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Trees, tight-spans and point configurations

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Tight-spans of metrics were first introduced by Isbell in 1964 and rediscovered and studied by others, most notably by Dress in 1984, who gave them this name. Subsequently, it has been found that tight-spans can be defined for more general maps, such as directed metrics and distances, and more recently for diversities. In this paper, we show that all of these tight-spans, as well as some related constructions, can be defined in terms of point configurations. This provides a useful way in which to study these objects in a unified and systematic way. We also show that by using point configurations we can recover results concerning one-dimensional tight-spans for all of the maps we consider, as well as extending these and other results to more general maps such as symmetric and asymmetric maps.

1. Introduction

Let V be a real vector space with some fixed basis B, and $\langle\cdot,\cdot\rangle$ denote the standard scalar product with respect to B (i.e., $\langle v, w\rangle = \sum_{b\in B}\lambda_b\mu_b$ if $v = \sum_{b\in B}\lambda_b b$, $w = \sum_{b\in B}\mu_b b$). A *point configuration* $\mathcal{A}$ in V is a finite subset of V; for technical reasons we shall always assume that the affine hull of any such configuration has codimension 1. Given a function $w : \mathcal{A} \to \mathbb{R}$, we define the *envelope* of $\mathcal{A}$ with respect to w to be the polyhedron

$$\mathcal{E}_w(\mathcal{A}) = \{x \in V\colon \langle a, x\rangle \geq -w \text{ for all } a \in \mathcal{A}\},$$

and the *tight-span* $\mathcal{T}_w(\mathcal{A})$ of $\mathcal{A}$ to be the union of the bounded faces of $\mathcal{E}_w(\mathcal{A})$. Tight-spans of point configurations were introduced in [15] for vertex sets of polytopes, as a tool for studying subdivisions of polytopes. Even so, they first appeared several years ago in a somewhat different guise.

More specifically, let X be a finite set, $V = \mathbb{R}^X$ be the vector space of functions $X \to \mathbb{R}$ and, for $x \in X$, let e_x denote the elementary function assigning 1 to x and 0 to all other $y \in X$. In addition, let D be a metric on X, that is, a symmetric map on $X \times X$ that vanishes on the diagonal and satisfies the triangle inequality. Then, as first remarked by Sturmfels and Yu [24], by setting $w(e_x + e_y) = -D(x, y)$, the tight-span $\mathcal{T}_w(\bar{\mathcal{A}}(X))$ of $\bar{\mathcal{A}}(X) = \{e_x + e_y\colon x, y \in X, x \neq y\}$ is nothing other than the *injective hull* of D that was first introduced by Isbell [20]. This object was subsequently rediscovered by Dress [8], who called it the *tight-span of* D, as well as by Chrobak and Larmore [4,5].

Since its discovery, the tight-span of a metric on a finite set has been intensively studied (see, e.g., [10,12] for overviews) and various related constructions have been introduced. These include tight-spans of *directed metrics* and *directed distances* [19], tight-spans of *polytopes* [15] and more recently the tight-span of a so-called *diversity* [3]. Note that, in contrast to the tight-span of a metric, it is not known whether or not all of these constructions are necessarily injective hulls (i.e., injective objects in some appropriate category), but for simplicity we shall still refer to them as tight-spans. Here we shall show that, as with metrics on finite sets, tight-spans of directed distances, diversities and some related maps can also all be described in terms of point configurations. This provides a useful way to systematically study these objects.

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More specifically, after presenting some preliminary results concerning point configurations in Sections 2 and 3, in Section 4 we shall show that the tight-span of a distance on X can be defined in terms of the configuration $\mathcal{A}(X) = \bar{\mathcal{A}}(X) \cup \{2e_x : x \in X\} = \{e_x + e_y : x, y \in X\}$ (Proposition 4.1). For Y a finite set with $X \cap Y = \emptyset$, let $\bar{\mathcal{B}}(X, Y) \subseteq \mathbb{R}^{X \cup Y}$ be the configuration of all points $e_x + e_y$ with $x \in X, y \in Y$ and $\mathcal{B}(X, Y) = \bar{\mathcal{B}}(X, Y) \cup \{2e_x : x \in X \cup Y\}$. We also show that the tight-span of a directed metric (distance) can be defined in terms of $\bar{\mathcal{B}}(X) = \bar{\mathcal{B}}(X, Y)$ or $\mathcal{B}(X) = \mathcal{B}(X, Y)$ if Y is considered to be a disjoint copy of X (Proposition 5.1). Using these point configurations, we will also extend this analysis to include arbitrary symmetric and even asymmetric maps (Section 5).

In Sections 6 and 7 we shall consider tight-spans of diversities, which were recently introduced in [3]. Using a relationship that we shall derive between metrics and diversities, in Section 7 we show that the tight-span of a diversity on X can be expressed in terms of the point configuration $\mathcal{C}(X) = \{\sum_{i \in A} e_i : A \in \mathcal{P}(X)\}$ (the vertices of a cube). Intriguingly, we also show that a very closely related object can also be associated with a diversity on X by considering the point configuration $\mathcal{A}(\mathcal{P}(X) \setminus \{\emptyset\})$ and that, for a special class of diversities (split system diversities) this object and the tight-span are in fact the same (Theorem 7.4).

