + D(b, c), D(a, c) + D(b, d), D(a, b) + D(c, d)$$

is attained at least twice. Moreover, the weighted  $X$ -tree  $(T, X, w)$  that realizes  $D$  is unique up to isomorphism.

### 3 Lipschitz polytopes and zonotopes

For any  $A \subseteq X$ , the *characteristic vector of  $A$  with respect to  $X$* , denoted by  $\chi_A$ , is the element in  $\mathbb{R}^X$  such that

$$\chi_A(x) = \begin{cases} 1 & \text{if } x \in A; \\ 0 & \text{otherwise.} \end{cases}$$

An ordered partition of a set  $X$  into two parts, say first  $A$  and then  $B$ , is called a *directed split* of  $X$  and denoted by  $A \vdash B$ . A partition of a set  $X$  into two parts  $A$  and  $B$  is called a *split* of  $X$  and denoted by  $A|B$ . We can think of  $A|B = B|A$  as an element representing the set  $\{A \vdash B, B \vdash A\}$  and we call  $A|B$  the *split corresponding to the directed split  $A \vdash B$* . For a directed split  $s = A \vdash B$  of  $X$ , the notation  $f_s$  stands for the element of  $\mathbb{R}^X$  such that

$$f_s(x) = \begin{cases} \frac{|B|}{|X|} & \text{if } x \in A; \\ \frac{-|A|}{|X|} & \text{if } x \in B. \end{cases} \quad (9)$$

That is,

$$f_{A \vdash B} = \frac{|B|\chi_A}{|X|} - \frac{|A|\chi_B}{|X|} = \chi_A - \frac{|A|}{|X|} = -f_{B \vdash A}.$$

For each split  $s = A|B = B|A$  of  $X$ , let  $D_s$  be the metric on  $X$  such that, for all  $x, y \in X$ ,

$$D_s(x, y) = \begin{cases} 1 & \text{if } |\{x, y\} \cap A| = 1; \\ 0 & \text{otherwise.} \end{cases}$$

We call  $D_s$  a *split metric* on  $X$ .

**Remark 3.1.** Let  $s = A|B$  be a split of a nonempty set  $X$ . Then  $L_{D_s} = \mathcal{Z}(\pm f_{A \vdash B}) = \mathcal{Z}(f_{A \vdash B}, f_{B \vdash A})$  is the line segment in  $\mathbb{R}^X$  connecting  $f_{A \vdash B}$  and  $f_{B \vdash A}$ .

Let  $(T, X)$  be an  $X$ -tree. For every  $\alpha \in A(T)$ , let

$$\begin{cases} \widehat{o_{T,X}(\alpha)} = \{x \in X : D_T(x, o_T(\alpha)) < D_T(x, t_T(\alpha))\}; \\ \widehat{t_{T,X}(\alpha)} = \{x \in X : D_T(x, o_T(\alpha)) > D_T(x, t_T(\alpha))\}. \end{cases}$$

Then let

$$s_\alpha^{T,X} = \widehat{o_{T,X}(\alpha)} \vdash \widehat{t_{T,X}(\alpha)}, \quad (10)$$

which is surely a directed split of  $X$ . For the two directed splits  $s_\alpha^{T,X}$  and  $s_{\bar{\alpha}}^{T,X}$ , we write  $s_e^{T,X}$  for the corresponding split of  $X$ , where  $e = [\alpha] = \{\alpha, \bar{\alpha}\}$ .

**Lemma 3.2.** [McS34, Theorem 1] Let  $(X, D_X)$  and  $(Y, D_Y)$  be two proper metric spaces such that  $X \subseteq Y$  and the restriction of  $D_Y$  on  $X \times X$  equals  $D_X$ . Then every function  $f : X \rightarrow \mathbb{R}$  can be extended to a function  $\tilde{f} : Y \rightarrow \mathbb{R}$  such that  $\tilde{f}|_X = f$  and  $\max\{\frac{|\tilde{f}(y_1) - \tilde{f}(y_2)|}{D_Y(y_1, y_2)} : y_1 \neq y_2 \in Y\} = \max\{\frac{|\tilde{f}(x_1) - \tilde{f}(x_2)|}{D_X(x_1, x_2)} : x_1 \neq x_2 \in X\}$ .

Zonotopes possess a high degree of symmetry and so allow various local characterizations. The Alexandrov characterization of zonotopes, [Ale33] [Bol69, Theorem 3.3] says that a polytope is a zonotope if and only if all its two-dimensional faces are centrally symmetric. More generally, McMullen [McM70] finds that for every  $d \geq 4$ , a dimension- $d$  polytope is a zonotope if and only if all its  $j$ -faces are centrally symmetric for one  $j$  satisfying  $2 \leq j \leq d - 2$ . As observed by Witsenhausen [Wit78, Lemma 2] [Zie95, Exercise 7.5], Alexandrov's characterization leads to the conclusion that, if all the 3-dimensional projections of a polytope  $P$  are zonotopes, then so is  $P$ . The next theorem suggests that Witsenhausen's observation may be viewed as a counterpart for Lemma 2.10.

**Theorem 3.3.** For every weighted  $X$ -tree  $(T, X, w)$ , we have

$$L_{D_{T,X,w}} = \sum_{e \in E(T)} w(e) L_{D_{s_e^T, X}} = \sum_{\alpha \in A(T)} w([\alpha]) \mathcal{Z}(f_{s_\alpha^T, X}), \quad (11)$$

which implies that the Lipschitz polytope of a tree metric is a zonotope.

*Proof.* By Remark 3.1, our task is to show

$$L_{D_{T,X,w}} = \sum_{e \in E(T)} w(e) L_{D_{s_e^T, X}}.$$

Take any  $f \in L_{D_{T,X,w}}$ . By Lemma 3.2, we can fix a map  $\tilde{f}$  on  $V(T) \times V(T)$  such that  $\tilde{f}|_{X \times X} = f$  and

$$|\tilde{f}(a) - \tilde{f}(b)| \leq D_{T,w}(a, b) \quad (12)$$

for all  $a, b \in V(T)$ . For each  $e = \{\vec{ab}, \vec{ba}\} \in E(T)$ , let

$$f_e = (\tilde{f}(a) - \tilde{f}(b)) f_{A \vdash B} = (\tilde{f}(b) - \tilde{f}(a)) f_{B \vdash A} \in \mathbb{R}^X,$$

where  $A \vdash B = s_{\vec{ab}}^{T,X}$ , as defined in (10). By (12),  $f_e \in L_{w(e) D_{s_e^T, X}} = w(e) L_{D_{s_e^T, X}}$  holds. For any path  $P = (\alpha_1, \dots, \alpha_\ell)$  in the tree  $T$  with  $\{o_T(P), t_T(P)\} \subseteq X$ ,

we have

$$\begin{aligned}
f(o_T(P)) - f(t_T(P)) &= \tilde{f}(o_T(P)) - \tilde{f}(t_T(P)) \\
&= \sum_{i=1}^{\ell} (\tilde{f}(o_T(\alpha_i)) - \tilde{f}(t_T(\alpha_i))) \tag{13} \\
&= \sum_{i=1}^{\ell} \left( \sum_{e \in E(T)} f_e(o_T(\alpha_i)) - \sum_{e \in E(T)} f_e(t_T(\alpha_i)) \right) \\
&= \sum_{e \in E(T)} (f_e(o_T(P)) - f_e(t_T(P))) \\
&= \left( \sum_{e \in E(T)} f_e \right)(o_T(P)) - \left( \sum_{e \in E(T)} f_e \right)(t_T(P)).
\end{aligned}$$

Since both  $f$  and  $\sum_{e \in E(T)} f_e$  are functions which sum to zero on  $X$ , (13) gives

$$f = \sum_{e \in E(T)} f_e$$

and henceforth

$$L_{D_{T,X,w}} \subseteq \sum_{e \in E(T)} L_{w(e)D_{s_e^T,X}} = \sum_{e \in E(T)} w(e) L_{D_{s_e^T,X}}. \tag{14}$$

It is not difficult to verify that

$$D_{T,X,w} = \sum_{e \in E(T)} w(e) D_{s_e^T,X}$$

and so

$$L_{D_{T,X,w}} \supseteq \sum_{e \in E(T)} w(e) L_{D_{s_e^T,X}} \tag{15}$$

follows. Now, (14) along with (15) implies what we want.  $\square$

**Theorem 3.4.** *Let  $(X, D)$  be a finite proper metric space. Then  $D$  is a tree metric if and only if  $L_D$  is a zonotope.*

*Proof.* In view of Theorem 3.3, we only need to establish the backward direction. We take arbitrarily  $U = \{a, b, c, d\} \in \binom{X}{4}$ . Without loss of generality, we assume that

$$D(a, d) + D(b, c) \geq D(a, b) + D(c, d) \tag{16}$$

and

$$D(a, c) + D(b, d) \geq D(a, b) + D(c, d). \tag{17}$$

By Lemma 2.10, it suffices to show that

$$D(a, d) + D(b, c) = D(a, c) + D(b, d). \tag{18}$$



Let  $D'$  be the restriction of  $D$  on  $U \times U$ . By Lemma 3.2, it holds that  $L_{D'}^a = p_a^U p_U(L_D)$ , where  $p_U : \mathbb{R}^X \rightarrow \mathbb{R}^U$  is the map that sends  $f \in \mathbb{R}^X$  to  $f|_U$ , and  $p_a^U : \mathbb{R}^U \rightarrow \mathbb{R}^U$  is as defined in (3). Note that both  $p_a^U$  and  $p_U$  are projection maps. Since we have assumed that  $L_D$  is a zonotope, we now see that so is  $L_{D'}^a$ . Let

$$\begin{aligned}
& F \\
& := \mathcal{F}_{\max}(L_{D'}^a, \chi_b - \chi_a) \\
& = \{f \in L_{D'} : f(a) = 0, f(b) = D(b, a)\} \\
& = \{f \in \mathbb{R}^U : f(a) = 0, f(b) = D(b, a), |f(c) - f(d)| \leq D(c, d), |f(c) - f(a)| \leq D(c, a), \\
& \quad |f(c) - f(b)| \leq D(c, b), |f(d) - f(a)| \leq D(d, a), |f(d) - f(b)| \leq D(d, b)\}.
\end{aligned} \tag{19}$$

As a face of the zonotope  $L_{D'}^a$ ,  $F$  must be centrally symmetric. Substituting  $f(c) = x$  and  $f(d) = y$  into (19), we then see that

$$\begin{aligned}
H & := \{(x, y) : |x - y| \leq D(c, d), |x| \leq D(c, a), \\
& \quad |x - D(b, a)| \leq D(c, b), |y| \leq D(d, a), |y - D(b, a)| \leq D(d, b)\}
\end{aligned}$$

should be a centrally symmetric subset of  $\mathbb{R}^2$ . Let

$$M_0 = D(b, a) - D(c, b), \quad M_1 = D(c, a),$$

and

$$I_x = [\max(D(b, a) - D(d, b), x - D(c, d)), \min(D(d, a), x + D(c, d))]$$

for all  $x \in [M_0, M_1]$ . Since  $D$  satisfies the triangle inequality, we can obtain

$$H = \{(x, y) : x \in [M_0, M_1], y \in I_x\}.$$

We further derive from the triangle inequality that

$$\begin{cases} I_{M_0} = [D(b, a) - D(d, b), D(b, a) - D(c, b) + D(c, d)], & \text{by (16)} \\ I_{M_1} = [D(c, a) - D(c, d), D(d, a)], & \text{by (17)}. \end{cases}$$

Applying the triangle inequality again shows that both  $I_{M_0}$  and  $I_{M_1}$  are nonempty and hence, because  $H$  is centrally symmetric,  $I_{M_0}$  and  $I_{M_1}$  should be of the same length. Comparing their lengths yields (18), as wanted.  $\square$

**Remark 3.5.** Let  $(X', D')$  be a metric space. For any  $x, y \in X'$ , we say that they are equivalent provided  $D'(x, y) = 0$ . Let  $X$  be the set of equivalence classes in  $X'$  and let  $D$  be the proper metric on it such that  $D(u, v)$  takes the value  $D'(x, y)$  for any  $x \in u$  and  $y \in v$ . Fix an  $x \in X'$  and let  $u$  be the equivalence class containing  $x$ . Let  $\pi$  be the injective linear map from  $\mathbb{R}^X$  to  $\mathbb{R}^{X'}$  such that  $\pi(\chi_u) = \sum_{x \in u} \chi_x$ . It is clear that  $\pi(L_D^u) = L_{D'}^x$ . By Remark 1.1 and Theorem 3.4, we obtain the equivalence of the following four claims:

- $L_{D'}$  is a zonotope;

- $p_x^{X'}(L_{D'}) = L_{D'}^x = \pi(L_D^u)$  is a zonotope;
- $L_D^u$  is a zonotope;
- $D$  is a tree metric.

**Remark 3.6.** According to a result of Godard [God10, Theorem 4.2 “(1) $\iff$ (3)”], a metric space  $(X, D)$  is a tree metric if and only if its Lipschitz-free space is  $L_1$ -embeddable and so, by [DL97, Theorem 8.3.2], if and only if  $L_D^x$ , where  $x$  is any fixed element of  $X$ , is a zonotope. This line of arguments could provide another indirect proof of Theorem 3.3. Conversely, surely Theorem 3.3 can be used to prove [God10, Theorem 4.2] as well. We mention that another proof of Theorem 3.3 is obtained by Delucchi and Hoessly [DH16, Theorem 3.5]. Theorem 3.4 is very close to [God10, Theorem 4.2]. Note that the backward direction of Theorem 3.3 just corresponds to the implication of [God10, Theorem 4.2 “(1) $\implies$ (2)”]. We can even talk about directed metric space (by dropping the symmetric condition for a metric space) and prove that the Lipschitz polytope of a directed metric is a zonotope if and only if the directed metric is read from a weighted directed  $X$ -tree [WX17].

#### 4 Oriented matroids and face posets

For any  $x \in X$  and any directed split  $s$  of  $X$ , say  $s = A \vdash B$ , we define  $f_{s,x} \in \mathbb{R}^X$  by setting

$$f_{s,x} = \begin{cases} -\chi_B & \text{if } x \in A; \\ \chi_A & \text{if } x \in B. \end{cases} \quad (20)$$

Let  $(T, X)$  be an  $X$ -tree. For any  $x \in X$  and  $\alpha \in A(T)$ , it follows from (10) and (20) that

$$f_{s_\alpha^{T,x}, x} = -f_{s_\alpha^{T,x}, x},$$

and it follows from (3), (9) and (20) that

$$p_x^X(f_{s_\alpha^{T,x}}) = f_{s_\alpha^{T,x}, x}.$$

Consequently, for any weighted  $X$ -tree  $(T, X, w)$  and  $x \in X$ , we can apply Remark 3.1 and Theorem 3.3 to get

$$L_{D_{T,X,w}}^x = \mathcal{Z}(w([\alpha])f_{s_\alpha^{T,x}, x} : \alpha \in A(T)). \quad (21)$$

Let  $(T, X)$  be an  $X$ -tree. Choose one  $x \in X$  and let  $\sigma = \sigma_{T,x}^-$ . Let  $\mathfrak{D}_{T,X,x}$  be the  $\sigma$ -indexed vector configuration in  $\mathbb{R}^X$  such that

$$\mathfrak{D}_{T,X,x}(\alpha) = f_{s_\alpha^{T,x}, x} \quad (22)$$

for each  $\alpha \in \sigma$ . From (21) we can believe that  $\mathfrak{D}_{T,X,x}$  is a vector configuration of special interest for our study of Lipschitz polytopes. Let  $\mathfrak{P}_{T,X,x} = \mathfrak{D}_{T,X,x}^\top$  be the  $X$ -indexed vector configuration in  $\mathbb{R}^\sigma$ . Note that

$$\mathfrak{P}_{T,X,x}(y) = \chi_Y \in \mathbb{R}^\sigma$$

where  $Y$  is the set of arcs on the unique path from  $y$  to  $x$  in  $T$ . We call  $\mathfrak{D}_{T,X,x}$  the *descendent matrix of  $(T, X)$  with origin  $x$*  and  $\mathfrak{P}_{T,X,x}$  the *path matrix of  $(T, X)$  with origin  $x$* . Using the terminology of phylogenetic combinatorics,  $\mathfrak{D}_{T,X,x}(\alpha)(y) = \mathfrak{P}_{T,X,x}(y)(\alpha) = 1$  if and only if the split  $x|y$  is compatible with  $S_{[\alpha]}^{T,X}$ .

**Lemma 4.1.** *Let  $(T, X)$  be an  $X$ -tree, let  $x \in X$  and let  $\sigma = \sigma_{T,x}^-$ . Then  $(\text{im } \mathfrak{P}_{T,X,x})^\perp = \ker \mathfrak{D}_{T,X,x}$  is equal to  $(\ker \mathfrak{I}_{T/X,\sigma})^\perp = \text{im } \partial_{T/X,\sigma}$ . More precisely,  $\text{im } \mathfrak{P}_{T,X,x}$  and  $\text{im } \partial_{T/X,\sigma}$  are the orthogonal complements to each other in  $\mathbb{R}^\sigma$  while  $\dim \text{im } \mathfrak{P}_{T,X,x} = |X| - 1$  and  $\dim \text{im } \partial_{T/X,\sigma} = |\mathbf{E}(T)| - |X| + 1 = |\mathbf{V}(T)| - |X|$ .*

*Proof.* We directly write  $\mathfrak{P}$  for  $\mathfrak{P}_{T,X,x}$  and  $\partial$  for  $\partial_{T/X,\sigma}$ . For each  $v \in \mathbf{V}(T) \setminus \{x\}$ , let  $\alpha_v$  denote the unique arc from  $o_T^{-1}(v) \cap \sigma$ .

For each  $v \in \mathbf{V}(T/X)$ , we have

$$\partial(v) = \begin{cases} \sum_{\alpha \in o_T^{-1}(v) \cap \sigma} \chi_\alpha - \sum_{\alpha \in t_T^{-1}(v) \cap \sigma} \chi_\alpha & \text{if } v \in \mathbf{V}(T) \setminus X; \\ \sum_{u \in X} \sum_{\alpha \in o_T^{-1}(u) \cap \sigma} \chi_\alpha - \sum_{u \in X} \sum_{\alpha \in t_T^{-1}(u) \cap \sigma} \chi_\alpha & \text{if } v = X. \end{cases}$$

Note that  $\sum_{v \in \mathbf{V}(T/X)} \partial(v) = 0 \in \mathbb{R}^\sigma$  and so

$$\text{im } \partial = \text{span}\{\partial(v) : v \in \mathbf{V}(T) \setminus X\}. \quad (23)$$

Let  $S$  be a subset of  $\mathbf{V}(T) \setminus X$  and assume that  $w$  is a vertex of shortest distance to  $x$  among elements of  $S$ . We can check that  $\partial(w)(\alpha_w) = 1$  and  $\partial(v)(\alpha_w) = 0$  for all  $v \in S \setminus \{w\}$ . This observation along with (23) implies  $\dim \text{im } \partial = |\mathbf{V}(T)| - |X|$ .

For every  $y \in X$ , we have  $\mathfrak{P}(y) = \chi_{P_y} \in \mathbb{R}^\sigma$ , where  $P_y$  is the set of arcs on the unique path from  $y \in X$  to  $x \in X$  in  $T$  and so is the union of several arc-disjoint cycles in  $T/X$  passing through  $X \in \mathbf{V}(T/X)$ . Note that  $\mathfrak{P}(x) = 0$  and so

$$\text{im } \mathfrak{P} = \text{span}\{\mathfrak{P}(y) : y \in X \setminus \{x\}\}. \quad (24)$$

Let  $S$  be a subset of  $X \setminus \{x\}$ . We assume that  $w$  is a vertex in  $T$  of largest distance to  $x$  among elements of  $S$ . We can check that  $\mathfrak{P}(w)(\alpha_w) = 1$  and  $\mathfrak{P}(v)(\alpha_w) = 0$  for all  $v \in S \setminus \{w\}$ . This observation along with (24) gives

$$\dim \text{im } \mathfrak{P} = |X| - 1. \quad (25)$$

For every  $y \in X$  and every  $v \in \mathbf{V}(T) \setminus X$ ,  $\mathfrak{P}(y)$  is in the cycle space of  $T/X$  while  $\partial(v)$  is from the cut space of  $T/X$  and so  $\mathfrak{P}(y)$  and  $\partial(v)$  are orthogonal to each other in  $\mathbb{R}^\sigma$ . Since  $\dim \text{im } \partial + \dim \text{im } \mathfrak{P} = (|\mathbf{V}(T)| - |X|) + (|X| - 1) = |\mathbf{E}(T)| = |\sigma|$ , we see that  $\text{im } \mathfrak{P}$  is the cycle space of  $T/X$  and  $\text{im } \partial$  coincides with the cut space of  $T/X$  and so they are the orthogonal complements of each other in  $\mathbb{R}^\sigma$ , as wanted.  $\square$

**Theorem 4.2.** *Let  $(T, X, w)$  be a weighted  $X$ -tree. Then,*

$$\mathcal{M}_{L_{D_{T,X,w}}} = \mathcal{M}_{T/X}^*, \quad (26)$$

and the face poset of  $L_{D_{T,X,w}}$  is anti-isomorphic with  $\mathcal{CF}(T/X)$ .

