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Optimal realizations of two-dimensional, totally-decomposable metrics

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ABSTRACT

A realization of a metric d on a finite set X is a weighted graph (G, w) whose vertex set contains X such that the shortest-path distance between elements of X considered as vertices in G is equal to d. Such a realization (G, w) is called optimal if the sum of its edge weights is minimal over all such realizations. Optimal realizations always exist, although it is NP-hard to compute them in general, and they have applications in areas such as phylogenetics, electrical networks and internet tomography. A. Dress (1984) showed that the optimal realizations of a metric d are closely related to a certain polytopal complex that can be canonically associated to d called its tight-span. Moreover, he conjectured that the (weighted) graph consisting of the zero- and one-dimensional faces of the tight-span of d must always contain an optimal realization as a homeomorphic subgraph. In this paper, we prove that this conjecture does indeed hold for a certain class of metrics, namely the class of totally-decomposable metrics whose tight-span has dimension two. As a corollary, it follows that the minimum Manhattan network problem is a special case of finding optimal realizations of two-dimensional totally-decomposable metrics.

1. Introduction

Let (X, d) be a finite metric space, that is, a finite set X, $|X| \geq 2$, together with a metric d (i.e., a symmetric map $d : X \times X \to \mathbb{R}_{\geq 0}$ that vanishes precisely on the diagonal and that satisfies the triangle inequality). A *realization* (G, w) of (X, d) consists of a graph $G = (V(G), E(G))$ with X a subset of the vertex set $V(G)$ of G, together with a weighting $w : E(G) \to \mathbb{R}_{>0}$ on the edge set $E(G)$ of G such that for all $x, y \in X$ the length of any shortest path in (G, w) between x and y equals $d(x, y)$. A realization (G, w) of d is called *optimal* if $\sum_{e\in E(G)} w(e)$ is minimal amongst all realizations of (X, d).

Realizing metrics by graphs has applications in fields such as phylogenetics, electrical networks and internet tomography. Optimal realizations were introduced by Hakimi and Yau [11] who also gave a polynomial algorithm for their computation in the special case where the metric space has a (necessarily unique) optimal realization that is a tree. Every finite metric space has an optimal realization [6,17], although they are not necessarily unique [1,6]. In general, it is NP-hard to compute optimal realizations [1,22], although recently some progress has been made in deriving heuristics for their computation [13,14].

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In [6], Dress pointed out an intriguing connection between optimal realizations and tight-spans, which we now recall. The *tight-span* $T(d)$ of the metric space (X, d) [6,18] is the set of all minimal elements (with respect to the product order) of the polyhedron

$$\mathbb{P}(d) := \{f \in \mathbb{R}^X : f(x) + f(y) \geq d(x, y) \text{ for all } x, y \in X\}.$$

Note that, in particular, $T(d)$ consists of the union of the bounded faces of $P(d)$. Moreover, the map d_∞, given by $d_\infty(f, g) = \sup_{x\in X} |f(x) - g(x)|$ for all $f, g \in \mathbb{P}(d)$, is a metric on $T(d)$ and the *Kuratowski map*

$$\kappa : X \to T(d) : x \to h_x; \qquad h_x(y) := d(x, y), \quad \text{for all } x \in X,$$

gives an isometric embedding of (X, d) into $(T(d), d_\infty)$; that is, κ is injective and preserves distances.

In [6, Theorem 5], Dress showed that the (necessarily finite and connected) weighted graph G_d consisting of the zero- and one-dimensional faces of $T(d)$ and weighting w_∞ defined by $w_\infty(\{f, g\}) := d_\infty(f, g)$, f, g zero-dimensional faces of $T(d)$, is homeomorphic to a realization of d (see Section 2 for relevant definitions). Moreover, he showed that if (G, w) is any optimal realization of (X, d), then there exists a certain map $\psi : V(G) \to T(d)$ of the vertices of G into $T(d)$ [6, Theorem 5] (see also Theorem 2.3). This led him to suspect that every optimal realization of (X, d) is homeomorphic to a subgraph of (G_d, w_∞). Even though this conjecture was disproven by Althöfer [1], the following related conjecture is still open:

Conjecture 1.1 (*cf.* (3.20) *in* [6]). *Let (X, d) be a finite metric space. Then there exists an optimal realization of (X, d) that is homeomorphic to a subgraph of (G_d, w_∞).*

Apart from having an intrinsic mathematical interest, if this conjecture were true, it could provide new strategies for computing optimal realizations, as it would provide a "search space" (albeit a rather large one in general) in which to systematically search for optimal realization [12].

Conjecture 1.1 is known to hold for metrics d that can be realized by a tree since in this case (G_d, w_∞) is precisely the tree that realizes d uniquely [17]. In this paper, we show that it also holds for a certain class of metrics that generalize tree metrics. More specifically, for a finite metric space (X, d) as above, define, for any four elements $x, y, u, v \in X$,

$$\beta(x, y; u, v) := \max\{d(x, u) + d(y, v), d(x, v) + d(y, u)\} - d(x, y) - d(u, v)$$

and put $\alpha(x, y; u, v) := \max(\beta(x, y; u, v), 0)$. The metric d is called *totally-decomposable* if for all $t, x, y, u, v \in X$ the inequality $\beta(x, y; u, v) \leq \alpha(x, t; u, v) + \alpha(x, y; u, t)$ holds [2]. Such metrics are commonly used to understand genetic data in phylogenetic analysis. Defining the *dimension* of d to be the dimension of $T(d)$ (regarded as a subset of $\mathbb{R}^X$), we shall prove the following result.

Theorem 1.2. *Let (X, d) be a totally-decomposable finite metric space with dimension two. Then there exists an optimal realization of (X, d) that is homeomorphic to a subgraph of (G_d, w_∞).*

In fact this immediately follows from a somewhat stronger theorem that we shall prove (Theorem 4.1), which shows that a certain special type of optimal realization of a two-dimensional, totally-decomposable metric d can be found as a homeomorphic subgraph of (G_d, w_∞). Note also that Theorem 1.2 implies that the optimal realization problem for l_1-planar metrics is equivalent to the Minimum Manhattan Network (MMN) problem; since the MMN problem is NP-hard [4], the optimal realization problem for two-dimensional metrics is also NP-hard (see [12, Section 5] for more details and some algorithmic consequences).

Our proof of Theorem 1.2 heavily relies on the two-dimensionality of the tight-span, and we do not know how to extend our arguments to totally-decomposable metrics. Even so, it might be of interest to try and extend our result to two-dimensional metrics in general, especially as a great deal is known concerning the structure of their tight-spans (e.g., [15,19]). Indeed, our proof of Theorem 1.2 relies on a close relationship between tight-spans and so-called Buneman or median complexes, and so results concerning median complexes and folder complexes [3] could potentially help yield a more general result for two-dimensional metrics.

The remainder of this paper is organized as follows. We recall some definitions and results in Section 2. We will then present a theorem about embeddings of realizations into the Buneman complex in Section 3 which uses the new notions of split-flow digraphs and split potentials. Finally, we establish our main result in Section 4, from which Theorem 1.2 follows.

2. Preliminaries and previous results

In this section, we will state the known definitions and results that are used in the rest of the paper.

2.1. Graphs

A *weighted graph* (G, w) is a graph G with vertex set $V(G)$ and edge set $E(G) \subseteq \binom{V(G)}{2}$ together with a weight function $w : E(G) \to \mathbb{R}_{>0}$ that assigns a positive weight or *length* to each edge. A weighted graph (G', w') is a *subgraph* of (G, w) if