In addition to providing some new insights on tight-spans using point configurations, we shall also pay special attention to one-dimensional tight-spans. These are important since, for example, they provide ways to generate phylogenetic trees and, more generally, phylogenetic networks (see, e.g., [9,11]). Indeed, a one-dimensional tight-span associated with a point configuration $\mathcal{A}$ and weight function w can also be regarded as a graph, with vertex set equal to that of $\mathcal{E}_w(\mathcal{A})$ and edge set consisting of precisely those pairs of vertices that both lie in a one-dimensional face of $\mathcal{E}_w(\mathcal{A})$. Since the union of bounded faces of an unbounded polyhedron is contractible (see, e.g., [18, Lemma 4.5]) it follows that a one-dimensional tight-span considered as a graph is, in fact, a tree.

The archetypal characterisation for one-dimensional tight-spans was first observed by Dress for metrics [8]:

Theorem 1.1 (*Tree Metric Theorem*)**.** *The tight-span of a metric D on a finite set X is a tree if and only if D satisfies*

$$D(x, y) + D(u, v) \leq \max\{D(x, u) + D(y, v), D(x, v) + D(y, u)\}$$

for any $x, y, u, v \in X$.

In this paper we will use point configurations to give various conditions for when tight-spans are trees in more general settings (Theorems 4.5, 5.5 and 7.3). This allows us to recover and extend various theorems connecting tight-spans and trees that arise in the literature. We conclude in Section 8 with a discussion on some possible future directions.

2. Tight-spans and splits of point configurations

In this section we shall recall some definitions and results concerning tight-spans and splits of general point configurations, as well as giving some elementary properties of these objects that we shall use later. For details, we refer the reader to [15] and [14, Section 2]. First we present a characterisation of the tight-span as the set of minimal elements of the envelope of a configuration for configurations that satisfy certain conditions. These conditions are fulfilled by all of the configurations that we shall consider. When tight-spans (of metric spaces, but also of diversities) are considered and thought of in a non-polyhedral way, this characterisation is normally used as a definition instead.

Now, as in the introduction, let V be a finite-dimensional vector space with a fixed basis B. An element of $v \in V$ is called *positive* (with respect to B) if in its representation $v = \sum_{b \in B} \lambda_b^v b$ with respect to B one has $\lambda_b^v \geq 0$ for all $b \in B$. In particular, we have a partial order $\preceq$ on V defined by $v \preceq v'$ if and only if $\lambda_b^v \leq \lambda_b^{v'}$ for all $b \in B$ (or, equivalently, $v' - v$ is positive). For a subset $A \subseteq V$ an element $a \in A$ is called *minimal* if $a \preceq a'$ implies $a = a'$ for all $a' \in A$. The set A is called *bounded from below* if there exists some $M \in \mathbb{R}$ such that $\lambda_b^v \geq M$ for all $b \in B$ and $v \in A$.

Let now $e \in \mathbb{N}$ and $\varphi : V \to \mathbb{R}^e$ be a linear map and $b \in \mathbb{R}^e$. In general, for a polyhedron $P = \{x \in V : \varphi(x) \geq b\}$, an element $x \in P$ is contained in a bounded face of P if and only if there does not exist some (non-trivial) $r \in \{x \in V : \varphi(x) \geq 0\}$ (a *ray* of P) and some $\lambda \in \mathbb{R}_{>0}$ with $x - \lambda r \in P$. Note that P is bounded from below if and only if all rays of P are positive. We now give a characterisation of tight-spans using these concepts.

Lemma 2.1. *Let $\mathcal{A} \subseteq V$ be a configuration of positive points. Then $\mathcal{T}_w(\mathcal{A})$ is a subset of the set of minimal elements of $\mathcal{E}_w(\mathcal{A})$. If, additionally, $\mathcal{E}_w(\mathcal{A})$ is bounded from below, then $\mathcal{T}_w(\mathcal{A})$ equals the set of minimal elements of $\mathcal{E}_w(\mathcal{A})$.*

Proof. Let $x \in \mathcal{T}_w(\mathcal{A})$ be non-minimal, that is, there exist $b \in B$ and $\lambda \in \mathbb{R}_{>0}$ such that $x - \lambda b \in P$. By positivity, we have $\langle a, b \rangle \geq 0$ for all $a \in \mathcal{A}$ and hence b is a ray of $\mathcal{E}_w(\mathcal{A})$ contradicting the assumption $x \in \mathcal{T}_w(\mathcal{A})$.

Conversely, let $x \in \mathcal{E}_w(\mathcal{A}) \setminus \mathcal{T}_w(\mathcal{A})$, r be a ray of $\mathcal{E}_w(\mathcal{A})$ and $\lambda \in \mathbb{R}_{>0}$ be such that $x - \lambda r \in \mathcal{E}_w(\mathcal{A})$. Since $\mathcal{E}_w(\mathcal{A})$ is bounded from below, r is positive and hence $x - \lambda r \preceq x$, so x is not minimal. However, then we have $x - \lambda_b^r b \in P$ which implies that x is not minimal. $\square$

Another simple but useful observation is the following:

Lemma 2.2. *Let $\mathcal{A} \subseteq V$ be a point configuration, $w : \mathcal{A} \to \mathbb{R}$ a weight function, $v \in V$, and $w' = w + \langle \cdot, v \rangle$. Then $\mathcal{T}_w(\mathcal{A}) = \mathcal{T}_{w'}(\mathcal{A}) + v$.*