*Proof.* Pick  $x \in X$ , let  $\sigma = \sigma_{T,x}^-$  and let  $\mathfrak{A} = \mathfrak{D}_{T,X,x}$  be a  $\sigma$ -indexed vector configuration in  $\mathbb{R}^X$ , which is multiplicity-free. In view of Remark 1.1, Remark 2.8 and (21), we know that

$$\mathcal{M}_{L_{D_{T,X,w}}} = \mathcal{M}_{L_{D_{T,X,w}}^x} = \mathcal{M}_{\mathcal{Z}(\mathfrak{A})} = \mathcal{M}_{\mathfrak{A}}, \quad (27)$$

and then, by Proposition 2.5, that the face poset of  $L_{D_{T,X,w}}$  is isomorphic with the face poset of  $\mathcal{Z}(\mathfrak{A})$ , namely

$$\mathcal{F}(L_{D_{T,X,w}}) = \mathcal{F}(\mathcal{Z}(\mathfrak{A})). \quad (28)$$

By Lemma 4.1,

$$\ker \mathfrak{A} = \ker \mathfrak{D}_{T,X,x} = (\ker \mathfrak{J}_{T/X,\sigma})^\perp. \quad (29)$$

Thanks to (27) and (29), we obtain (26). By Proposition 2.9, (28) along with (29) implies that  $\mathcal{F}(L_{D_{T,X,w}})$  is anti-isomorphic with  $\mathcal{CF}(T/X)$ .  $\square$

**Remark 4.3.** *Let  $(T, X)$  be an  $X$ -tree with  $|\mathbf{V}(T)| \geq 2$ .*

- (a) *No vertex other than  $X$  could be a cut vertex of  $T/X$ . If  $(T, X)$  is a phylogenetic  $X$ -tree, then  $T/X$  has no cut vertices.*
- (b) *All cycles of  $T/X$  pass through the vertex  $X$ . Moreover,  $X$  is the unique vertex of  $T/X$  that falls into all cycles of  $T/X$  unless  $T$  is a star tree, i.e., a phylogenetic  $X$ -tree with exactly one interior vertex.*
- (c) *Every phylogenetic  $X$ -tree  $T$  can be recovered from  $T/X$  as follows: If  $|\mathbf{V}(T/X)| \leq 2$ , then  $T$  is the star tree with  $\mathbf{E}(T) = \mathbf{E}(T/X)$ ; otherwise, we find the unique vertex  $v$  of  $T/X$  satisfying the property claimed in (b), for each edge  $e$  of  $T/X$  such that  $\text{bd}_{T/X}(e) = \{v, u\}$  we add a new vertex  $v_e$  to  $T/X$  and change the endpoints of  $e$  to be  $u$  and  $v_e$ , and finally delete vertex  $v$  to get  $T$ .*

For any two posets  $P$  and  $Q$ , we define their *Cartesian product* to be the poset  $P \times Q$  on ground set  $\{(p, q) : p \in P, q \in Q\}$  such that  $(a, b) \leq (c, d)$  if and only if  $a \leq c$  in  $P$  and  $b \leq d$  in  $Q$ . For any two graphs  $G_1$  and  $G_2$ , their *disjoint union* is the graph  $G_1 \cup G_2$  such that  $\mathbf{V}(G_1 \cup G_2)$  is the disjoint union of  $\mathbf{V}(G_1)$  and  $\mathbf{V}(G_2)$ ,  $\mathbf{E}(G_1 \cup G_2)$  is the disjoint union of  $\mathbf{E}(G_1)$  and  $\mathbf{E}(G_2)$ , and for every  $e \in \mathbf{E}(G_1 \cup G_2)$  it holds

$$\text{bd}_{G_1 \cup G_2}(e) = \begin{cases} \text{bd}_{G_1}(e) & \text{if } e \in \mathbf{E}(G_1); \\ \text{bd}_{G_2}(e) & \text{if } e \in \mathbf{E}(G_2). \end{cases}$$

**Remark 4.4.** Let  $G_1$  and  $G_2$  be two graphs and let  $(v_1, v_2) \in V(G_1) \times V(G_2)$ . Then  $\mathcal{CF}((G_1 \cup G_2)/\{v_1, v_2\})$  is isomorphic with  $\mathcal{CF}(G_1) \times \mathcal{CF}(G_2)$  as a poset.

**Proposition 4.5.** Let  $T_1$  be an  $X_1$ -tree and  $T_2$  be an  $X_2$ -tree. Take  $x_1 \in X_1$  and  $x_2 \in X_2$ . We write  $x$  for the new vertex of  $T = (T_1 \cup T_2)/\{x_1, x_2\}$  obtained by contracting  $\{x_1, x_2\}$ . For  $X = (X_1 \cup X_2 \cup \{x\}) \setminus \{x_1, x_2\}$ , the face poset of  $L_{D_{T,X}}$  is the product of the face posets of  $L_{D_{T_1, X_1}}$  and  $L_{D_{T_2, X_2}}$ .

*Proof.* It is a consequence of Theorem 4.2, Remark 4.3 and Remark 4.4.  $\square$

Let  $(T, X)$  be an  $X$ -tree. We construct a graph  $G$  on the vertex set  $X$  where  $uv \in E(G)$  if and only if  $u$  and  $v$  are two different elements from  $X$  such that the path running from  $u$  to  $v$  in  $T$  has no interior vertices from  $X$ . Let  $X_1, \dots, X_k$  be all the maximal cliques of  $G$ . For  $i = 1, \dots, k$ , let  $T_i$  be the subgraph of  $T$  induced by the set of vertices on paths in  $T$  connecting vertices in  $X_i$  and thus we have a phylogenetic  $X_i$ -tree  $(T_i, X_i)$ . We call  $(T_i, X_i), i = 1, \dots, k$ , the set of phylogenetic trees generated by  $(T, X)$ . For the example as displayed in Figure 1, we can see that the phylogenetic trees generated by  $(T, X)$  are  $(T_1, X_1)$  and  $(T_2, X_2)$ , and that  $T/X = ((T_1/X_1) \cup (T_2/X_2))/\{X_1, X_2\}$ .

**Remark 4.6.** By virtue of Remark 4.4 and Proposition 4.5, the face poset of  $L_{D_{T,X}}$  is the product of the face posets of the Lipschitz polytopes of those phylogenetic trees generated by  $(T, X)$ .

**Lemma 4.7.** Let  $(T, X)$  be an  $X$ -tree and let  $(T_i, X_i), i = 1, \dots, k$ , be the set of phylogenetic trees generated by  $(T, X)$ . Then

- (a) The oriented matroid structure of  $\mathcal{M}_{T_i/X_i}$  for  $i = 1, \dots, k$  are uniquely determined by the oriented matroid structure of  $\mathcal{M}_{T/X}$ .
- (b) If  $k = 1$ , namely  $(T, X)$  is a phylogenetic tree, then the oriented matroid structure of  $\mathcal{M}_{T/X}$  uniquely determines the graph structure of  $T$ .

*Proof.* (a). Let  $\mathcal{M}_{T/X} = (E, \mathcal{V})$  and  $\mathcal{M}_{T_i/X_i} = (E_i, \mathcal{V}_i)$  for  $i = 1, \dots, k$ . For  $e, f \in E$ , we say that  $e$  and  $f$  are equivalent if there is a circuit  $\Sigma$  of  $\mathcal{M}_{T/X}$  such that  $\{e, f\} \subseteq \Sigma^+ \cup \Sigma^-$ . It is clear that the resulting equivalence classes of  $E$  are just  $E_1, \dots, E_k$ , and

$$\mathcal{V}_i = \{(\Sigma^+ \cap E_i, \Sigma^- \cap E_i) : \Sigma \in \mathcal{V}\}$$

for  $i = 1, \dots, k$ . This proves (a).

(b). Let  $\mathcal{M}_{T/X} = (E, \mathcal{V})$ . Let  $\mathcal{C}$  be the set of circuits of the underlying matroid of  $\mathcal{M}_{T/X}$ . We can naturally assume  $E = E(T/X) = E(T)$ . Then each set in  $\mathcal{C}$  is the edge set of a cycle of  $T/X$ , or equivalently, edge set of a path of  $T$  from  $X$  to  $X$ . Note that  $T$  is a two-vertex tree if and only if  $|E| = 1$  and so the result is trivial. Assume now  $|V(T)| \geq 3$ . Let  $F = \{e_1, \dots, e_{|X|}\} \subseteq E$  be the edges contained in exactly  $|X| - 1$  sets of  $\mathcal{C}$ , which must be the edges of  $T$  which are incident with leaves of  $T$ . We define a metric  $D$  on  $F$  by setting  $D(e_i, e_j)$

to be the size of the unique set in  $\underline{\mathcal{C}}$  containing  $e_i$  and  $e_j$ , for all  $e_i, e_j \in F$ . It is obvious that  $(F, D)$  and  $(X, D_{T,X})$  are isometric metric spaces. So, in view of Lemma 2.10, the structure of  $T$  is uniquely determined by  $(F, D)$ , which has been read from  $\mathcal{M}_{T/X}$  as above. The proof of (b) is now completed.  $\square$

**Theorem 4.8.** *Let  $(T, X)$  be an  $X$ -tree and  $(T', X')$  be an  $X'$ -tree. Then, the following hold:*

- (a)  $L_{D_{T,X}}$  and  $L_{D_{T',X'}}$  are combinatorially equivalent if and only if  $T/X$  and  $T'/X'$  are isomorphic up to graph isomorphism.
- (b) If we further assume that  $(T, X)$  and  $(T', X')$  are phylogenetic trees, then  $\mathcal{CF}(T/X)$  and  $\mathcal{CF}(T'/X')$  are combinatorially equivalent if and only if  $T$  and  $T'$  are isomorphic as graphs.

*Proof.* The backward direction of (a) is due to Theorem 4.2 and the backward direction of (b) is trivial. So, we only need to consider the forward direction of (a) and (b).

We first prove (a). Assume that  $L_{D_{T,X}}$  and  $L_{D_{T',X'}}$  are combinatorially equivalent. As a consequence of Lemma 2.1, Proposition 2.5 and Theorem 3.3,  $\mathcal{M}_{L_{D_{T,X}}}$  is isomorphic with  $\mathcal{M}_{L_{D_{T',X'}}}$ . By Theorem 4.2, we then see that  $\mathcal{M}_{T/X}$  is isomorphic with  $\mathcal{M}_{T'/X'}$ . It is clear that our task now is to show that  $\mathcal{M}_{T/X}$  uniquely determines  $T/X$ . Let  $(T_i, X_i), i = 1, \dots, k$ , be the set of phylogenetic trees generated by  $(T, X)$ . Then  $T/X = (\cup_{i=1}^k T_i/X_i)/\{X_1, \dots, X_k\}$ . By Lemma 4.7(b), every phylogenetic tree  $(T_i, X_i)$  can be determined by  $\mathcal{M}_{T_i/X_i}$ ; by Lemma 4.7(a),  $\mathcal{M}_{T/X}$  determines the collection of oriented matroids  $\mathcal{M}_{T_i/X_i}, i = 1, \dots, k$ . This means that  $\mathcal{M}_{T/X}$  uniquely determines  $T/X$  and so we are done.

We now turn to (b). Assume that  $\mathcal{CF}(T/X)$  and  $\mathcal{CF}(T'/X')$  are isomorphic posets. By Theorem 4.2,  $L_{D_{T,X}}$  and  $L_{D_{T',X'}}$  are combinatorially equivalent; it then follows from Lemma 2.1, Proposition 2.5 and Theorem 3.3 that  $\mathcal{M}_{L_{D_{T,X}}}$  is isomorphic with  $\mathcal{M}_{L_{D_{T',X'}}}$ ; now, applying Theorem 4.2 again yields that  $\mathcal{M}_{T/X}$  and  $\mathcal{M}_{T'/X'}$  are isomorphic; finally, Lemma 4.7(b) concludes the proof. Another way to derive (b) is to make use of (a) and Remark 4.3(c).  $\square$

**Example 4.9.** *Let  $T$  be an  $X$ -tree with  $X = V(T)$ . Then  $L_{D_{T,X}}$  is affine equivalent with the  $(|X| - 1)$ -dimensional hypercube. This shows that the combinatorial type of  $L_{D_{T,X}}$  is not related to the structure of the tree. Note that what we see here confirms Theorem 4.8(a) and also demonstrates that Theorem 4.8(b) does not hold when we replace phylogenetic  $X$ -trees by general  $X$ -trees.*

## 5 Face posets and flow posets

**5.1 Some facts** A *ranked poset* is a poset in which all maximal chains have the same length. In a ranked poset, we define the *rank* of an element  $x$  to be the length of its longest chains in which  $x$  is the biggest element. Note that a minimal element in a ranked poset has rank 0. Let  $P$  be a ranked poset. The

maximum rank of the elements from  $P$ , if any, is called the *dimension* of this poset and denoted by  $\dim(P)$ .

**Lemma 5.1.** *If  $(X, D)$  is a proper metric space, then  $\mathcal{F}(L_D)$  is a ranked poset with dimension  $|X| - 1$ .*

*Proof.* The face poset of  $L_D$  is clearly a ranked poset in which the rank of a face  $F$  is given by  $\dim(F)$ . Since  $L_D$  falls into  $\{f \in \mathbb{R}^X : \sum_{x \in X} f(x) = 0\}$ , it follows  $\dim(\mathcal{F}(L_D)) \leq |X| - 1$ . For a sufficiently small positive real number  $\epsilon$  and any fixed  $a \in X$ , the  $|X|$  vectors,  $\epsilon(\chi_a - \chi_b)$ ,  $b \in X$ , is a set of affinely independent points from  $L_D$ , showing that the dimension of  $\mathcal{F}(L_D)$  is  $|X| - 1$ .  $\square$

Let  $G$  be a graph. The *zero-th Betti number*  $b_0(G)$  of  $G$  is the number of connected components of  $G$ , and the *first Betti number*  $b_1(G)$  of  $G$ , also called the *cyclomatic number* of  $G$ , is the value  $|E(G)| - |V(G)| + b_0(G)$ . They are known to be the ranks of the 0th and 1st homology groups of  $G$ , namely, the number of 0-holes and 1-holes of  $G$ . For a digraph  $G$ , let  $b_0(G)$  represent the number of its weakly connected components.

Let  $G$  be a digraph and  $H$  a subgraph of  $G$ , which we record as  $H \leq G$ . We say that a path  $P$  of  $G$  is an *ear* of  $(G, H)$  if  $A(G) \setminus A(H)$  consists of all those arcs from  $P$  and  $V(G) \setminus V(H)$  consists of all those interior vertices of  $P$ . If both  $G$  and  $H$  are strongly connected and  $G \neq H$ , the *Ear Decomposition Theorem* in the folklore [Bab06, Theorem 1.3][BM08, Proposition 5.11, Proposition 5.12, Theorem 5.13] [LM01] says that we can find an ear  $P$  for  $(G, H)$  and so the digraph  $J$  obtained from  $H$  by adding this ear is a minimal strongly connected extension of  $H$ , meaning that  $I = J$  and  $I = H$  are the only possible strongly connected digraphs satisfying  $H \leq I \leq J$ . Because of the pioneering work of Whitney [Whi32] and Robbins [Rob39] on ear decompositions, an ear decomposition is also known as a Whitney-Robbins synthesis.

**Lemma 5.2.** *Let  $G$  be a graph. Then  $\mathcal{CF}(G)$  is a ranked poset in which the rank of each element  $\sigma \in \mathcal{CF}(G)$  is given by  $b_1(G^\sigma)$ .*

*Proof.* Let  $\sigma$  be a combinatorial flow on  $G$ . Assume that  $(V(G), \sigma)$  has  $c$  strongly connected components and we take one vertex from each of them to form a set  $V_0 = \{v_1, \dots, v_c\}$ . Applying the Ear Decomposition Theorem, we see that

$$\sigma_0 < \sigma_1 < \dots < \sigma_r \tag{30}$$

is a saturated chain in  $\mathcal{CF}(G)$  with  $\sigma$  as its top element if and only if, along with the nested sequence of partial orientations of  $G$ ,

$$\emptyset = \sigma_0 \subsetneq \sigma_1 \subsetneq \dots \subsetneq \sigma_r = \sigma,$$

there is a nested sequence of subsets of  $V(G)$ , say

$$\{v_1, \dots, v_c\} = V_0 \subseteq V_1 \subseteq \dots \subseteq V_r = V(G)$$

such that  $G_m$  is obtained from  $G_{m-1}$  by adding an ear for  $m = 1, \dots, r$ , where  $G_m = (V_m, \sigma_m)$  for  $m = 0, \dots, r$ . Note that the number of strongly connected components of  $G_m$ ,  $m = 0, \dots, r$ , is always  $c$ ; while  $|A(G_m)| - |V(G_m)| = 1 + |A(G_{m-1})| - |V(G_{m-1})|$  for  $m = 1, \dots, r$ . This implies

$$\begin{aligned} r &= r + |A(G_0)| - |V(G_0)| + c \\ &= |A(G_r)| - |V(G_r)| + c \\ &= |\sigma| - |V(G)| + c \\ &= b_1(G^\sigma), \end{aligned}$$

namely, the length of the saturated chain displayed in (30) is totally determined by  $\sigma$ . We now find that  $\mathcal{CF}(G)$  is a ranked poset in which  $\sigma \in \mathcal{CF}(G)$  has rank  $b_1(G^\sigma)$ .  $\square$

Let  $(T, X)$  be an  $X$ -tree and let  $\sigma$  be a partial orientation of  $T$ . We define  $(T, X)^\sigma$  to be the subgraph of  $T$  such that  $V((T, X)^\sigma) = \{\text{bd}_T([\alpha]) : \alpha \in \sigma\} \cup X$  and  $E((T, X)^\sigma) = E(T^\sigma) = \{[\alpha] : \alpha \in \sigma\}$ .

**Lemma 5.3.** *Let  $(T, X)$  be an  $X$ -tree. For each  $\sigma \in \mathcal{CF}(T, X)$ , it holds*

$$b_1((T/X)^\sigma) = |X| - b_0((T, X)^\sigma).$$

*Proof.* Let  $T_1, \dots, T_k$ ,  $k \geq 1$ , be the connected components of  $(T, X)^\sigma$ . For  $i = 1, \dots, k$ , let  $X_i = V(T_i) \cap X$ . Then  $(T/X)^\sigma$  is the graph obtained from the disjoint union of  $T_1/X_1, \dots, T_k/X_k$  by contracting  $\{X_1, \dots, X_k\}$ . We now find that

$$\begin{aligned} b_1((T/X)^\sigma) &= \sum_{i=1}^k b_1(T_i/X_i) \\ &= \sum_{i=1}^k (|E(T_i/X_i)| - |V(T_i/X_i)| + 1) \\ &= \sum_{i=1}^k (|E(T_i)| - (|V(T_i)| - |X_i| + 1) + 1) \\ &= \sum_{i=1}^k (|X_i| - 1) \\ &= |X| - b_0((T, X)^\sigma), \end{aligned}$$

finishing the proof.  $\square$

Let  $T$  be an  $X$ -tree. Lemma 2.3 together with Theorem 3.3 claims that all combinatorial information about the Lipschitz polytope of  $(T, X)$  is encoded in the 1-skeleton graph  $\text{SG}_{\text{LD}_{T,X}}$ . We adopt the shorthand  $\text{SG}_{T,X}$  for  $\text{SG}_{\text{LD}_{T,X}}$ .

**Lemma 5.4.** *Let  $T$  be an  $X$ -tree. The graph  $\text{SG}_{T,X}$  is isomorphic to the one with  $\mathcal{CF}^*(T, X)$  as vertex set where two full combinatorial flows are adjacent if and only if they differ at exactly one edge of  $T$ .*



*Proof.* Apply Theorem 4.2, Lemma 5.2 and Lemma 5.3.  $\square$

**Remark 5.5.** Let  $T$  be an  $X$ -tree and take  $\sigma \in \mathcal{CF}^*(T, X)$ . An arc  $\alpha \in \sigma$  is flippable for  $\sigma$  if  $\sigma \Delta [\alpha] = (\sigma \setminus \{\alpha\}) \cup \{\bar{\alpha}\} \in \mathcal{CF}^*(T, X)$ . By Lemma 5.4, viewing  $\sigma$  as a vertex of  $\text{SG}_{T,X}$ , the degree of  $\sigma$  in  $\text{SG}_{T,X}$  is exactly the number of flippable arcs of  $\sigma$ .

**Remark 5.6.** According to Lemma 2.3, Theorem 3.3, Theorem 4.2, Theorem 4.8(b) and Lemma 5.4, we conclude that a phylogenetic  $X$ -tree could be “seen” by watching its full combinatorial flows to the detail of knowing which two differ at exactly one place.

**5.2 An explicit anti-isomorphism** In the rest of this section, for any weighted  $X$ -tree  $(T, X, w)$ , we try to derive an explicit anti-isomorphism between the face poset of  $\text{L}_{D_{T,X,w}}$  and the flow poset  $\mathcal{CF}(T, X)$ .

Let  $(G, X)$  be an  $X$ -network. For every  $\sigma \in \mathcal{CF}(G, X)$ , we define its *tight digraph* to be the digraph  $\mathcal{T}_{G,X}(\sigma)$  with vertex set  $X$  such that  $(a, b) \in \mathcal{A}(\mathcal{T}_{G,X}(\sigma))$  if and only if there is a path in  $(V(G), \sigma)$  from  $a$  to  $b$ . Let  $(G, w)$  be a connected weighted graph and let  $a, b$  be two vertices of  $G$ . We say that  $\alpha \in \mathcal{A}(G)$  supports traffic from  $a$  to  $b$  in  $(G, w)$  provided

$$D_{G,w}(a, b) = D_{G,w}(a, o_G(\alpha)) + w([\alpha]) + D_{G,w}(t_G(\alpha), b), \quad (31)$$

and we designate by  $P_{a,b}(G, w)$  the set of all those arcs of  $G$  which support traffic from  $a$  to  $b$  in  $(G, w)$ .

Let  $G$  be a graph, let  $\sigma$  be a partial orientation of  $G$ , and let  $w \in \mathbb{R}_{>0}^{E(G)}$ . For any  $\alpha \in \mathcal{A}(G)$ , we set

$$\int_{\alpha} w d\sigma = \begin{cases} w([\alpha]) & \text{if } \alpha \in \sigma; \\ -w([\alpha]) & \text{if } \bar{\alpha} \in \sigma; \\ 0 & \text{else.} \end{cases}$$

For any path  $P = (\alpha_1, \dots, \alpha_{\ell})$  of  $G$ , the *integral with respect to  $\sigma$  of the weight function  $w$  along the path  $P$*  is defined to be

$$\sum_{i=1}^{\ell} \int_{\alpha_i} w d\sigma,$$

which we denote by  $\int_P w d\sigma$ . We call the partial orientation  $\sigma$  a *potential difference* with respect to  $(G, w)$  if there is a point  $\tilde{f} \in \mathbb{R}^{V(G)}$  such that

$$w([\alpha]) = \tilde{f}(o(\alpha)) - \tilde{f}(t(\alpha))$$

for all  $\alpha \in \sigma$ .

Let  $(G, X, w)$  be a connected weighted  $X$ -network. Recall from (4) the definition of the tight digraph of a point in the Lipschitz polytope. For the metric space  $(X, D_{G,X,w})$ , we often write the tight digraph operator  $\mathcal{T}_{D_{G,X,w}}$  as

$\mathcal{T}_{G,X,w}$  and we use  $A_{G,X,w}$  for  $A_{D_{G,X,w}}$ . For any  $f \in L_{D_{G,X,w}}$ , we define the flow of  $(G, X)$  determined by  $f$  to be

$$\zeta_f^{G,X,w} := \cup_{(a,b) \in A_{G,X,w}(f)} P_{a,b}(G, w). \quad (32)$$

For any  $F \in \mathcal{F}(L_{D_{G,X,w}})$ ,  $\zeta_f^{G,X,w}$  take constant value when  $f$  runs through interior points of  $F$ , and we will record this common value as  $\zeta_F^{G,X,w}$ .

**Lemma 5.7.** *Let  $(G, X, w)$  be a connected weighted  $X$ -network with  $X \neq \emptyset$ , let  $F$  be a face of  $L_{D_{G,X,w}}$  and let  $\sigma = \zeta_F^{G,X,w}$ . Then the following hold:*

- (a)  $\sigma$  is a combinatorial flow on  $(G, X)$ .
- (b)  $\mathcal{T}_{G,X}(\sigma) = \mathcal{T}_{G,X,w}(F)$ .
- (c)  $\sigma$  is a potential difference with respect to  $(G, w)$ .
- (d) Let  $f$  be an interior point of  $F$  and take  $a, b \in X$  which appear in the same connected component of  $G^\sigma$ . Then  $\int_P w d\sigma = f(a) - f(b)$  for any path in  $G^\sigma$  leading from  $a$  to  $b$ .
- (e)  $\sigma = \cup_{(a,b) \in A(\mathcal{T}_{G,X}(\sigma))} P_{a,b}(G, w)$ .

*Proof.* Let  $f$  be a point in the relative interior of  $F$ . By Lemma 3.2, we can extend this 1-Lipschitz function  $f$  on  $(X, D_{G,X,w})$  to be a 1-Lipschitz function  $\tilde{f}$  on  $(V(G), D_{G,w})$ .

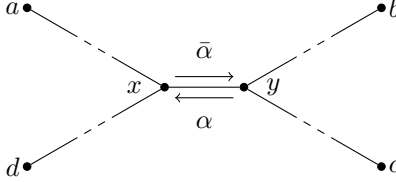


Figure 2: Opposite orientations on an edge induced by two directed paths.

We now try to establish claim (a), namely,  $\sigma \in \mathcal{CF}(G, X)$ . It is clear that  $P_{a,b}(G, w)$  is a combinatorial flow on  $(G, X)$  for every  $(a, b) \in X \times X$ . So, our task is to demonstrate that  $\sigma$  is a partial orientation of  $G$ . If this were not true, we can find  $(a, b), (c, d) \in A_{G,X,w}(F)$  and  $\alpha \in A(G)$  such that  $\bar{\alpha} \in P_{a,b}(G, w)$  and  $\alpha \in P_{c,d}(G, w)$ . Let  $(x, y) = (t(\alpha), o(\alpha))$ ; see Figure 2. We then obtain

$$\begin{aligned} & D_{G,w}(a, d) + D_{G,w}(c, b) + 2D_{G,w}(x, y) \\ \leq & (D_{G,w}(a, x) + D_{G,w}(x, d)) + (D_{G,w}(c, y) + D_{G,w}(y, b)) + 2D_{G,w}(x, y) \\ = & (D_{G,w}(a, x) + D_{G,w}(x, y) + D_{G,w}(y, b)) + (D_{G,w}(c, y) + D_{G,w}(y, x) + D_{G,w}(x, d)) \\ = & D_{G,w}(a, b) + D_{G,w}(c, d) \\ = & (f(a) - f(b)) + (f(c) - f(d)) \\ = & (f(a) - f(d)) + (f(c) - f(b)) \\ \leq & D_{G,w}(a, d) + D_{G,w}(c, b). \end{aligned}$$

Since  $D_{G,w}(x, y) = w([\alpha]) > 0$ , the above inequality is impossible.

We continue to check claim (b), which is equivalent to  $A(\mathcal{T}_{G,X}(\sigma)) = A_{G,X,w}(f)$ . If  $(u, v) \in A_{G,X,w}(f)$ , then  $P_{u,v}(G, w) \subseteq \zeta_f^{G,X,w}$  and so  $(u, v) \in A(\mathcal{T}_{G,X}(\sigma))$  follows. Conversely, we assume  $(u, v) \in A(\mathcal{T}_{G,X}(\sigma)) \subseteq X \times X$  and aim to show that

$$f(u) - f(v) = D_{G,X,w}(u, v). \quad (33)$$

Our assumption means that there is a path in

$$(V(G), \sigma) = (V(G), \cup_{(a,b) \in A_{G,X,w}(f)} P_{a,b}(G, w))$$

leading from  $u \in X$  to  $v \in X$ , say  $(\alpha_1, \alpha_2, \dots, \alpha_\ell)$ , where  $o(\alpha_0) = u$ ,  $t(\alpha_1) = o(\alpha_2)$ ,  $\dots$ ,  $t(\alpha_{\ell-1}) = o(\alpha_\ell)$ ,  $t(\alpha_\ell) = v$ . For each  $i \in \{1, \dots, \ell\}$ , we can find  $(a_i, b_i) \in A_{G,X,w}(f)$  such that  $\alpha_i \in P_{a_i, b_i}(G, w)$ , and so, by (31) and the fact that  $\tilde{f} \in L_{D_{G,w}}$ , we derive

$$\begin{aligned} 0 &= D_{G,w}(a_i, b_i) - (f(a_i) - f(b_i)) \\ &= D_{G,w}(a_i, o(\alpha_i)) + w([\alpha]) + D_{G,w}(t(\alpha_i), b_i) - (\tilde{f}(a_i) - \tilde{f}(b_i)) \\ &\geq (\tilde{f}(a_i) - \tilde{f}(o(\alpha_i))) + (\tilde{f}(t(\alpha_i)) - \tilde{f}(b_i)) - (\tilde{f}(a_i) - \tilde{f}(b_i)) + w([\alpha]) \\ &= w([\alpha]) - (\tilde{f}(o(\alpha_i)) - \tilde{f}(t(\alpha_i))) \\ &\geq D_{G,w}(o(\alpha_i), t(\alpha_i)) - (\tilde{f}(o(\alpha_i)) - \tilde{f}(t(\alpha_i))) \\ &\geq 0, \end{aligned}$$

yielding

$$w([\alpha]) = D_{G,w}(o(\alpha_i), t(\alpha_i)) = \tilde{f}(o(\alpha_i)) - \tilde{f}(t(\alpha_i)). \quad (34)$$

This gives

$$\begin{aligned} D_{G,w}(u, v) &= D_{G,w}(o(\alpha_1), t(\alpha_\ell)) \\ &\leq \sum_{i=1}^{\ell} D_{G,w}(o(\alpha_i), t(\alpha_i)) \\ &= \sum_{i=1}^{\ell} (\tilde{f}(o(\alpha_i)) - \tilde{f}(t(\alpha_i))) \\ &= \tilde{f}(o(\alpha_1)) - \tilde{f}(t(\alpha_\ell)) \\ &= \tilde{f}(u) - \tilde{f}(v) \\ &= f(u) - f(v) \\ &\leq D_{G,w}(u, v), \end{aligned}$$

from which (33) follows, as wanted.

Finally, (34) establishes claim (c) and claim (d); while, by checking (32), claim (b) implies claim (e).  $\square$

Let  $(G, X)$  be a connected  $X$ -network. For any  $w \in \mathbb{R}_{>0}^{E(G)}$ , Lemma 5.7(a) says that  $\{\zeta_F^{G,X,w} : F \in \mathcal{F}(\mathbb{L}_{D_{G,X,w}})\}$ , which we denote by  $\mathcal{CF}(G, X, w)$ , is a subset of  $\mathcal{CF}(G, X)$  and inherits its natural poset structure.

**Theorem 5.8.** *Let  $(G, X, w)$  be a connected weighted  $X$ -network. Then, the map from  $\mathcal{F}(\mathbb{L}_{D_{G,X,w}})$  to  $\mathcal{CF}(G, X, w)$  which sends  $F$  to  $\zeta_F^{G,X,w}$  is an anti-isomorphism from the face poset of  $\mathbb{L}_{D_{G,X,w}}$  to the subposet  $\mathcal{CF}(G, X, w)$  of the flow poset  $\mathcal{CF}(G, X)$ .*

*Proof.* For any two faces  $F$  and  $F'$  of  $\mathbb{L}_{D_{G,X,w}}$ , it is clear that  $F \subseteq F'$  if and only if  $A_{G,X,w}(F) \supseteq A_{G,X,w}(F')$  and if and only if  $\zeta_F^{G,X,w} \supseteq \zeta_{F'}^{G,X,w}$ . Lemma 5.7(b) says that the map from  $\mathcal{F}(\mathbb{L}_{D_{G,X,w}})$  to  $\mathcal{CF}(G, X, w)$  that sends  $F \in \mathcal{F}(\mathbb{L}_{D_{G,X,w}})$  to  $\zeta_F^{G,X,w}$  is an injective map and so the result follows.  $\square$

Let  $(T, X, w)$  be a weighted  $X$ -tree. We recall our notation from (9) and (10) and define for any  $\alpha \in A(T)$  that

$$f_\alpha^{T,X,w} = w([\alpha]) f_{s_\alpha^{T,X}} = w([\alpha]) f_{\widehat{o_{T,X}(\alpha)} \vdash \widehat{t_{T,X}(\alpha)}} \in \mathbb{R}^X. \quad (35)$$

Then, for every  $\sigma \subseteq A(T)$ , let

$$f_\sigma^{T,X,w} = \sum_{\alpha \in \sigma} f_\alpha^{T,X,w}. \quad (36)$$

**Theorem 5.9.** *Let  $(T, X, w)$  be a weighted  $X$ -tree. Then, the map*

$$\zeta^{T,X,w} : \mathcal{F}(\mathbb{L}_{D_{T,X,w}}) \rightarrow \mathcal{CF}(T, X) : F \mapsto \zeta_F^{T,X,w}$$

and the map

$$[f^{T,X,w}] : \mathcal{CF}(T, X) \rightarrow \mathcal{F}(\mathbb{L}_{D_{T,X,w}}) : \sigma \mapsto [f_\sigma^{T,X,w}]_{\mathbb{L}_{D_{T,X,w}}}$$

are reverses to each other. This says that both  $\zeta^{T,X,w}$  and  $[f^{T,X,w}]$  give anti-isomorphism between the face poset of the Lipschitz polytope  $\mathbb{L}_{D_{T,X,w}}$  and the flow poset  $\mathcal{CF}(T, X)$ , which further implies that the normal poset  $\mathcal{N}(\mathbb{L}_{D_{T,X,w}})$  and the flow poset  $\mathcal{CF}(T, X)$  are isomorphic.

*Proof.* Take  $\sigma \in \mathcal{CF}(T, X)$ . Owing to Theorem 3.3, we see that  $f_\sigma^{T,X,w} \in \mathbb{L}_{D_{T,X,w}}$ . In the light of Theorem 5.8, our task is to show  $\zeta_F^{T,X,w} = \zeta_{f_\sigma^{T,X,w}}^{T,X,w} = \sigma$  where  $F = [f_\sigma^{T,X,w}]_{\mathbb{L}_{D_{T,X,w}}}$ .

Since  $T$  is acyclic, from  $\sigma \in \mathcal{CF}(T, X)$  we derive that

$$\sigma = \bigcup_{(a,b) \in A} (\mathcal{T}_{T,X}(\sigma)) P_{a,b}(T, w).$$

By (32),  $\zeta_{f_\sigma^{T,X,w}}^{T,X,w}$  is given by

$$\bigcup_{(a,b) \in A_{T,X,w}(f_\sigma^{T,X,w})} P_{a,b}(T, w).$$

Therefore, we are reduced to showing that the tight digraph of  $f_\sigma^{T,X,w} = \sum_{\alpha \in \sigma} f_\alpha^{T,X,w}$  equals the tight digraph of  $\sigma$ . For any  $(a, b) \in X \times X$  with  $a \neq b$ ,  $(a, b) \in A_{T,X,w}(f_\sigma^{T,X,w})$  holds if and only if

$$\sum_{\alpha \in \sigma} f_\alpha^{T,X,w}(a) - \sum_{\alpha \in \sigma} f_\alpha^{T,X,w}(b) = D_{T,X,w}(a, b),$$

which, by the same process of getting (13), will be possible if and only if  $P_{a,b}(T, w)$ , the unique path from  $a$  to  $b$  in the tree  $T$ , is a subset of  $\sigma$ , that is, if and only if  $(a, b) \in A(\mathcal{T}_{T,X}(\sigma))$ . This completes the proof.  $\square$

**Remark 5.10.** *Let  $(T, X, w)$  be a weighted  $X$ -tree. In view of Theorem 5.9, we will often identify the vertices of  $L_{D_{T,X,w}}$  with elements of  $\mathcal{CF}^*(T, X)$ . Especially, for each  $x \in X$ ,  $\sigma_{T,x}^+$  and  $\sigma_{T,x}^-$  defined in (7) and (8) will often be directly viewed as corresponding vertices of  $L_{D_{T,X,w}}$  from now on. For the metric space  $(X, D_{T,X,w})$ , the elements  $x^-$  and  $x^+$  introduced in Example 1.2 have been claimed to be vertices of  $L_{D_{T,X,w}}$  in Remark 2.2. We can check that the orientation  $\sigma_{T,x}^+$  corresponds to vertex  $x^+$  while orientation  $\sigma_{T,x}^-$  corresponds to vertex  $x^-$ .*

**Question 5.11.** *Take a nonempty finite set  $X$ . Given an  $X$ -tree  $T$ , regardless of in which way we assign positive weights to  $E(T)$ , the combinatorial type of the resulting Lipschitz polytopes will keep the same. Is there any other  $X$ -network sharing this property?*

## 6 Albanese tori and flow posets

Let  $X$  be a finite set, and let  $\Gamma$  be a subgroup of  $\mathbb{Z}^X$ , which is often referred to as a *lattice*. For each  $\lambda \in \Gamma$ , the *Voronoi cell*  $V(\Gamma, \lambda)$  is the set of points in  $\mathbb{R}^X$  whose distance to  $\lambda$  is not greater than its distance to any other points in  $\Gamma$ .

Let  $G$  be a graph and fix an orientation  $\sigma$  of  $G$ . Let

$$H_1(G, \mathbb{R}) = \ker(\mathfrak{J}_{G,\sigma}),$$

and let

$$H_1(G, \mathbb{Z}) = \ker(\mathfrak{J}_{G,\sigma}) \cap \mathbb{Z}^\sigma,$$

the latter being known as the *lattice of integer flows of  $G$* . Let  $\mathbb{R}^\sigma$  be the vector space endowed with the scalar product  $\langle \cdot, \cdot \rangle$  such that  $\langle f, g \rangle = \sum_{\alpha \in \sigma} f(\alpha)g(\alpha)$ . The *Albanese torus*  $\text{Alb}(G)$  of  $G$  is defined as  $\text{Alb}(G) = (H_1(G, \mathbb{R})/H_1(G, \mathbb{Z}); \langle \cdot, \cdot \rangle)$  with the flat metric derived from the scalar product  $\langle \cdot, \cdot \rangle$  on  $\mathbb{R}^\sigma$  [KS00, p. 94]. Note that  $\dim \text{Alb}(G) = b_1(G)$ . For two graphs  $G_1$  and  $G_2$ , we say  $\text{Alb}(G_1)$  and  $\text{Alb}(G_2)$  are isomorphic, denoted as  $\text{Alb}(G_1) \cong \text{Alb}(G_2)$ , if there exists a linear isomorphism  $f : \text{Alb}(G_1) \rightarrow \text{Alb}(G_2)$  such that  $\langle x, y \rangle = \langle f(x), f(y) \rangle$  for all  $x, y \in \text{Alb}(G_1)$ .

For every graph  $G$ , it follows from Proposition 2.9 that the flow poset  $\mathcal{CF}(G)$  can be realized as the face poset of a zonotope up to anti-isomorphism. Solving a conjecture of Caporaso and Viviani [CV10, Conjecture 5.2.8] and answering a

question of Bacher, La Harpe and Nagnibeda [BdlHN97], Amini [Ami10] proved that there is an interesting explicit zonotope construction to realize any graph flow poset.

**Theorem 6.1.** [Ami10, Theorem 1] *Let  $G$  be a connected graph. Then the face poset of  $V(H_1(G, \mathbb{Z}), 0)$  is anti-isomorphic with  $\mathcal{CF}(G)$ .*

Let  $G$  be a graph. A *bridge* of  $G$  is one of its edges whose deletion from  $G$  will increase the number of connected components. For any bridge  $uv$  of  $G$ , we can delete the edge  $uv$  to form the graph  $G' = G - uv$  and then contract the two nonadjacent vertices  $u$  and  $v$  in  $G'$  to obtain a new graph, which is said to be the graph obtained from  $G$  by *shrinking* the edge  $uv$ .

For each graph  $G$ , we let  $\tilde{G}$  be the graph obtained from  $G$  by shrinking all the bridges of  $G$ . Assume that  $H_1$  and  $H_2$  are two graphs on disjoint vertex sets,  $\{v_1, u_1\} \in \binom{V(H_1)}{2}$  and  $\{v_2, u_2\} \in \binom{V(H_2)}{2}$ . Then we say that  $((H_1 \cup H_2)_{\{v_1, v_2\}})_{\{u_1, u_2\}}$  is a *twisting* of  $((H_1 \cup H_2)_{\{v_1, u_2\}})_{\{u_1, v_2\}}$ .

The equivalence (a) $\Leftrightarrow$ (d) in Theorem 6.2 is known as the Torelli theorem for graphs and proved by Caporaso and Viviani [CV10, Theorem 3.1.1]. Note that Su and Wagner obtained a stronger result [SW10, Theorem 1] which could be said to be the Torelli theorem for regular matroids.

**Theorem 6.2.** *Let  $G_1$  and  $G_2$  be two connected graphs. Then the following are equivalent:*

- (a)  $\text{Alb}(G_1) \cong \text{Alb}(G_2)$ .
- (b) The two flow posets  $\mathcal{CF}(G_1)$  and  $\mathcal{CF}(G_2)$  are isomorphic.
- (c) The oriented matroids  $\mathcal{M}_{\tilde{G}_1}$  and  $\mathcal{M}_{\tilde{G}_2}$  are isomorphic.
- (d) The matroids  $\underline{\mathcal{M}}_{\tilde{G}_1}$  and  $\underline{\mathcal{M}}_{\tilde{G}_2}$  are isomorphic.
- (e) The graph  $\tilde{G}_1$  is obtained from  $\tilde{G}_2$  by repeated twisting operations.

*Proof.* (a) $\Rightarrow$ (b). If  $\text{Alb}(G_1) \cong \text{Alb}(G_2)$ , then  $V(H_1(G_1, \mathbb{Z}), 0)$  and  $V(H_1(G_2, \mathbb{Z}), 0)$  are affinely equivalent, and are thus combinatorially equivalent. Applying Theorem 6.1, we have  $\mathcal{CF}(G_1) \cong \mathcal{CF}(G_2)$ .

(b) $\Leftrightarrow$ (c). Note that for a graph  $G$ ,  $\mathcal{CF}(G) = \mathcal{V}(\mathcal{M}_G) = \mathcal{V}(\mathcal{M}_{\tilde{G}}) = \mathcal{V}^*(\mathcal{M}_{\tilde{G}}^*)$ . By Lemma 2.1, the posets  $\mathcal{CF}(G_1)$  and  $\mathcal{CF}(G_2)$  are isomorphic if and only if  $\mathcal{M}_{\tilde{G}_1}^*$  and  $\mathcal{M}_{\tilde{G}_2}^*$  are isomorphic, which, by [BLVS+99, Proposition 3.4.1], is equivalent to the fact that  $\mathcal{M}_{\tilde{G}_1}$  and  $\mathcal{M}_{\tilde{G}_2}$  are isomorphic.

(c) $\Leftrightarrow$ (d). This is obvious.

(d) $\Rightarrow$ (a). This is proved in [BdlHN97, Proposition 5]. Also see [CV10, Proposition 3.1.3].

(d) $\Leftrightarrow$ (e). This is Whitney's Theorem [Whi33]. □

**Corollary 6.3.** *Let  $(T_1, X_1)$  and  $(T_2, X_2)$  be two phylogenetic trees. Then  $T_1$  and  $T_2$  are isomorphic if and only if  $\text{Alb}(T_1/X_1) \cong \text{Alb}(T_2/X_2)$ .*

*Proof.* Theorem 4.8(b) and Theorem 6.2 (a) $\Leftrightarrow$ (b). □

## 7 Lipschitz polytopes of trees and flow posets of graphs

Let  $G$  be a connected graph with  $n$  vertices and  $m$  edges. In Theorem 6.1, we see that  $\mathcal{CF}(G)$  can be realized up to anti-isomorphism as the face poset of an explicitly given zonotope living in  $\mathbb{R}^m$ . This section aims to provide another description of this poset  $\mathcal{CF}(G)$  via a zonotope living in  $\mathbb{R}^{m-n+1}$  which are precisely given in terms of the original graph  $G$ ; see Theorem 7.2 and its proof.

A graph is *reduced* if its minimum degree is at least three. For any graph, its flow poset must be isomorphic with the flow poset of a reduced graph or an empty graph.

**Definition 7.1 (Cleaving a graph into a tree).** *Let  $G$  be a connected reduced graph. Take  $U \subseteq E(G)$  such that  $(V(G), E(G) \setminus U)$  is a tree  $T$ . Let  $\dot{U} = \{\alpha \in A(G) : [\alpha] \in U\}$ . For each arc  $\alpha \in \dot{U}$ , create a new vertex  $v_\alpha$  and a new edge  $e_\alpha$  such that the boundary of  $e_\alpha$  contains two different vertices  $\text{o}_G(\alpha)$  and  $v_\alpha$ . Let*

$$\mathcal{U} = \{v_\alpha : \alpha \in \dot{U}\} = \{v_\alpha, v_{\bar{\alpha}} : [\alpha] \in U\}$$

and

$$U^\diamond = \{\overrightarrow{\text{o}_G(\alpha)v_\alpha}, \overrightarrow{v_\alpha \text{o}_G(\alpha)} : \alpha \in \dot{U}\},$$

After adding the new vertex set  $\mathcal{U}$  and new arc set  $U^\diamond$  to  $T$ , we get a new graph, which is dubbed  $\ddot{\mathbf{T}}$ . That is,  $A(\ddot{\mathbf{T}})$  is the disjoint union of  $A(T) = A(G) \setminus \dot{U}$  and  $U^\diamond$ , while  $V(\ddot{\mathbf{T}})$  coincides with  $V(G) \cup \mathcal{U} = V(T) \cup \mathcal{U}$ . Considering that  $G$  is reduced,  $\ddot{\mathbf{T}}$  is surely a phylogenetic  $\mathcal{U}$ -tree. See Figure 3 for an illustration of the above-mentioned process of cleaving  $G$  into the phylogenetic  $\mathcal{U}$ -tree  $\ddot{\mathbf{T}}$ .

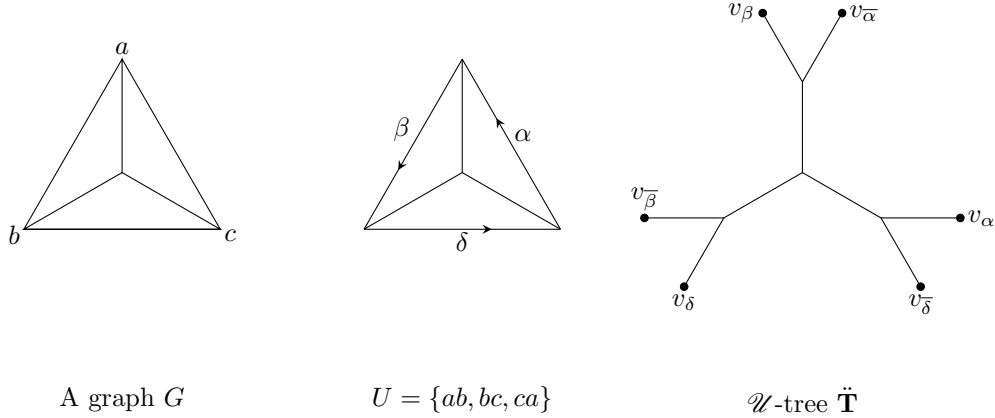


Figure 3: Cleaving a reduced connected graph  $G$  into a phylogenetic  $\mathcal{U}$ -tree  $\ddot{\mathbf{T}}$ .

**Theorem 7.2.** *We follow the notation and assumption in Definition 7.1. There is an orthogonal projection  $\mathfrak{p}$  from  $\mathbb{R}^{\mathcal{U}}$  to one of its subspaces of dimension  $|U|$  such that the face poset of the polytope  $\mathfrak{p}(L_{D_{\ddot{\mathbf{T}}, \mathcal{U}}})$  is anti-isomorphic with  $\mathcal{CF}(G)$ .*

*Proof.* We divide the proof into five steps. At the beginning, we define explicitly the projection  $p$  and then we show that  $\mathcal{F}(p(L_{D_{\mathbf{T}, \mathcal{U}}}))$  is isomorphic to the face posets of another four zonotopes in four steps. Indeed, the first four steps aim to obtain that  $\mathcal{F}(p(L_{D_{\mathbf{T}, \mathcal{U}}}))$  is isomorphic with  $\mathcal{F}(\mathcal{Z}(\mathfrak{M} \circ \theta))$  (See below for the definition of  $\mathfrak{M}$  and  $\theta$ ). In the last step, we verify that  $\mathcal{F}(\mathcal{Z}(\mathfrak{M} \circ \theta))$  is anti-isomorphic with  $\mathcal{CF}(G)$ , thus completing the proof.

**Step 1.** For any  $y = v_\alpha \in \mathcal{U}$ , we directly write  $\bar{y}$  for  $v_{\bar{\alpha}}$ . More generally, for any  $A \subseteq \mathcal{U}$ , we use  $\bar{A}$  to stand for the set  $\{\bar{y} : y \in A\}$ . Let  $W_1 = \text{span}\{\chi_y + \chi_{\bar{y}} : y \in \mathcal{U}\}$  and  $W_0 = \text{span}\{\chi_y - \chi_{\bar{y}} : y \in \mathcal{U}\}$  be two subspaces of  $\mathbb{R}^{\mathcal{U}}$ . It is easy to see that  $W_1 = W_0^\perp$  in  $\mathbb{R}^{\mathcal{U}}$  and  $\dim W_1 = \dim W_0 = \frac{|\dot{U}|}{2} = \frac{|\mathcal{U}|}{2} = |U|$ . We let  $p$  be the orthogonal projection from  $\mathbb{R}^{\mathcal{U}}$  to  $W_0$  along the direction of  $W_1$ .

We fix  $\beta \in \ddot{U}$ , let  $x = v_\beta \in \mathcal{U}$ ,  $\sigma = \sigma_{\mathbf{T}, x}^-$  and write  $\mathfrak{A}$  for the descendent matrix of  $(\ddot{\mathbf{T}}, \mathcal{U})$  with origin  $x$ , namely  $\mathfrak{A} = \mathfrak{D}_{\mathbf{T}, \mathcal{U}, x}$  is a  $\sigma$ -indexed vector configuration in  $\mathbb{R}^{\mathcal{U}}$ .

It follows from (21) and (22) that

$$L_{D_{\mathbf{T}, \mathcal{U}}}^x = \mathcal{Z}(\pm \mathfrak{A}). \quad (37)$$

Note that the constant function  $1 = \chi_{\mathcal{U}}$  falls into  $W_1$ . Henceforth, using the notation introduced in (3), we have  $p \circ p_x^{\mathcal{U}} = p$ . It then follows from Remark 1.1 and (37) that

$$p(L_{D_{\mathbf{T}, \mathcal{U}}}) = p \circ p_x^{\mathcal{U}}(L_{D_{\mathbf{T}, \mathcal{U}}}) = p(L_{D_{\mathbf{T}, \mathcal{U}}}^x) = p(\mathcal{Z}(\pm \mathfrak{A})) = \mathcal{Z}(\pm p \circ \mathfrak{A}).$$

By Remark 2.6,  $\mathcal{Z}(\pm p \circ \mathfrak{A})$  is combinatorially equivalent with  $\mathcal{Z}(p \circ \mathfrak{A})$ . So far, we find that the face poset of  $p(L_{D_{\mathbf{T}, \mathcal{U}}})$  is isomorphic with the face poset of  $\mathcal{Z}(p \circ \mathfrak{A})$ .

**Step 2.** For any  $A \subseteq \mathcal{U}$ , we have

$$\frac{1}{2}(\chi_A - \chi_{\bar{A}}) + \frac{1}{2}(\chi_A + \chi_{\bar{A}}) = \chi_A \in \mathbb{R}^{\mathcal{U}},$$

where  $\frac{1}{2}(\chi_A - \chi_{\bar{A}}) \in W_0$  and  $\frac{1}{2}(\chi_A + \chi_{\bar{A}}) \in W_1$ , and consequently it holds

$$p(\chi_A) = \frac{1}{2}(\chi_A - \chi_{\bar{A}}). \quad (38)$$

We write  $\alpha_x$  for the unique element in  $\sigma \cap t_{\mathbf{T}}^{-1}(x)$  and we write  $\alpha_y$  for the unique element in  $\sigma \cap o_{\mathbf{T}}^{-1}(y)$  for every  $y \in \mathcal{U} \setminus \{x\}$ . Then we find that

$$\begin{cases} \mathfrak{A}(\alpha_y) = \chi_y & \text{if } y \in \mathcal{U} \setminus \{x\}; \\ \mathfrak{A}(\alpha_y) = 1 - \chi_x & \text{if } y = x. \end{cases} \quad (39)$$

Applying (38) and (39) yields

$$\begin{cases} p(\mathfrak{A}(\alpha_y)) = \frac{1}{2}(\chi_y - \chi_{\bar{y}}) & \text{if } y \in \mathcal{U} \setminus \{x\}; \\ p(\mathfrak{A}(\alpha_y)) = -\frac{1}{2}(\chi_x - \chi_{\bar{x}}) & \text{if } y = x. \end{cases} \quad (40)$$



We fix an orientation  $\lambda$  of  $G$  satisfying  $\lambda \setminus \ddot{U} \subseteq \sigma$  and  $\beta \in \lambda$ . Consider the injective map  $\theta$  from  $A(G)$  to  $A(\ddot{\mathbf{T}})$  given by

$$\theta(\alpha) = \begin{cases} \alpha & \text{if } \alpha \in A(G) \setminus \ddot{U} = A(T); \\ v_{\bar{\alpha}} t_G(\alpha) & \text{if } \alpha \in \ddot{U}. \end{cases}$$

Let  $\ddot{\lambda} = \{\theta(\alpha) : \alpha \in \lambda\} \subseteq A(\ddot{\mathbf{T}})$ . Note that the restriction of  $\theta$  on  $\lambda$ , denoted by  $\theta$ , is a bijection from  $\lambda$  to  $\ddot{\lambda}$ .

For every  $u \in U$ , we denote  $v_\alpha$  by  $u_0$  and  $v_{\bar{\alpha}}$  by  $u_1$ , where  $\alpha$  is the only element in  $u \cap \lambda$ . For example,  $[\beta]_1 = \bar{x}$  and  $[\beta]_0 = x$ . One can see that

$$\ddot{\lambda} = (\lambda \setminus U^\diamond) \cup \{\alpha_{u_1} : u \in U\} = (\sigma \setminus U^\diamond) \cup \{\alpha_{u_1} : u \in U\} \subseteq \sigma. \quad (41)$$

Restricting  $\mathfrak{A}$  on  $\ddot{\lambda} \subseteq \sigma$ , we obtain a  $\ddot{\lambda}$ -indexed vector configuration  $\ddot{\mathfrak{A}}$  in  $\mathbb{R}^{\mathcal{U}}$ . As a consequence of Remark 2.6, (40) and (41),  $\mathcal{Z}(\text{p} \circ \ddot{\mathfrak{A}})$  is combinatorially equivalent with  $\mathcal{Z}(\mathfrak{B})$ , where  $\mathfrak{B} = \text{p} \circ \ddot{\mathfrak{A}}$  is a  $\ddot{\lambda}$ -indexed vector configuration in  $W_0$ .

**Step 3.** Define  $\mathfrak{C} : \mathbb{R}^U \rightarrow W_0 \subset \mathbb{R}^{\mathcal{U}}$  such that

$$\mathfrak{C}(f) = \sum_{u \in U} \frac{f(u)}{2} (\chi_{u_1} - \chi_{u_0}) \quad (42)$$

for all  $f \in \mathbb{R}^U$ . Since  $\{\frac{1}{2}(\chi_{u_1} - \chi_{u_0}) : u \in U\}$  is a basis of  $W_0$ ,  $\mathfrak{C}$  is a linear isomorphism from  $\mathbb{R}^U$  to  $W_0$  and so we arrive at

$$\mathcal{M}_{\mathfrak{B}} = \mathcal{M}_{\mathfrak{M}}$$

where  $\mathfrak{M} = \mathfrak{C}^{-1} \mathfrak{B}$  is the  $\ddot{\lambda}$ -indexed vector configuration in  $\mathbb{R}^U$  which sends  $\alpha \in \ddot{\lambda}$  to  $\mathfrak{C}^{-1} \mathfrak{B}(\alpha) \in \mathbb{R}^U$ . It follows from Proposition 2.5 that  $\mathcal{Z}(\mathfrak{B})$  and  $\mathcal{Z}(\mathfrak{M})$  are combinatorially equivalent.

**Step 4.** Surely,  $\mathcal{Z}(\mathfrak{M})$  and  $\mathcal{Z}(\mathfrak{M} \circ \theta)$  are the same zonotope in  $\mathbb{R}^U$ . So, we can focus on  $\mathfrak{M} \circ \theta$ , which is a  $\lambda$ -indexed vector configuration in  $\mathbb{R}^U$ .

**Step 5.** To conclude the proof, we need to verify that the face poset of  $\mathcal{Z}(\mathfrak{M} \circ \theta)$  is anti-isomorphic with  $\mathcal{CF}(G)$ . By Proposition 2.9, our task is to show that  $\text{im}(\mathfrak{M} \circ \theta)^\top$  is the cycle space of  $G$ .

For every  $z, w \in V(\ddot{\mathbf{T}})$ , let  $P_{z,y}$  denote the set of arcs on the unique path from  $z$  to  $y$  in  $\ddot{\mathbf{T}}$ . For every  $\alpha \in \lambda$ , let  $D_\alpha$  be the set of elements  $z \in \mathcal{U}$  such

that  $P_{z,x}$  contains  $\alpha$ . In view of (22), (38) and (42), for each  $\alpha \in \lambda$ ,

$$\begin{aligned}
\mathfrak{M} \circ \theta(\alpha) &= \mathfrak{C}^{-1} \mathfrak{B}(\theta(\alpha)) \\
&= \mathfrak{C}^{-1} \mathfrak{p}(\check{\mathfrak{A}}(\theta(\alpha))) \\
&= \mathfrak{C}^{-1} \left( \sum_{\substack{u \in U \\ u \cap D_{\theta(\alpha)} = \{u_1\}}} \frac{1}{2}(\chi_{u_1} - \chi_{u_0}) + \sum_{\substack{u \in U \\ u \cap D_{\theta(\alpha)} = \{u_0\}}} \frac{1}{2}(\chi_{u_0} - \chi_{u_1}) \right) \\
&= \sum_{\substack{u \in U \\ u \cap D_{\theta(\alpha)} = \{u_1\}}} \chi_u - \sum_{\substack{u \in U \\ u \cap D_{\theta(\alpha)} = \{u_0\}}} \chi_u \\
&= \sum_{\substack{u \in U \\ \theta(\alpha) \in P_{u_1, u_0}}} \chi_u - \sum_{\substack{u \in U \\ \theta(\alpha) \in P_{u_0, u_1}}} \chi_u \\
&\in \mathbb{R}^U.
\end{aligned}$$

Therefore, as a  $U$ -indexed vector configuration in  $\mathbb{R}^\lambda$ ,  $(\mathfrak{M} \circ \theta)^\top$  sends  $u \in U$  to  $\chi_{A_u^0} - \chi_{A_u^1}$ , where  $A_u^0 = \{\theta^{-1}(\gamma) : \gamma \in P_{u_1, u_0} \cap \check{\lambda}\}$  and  $A_u^1 = \{\theta^{-1}(\gamma) : \gamma \in P_{u_0, u_1} \cap \check{\lambda}\}$ . For each  $u \in U$ ,  $\chi_{A_u^0} - \chi_{A_u^1} \in \mathbb{R}^\lambda$  is nothing but the fundamental cycle of  $G$  corresponding to the tree  $T$  and the only arc in  $u \cap \lambda$ . This proves that  $\text{im}(\mathfrak{M} \circ \theta)^\top$  is the cycle space of  $G$ , as was to be shown.  $\square$

## 8 Isometric embeddings

A *metric pair*  $(Y, X, D)$  is a metric space  $(Y, D)$  together with a subset  $X \subset Y$  which has a metric space structure by restricting the map  $D$  to  $X \times X$ . A metric space  $M$  is called an *injective metric space*, or an *absolute 1-Lipschitz retract* [Lan13, Proposition 2.2], provided that for every metric pair  $(Y, X, D)$  and every 1-Lipschitz map  $g$  from  $X$  to  $M$ , we can find a 1-Lipschitz map  $f$  from  $Y$  to  $M$  that is an extension of  $g$ . Note that Lemma 3.2 just says that the real line is an injective metric space. It is known that every metric space  $(X, D)$  possesses an injective hull, namely a smallest injective metric space containing an isometric copy of  $(X, D)$  [Isb64, Dre84]. Following Dress [Dre84], we call the injective hull of a metric space its *tight span*.

For any two points  $f, g \in \mathbb{R}^X$ , the  $L_\infty$ -distance between them is the  $L_\infty$ -norm of  $f - g$ , namely,  $|f - g|_\infty := \sup_{x \in X} |f(x) - g(x)|$ . For any metric space  $(X, D)$ , the following set

$$\{f \in \mathbb{R}^X : f(x) = \sup_{y \in X} \{D(x, y) - f(y)\}, \forall x \in X\}$$

endowed with the  $L_\infty$ -distance is the *tight span* of  $(X, D)$  and will be denoted by  $T_{X, D}$  [CL94, Dre84, Isb64].

Let  $(X, D)$  be a metric space. For each  $x \in X$ , we define the *Kuratowski map*  $k_{D;x} \in \mathbb{R}^X$  by putting

$$k_{D;x}(y) = D(x, y)$$

for all  $y \in X$ . It is clear that the mapping  $\kappa : (X, D) \rightarrow T_{X,D} : x \mapsto k_{D;x}$  is an isometric embedding. For every  $f \in T_{X,D}$ , it holds [DHK<sup>+</sup>12, Proposition 5.2(ii)]

$$\sup\{f(y) - D(x, y) : y \in X\} = f(x)$$

for all  $x \in X$ . Especially, this implies that

$$f(y) - f(x) \leq D(x, y) \tag{43}$$

for  $f \in T_{X,D}$  and  $x, y \in X$ . To see (43) directly, we assume for contradiction that there exist  $x, y \in X$  such that  $f(x) - f(y) > D(x, y)$ , and then, by definition, we can find  $y' \in X$  such that  $f(x) - (D(x, y') - f(y')) < (f(x) - f(y)) - D(x, y)$ , implying  $f(y) < D(x, y') - D(x, y) - f(y') \leq D(y, y') - f(y')$ , a contradiction with  $f \in T_{X,D}$ .

For a finite set  $X$ , we use  $q_X$  for the linear transformation on  $\mathbb{R}^X$  such that, for every  $f \in \mathbb{R}^X$  and  $x \in X$ ,

$$q_X(f)(x) = f(x) - \frac{\sum_{y \in X} f(y)}{|X|}.$$

Note that  $q_X$  is an orthogonal projection of  $\mathbb{R}^X$  along the subspace of constant functions to its orthogonal complement. This together with (43) shows that

$$q_X(T_{X,D}) \subseteq L_D \tag{44}$$

for every finite metric space  $(X, D)$ .

**Proposition 8.1.** *Let  $(X, D)$  be a finite metric space. Then  $q_X$  induces an injective map from  $T_{X,D}$  to  $L_D$ . Moreover,  $q_X(k_{D,x})$  is a vertex of  $L_D$  for all  $x \in X$ .*

*Proof.* It is clear that no two different points from  $T_{X,D}$  can have the same image under the map  $q_X$ . The first claim thus follows from (44).

For each  $x \in X$ , let  $f_x := 1 - |X|\chi_x \in \mathbb{R}^X$ . Then for each  $p \in L_D$ ,

$$\begin{aligned} \langle f_x, p \rangle &= \sum_{y \in X} (p(y) - p(x)) \\ &\leq \sum_{y \in X} D(x, y), \end{aligned}$$

with equality if and only if  $p(y) - p(x) = D(x, y)$  for all  $y \in X$  and if and only if  $p = q_X(k_{D,x})$ . This proves the second claim.  $\square$

For any two full orientations  $\sigma_1$  and  $\sigma_2$  of a graph  $G$ , we define their *separation set*  $S(\sigma_1, \sigma_2)$  to be  $\{e \in E(G), e \cap \sigma_1 \neq e \cap \sigma_2\}$ .

**Lemma 8.2.** *Let  $(T, X)$  be an  $X$ -tree. For any  $\sigma_1, \sigma_2 \in V(\text{SG}_{T,X}) = \mathcal{CF}^*(T, X)$ ,  $D_{\text{SG}_{T,X}}(\sigma_1, \sigma_2) = |S(\sigma_1, \sigma_2)|$ , and so the diameter of  $\text{SG}_{T,X}$  is exactly  $|E(T)|$ .*

*Proof.* Lemma 5.4 and [BLVS<sup>+</sup>99, Proposition 4.2.3].  $\square$

Let  $(T, X, w)$  be a weighted  $X$ -tree. For each edge  $e$  of  $\text{SG}_{T,X,w}$ , according to Theorem 3.3, there exists a unique edge  $e' = e_{T,X} \in \text{E}(T)$  such that the 1-face of  $\text{L}_{D_{T,X,w}}$  that corresponds to  $e$  is a translation of  $w(e') \text{L}_{D_{e'}^{T,X}}$  in  $\mathbb{R}^X$ .

We let  $w_{T,X} \in \mathbb{R}_{>0}^{\text{E}(\text{SG}_{T,X,w})}$  be the function such that  $w_{T,X}(e) = w(e_{T,X})$  for every  $e \in \text{E}(\text{SG}_{T,X,w})$ . We write  $w(T)$  for  $\sum_{e \in \text{E}(T)} w(e)$ . To proceed with the next lemma, the reader may like to review our convention from Remark 5.10.

**Lemma 8.3.** *Let  $(T, X, w)$  be a weighted  $X$ -tree. In the weighted graph  $(\text{SG}_{T,X,w}, w_{T,X})$ , it holds for any  $a, b \in X$  that*

$$\begin{cases} \text{D}_{\text{SG}_{T,X,w}, w_{T,X}}(\sigma_{T,a}^+, \sigma_{T,b}^+) = \text{D}_{\text{SG}_{T,X,w}, w_{T,X}}(\sigma_{T,a}^-, \sigma_{T,b}^-) = \text{D}_{T,w}(a, b), \\ \text{D}_{\text{SG}_{T,X,w}, w_{T,X}}(\sigma_{T,a}^+, \sigma_{T,b}^-) = \text{D}_{\text{SG}_{T,X,w}, w_{T,X}}(\sigma_{T,a}^-, \sigma_{T,b}^+) = w(T) - \text{D}_{T,w}(a, b). \end{cases}$$

*Proof.* By Lemma 8.2 and the definition of  $w_{T,X}$ ,

$$\text{D}_{\text{SG}_{T,X,w}, w_{T,X}}(\sigma_1, \sigma_2) = \sum_{e \in \text{S}(\sigma_1, \sigma_2)} w(e)$$

for all  $\sigma_1, \sigma_2 \in \text{V}(\text{SG}_{T,X,w})$ . Note that  $\text{S}(\sigma_{T,a}^+, \sigma_{T,b}^+) = \text{S}(\sigma_{T,a}^-, \sigma_{T,b}^-)$  consists of all the edges on the unique path of  $T$  connecting  $a$  and  $b$ , and  $\text{S}(\sigma_{T,a}^+, \sigma_{T,b}^-) = \text{S}(\sigma_{T,a}^-, \sigma_{T,b}^+)$  is the complement of  $\text{S}(\sigma_{T,a}^+, \sigma_{T,b}^+) = \text{S}(\sigma_{T,a}^-, \sigma_{T,b}^-)$  in  $\text{E}(T)$ . The result thus follows.  $\square$

Figure 4 is a graphical presentation of Lemma 8.3. Note that, taking  $a = b$  in Lemma 8.3, we see that

$$\text{D}_{\text{SG}_{T,X,w}, w_{T,X}}(\sigma_{T,a}^+, \sigma_{T,a}^-) = \text{D}_{\text{SG}_{T,X,w}, w_{T,X}}(\sigma_{T,b}^+, \sigma_{T,b}^-) = w(T)$$

and so the weighted 4-cycle in Figure 4 can be embedded into  $(\text{SG}_{T,X,w}, w_{T,X})$  isometrically.

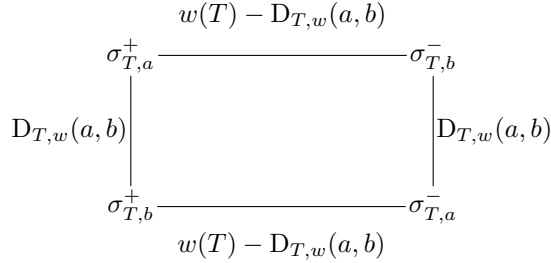


Figure 4: An isometry from the metric of a weighted 4-cycle to  $\text{D}_{\text{SG}_{T,X,w}, w_{T,X}}$ .

**Theorem 8.4.** *For each weighted  $X$ -tree  $(T, X, w)$ , there exist two isometric embeddings of  $(X, D_{T,X,w})$  into the weighted graph  $(\text{SG}_{T,X,w}, w_{T,X})$ .*

	$v_0$	$v_1$	$v_2$	$v_3$
$f_0$	0	1	0	-1
$f_1$	1	0	-1	0
$f_2$	0	-1	0	1
$f_3$	-1	0	1	0
$f_4$	1/2	-1/2	1/2	-1/2
$f_5$	-1/2	1/2	-1/2	1/2

Table 1: Coordinates of vertices of  $L_{D_G}$  in Figure 5.

*Proof.* Lemma 8.3 shows that the map from  $x \in X$  to  $\sigma_{T,x}^+$  is an isometric embedding of  $(X, D_{T,X,w})$  into the weighted graph  $(SG_{L_{D_{T,X,w}}}, w_{T,X})$ , and the map from  $x \in X$  to  $\sigma_{T,x}^-$  is another isometric embedding of  $(X, D_{T,X,w})$  into the weighted graph  $(SG_{L_{D_{T,X,w}}}, w_{T,X})$ .  $\square$

**Question 8.5.** For any weighted  $X$ -tree  $(T, X, w)$  and  $x \in X$ , Remark 5.10 claims that the orientation  $\sigma_{T,x}^-$  actually corresponds to the vertex  $x^- = q_X(k_{D_{T,X,w},x})$  of  $L_{D_{T,X,w}}$ . For which metric space  $(X, D)$  can we find a weight function  $w'$  on  $E(SG_{L_D})$  such that the map from  $x \in X$  to  $x^- = q_X(k_{D,x})$  induces an isometric embedding of  $(X, D)$  into  $(V(SG_{L_D}), D_{SG_{L_D},w'})$ ?

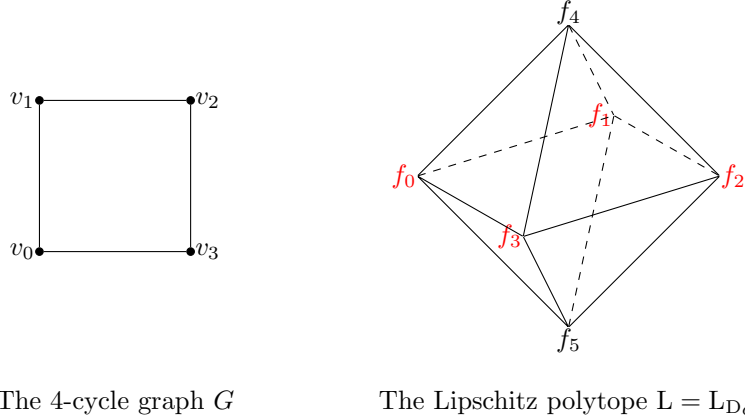


Figure 5: An isometric embedding from  $D_G$  to  $D_{SGL}$  (Example 8.6).

**Example 8.6.** Let  $X = \{v_0, v_1, v_2, v_3\}$ . On the left of Figure 5, we draw the 4-cycle graph  $G$  with  $V(G) = X$ ; on the right of Figure 5, we depict the Lipschitz polytope  $L = L_{D_G}$ . The vertex set of  $L$  is  $Y = \{f_0, \dots, f_5\}$  and their coordinates are given in Table 1. Note that  $D_G$  is not any tree metric while  $f_i = q_X(k_{D,v_i})$  for  $i = 0, 1, 2, 3$ . We can check that the map from  $X$  to  $Y$ , sending  $v_i \in X$  to  $f_i \in Y$ ,  $0 \leq i \leq 3$ , is an isometric embedding of  $(X, D_G)$  into  $(Y, D_{SGL})$ .

**Example 8.7.** On the left of Figure 6, we display a 4-cycle graph  $G$  with  $V(G) = X = \{v_0, v_1, v_2, v_3\}$  and with a non-constant weight function  $w$ . Note that  $D_{G,w}$  is not any tree metric. In the middle of Figure 6 we draw the Lipschitz polytope  $L_{D_{G,w}}$  whose set of vertices is  $Y = \{f_i : 0 \leq i \leq 11\}$ . The coordinates of those functions from  $Y$  are listed in Table 2. For  $i = 0, 1, 2, 3$ , we have  $q_X(k_{D_{G,w}, v_i}) = f_i$ . Let  $w' \in \mathbb{R}^{\text{E}(\text{SG}_{L_{D_{G,w}}})}$  be the weight function which assigns weight 1 to edges  $f_0f_1, f_1f_8, f_8f_4, f_4f_5, f_5f_9, f_9f_0$  and assigns weight  $\frac{1}{2}$  to the remaining edges. Then the map from  $X$  to  $Y$ , sending  $v_i$  to  $f_i, 0 \leq i \leq 3$ , is an isometric embedding of  $(X, D_{G,w})$  to  $(Y, D_{\text{SG}_{L_{D_{G,w}}}, w'})$ . The polar of  $L_{D_{G,w}}$ , which is just the fundamental polytope of  $D_{G,w}$ , is demonstrated on the right of Figure 6. Since each vertex  $f$  of  $L_{D_{G,w}}^\Delta$  corresponds to a facet  $F$  of  $L_{D_{G,w}}$ , we label the vertex  $f$  of  $L_{D_{G,w}}^\Delta$  by  $A_{D_{G,w}}(F)$ , the arc set of the corresponding tight digraph.

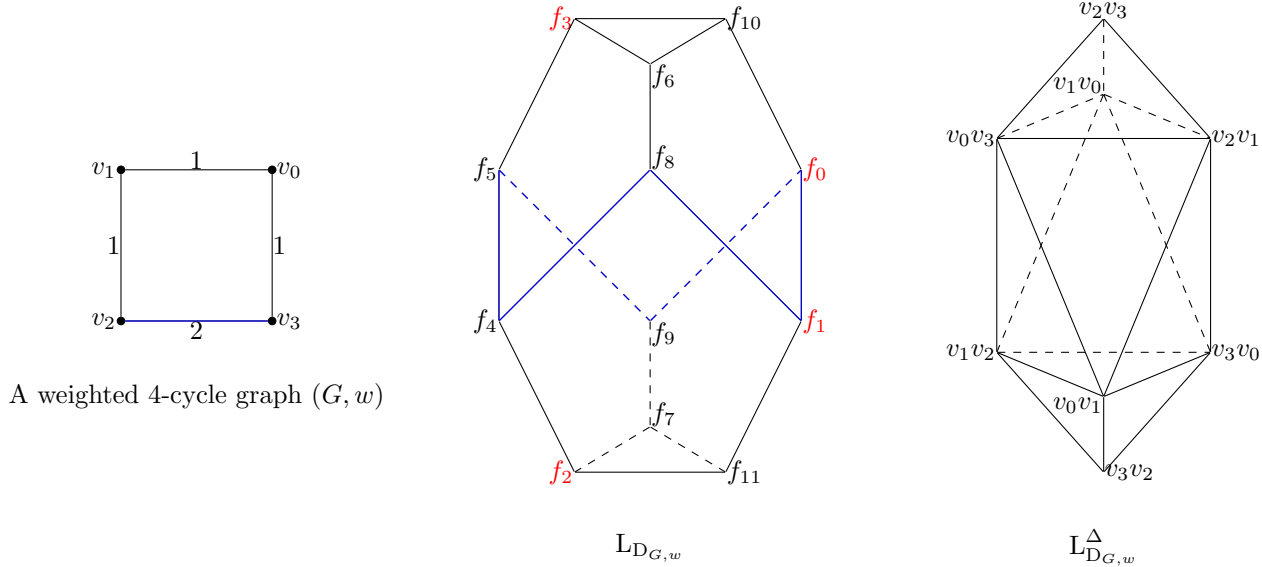


Figure 6: A graph metric space  $(V(G), D_{G,w})$ , its Lipschitz polytope and fundamental polytope. See Example 8.7 for relevant isometry and tight digraphs.

## 9 Face vectors

For a ranked poset  $P$ , the *Whitney number*  $W_i(P)$  of  $P$  refers to the number of rank- $i$  elements in  $P$  and the *face vector*, also known as *f-vector*, of  $P$  is

$$W(P) = (W_0(P), \dots, W_{\dim(P)}(P)).$$

For any polytope  $P$ , we also use  $W_i(P)$  for the number of  $i$ -faces of  $P$ , which clearly coincides with  $W_i(\mathcal{F}(P))$ .

	$v_0$	$v_1$	$v_2$	$v_3$
$f_0$	-1	0	1	0
$f_1$	0	-1	0	1
$f_2$	3/4	-1/4	-5/4	3/4
$f_3$	-1/4	3/4	3/4	-5/4
$f_4$	1	0	-1	0
$f_5$	0	1	0	-1
$f_6$	0	0	1	-1
$f_7$	0	0	-1	1
$f_8$	1/2	-1/2	1/2	-1/2
$f_9$	-1/2	1/2	-1/2	1/2
$f_{10}$	-3/4	1/4	5/4	-3/4
$f_{11}$	1/4	-3/4	-3/4	5/4

Table 2: Coordinates of vertices of  $L_{D_{G,w}}$  in Figure 6.

This section aims to understand the face vectors of the face poset of the Lipschitz polytope of a tree metric. For a weighted  $X$ -tree  $(T, X, w)$ , Theorem 4.2 tells us that  $\mathcal{F}(L_{D_{T,X,w}})$  is determined by  $(T, X)$  or  $T/X$ . So, we will sometimes simply talk about  $\mathcal{F}(L_{D_{T,X,w}})$  and  $W_i(\mathcal{F}(L_{D_{T,X,w}}))$  as the face poset and the Whitney numbers of the  $X$ -tree  $(T, X)$  or the graph  $T/X$ . Lemma 9.1 says that the degree sequence of a phylogenetic tree determines the number of vertices of the corresponding Lipschitz polytope while Lemma 9.4 asserts that the Whitney numbers of binary phylogenetic  $X$ -trees is solely determined by  $|X|$ . Via repeated applications of Lemma 5.3, we will reach the main goal of this section, Theorem 9.9, which gives lower bound and upper bound estimates of the Whitney numbers of  $X$ -trees and phylogenetic  $X$ -trees.

Note that a partial orientation  $\sigma$  of  $T$  lies inside  $\mathcal{CF}(T, X)$  if and only if every arc  $\alpha \in \sigma$  belongs to a path  $P$  in  $T$  that runs from an element of  $X$  to another element of  $X$  and satisfies  $P \subseteq \sigma$ . Let  $\sigma$  be a partial orientation of an  $X$ -tree  $T$ . We say that a vertex  $v \in V(T)$  is *good with respect to  $X$  for  $\sigma$*  provided either  $v \in X$  or  $v \notin (\cup_{\alpha \in \sigma} o_G(\alpha)) \Delta (\cup_{\alpha \in \sigma} t_G(\alpha))$ . Note that  $\sigma \in \mathcal{CF}(T, X)$  if and only if all vertices of  $T$  are good with respect to  $X$  for  $\sigma$ .

For the  $X$ -tree  $(T, X)$ , the arc set of  $T/X$  coincides with the arc set of  $T$  and so there is a one-to-one correspondence between partial orientations of  $T$  and partial orientations of  $T/X$ . Although  $\mathcal{CF}(T, X)$  is the same as  $\mathcal{CF}(T/X)$  as a set/poset, when we call a partial orientation an element from  $\mathcal{CF}(T, X)$  we are emphasizing that we will make use of the boundary map on  $T$ , instead of the boundary map on  $T/X$ , for relevant analysis. We may prefer to work on the tree  $T$  than the graph  $T/X$  simply because the tree structure of  $T$  is simpler to visualize than the structure of  $T/X$ .

For any tree  $T$ , we write  $\mathcal{L}(T)$  for the set of leaves of  $T$ , that is,  $\mathcal{L}(T) = \{v \in V(T) : \deg_T(v) = 1\}$ . For a metric space consisting of one point, its Lipschitz polytope also has one point and so one vertex. This means that the formula in Lemma 9.1 cannot be applied to the case of  $|X| = 1$ . A *star tree* is a

phylogenetic  $X$ -tree with exactly one interior vertex. Note that a star tree has at least three leaves. As with many simple results on trees, the next result is also proved with a simple idea as explained by Steel in [Ste16, p. 4].

**Lemma 9.1.** *Let  $X$  be a set of size at least two and let  $T$  be a phylogenetic  $X$ -tree. Then the number of vertices of  $L_{D_{T,X}}$ , namely,  $W_0(L_{D_{T,X}})$ , is  $2 \prod_{v \in V(T) \setminus X} (2^{\deg_T(v)-1} - 1)$ .*

*Proof.* By Theorem 4.2, Lemma 5.2 and Lemma 5.3, what we intend to count is the size of  $\mathcal{CF}^*(T, X)$ . We use induction on the size of  $V(T) \setminus \mathcal{L}(T) = V(T) \setminus X$ . When  $|V(T) \setminus X| = 0$ , it is trivial to see that  $|\mathcal{CF}^*(T, X)| = 2$ , as claimed. When  $|V(T) \setminus X| = 1$ , namely, when  $T$  is a star tree,  $|\mathcal{CF}^*(T, X)| = 2^{|X|} - 2 = 2 \prod_{v \in V(T) \setminus X} (2^{\deg_T(v)-1} - 1)$ , also as claimed. Now assume that  $T$  has  $k \geq 2$  interior vertices and our formula holds when  $k$  is smaller. The set of interior vertices of  $T$ , namely  $V(T) \setminus X$ , induces a subtree of  $T$  and we choose a leaf  $b$  of this subtree. Let  $T'$  be the subtree of  $T$  obtained by removing the set  $B$  of all leaves of  $T$  adjacent to  $b$ . Since  $T'$  only has  $k - 1$  interior vertices, we can use induction hypothesis to see that it, as a phylogenetic  $X'$ -tree where  $X' = (X \setminus B) \cup \{b\}$ , has in total

$$2 \prod_{w \in V(T) \setminus (X \cup \{b\})} (2^{\deg_T(w)-1} - 1)$$

full combinatorial flows. As a combinatorial flow on  $(T, X)$ , there should be both incoming and outgoing arcs at  $b$  and so we see that for any full combinatorial flow  $\sigma'$  of  $(T', X')$ , there are exactly  $2^{\deg_T(b)-1} - 1$  ways to extend it to a full combinatorial flow on  $(T, X)$ , which is the way to choose a suitable orientation for each of those  $\deg_T(b) - 1$  edges connecting a leaf to  $b$  in  $T$ . Since every full combinatorial flow on  $(T, X)$  must come from a full combinatorial flow on  $(T', X')$  in this way, we get the required result.  $\square$

For any two positive integers  $n$  and  $m$ , let  $t_{n,m} = \binom{n-m}{m}$ . By an  $m$ -subdivision of a tree  $T$  we mean a set  $\mathbb{T} = \{T_1, \dots, T_m\}$  of subtrees of  $T$  such that  $V(T_1), \dots, V(T_m)$  are disjoint subsets of  $V(T)$ ,  $\cup_{i=1}^m \mathcal{L}(T_i) = \mathcal{L}(T)$ , and  $\mathcal{L}(T_i) \in \binom{\mathcal{L}(T)}{\geq 2}$  for  $i \in \{1, \dots, m\}$ . Note that this concept of  $m$ -subdivision is very similar to the concept of convex-state character of a phylogenetic tree studied in phylogenetic combinatorics [KS17, Ste92]. Indeed, [Ste92, Proposition 1(4)] is a result quite similar to the following Lemma 9.2 on  $m$ -subdivisions.

**Lemma 9.2.** *Let  $n \geq 2$  and  $m \geq 1$  be two integers. For every  $n$ -leaf binary tree, the number of its  $m$ -subdivisions is  $t_{n-2,m-1} = \binom{n-m-1}{m-1}$ .*

*Proof.* Denote the number of  $m$ -subdivisions of a given  $n$ -leaf binary tree  $T$  by  $c_{n,m}(T)$ . We need to show that  $c_{n,m}(T)$  is totally determined by  $n$  and  $m$  and will indeed equal to  $t_{n-2,m-1}$ . When  $m > \frac{n}{2}$ , it is clear that  $c_{n,m}(T) = t_{n-2,m-1} = 0$ . Accordingly, we shall always assume below  $m \leq \lfloor \frac{n}{2} \rfloor$ .

We do induction on  $n$ . When  $n = 2$ ,  $m$  can only be 1 and  $T$  must be the two-vertex tree. So  $c_{n,m}(T) = t_{n-2,m-1} = 1$ . When  $n = 3$ ,  $m$  also can only



take value 1 while  $T$  is a star tree with three leaves. We hence find  $c_{n,m}(T) = t_{n-2,m-1} = 1$ .

Assume now  $n > 3$  and the result holds for smaller  $n$ . Let  $T$  be a binary tree with  $n$  leaves and hence  $n - 2 \geq 2$  interior vertices. Then the subtree of  $T$  induced by its interior vertices has a leaf  $b$ . Let  $b'$  be the interior vertex of  $T$  which is adjacent to  $b$  in  $T$  and let  $c_1$  and  $c_2$  be the vertices other than  $b$  which are adjacent to  $b'$  in  $T$ . Since  $T$  is binary, there are exactly two leaves  $a_1, a_2$  of  $T$  which are adjacent to  $b$ . Let  $S$  be the set of  $m$ -subdivisions of  $T$ , which is the disjoint union of  $S_1$  and  $S_2$ , where  $S_1$  represent the set of those  $m$ -subdivisions  $\mathbb{T}$  of  $T$  in which the subtree induced by  $\{a_1, a_2, b\}$  is an element and  $S_2$  represent the set of those  $m$ -subdivisions  $\mathbb{T}$  of  $T$  in which the subtree induced by  $\{a_1, a_2, b\}$  is not any element. Let  $T'$  be the binary tree obtained from  $T$  by deleting vertices  $a_1, a_2, b$  and  $b'$  and adding a new edge connecting  $c_1$  and  $c_2$ , and let  $T''$  be the binary tree obtained from  $T$  by deleting vertices  $a_1$  and  $a_2$ . The size of  $S_1$  is  $c_{n-2,m-1}(T')$ , which is equal to  $t_{n-4,m-2}$  by induction assumption; The size of  $S_2$  is  $c_{n-1,m}(T'')$ , which is equal to  $t_{n-3,m-1}$  by induction assumption. For  $n \geq 4$  and  $m \leq \lfloor \frac{n}{2} \rfloor$ , we can check that

$$t_{n-2,m-1} = t_{n-4,m-2} + t_{n-3,m-1}.$$

This proves  $c_{n,m}(T) = |S| = |S_1| + |S_2| = t_{n-2,m-1}$ , as desired.  $\square$

**Remark 9.3.** Note that  $t_{n,m}$  is the number of sequences of 1's and 2's that sums to  $n$  and has  $m$  appearances of 2 and hence

$$\sum_{m=0}^{\lfloor \frac{n}{2} \rfloor} t_{n,m}$$

counts the number of walks of length  $n$  from  $u$  to  $u$  in the digraph shown in Figure 7. The digraph in Figure 7 represents the famous golden mean shift and it is known that the number of walks of length  $n$  from  $u$  to  $u$  in it is the  $(n+1)$ th Fibonacci number; see [LM95, Example 4.14]. Considering that every  $n$ -leaf binary tree has  $n - 2$  interior vertices, we are thus wondering if there should exist a simple bijective proof of Lemma 9.2.



Figure 7: Graph for the golden mean shift.

Let  $T$  be a tree with maximum degree at most three. If  $T$  is not binary, we can find a vertex  $v$  with degree two and choose one of its adjacent vertices, say,  $u$ . We shrink the edge  $uv$  and the resulting graph will have one less degree-two vertex. By a series of such shrinking operation, we will finally obtain from  $T$  a binary tree, which is unique up to isomorphism and will be referred to as *the binary tree presented in  $T$* .

**Lemma 9.4.** *Let  $n$  be a positive integer, let  $X$  be a set of  $n \geq 2$  elements and let  $T$  be a binary phylogenetic  $X$ -tree. For any nonnegative integer  $i$ , it holds that*

$$W_i = \sum_{m=1}^{+\infty} 2^m 3^{n-m-i-1} \binom{n-i-2}{m-1} \binom{n}{n+m-i-1},$$

where  $W_i$  denotes the number of  $i$ -faces of the Lipschitz polytope of  $D_{T,X}$ .

*Proof.* Let  $\sigma$  be a combinatorial flow on  $(T, X)$  such that

$$i = b_0((T, X)^\sigma) - 1. \quad (45)$$

Let us assume that among all the connected components of  $(T, X)^\sigma$ , exactly  $m$  of them, say  $(T_1, X_1), \dots, (T_m, X_m)$ , are not isolated vertices, where  $|X_1| \geq |X_2| \geq \dots \geq |X_m|$ . Let  $k = \sum_{j=1}^m |X_j|$  and note that  $(T, X)^\sigma$  has exactly  $n - k$  isolated vertices. It follows from (45) that  $(n - k) + m = i + 1$  and so  $k = n + m - i - 1$ .

By Theorem 4.2, Lemma 5.2 and Lemma 5.3,  $W_i$  is the number of combinatorial flows  $\sigma$  on  $(T, X)$  such that (45) holds. Fix the number  $m$  of the weakly connected components of  $(T, X)^\sigma$  with size greater than one. There are  $\binom{n}{k} = \binom{n}{n+m-i-1}$  ways to choose a set  $S$  of  $n - k$  leaves as isolated vertices in  $(T, X)^\sigma$ .

We delete vertex set  $S$  from  $T$  to get another tree and then look at the binary tree  $T'$  presented by it. In an obvious way, the components of  $T^\sigma$  which contain nonempty edge sets give rise to an  $m$ -subdivision  $\mathbb{T} = \{T_1, \dots, T_m\}$  of  $T'$ . By Lemma 9.2, the number of  $m$ -subdivisions of  $T'$  is  $t_{k-2, m-1} = \binom{k-m-1}{m-1} = \binom{n-i-2}{m-1}$ .

For any such  $m$ -subdivision  $\mathbb{T} = \{T_1, \dots, T_m\}$  of  $T'$ , we consider the binary trees  $T'_1, \dots, T'_m$  presented by  $T_1, \dots, T_m$  and we can assume that  $T'_j$  has  $|X_j|$  leaves for  $j = 1, \dots, m$ . Recall that a binary tree with  $r$  leaves has  $r - 2$  interior vertices. By the proof of Lemma 9.1, we thus see that the number of full combinatorial flows on the binary phylogenetic tree  $T'_j$  is  $2 \cdot (2^2 - 1)^{|X_j|-2} = 2 \cdot 3^{|X_j|-2}$ . This means that the number of such possible  $\sigma$  which corresponds to this same  $m$ -subdivision  $\mathbb{T}$  of  $T'$  is

$$\prod_{j=1}^m 2 \cdot 3^{|X_j|-2} = 2^m \cdot 3^{|X_1|+\dots+|X_m|-2m} = 2^m \cdot 3^{k-2m} = 2^m \cdot 3^{n-m-i-1}.$$

To sum up, we now find that the total number of combinatorial flows on  $(T, X)$  fulfilling (45) is

$$\sum_{m=1}^{+\infty} 2^m 3^{n-m-i-1} \binom{n-i-2}{m-1} \binom{n}{n+m-i-1},$$

as desired.  $\square$

Let  $(T, X)$  be an  $X$ -tree. A *quartet* of  $(T, X)$  is a partition  $ab|cd$  of a four element subset  $\{a, b, c, d\}$  of  $X$  such that the path connecting  $a$  and  $b$  in  $T$  is vertex-disjoint with the path connecting  $c$  and  $d$  in  $T$  [DHK<sup>+</sup>12, § 2.4]. We use  $q(T, X)$  to denote the number of quartets of  $(T, X)$ . Assume that  $|X| \geq 4$  and  $T$  is a phylogenetic  $X$ -tree. By Theorem 4.2, Lemma 5.2 and Lemma 5.3, we can obtain

$$W_{|X|-3}(\mathbb{L}_{D_T}) = |X|(|X| - 1)(|X| - 2) + 4q(T, X). \quad (46)$$

**Example 9.5.** Figure 8 shows two different 4-nary phylogenetic  $X$ -trees  $T_1$  and  $T_2$  with  $|X| = 10$  leaves. We can directly check that  $q(T_1, X) = 166$  and  $q(T_2, X) = 162$  and so, by (46),  $W_7(\mathbb{L}_{D_{T_1}}) \neq W_7(\mathbb{L}_{D_{T_2}})$ . This example says that in general the face vector of the Lipschitz polytope of a phylogenetic  $X$ -tree  $T$  is not determined by the degree sequence of  $T$ . Note that Lemma 9.1 and Lemma 9.4 suggest some nice cases in which we can really read some information of the face vectors from the degree sequences.

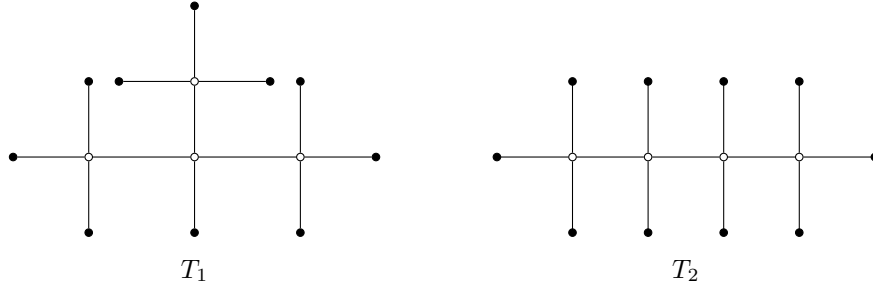


Figure 8: Two non-isomorphic 4-nary phylogenetic  $X$ -trees with  $|X| = 10$ .

By Theorem 4.2 and Remark 4.6, for the study of combinatorial type of the Lipschitz polytopes of tree metrics, we shall be concerned with all phylogenetic trees. Lemma 9.1 is a result in this direction about the number of vertices. With the help of Lemma 9.2, we determine explicitly in Lemma 9.4 the whole face vectors for the Lipschitz polytopes coming from binary phylogenetic trees. Example 9.5 indicates the subtlety of pursuing a general explicit formula for all phylogenetic trees. In the remainder of this section, let us turn to establish extremal results instead.

**Lemma 9.6.** *Let  $T$  and  $T'$  be two  $X$ -trees such that  $T$  is obtained from  $T'$  by shrinking an edge. Then  $W(\mathbb{L}_{D_{T',X}}) \neq W(\mathbb{L}_{D_{T,X}})$  and  $W_i(\mathbb{L}_{D_{T',X}}) \geq W_i(\mathbb{L}_{D_{T,X}})$  for all  $i$  satisfying  $0 \leq i \leq |X| - 1 = \dim(\mathbb{L}_{D_{T,X}}) = \dim(\mathbb{L}_{D_{T',X}})$ .*

*Proof.* Let  $e = uv$  be the edge of  $T'$  such that  $T$  is obtained from  $T'$  by shrinking  $e$ . We denote the vertex of  $T$  which corresponds to the set  $\{u, v\}$  by  $w$ . Note that  $\{u, v\} \cap X$  has size at most 1 and that  $w$  should be the unique element in  $\{u, v\} \cap X$  when  $\{u, v\} \cap X$  is nonempty. Let  $E_u = \{e' \in E(T') : u \in$

$\text{bd}_{T'}(e'), v \notin \text{bd}_{T'}(e')\}$  and  $E_v = \{e' \in \mathbb{E}(T') : v \in \text{bd}_{T'}(e'), u \notin \text{bd}_{T'}(e')\}$ . Note that  $\mathbb{E}(T) = \mathbb{E}(T') \setminus \{e\}$  and  $\mathbb{A}(T) = \mathbb{A}(T') \setminus \{\overrightarrow{uv}, \overrightarrow{vu}\}$ .

By Theorem 4.2, Lemma 5.2 and Lemma 5.3, we need to find an injective map  $\pi$  from  $\mathcal{CF}(T, X)$  to  $\mathcal{CF}(T', X)$  which preserves the rank and also show that this map is not a bijection. Take  $\sigma \in \mathcal{CF}(T, X)$ . Let us construct  $\pi(\sigma) \in \mathcal{CF}(T', X)$  such that  $\text{b}_0((T, X)^\sigma) = \text{b}_0((T', X)^{\pi(\sigma)})$  and  $\pi(\sigma) \cap \mathbb{A}(T) = \sigma$ .

**Case 1.** Either  $w = u \in X$  or  $w = v \in X$ .

Without loss of generality, assume that  $w = u \in X$ . If  $\sigma \cap E_v = \emptyset$ , we let  $\pi(\sigma) = \sigma$ . If  $\sigma \cap E_v \neq \emptyset$ , we let  $\pi(\sigma) = \sigma \cup \overrightarrow{uv}$  provided there exists  $\alpha \in \sigma$  such that  $\text{o}_G(\alpha) = v$  and let  $\pi(\sigma) = \sigma \cup \overrightarrow{vu}$  otherwise.

**Case 2.**  $\{u, v\} \cap X = \emptyset$ , to wit,  $w \notin V(T)$ .

Since  $\sigma$  is good at  $w \notin X$ , there are  $\alpha, \beta \in E_u \cup E_v$  such that  $\text{o}_T(\alpha) = w$  and  $\text{t}_T(\alpha) = w$ . Due to the symmetry between  $u$  and  $v$ , we need only consider the following two cases.

**Case 2.1.**  $[\alpha] \in E_u, [\beta] \in E_v$ .

Let  $\gamma = \overrightarrow{vu}$  be the arc in  $e$  that goes from  $v$  to  $u$  and let  $\pi(\sigma) = \sigma \cup \{\gamma\}$ .

**Case 2.2.**  $\alpha, \beta \in E_u, \sigma \cap E_v = \emptyset$ .

Let  $\pi(\sigma) = \sigma$ .

Since we have obtained the required map  $\pi$  from  $\mathcal{CF}(T, X)$  to  $\mathcal{CF}(T', X)$ , which must be injective, we see that  $\text{W}(\text{L}_{D_{T', X}}) - \text{W}(\text{L}_{D_{T, X}})$  is nonnegative componentwise.

To show that  $\text{W}(\text{L}_{D_{T', X}}) \neq \text{W}(\text{L}_{D_{T, X}})$ , it remains to show that the sum of entries in  $\text{W}(\text{L}_{D_{T', X}})$  is bigger than the sum of entries in  $\text{W}(\text{L}_{D_{T, X}})$ . Therefore, we just need to find a  $\sigma \in \mathcal{CF}(T, X)$  and at least two different flows  $\sigma' \in \mathcal{CF}(T', X)$  such that  $\sigma' \cap \mathbb{A}(T) = \sigma$ . As both  $T$  and  $T'$  are  $X$ -trees, we may assume that  $\text{deg}_{T'}(u) \geq 3$ . This enables the existence of  $\sigma \in \mathcal{CF}(T, X)$  such that  $\sigma \cap E_u$  contains both incoming and outgoing arcs at  $w$ . In the case that  $v \in X$ , it is easy to see that  $\sigma, \sigma \cup \{\overrightarrow{uv}\}$  and  $\sigma \cup \{\overrightarrow{vu}\}$  could all be our  $\sigma'$ . Otherwise, we have  $\text{deg}_{T'}(v) \geq 3$  as well and so we could assume in addition that  $\sigma \cap E_v$  contains both incoming and outgoing arcs at  $w$ . This again guarantees that  $\sigma, \sigma \cup \{\overrightarrow{uv}\}$  and  $\sigma \cup \{\overrightarrow{vu}\}$  could all be chosen as  $\sigma'$  for this suitable  $\sigma$ , completing the proof.  $\square$

**Lemma 9.7.** *Let  $n \geq 3$  and let  $(T, X)$  be a star tree on  $n + 1$  vertices. Then*

$$\text{W}_i(\text{L}_{D_{T, X}}) = \begin{cases} \binom{n}{i}(2^{n-i} - 2) & \text{if } i = 0, \dots, n-2; \\ 1 & \text{if } i = n-1. \end{cases}$$

*Proof.* For any  $\sigma \in \mathcal{CF}(T, X)$ , it clearly holds

$$\text{b}_0((T, X)^\sigma) = \begin{cases} n - |\sigma| = n & \text{if } |\sigma| = 0; \\ n - |\sigma| + 1 & \text{if } |\sigma| = 2, \dots, n. \end{cases}$$

Accordingly, an application of Theorem 4.2, Lemma 5.2 and Lemma 5.3 shows that  $\text{W}_{n-1}(\text{L}_{D_{T, X}})$  equals 1 while  $\text{W}_i(\text{L}_{D_{T, X}})$  is the number of  $\sigma \in \mathcal{CF}(T, X)$  with  $|\sigma| = n - i$  for  $i = 0, \dots, n - 2$ . Fixing any  $i \in \{0, \dots, n - 2\}$ , to find such a  $\sigma$ , we choose any  $n - i$  of the  $n$  edges of the star tree and then assign orientations

to them in an arbitrary way, excepting the two ways for which the interior vertex of the tree will not be good. This shows that  $W_i(\mathbb{L}_{\mathbb{D}_{T,X}}) = \binom{n}{i}(2^{n-i} - 2)$  for  $i \in \{0, \dots, n-2\}$ .  $\square$

**Lemma 9.8.** *Let  $T$  be an  $X$ -tree with  $X = V(T)$  and let  $n = |X|$ . Then  $W_i(\mathbb{L}_{\mathbb{D}_{T,X}}) = \binom{n-1}{i}2^{n-i-1}$  for  $i = 0, \dots, n-1$ .*

*Proof.* For any  $\sigma \in \mathcal{CF}(T, X)$ , it clearly holds

$$b_0((T, X)^\sigma) = n - |\sigma|.$$

It thus follows from Theorem 4.2, Lemma 5.2 and Lemma 5.3 that  $W_i(\mathbb{L}_{\mathbb{D}_{T,X}})$  is the number of  $\sigma \in \mathcal{CF}(T, X)$  such that  $|\sigma| = n - i - 1$ . Consequently,  $W_i(\mathbb{L}_{\mathbb{D}_{T,X}}) = \binom{n-1}{i}2^{n-i-1}$ .  $\square$

$ X  \backslash i$	0	1	2	3	4	5	6
3	6	6					
4	18	28	12				
5	54	114	80	20			
6	162	432	422	180	30		
7	486	1566	1962	1190	350	42	
8	1458	5508	8424	6640	2828	616	56

Figure 9: The number of  $i$ -faces of the Lipschitz polytopes of binary phylogenetic  $X$ -trees with  $|X| = 3, \dots, 8$ .

We write  $\delta_{i,j}$  for the Kronecker function, which equals 1 if  $i = j$  and equals 0 otherwise.

**Theorem 9.9.** *Let  $T$  be an  $X$ -tree and let  $n = |X|$ . For  $i = 0, \dots, n-1$ , let*

$$\begin{cases} u_i = \sum_{m=1}^{+\infty} 2^m 3^{n-m-i-1} \binom{n-i-2}{m-1} \binom{n}{n+m-i-1}, \\ y_i = \binom{n-1}{i} 2^{n-i-1}, \\ z_i = \binom{n}{i} (2^{n-i} - 2) + \delta_{i,n-1}. \end{cases}$$

Let  $U, Y, Z$  be three vectors of length  $n$  whose  $i$ th entry is  $u_i, y_i, z_i$  respectively. Let  $W$  be the face vector of  $\mathbb{L}_{\mathbb{D}_{T,X}}$ , that is, its  $i$ th entry is  $W_i(\mathbb{L}_{\mathbb{D}_{T,X}})$ .

- It holds that  $Y \leq W \leq U$ . Moreover,  $W = U$  if and only if  $T$  is a binary phylogenetic  $X$ -tree and  $Y = W$  if and only if  $V(T) = X$ .
- Assume that  $T$  is a phylogenetic  $X$ -tree. Then  $Z \leq W \leq U$ , with  $W = U$  if and only if  $T$  is a binary phylogenetic  $X$ -tree and with  $Z = W$  if and only if  $T$  is a star tree or  $n = 2$ .

*Proof.* (a) It is not hard to see that we can find a binary phylogenetic  $X$ -tree  $T'$  such that  $T$  is obtained from  $T'$  by a sequence of operations of shrinking edges.

By Lemma 9.4 and Lemma 9.6, we know that  $W = W(L_{D_{T,X}}) \leq W(L_{D_{T',X}}) = U$  with equality if and only if  $T$  itself is a binary phylogenetic  $X$ -tree.

By a sequence of operations of shrinking edges, we can transform  $T$  into an  $X$ -tree  $T''$  with  $X = V(T'')$ . Applying Lemma 9.6 and Lemma 9.8, we know that  $W = W(L_{D_{T,X}}) \geq W(L_{D_{T'',X}}) = Y$  and equality happens if and only if  $V(T) = X$ .

(b) The relationship between  $U$  and  $W$  is obtained already in (a). We now turn to discuss the relationship between  $W$  and  $Z$ . If  $n = 2$ , we have  $X = V(T)$  and  $Z = U$  and so the result trivially holds. We now assume  $n \geq 3$ . Since  $T$  is a phylogenetic  $X$ -tree and  $|X| \geq 3$ , by shrinking edges successively, we can go from  $T$  to a star tree  $T^*$  with  $X$  as its leaf set. In view of Lemma 9.4, Lemma 9.6 and Lemma 9.7, we then find that  $W = W(L_{D_{T,X}}) \geq W(L_{D_{T^*,X}}) = Z$ , with equality if and only if  $T = T^*$ , namely,  $(T, X)$  is a star tree.  $\square$

## 10 Simple vertices

We say that a proper metric  $(X, D)$  is *generic* [GP17], if  $L_D$  is simple and  $D(x, y) + D(z, y) > D(x, z)$  for all  $\{x, y, z\} \in \binom{X}{3}$ . For any generic metric space, Gordon and Petrov [GP17] deduced general formula for the face numbers of its Lipschitz polytope. For phylogenetic  $X$ -tree  $T$  with at least four leaves, we will find in this section that  $L_{D_{T,X}}$  is not simple (Corollary 10.3) and so our Lemma 9.1 and Lemma 9.4 are not covered by their results on generic metrics.

**Lemma 10.1 (Balinski's Theorem).** [Bal61] [Zie95, Theorem 3.14] *For every  $d$ -dimension polytope  $P$ , its 1-skeleton graph  $SG_P$  is  $d$ -connected.*

By Lemma 10.1, simple vertices of  $SG_P$  are those whose degree attains the absolute lower bound  $d$ . In the same spirit of Lemma 2.3, the face poset of a simple polytope is determined by its 1-skeleton graph [BML87, Kal88]. But, simple zonotopes correspond to simplicial arrangements of hyperplanes and they are rare [Zie95, p. 224], This section confirms this general observation by characterizing simple vertices of Lipschitz polytopes of phylogenetic  $X$ -trees.

**Theorem 10.2.** (a) *For every  $X$ -tree  $T$ , the dimension of  $L_{D_{T,X}}$  and the minimum degree of  $SG_{T,X}$  are both  $|X| - 1$ .*

(b) *Let  $T$  be a phylogenetic  $X$ -tree and take  $\sigma \in V(SG_{T,X}) = \mathcal{CF}^*(T, X)$  (see Lemma 5.4). Then,  $\deg_{SG_{T,X}}(\sigma) \geq |X| - 1$ , with equality if and only if  $\sigma$  is both  $H_1$ -free and  $H_2$ -free, where  $H_1$  and  $H_2$  are the two digraphs as shown in Figure 10.*

*Proof.* (a) By Lemma 5.1,  $L_{D_{T,X}}$  has dimension  $|X| - 1$ . By Lemma 10.1,  $SG_{T,X}$  is  $(|X| - 1)$ -connected and so its minimum degree is at least  $|X| - 1$ . Take  $x \in X$  and consider the elements  $\sigma_{T,x}^+$  and  $\sigma_{T,x}^-$ . An arc  $\alpha \in \sigma_{T,x}^+$  is flippable for  $\sigma_{T,x}^+$  if and only if  $t_T(\alpha) \in X$  while an arc  $\alpha \in \sigma_{T,x}^-$  is flippable for  $\sigma_{T,x}^-$  if and only if  $o_T(\alpha) \in X$ . In view of Remark 5.5, we see that  $\deg_{SG_{T,X}}(\sigma_{T,x}^+) = \deg_{SG_{T,X}}(\sigma_{T,x}^-) = |X| - 1$ .

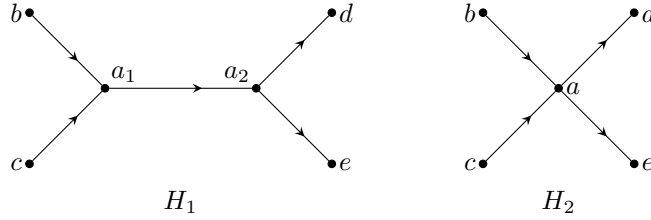


Figure 10: Two forbidden digraphs.

(b) If  $|V(T)| \leq 5$ , the result can be directly checked. We assume now  $|V(T)| \geq 6$  and the result is valid when  $|V(T)|$  is smaller. Let  $H = (V(T), \sigma)$ .

**Case 1.** The digraph  $H$  has  $H_1$  as an induced subgraph.

We may assume that  $S = \{a_1, a_2, b, c, d, e\}$  is a subset of  $V(T)$  and  $H[S] = H_1$ . Let  $T'$  be obtained from  $T$  by shrinking  $a_1 a_2$  into a new vertex  $a$  and let  $\sigma' = \sigma \cap A(T')$ . It is clear that  $\sigma'$  restricted on  $\{a, b, c, d, e\}$  is just  $H_2$ . By induction hypothesis,  $\deg_{\text{SG}_{T',X}}(\sigma') > |X| - 1$ . Since every flippable arc of  $\sigma'$  is also a flippable arc of  $\sigma$ , we can infer that  $\deg_{\text{SG}_{T,X}}(\sigma) \geq \deg_{\text{SG}_{T',X}}(\sigma') > |X| - 1$ .

**Case 2.** The  $X$ -tree  $(T, X)$  is a star tree.

Since  $T$  is a star tree,  $\sigma$  cannot contain  $H_1$  as a subgraph,  $\sigma$  contains  $H_2$  as a subgraph if and only if  $\sigma \notin \{\sigma_{T,x}^+, \sigma_{T,x}^- : x \in X\}$  while  $\{\sigma_{T,x}^+, \sigma_{T,x}^- : x \in X\}$  is the set of all those vertices of  $\text{SG}_{T,X}$  having degree  $|X| - 1$ .

**Case 3.** The  $X$ -tree  $(T, X)$  is not a star tree, the digraph  $H$  contains  $H_2$  as an induced subgraph but does not contain  $H_1$  as an induced subgraph.

Since  $T$  is not a star tree, we may assume that  $S = \{a, b, c, d, e\}$  is a subset of  $V(T)$ ,  $H[S] = H_2$  and either  $b$  or  $d$  is not a leaf of  $T$ . By symmetry, let us only consider the case of  $d \notin \mathcal{L}(T) = X$ . Since  $d$  is good for the flow  $\sigma$  and  $H$  does not contain  $H_1$  as an induced subgraph, there is exactly one vertex  $d' \in V(T)$  such that  $\overrightarrow{dd'} \in \sigma$ . As a phylogenetic  $X$ -tree,  $\deg_T(d) \geq 3$  holds and so we can find a vertex  $d'' \neq a$  such that  $\overrightarrow{d''d} \in \sigma$ . Accordingly, we see now  $H$  contains the digraph shown in Figure 11 as an induced subgraph.

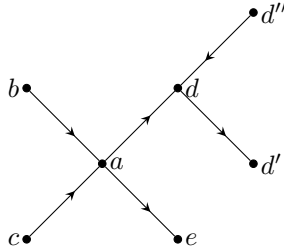


Figure 11: An induced subgraph of  $H$ .

We shrink  $ad$  into a new vertex  $a'$  and thus obtain from  $T$  a new tree  $T'$ .

Let  $\sigma' = \sigma \cap A(T')$ . Since  $H_2$  is isomorphic with the subgraph of  $\sigma'$  induced by  $\{a', b, c, d', e\}$ , the induction hypothesis implies  $\deg_{\text{SG}_{T',X}}(\sigma') > |X| - 1$ . A look at Figure 11 shows that  $\overrightarrow{ad} \notin \sigma'$  is a flippable arc for  $\sigma$  and that every arc which is flippable for  $\sigma'$ , must be also flippable for  $\sigma$  as long as it is not  $\overrightarrow{ad'}$ . It follows  $\deg_{\text{SG}_{T,X}}(\sigma) \geq \deg_{\text{SG}_{T',X}}(\sigma') - 1 + 1 = \deg_{\text{SG}_{T',X}}(\sigma') > |X| - 1$ .

**Case 4.** The digraph  $H$  contains neither  $H_1$  nor  $H_2$  as an induced subgraph.

Let  $b$  be a leaf of the subgraph of  $T$  induced by its interior vertices. Let  $a_1, \dots, a_k$  be all the leaves of  $T$  which are adjacent to  $b$ , let  $T'$  be the tree obtained from  $T$  by deleting  $a_1, \dots, a_k$ , let  $c$  be the only vertex adjacent to  $b$  in  $T'$ , and let  $f_1, \dots, f_m$  be all the edges of  $T$  other than  $bc$  whose boundaries contain  $c$ . Note that  $\min\{k, m\} \geq 2$ . Let the subgraph of  $T$  induced by  $\{c, b, a_1, \dots, a_k\}$  be  $\tilde{T}$ .

Let  $X' = (X \setminus \{a_1, \dots, a_k\}) \cup \{b\}$  and let  $\sigma' = \sigma \cap A(T')$ . Since  $\sigma'$  has neither  $H_1$  nor  $H_2$  as its induced subgraph, the induction hypothesis leads to  $\deg_{\text{SG}_{T',X'}}(\sigma') = |X'| - 1 = |X| - k$ .

**Case 4.1.**  $\sigma \cap A(\tilde{T}) \in \{\sigma_{\tilde{T},c}^-, \sigma_{\tilde{T},c}^+\}$ .

Since  $\sigma$  does not have  $H_1$  as an induced subgraph, there exist two distinct edges  $f_i$  and  $f_j$  from  $\{f_1, \dots, f_m\}$  such that  $c = o_T(\sigma \cap f_i)$  and  $c = t_T(\sigma \cap f_j)$ . Let the set of edges flippable for  $\sigma$  be  $F$  and let the set of edges flippable for  $\sigma$  be  $F'$ . Let  $S$  denote the singleton set  $\{\overrightarrow{cb}, \overrightarrow{bc}\} \cap \sigma$  and let  $R$  denote the  $k$ -element set  $\sigma \cap \{\overrightarrow{ba_1}, \overrightarrow{a_1b}, \dots, \overrightarrow{ba_k}, \overrightarrow{a_kb}\}$ . We can check that  $F = (F' \setminus S) \cup R$  and  $S \subseteq \sigma$ . This shows that  $|F| = |F'| - 1 + k$  and so  $\deg_{\text{SG}_{T,X}}(\sigma) = \deg_{\text{SG}_{T',X'}}(\sigma') - 1 + k = |X| - 1$ .

**Case 4.2.**  $\sigma \cap A(\tilde{T}) \notin \{\sigma_{\tilde{T},c}^-, \sigma_{\tilde{T},c}^+\}$ .

Without loss of generality, we assume  $\overrightarrow{cb} \in \sigma$  and so there are at least two incoming arcs at  $b$  from  $\sigma$ . Since  $\sigma$  does not have  $H_2$  as an induced subgraph, there is exactly one outgoing arc at  $b$  from  $\sigma$ , say  $\overrightarrow{ba_1}$ . Note that every arc which are flippable for  $\sigma'$  must be flippable for  $\sigma$  as well. Also,  $\overrightarrow{a_2b}, \dots, \overrightarrow{a_kb}$  are  $k - 1$  arcs flippable for  $\sigma$  while  $\overrightarrow{ba_1}$  is not flippable for  $\sigma$ . Therefore, we can conclude that  $\deg_{\text{SG}_{T,X}}(\sigma) = \deg_{\text{SG}_{T',X'}}(\sigma') + k - 1 = |X| - 1$ .  $\square$

**Corollary 10.3.** *Let  $T$  be a phylogenetic  $X$ -tree. Then  $L_{D_{T,X}}$  is simple if and only if  $|X| \leq 3$ .*

*Proof.* If  $T$  has at least two interior vertices, then  $|X| \geq 4$  and there exists  $\sigma \in \mathcal{CF}^*(T, X)$  which contains  $H_1$  as an induced subgraph; If  $T$  has at most one interior vertex, then no  $\sigma \in \mathcal{CF}^*(T, X)$  can contain  $H_1$  as an induced subgraph while there exists  $\sigma \in \mathcal{CF}^*(T, X)$  which contains  $H_2$  as an induced subgraph if and only if  $T$  is a star tree with at least four leaves. Henceforth, the result is a consequence of Theorem 10.2.  $\square$



## 11 Integral points in skew Lipschitz polytopes

An element of  $\mathbb{R}^X$  is called *integral* if it lies in  $\mathbb{Z}^X$ . We call a polytope  $P \subseteq \mathbb{R}^X$  an *integral polytope* if all the vertices of  $P$  are integral. The *Ehrhart series* of an integral polytope  $P \subseteq \mathbb{R}^X$  is a series in an indeterminate, say  $z$ , such that

$$\text{Ehr}_P(z) = \sum_{t=0}^{\infty} \text{Ehr}(P, t) z^t,$$

where  $\text{Ehr}(P, t)$  enumerates the number of integral points in  $tP = \{tv : v \in P \subseteq \mathbb{R}^X\}$ . For each integral polytope  $P$  of dimension  $d$ , Ehrhart [Ehr62] proved that  $\text{Ehr}(P, t)$  is a rational polynomial of degree  $d$  in  $t$ , called the *Ehrhart polynomial* of  $P$ , and that there exists complex numbers  $h_j^*$ ,  $0 \leq j \leq d$ , such that

$$\text{Ehr}_P(z) = \frac{\sum_{j=0}^d h_j^* z^j}{(1-z)^{d+1}}.$$

The vector  $(h_0^*, \dots, h_d^*)$  is called the  *$h^*$ -vector* of the integral polytope  $P$ . For any integral polytope  $P$  of dimension  $d$ , we know that the leading coefficient of  $\text{Ehr}(P, t)$ , namely, the coefficient of  $t^d$ , equals the  $d$ -volume of  $P$  [BR15, Corollary 3.20] while the constant term of it is 1 [BR15, Corollary 3.15].

Let  $\mathfrak{A}$  be an  $I$ -indexed vector configuration in  $\mathbb{Z}^X$ . We denote the greatest common divisor of the set

$$\{|\det(\mathfrak{A}_Y)| : Y \in \binom{X}{|I|}\} \subseteq \mathbb{Z}$$

by

$$\underline{\text{gcd}}(\mathfrak{A}),$$

where, for any  $Y \in \binom{X}{|I|}$ ,  $\mathfrak{A}_Y$  is the  $Y \times I$  matrix whose  $(y, i)$ -entry is  $\mathfrak{A}(i)(y)$  for any  $(y, i) \in Y \times I$ . By convention,  $\underline{\text{gcd}}(\mathfrak{A}) = 0$  provided  $\sum_{i \in I} t_i \mathfrak{A}(i) = 0$  possesses a nonzero solution  $(t_i)_{i \in I}$ , say when  $|X| < |I|$ .

**Lemma 11.1.** [She74] [Sta80, Example 3.1] [Sta91, Theorem 2.2] [BR15, Theorem 9.9] *Let  $X$  and  $I$  be two finite sets and let  $\mathfrak{A}$  be an  $I$ -indexed vector configuration in  $\mathbb{Z}^X$ . Then the Ehrhart polynomial of  $\mathcal{Z}(\mathfrak{A})$  is given by*

$$\text{Ehr}(\mathcal{Z}(\mathfrak{A}), t) = \sum_{m=0}^{|X|} \sum_{Y \in \binom{I}{m}} \underline{\text{gcd}}(\mathfrak{A}(Y)) t^m = 1 + \sum_{m=1}^{|X|} \sum_{Y \in \binom{I}{m}} \underline{\text{gcd}}(\mathfrak{A}(Y)) t^m,$$

where  $\mathfrak{A}(Y)$  stands for the  $Y$ -indexed vector configuration in  $\mathbb{Z}^X$  obtained as the restriction of  $\mathfrak{A}$  on  $Y \subseteq I$ .

A matrix is *totally unimodular* provided all its minors are 1, 0 or  $-1$ . To make our paper self-contained, let us recall some simply property about totally

unimodular matrices. We first note that, as observed already by Poincaré, a  $(0, \pm 1)$ -matrix in which each column has at most one 1 and at most one  $-1$  must be totally unimodular [Poi00] [Sch86, p. 274]. A  $(0, 1)$ -matrix is said to have the *consecutive-ones property* for columns [BL76] if its rows can be permuted in such a way that the ones in each column occur consecutively. Going further from the result of Poincaré, we mention that a  $(0, 1)$ -matrix with the consecutive-ones property must be totally unimodular. Indeed, a minor of a  $(0, 1)$ -matrix with the consecutive-ones property for columns is the determinant of a matrix with the consecutive-ones property for columns and so is the determinant of a  $(0, \pm 1)$ -matrix in which each column has at most one 1 and at most one  $-1$  and so must fall into  $\{-1, 0, 1\}$ . Matrices with consecutive-ones property are some special network matrices while Seymour [Sey80] found in 1980 that a matrix is totally unimodular if and only if it is a natural combination of some network matrices and some copies of two particular 5 by 5 matrices [Sch86, Theorem 19.6].

**Lemma 11.2.** *Let  $(X, D)$  be a metric space such that  $D(a, b)$  are integers for all  $a, b \in X$ . Then  $L_D^x$  is an integral polytope for any  $x \in X$ .*

*Proof.* Let  $I = \{(a, b) : \{a, b\} \in \binom{X}{2}\} \cup \{x_1, x_2\}$  and let  $\mathfrak{A}$  be the  $I$ -indexed vector configuration in  $\mathbb{R}^X$  such that  $\mathfrak{A}((a, b)) = \chi_a - \chi_b$  for  $\{a, b\} \in \binom{X}{2}$  and  $\mathfrak{A}(x_1) = -\mathfrak{A}(x_2) = \chi_x$ . As a matrix,  $\mathfrak{A}$  is totally unimodular, simply because each column of it, namely every vector in  $\mathfrak{A}$ , has all entries being zeros, excepting at most one  $+1$  and at most one  $-1$  [Poi00] [Sch86, p. 274]. Recall that  $L_D^x$  is defined via a set of linear inequalities as shown in (2). That is,  $L_D^x = \{f \in \mathbb{R}^X : \mathfrak{A}^\top f \leq \varrho\}$  where  $\varrho \in \mathbb{R}^I$  is the integral vector such that  $\varrho(a, b) = D(a, b)$  for  $\{a, b\} \in \binom{X}{2}$  and  $\varrho(x_1) = \varrho(x_2) = 0$ . If  $f$  is a vertex of  $L_D^x$ , there should be a subset  $I' \in \binom{I}{|X|}$  so that  $f$  is the unique solution to  $(\mathfrak{A}|_{I'})^\top f = \varrho|_{I'}$  [Lau13, Proposition 4.3]. Since  $\mathfrak{A}$  is totally unimodular,  $\mathfrak{A}|_{I'}$  must have an integral matrix as its inverse. This shows that  $f \in \mathbb{Z}^X$ , as wanted.  $\square$

Let  $(T, X)$  be an  $X$ -tree and  $x \in X$ . Let  $\sigma = \sigma_{T,x}^-$  and recall from (22) that  $\mathfrak{D}_{T,X,x}$ , the descendent matrix of  $(T, X)$  with origin  $x$ , is a  $\sigma$ -indexed vector configuration in  $\mathbb{R}^X$ . Note that  $\mathfrak{D}_{T,X,x}$  can be viewed as an  $X \times \sigma$  matrix whose  $(x, \alpha)$ -entry is  $\mathfrak{D}_{T,X,x}(\alpha)(x)$ .

**Lemma 11.3.** *If  $(T, X)$  is an  $X$ -tree and  $x \in X$ , then the matrix  $\mathfrak{D}_{T,X,x}$  is totally unimodular.*

*Proof.* We can view  $T' = (V(T), \sigma_{T,x}^-)$  as a directed in-tree rooted at  $x$ . For every two vertices  $v$  and  $w$  of  $T'$ , let  $v \vee w$  be the vertex which is of longest distance from  $x$  in the tree  $T$  and is on both the path from  $v$  to  $x$  and the path from  $w$  to  $x$  in  $T'$ . For each  $v \in V(T)$ , let  $H_v$  be the set of elements  $u \in X$  such that there is a path in  $T'$  leading from  $u$  to  $v$ . Note that the columns of  $\mathfrak{D}_{T,X,x}$  are of the form  $\chi_A \in \mathbb{R}^{X \setminus \{x\}}$  where  $A = H_v$  for some  $v \in V(T) \setminus \{x\}$ . We make use of the so-called postorder transversal to get an ordering of  $V(T)$ : For each

$v \in V(T)$ , fix a total ordering  $\prec_v$  of the connected components of  $T - v$ ; Let  $\pi(1), \dots, \pi(n)$ , where  $n = |V(T)|$ , be the total ordering of  $V(T)$  such that, for every two vertices  $v$  and  $w$ , we have  $\pi^{-1}(v) < \pi^{-1}(w)$  if  $w = v \vee w$ , or if  $v$  and  $w$  fall into different components of  $T - (v \vee w)$  while the one containing  $v$  comes earlier than that containing  $w$  in the total order  $\prec_{v \vee w}$ . This ordering  $\pi$  naturally induces a total order  $\mu$  on  $X \setminus \{x\} \subseteq V(T)$ , where  $\hat{x} \in X \setminus \{x\}$  appears earlier than  $x' \in X \setminus \{x\}$  in  $\mu$  if and only if that happens in  $\pi$ . It is clear that  $H_v$  is always consecutive in  $\mu$  for each  $v \in V(T)$ , completing the proof.  $\square$

**Remark 11.4.** *Our proof of Lemma 11.3 indeed shows that  $\mathfrak{D}_{T,X,x}$  has consecutive-ones property for columns. We mention that this fact is already observed implicitly in phylogenetic combinatorics; see [KHP13, Proposition 3.5] and [Ste16, p. 130].*

*Note that  $\mathfrak{D}_{T,X,x}$  is totally unimodular if and only if its transpose,  $\mathfrak{P}_{T,X,x}$ , the path matrix of  $(T, X)$  with origin  $x$ , is totally unimodular. From this view point, Lemma 11.3 is just [Fra11, Corollary 4.2.6], which is obtained from a result of Tutte [Fra11, Theorem 4.2.5] that all network matrices are totally unimodular.*

The *independence complex*  $\text{IC}(\mathfrak{A})$  of an  $E$ -indexed vector configuration  $\mathfrak{A}$  in  $\mathbb{R}^X$  is the simplicial complex whose faces are subsets of  $E$  which are mapped by  $\mathfrak{A}$  to a set of linearly independent set of vectors. Similarly, the *independence complex* of a matroid  $\mathcal{M}$  is the simplicial complex whose faces are independent sets of  $\mathcal{M}$ . It is easy to see that  $\text{IC}(\mathfrak{A}) = \text{IC}(\mathcal{M}_{\mathfrak{A}})$ .

Assume that  $P = \mathcal{Z}(u_1, \dots, u_m)$  and  $P' = \mathcal{Z}(\pm u_1, \dots, \pm u_m)$  where  $u_i \in \mathbb{Z}^X$  for  $i = 1, \dots, m$ . It is easy to see that

$$\text{Ehr}(P', t) = \text{Ehr}(P, 2t) \quad (47)$$

for all nonnegative integers  $t$ .

**Theorem 11.5.** *Let  $(T, X)$  be an  $X$ -tree and take  $x \in X$ . Then*

$$\text{Ehr}(\text{L}_{\mathfrak{D}_{T,X}}^x, t) = c_0 + c_1 \times 2t + \dots + c_{|X|-1} \times (2t)^{|X|-1}, \quad (48)$$

where  $(c_0, \dots, c_{|X|-1})$  is the face vector of the independence complex of  $\mathcal{M}_{T/X}^*$ . In particular, the  $(|X| - 1)$ -volume of  $\text{L}_{\mathfrak{D}_{T,X}}^x$  equals  $2^{|X|-1}$  times the number of spanning trees of  $T/X$ .

*Proof.* Recall from Lemma 5.1 that  $\text{L}_{\mathfrak{D}_{T,X}}^x$  has dimension  $|X| - 1$ . By Lemma 11.2, we can assume that (48) holds for some numbers  $c_0, \dots, c_{|X|-1}$ . It follows from (21) that  $\text{L}_{\mathfrak{D}_{T,X}}^x = \mathcal{Z}(\pm \mathfrak{D}_{T,X,x})$  and so, by (47),

$$\text{Ehr}(\mathcal{Z}(\mathfrak{D}_{T,X,x}), t) = c_0 + c_1 \times t + \dots + c_{|X|-1} \times t^{|X|-1}.$$

Applying Lemma 11.1 and Lemma 11.3, we now find that  $(c_0, \dots, c_{|X|-1})$  is the face vector of  $\text{IC}(\mathfrak{D}_{T,X,x})$ . By virtue of (26) and (27),  $\mathcal{M}_{\mathfrak{D}_{T,X,x}} = \mathcal{M}_{T/X}^*$ . This implies that  $(c_0, \dots, c_{|X|-1})$  is the face vector of  $\text{IC}(\mathcal{M}_{T/X}^*)$ .

By [BR15, Corollary 3.20], the volume of  $L_{D_{T,X}}^x$  is given by the leading term of  $\text{Ehr}(L_{D_{T,X}}^x, t)$ , i.e.  $2^{|X|-1}c_{|X|-1}$ . But  $c_{|X|-1}$  enumerates the number of bases of  $\mathcal{M}_{T/X}^*$ , which is equal to the number of bases of  $\mathcal{M}_{T/X}$  and so, the number of spanning trees of  $T/X$ .  $\square$

A consequence of Theorem 11.5 is that it is easy to compute the volume of  $L_{D_{T,X}}^x$ . Note that the problem of calculating the volume of a general zonotope is #P-hard [DGH98, Theorem 1]. From Theorem 11.5 we also see that  $\text{Ehr}(L_{D_{T,X}}^x, t)$  is independent with the choice of  $x \in X$  and so we will write  $\text{Ehr}(T, X, t)$  for  $\text{Ehr}(L_{D_{T,X}}^x, t)$  and write  $\text{Ehr}_{T,X}(z)$  for  $\text{Ehr}_{L_{D_{T,X}}^x}(z)$ .

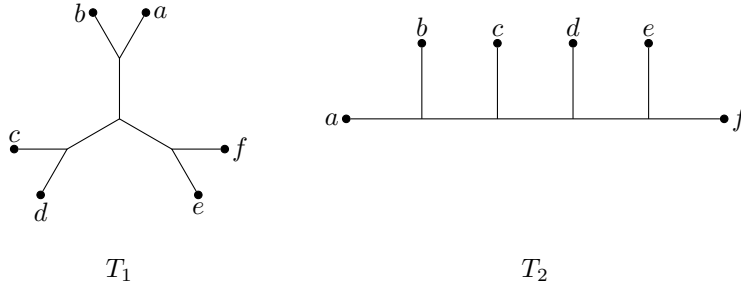


Figure 12: Two binary phylogenetic  $X$ -trees.

**Example 11.6.** Let  $T_1$  and  $T_2$  be the two binary phylogenetic  $X$ -trees shown in Figure 12. Then, a computation with the software Polymake [GJ00] tells us that

$$\begin{cases} \text{Ehr}(T_1, X, t) = 1 + 9 \times (2t) + 36 \times (2t)^2 + 80 \times (2t)^3 + 99 \times (2t)^4 + 54 \times (2t)^5, \\ \text{Ehr}(T_2, X, t) = 1 + 9 \times (2t) + 36 \times (2t)^2 + 80 \times (2t)^3 + 99 \times (2t)^4 + 55 \times (2t)^5; \end{cases}$$

and that

$$\begin{cases} \text{Ehr}_{T_1, X}(z) = \frac{1+4109z+61698z^2+110306z^3+30589z^4+657z^5}{(1-z)^6}, \\ \text{Ehr}_{T_2, X}(z) = \frac{1+4141z+62530z^2+112418z^3+31421z^4+689z^5}{(1-z)^6}. \end{cases}$$

Stanley's Monotonicity Theorem [Sta93, Theorem 3.3] says that if  $P_1$  and  $P_2$  are integral polytopes and  $P_1 \subseteq P_2$ , then  $h^*(P_2) - h^*(P_1)$  is a nonnegative vector. Though the  $h^*$ -vector of  $L_{D_{T_2, X}}$  dominates the  $h^*$ -vector of  $L_{D_{T_1, X}}$ ,  $L_{D_{T_1, X}}$  is not a subset of  $L_{D_{T_2, X}}$ . This suggests that we may need a new Monotonicity Theorem to explain this comparison result for  $T_1$  and  $T_2$ .

**Question 11.7.** If  $(T_1, X)$  and  $(T_2, X)$  are two phylogenetic  $X$ -trees satisfying  $\text{Ehr}_{T_1, X} = \text{Ehr}_{T_2, X}$ , can we conclude that  $T_1$  and  $T_2$  are isomorphic graphs?

## 12 Lipschitz heights

For any finite set  $X$  and any function  $f \in \mathbb{R}^X$ , we define the *height* of  $f$  to be

$$h(f) = \max_{x \in X} f(x) - \min_{x \in X} f(x).$$

Let  $(X, D)$  be a proper finite metric space. Taking any  $x \in X$ , we define the *Lipschitz height* of  $(X, D)$  to be

$$\text{LipH}(X, D) = \frac{\int_{L_D^x} h(f) \, d f}{\text{Vol}_{|X|-1}(L_D^x)}, \quad (49)$$

and define the *integral Lipschitz height* of  $(X, D)$  to be

$$\text{IntLipH}(X, D) = \frac{\sum_{f \in L_D^x \cap \mathbb{Z}^X} h(f)}{|L_D^x \cap \mathbb{Z}^X|}.$$

Note that the parameters  $\text{LipH}(X, D)$  and  $\text{IntLipH}(X, D)$  are indeed independent of the choice of  $x \in X$  and they measure the average height of the 1-Lipschitz functions on  $(X, D)$  and the average height of the integral 1-Lipschitz functions on  $(X, D)$  respectively. In addition, by the linearity of expectation, we have

$$\text{LipH}(X, D) = \frac{\int_{L_D^x} \max_{x \in X} f(x) \, d f}{\text{Vol}_{|X|-1}(L_D^x)} - \frac{\int_{L_D^x} \min_{x \in X} f(x) \, d f}{\text{Vol}_{|X|-1}(L_D^x)} = 2 \frac{\int_{L_D^x} \max_{x \in X} f(x) \, d f}{\text{Vol}_{|X|-1}(L_D^x)};$$

similarly, we have

$$\text{IntLipH}(X, D) = \frac{2 \sum_{f \in L_D^x \cap \mathbb{Z}^X} \max_{x \in X} f(x)}{|L_D^x \cap \mathbb{Z}^X|}.$$

For a connected graph  $G$  and the shortest path metric  $D_G$  on  $V(G)$ , we write  $\text{LipH}(G)$  and  $\text{IntLipH}(G)$  for  $\text{LipH}(V(G), D_G)$  and  $\text{IntLipH}(V(G), D_G)$ , respectively. Note that what we call an integral Lipschitz height of a graph metric space is named by Loeb, Nešetřil and Reed the Lipschitz height of a graph [LNR03].

In (49) we assign the expected value of the height of a random 1-Lipschitz function to a proper metric space, assuming that the random Lipschitz functions are uniformly distributed in the Lipschitz polytope. This parameter looks natural but it lacks scaling invariance. For any proper finite metric space  $(X, D)$ , we define its *scale-invariant Lipschitz height* to be

$$\text{SLipH}(X, D) = \frac{\int_{L_D^x} h(f) \, d f}{(\text{Vol}_{|X|-1}(L_D^x))^{\frac{2}{|X|-1}}}.$$

This new parameter is scale-invariant, namely  $\text{SLipH}(X, tD) = \text{SLipH}(X, D)$  for all positive real  $t$ . As a consequence,  $\max \text{SLipH}(X, D)$  and  $\min \text{SLipH}(X, D)$  exist where  $D$  runs through all proper metrics on the fixed finite set  $X$ .

**Question 12.1.** *Let  $(X, D)$  be a proper metric space. Find an upper/lower bound estimates of  $\text{SLipH}(X, D)$  in terms of  $|X|$ . If  $(X, D)$  is a tree metric, what are the corresponding upper and lower bounds?*

The rest of this section will focus on Question 12.1 and related issues for some special tree metrics. Let  $\mathcal{T}_n$  denote the set of all  $n$ -vertex trees up to graph isomorphism. For any connected graph  $G$  and  $x, y \in V(G)$ , we use the notation  $[x, y]_G$  for the set  $\{z \in V(G) : D_G(x, z) + D_G(z, y) = D_G(x, y)\}$  and we use the notation  $(x, y)_G$  for  $[x, y]_G \setminus \{x, y\}$ . Let  $T$  be a tree and let  $x, y$  be two interior vertices of  $T$  such that  $(x, y)_T$  only contains degree-two vertices of  $T$ . We now define  $\text{KC}_{x \rightarrow y}(T)$  to be the tree having  $V(T)$  and  $A(T)$  as its vertex set and arc set, respectively, but having a new boundary relation that, for each  $\alpha \in A(\text{KC}_{x \rightarrow y}(T)) = A(T)$ , it holds  $o_{\text{KC}_{x \rightarrow y}(T)}(\alpha) = o_T(\alpha)$  and  $t_{\text{KC}_{x \rightarrow y}(T)}(\alpha) = t_T(\alpha)$ , with the exception of

$$\begin{cases} o_{\text{KC}_{x \rightarrow y}(T)}(\alpha) = y & \text{if } o_T(\alpha) = x \text{ and } t_T(\alpha) \notin (x, y)_T; \\ t_{\text{KC}_{x \rightarrow y}(T)}(\alpha) = y & \text{if } t_T(\alpha) = x \text{ and } o_T(\alpha) \notin (x, y)_T. \end{cases}$$

This transformation from  $T$  to  $\text{KC}_{x \rightarrow y}(T)$  is called a *KC-transformation*, in honor of Kelmans [Kel81] and Csikvári [Csi10]; see [WXZ16, Figure 4] for an illustration of this transformation. For any two trees  $T_1, T_2 \in \mathcal{T}_n$ , we say that  $T_1$  is *less than*  $T_2$  and write  $T_1 \leq T_2$  if we can obtain  $T_1$  from  $T_2$  by a sequence of KC-transformations. It is apparent that  $(\mathcal{T}_n, \leq)$  is a poset. Let  $P_n, S_n \in \mathcal{T}_n$  be the path and the star with  $n$  vertices, respectively.

**Lemma 12.2.** [Csi10, Theorem 2.4] *For any positive integer  $n$ ,  $(\mathcal{T}_n, \leq)$  is a ranked poset with  $S_n$  and  $P_n$  being the minimum and maximum elements, respectively.*

A graph automorphism  $\rho$  of a graph  $G$  is a pair of maps  $(\rho_0, \rho_1)$ , where  $\rho_0 \in V(G)^{V(G)}$  and  $\rho_1 \in A(G)^{A(G)}$  are two bijective maps such that  $\rho_1 o_G(\alpha) = o_G \rho_1(\alpha)$ ,  $\rho_1 t_G(\alpha) = t_G \rho_1(\alpha)$  and  $\rho_1(\bar{\alpha}) = \overline{\rho_1(\alpha)}$  for all  $\alpha \in A(G)$ . We call  $\rho_0$  and  $\rho_1$  the *vertex map* and the *arc map* of  $\rho$ . It is clear that  $\rho_1$  induces a bijective map from  $E(G)$  to  $E(G)$  which we often also refer to as  $\rho_1$ .

**Theorem 12.3.** *Let  $n$  be a positive integer and take  $T \in \mathcal{T}_n$ .*

(a) [WXZ16, Corollary 2.6] *It holds  $\text{IntLipH}(S_n) \leq \text{IntLipH}(T) \leq \text{IntLipH}(P_n)$ . The first equality holds if and only if  $T = S_n$  and the second equality holds if and only if  $T = P_n$ .*

(b) *It holds  $\text{LipH}(S_n) \leq \text{LipH}(T) \leq \text{LipH}(P_n)$ . The first equality holds if and only if  $T = S_n$  and the second equality holds if and only if  $T = P_n$ .*

*Proof.* Our task is to prove claim (b). We will show that we can follow the same arguments in [WXZ16] for proving (a) to prove (b).

When  $n \leq 3$ ,  $|\mathcal{T}_n| = 1$  and so there is nothing to prove. We now assume that  $n > 3$ . In view of Lemma 12.2, we will be done if we can obtain

$$\text{LipH}(T) - \text{LipH}(T') > 0, \tag{50}$$

where  $T \in \mathcal{T}_n$ ,  $x$  and  $y$  are two interior vertices of  $T$  such that  $(x, y)_T$  only contains degree-two vertices of  $T$ , and  $T' = \text{KC}_{x \rightarrow y}(T)$ .

Let us write  $L_T^x$  for  $L_{D_T, V(T)}^x$ . Let  $p = p_x^{V(T)}$  be the projection from  $\mathbb{R}^{V(T)}$  to  $\mathbb{R}^{V(T) \setminus \{x\}}$  as defined in (3). For each  $g \in \mathbb{R}^{V(T) \setminus \{x\}}$ , let  $\widehat{g}$  denote the unique element  $f \in \mathbb{R}^{V(T)}$  such that  $f(x) = 0$  and  $p(f) = g$ . Recall the definition of the descendent matrix of  $(T, V(T))$  with origin  $x$  as given in (22). Let  $\sigma = \sigma_{T,x}^-$  and consider the  $\sigma$ -indexed vector configuration  $\mathfrak{D}_T$  in  $\mathbb{R}^{V(T) \setminus \{x\}}$  defined by  $\mathfrak{D}_T = p \circ \mathfrak{D}_{T, V(T), x}$ . It follows from (21) that

$$p(L_T^x) = \mathfrak{D}_T[-1, 1]^\sigma = \{ \mathfrak{D}_T \xi = \sum_{\alpha \in \sigma} \xi(\alpha) \mathfrak{D}_T(\alpha) : \xi \in [-1, 1]^\sigma \} \subseteq \mathbb{R}^{V(T) \setminus \{x\}}. \quad (51)$$

By (25),  $\mathfrak{D}_T$  is a nonsingular linear map from  $\mathbb{R}^\sigma$  to  $\mathbb{R}^{V(T) \setminus \{x\}}$ . This and Remark 1.1 allow us deduce from (51) that

$$\begin{aligned} \text{LipH}(T) &= \frac{\int_{L_T^x} h(f) \, d f}{\text{Vol}_{n-1}(L_T^x)} \\ &= \frac{\int_{p(L_T^x)} h(\widehat{g}) \, d g}{\text{Vol}_{n-1}(p(L_T^x))} \\ &= \frac{\int_{[-1, 1]^\sigma} h(\widehat{\mathfrak{D}_T \xi}) \det(\mathfrak{D}_T) \, d \xi}{\det(\mathfrak{D}_T) \text{Vol}_{n-1}([-1, 1]^\sigma)} \\ &= \frac{\int_{[-1, 1]^\sigma} h(\widehat{\mathfrak{D}_T \xi}) \, d \xi}{\text{Vol}_{n-1}([-1, 1]^\sigma)} \\ &= \frac{1}{2^{n-1}} \int_{[-1, 1]^\sigma} h(\widehat{\mathfrak{D}_T \xi}) \, d \xi. \end{aligned} \quad (52)$$

The subgraph of  $T$  induced by the set  $[x, y]_T$  is a path graph  $H$  and hence has a unique automorphism  $\rho$  whose vertex map  $\rho_0$  swaps  $x$  and  $y$ . For any  $\xi \in [-1, 1]^\sigma$ , we define  $\Phi(\xi)$  to be the element in  $[-1, 1]^\sigma$  such that

$$\Phi(\xi)(\alpha) = \begin{cases} -\xi(\overline{\rho_1(\alpha)}) & \text{if } \alpha \in \sigma \cap A(H); \\ \xi(\alpha) & \text{if } \alpha \in \sigma \setminus A(H). \end{cases}$$

Let  $\Delta_\xi$  represent

$$h(\widehat{\mathfrak{D}_T \xi}) - h(\widehat{\mathfrak{D}_{T'} \xi})$$

for every  $\xi \in [-1, 1]^\sigma$ . We proceed to show that

$$\Delta_\xi + \Delta_{\Phi(\xi)} \geq 0 \quad (53)$$

holds for all  $\xi \in [-1, 1]^\sigma$  while

$$\Delta_\xi + \Delta_{\Phi(\xi)} \geq 0 \quad (54)$$

holds for some  $\xi \in [-1, 1]^\sigma$ . When we replace  $\xi \in [-1, 1]^\sigma$  by  $\xi \in \{0, \pm 1\}^\sigma$ , the statements corresponding to (53) and (54) are proved in [WXZ16, pp. 109–114].

Especially, this shows the truth of (54). Moreover, the reader can check that the range of  $\xi$  does not make any difference to the proof of [WXZ16, Eq. (4)] and so the same argument as there establishes the validity of (53).

Finally, we are ready to derive that

$$\begin{aligned}
& 2^n (\text{LipH}(T) - \text{LipH}(T')) \\
&= 2 \int_{[-1,1]^\sigma} \overbrace{h(\mathfrak{D}_T \xi)} \, d\xi - 2 \int_{[-1,1]^\sigma} \overbrace{h(\mathfrak{D}_{T'} \xi)} \, d\xi \quad \text{by (52)} \\
&= \int_{[-1,1]^\sigma} (\overbrace{h(\mathfrak{D}_T \xi)} + \overbrace{h(\mathfrak{D}_T \Phi(\xi))}) \, d\xi - \int_{[-1,1]^\sigma} (\overbrace{h(\mathfrak{D}_{T'} \xi)} + \overbrace{h(\mathfrak{D}_{T'} \Phi(\xi))}) \, d\xi \\
&= \int_{[-1,1]^\sigma} (\Delta_\xi + \Delta_{\Phi(\xi)}) \, d\xi \\
&> 0, \quad \text{by (53) and (54)} \quad \square
\end{aligned}$$

proving (50), as wanted.

**Theorem 12.4.** *Let  $n$  be a positive integer and take  $T \in \mathcal{T}_n$ . It holds*

$$\text{SLipH}(S_n) \leq \text{SLipH}(T) \leq \text{SLipH}(P_n).$$

*The first equality holds if and only if  $T = S_n$  and the second equality holds if and only if  $T = P_n$ .*

*Proof.* By Theorem 11.5 we have  $\text{Vol}(L_T^x) = 2^{n-1}$  for all  $T \in \mathcal{T}_n$  and  $x \in V(T)$ . Accordingly, we can check that  $\text{SLipH}(T) = 2^{n-3} \text{LipH}(T)$ . Thus the result follows from Theorem 12.3(b) directly.  $\square$

**Conjecture 12.5.** *Let  $n$  be a positive integer and let  $G$  be a connected graph with  $n$  vertices.*

- (a) [LNR03, Conjecture 1]  $\text{IntLipH}(G) \leq \text{IntLipH}(P_n)$  holds.
- (b)  $\text{LipH}(G) \leq \text{LipH}(P_n)$  holds, with equality if and only if  $G = P_n$ .
- (c)  $\text{SLipH}(G) \leq \text{SLipH}(P_n)$  holds, with equality if and only if  $G = P_n$ .

Conjecture 12.5 is a statement about the real line. If we consider a general injective metric space and the corresponding Lipschitz maps, there may be even more interesting mathematics ahead.

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