

OPTIMAL REALISATIONS OF TWO-DIMENSIONAL, TOTALLY-DECOMPOSABLE METRICS

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ABSTRACT. A realisation 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 realisation (G, w) is called optimal if the sum of its edge weights is minimal over all such realisations. Optimal realisations 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. In [Adv. in Math. **53**, 1984, 321-402] A. Dress showed that the optimal realisations 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 realisation 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.

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 $d : X \times X \rightarrow \mathbb{R}_{\geq 0}$ that vanishes precisely on the diagonal and that satisfies the triangle inequality). A *realisation* (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 $w : E(G) \rightarrow \mathbb{R}_{> 0}$ 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 realisation (G, w) of d is called *optimal* if $\sum_{e \in E(G)} w(e)$ is minimal amongst all realisations of (X, d) .

Realising metrics by graphs has applications in fields such as phylogenetics [26, 28], electrical networks [16], psychology [8], compression software [27] and internet tomography [7]. Optimal realisations were introduced by Hakimi and Yau [16] who also gave a polynomial algorithm for their computation in the special case where the metric space has a (necessarily unique) optimal realisation that is a

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tree. Every finite metric space has an optimal realisation [11, 22], although they are not necessarily unique [11, 2]. In general, it is NP-hard to compute optimal realisations [2, 29], although recently some progress has been made in deriving heuristics for their computation [17, 18] (see also [1, 3]).

In [11], Dress pointed out an intriguing connection between optimal realisations and tight-spans, which we now recall. The *tight-span* $T(d)$ of the metric space (X, d) [23] (see also [11] and [6]) is the set of all minimal elements (with respect to the product order) of

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

The map d_∞ , given by $d_\infty(f, g) = \sup_{x \in X} |f(x) - g(x)|$ for all $f, g \in P(d)$, is a metric on $T(d)$ and the *Kuratowski map*

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

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

Regarding $T(d)$ as a polytopal complex (see Section 2.4 for details), 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 realisation of d [11, Theorem 5] (see Section 2.1 for relevant definitions). Moreover, he showed that if (G, w) is any optimal realisation of (X, d) , then there exists a certain map $\psi : V(G) \rightarrow T(d)$ of the vertices of G into $T(d)$ [11, Theorem 5] (see also Theorem 2.3 below). This led him to suspect that every optimal realisation of (X, d) is homeomorphic to a subgraph of (G_d, w_∞) . Even though this conjecture was disproven by Althöfer [2], the following related conjecture is still open:

Conjecture 1.1 ((3.20) in [11]). Let (X, d) be a finite metric space. Then there exists an optimal realisation of (X, d) that is homeomorphic to a subgraph of (G_d, w_∞) .

If this conjecture were true, it could provide interesting new strategies for computing optimal realisations, as it would provide a “search space” (albeit a rather large one in general!) in which to look for optimal realisations. This strategy has already been exploited in [10], where it is pointed out that the cut-vertices of *any* optimal realisation of a metric d must be contained in the tight-span of d .

Conjecture 1.1 is known to hold for metrics d that can be realised by a tree since in this case (G_d, w_∞) is precisely the tree that realises d . In this paper, we will show that it also holds for a certain class of metrics that generalise 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 $\alpha(x, y; u, v) := \max(\beta(x, y; u, v), 0)$. Then 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. Such metrics were introduced by Bandelt and Dress [4], and they are commonly used by evolutionary biologists to construct phylogenetic networks (see, e.g., [5, 21]). 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:

Theorem 1.2. *Let (X, d) be a totally-decomposable finite metric space with dimension two. Then there exists an optimal realisation 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 5.1), which essentially states that any “well-behaved” optimal realisation of a two-dimensional, totally-decomposable metric d can be found as a homeomorphic subgraph of (G_d, w_∞) .

The proof of this theorem heavily relies on the two-dimensionality of the tight-span. Indeed, we do not know how to extend Theorem 1.2 to even three-dimensional totally-decomposable metrics (see Example 3.2). In another direction, it might be of interest to try and extend this result to two-dimensional metrics in general, for which a fair amount is known concerning the structure of their tight-span [24, 19].

The remainder of this paper is organised as follows. We recall some definitions and results in Section 2. Section 3 discusses embeddings of realisations into the Buneman complex, a polytopal complex which is closely related to the tight-span, and which is precisely the tight-span for the metrics that we consider. We will also present a theorem about embeddings of realisations into the Buneman complex in Section 4 which uses the new notions of split-flow graphs and split potentials. Finally, we establish Theorem 1.2 in Section 5.

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 $w : E(G) \rightarrow \mathbb{R}_{>0}$ that assigns a positive weight or *length* to each edge. A weighted graph (G', w') is a *subgraph* of (G, w) if $V(G') \subseteq V(G)$, $E(G') \subseteq \{e \in E(G) \mid e \subseteq V(G')\}$ and $w' = w|_{E(G')}$. The *length* of (G, w) is $l(G, w) := \sum_{e \in E(G)} w(e)$. A *path* P from u to v in G is a sequence $u = v_0, v_1, \dots, v_{k-1}, v_k = v$ of vertices in G such that $\{v_{i-1}, v_i\} \in E(G)$ for all $1 \leq i \leq k$ and the *length* of P is defined as $w(P) := \sum_{i=1}^k w(\{v_{i-1}, v_i\})$. It is easily observed that for any $W \subseteq V(G)$ the map setting $d_{(G,w)}(u, v)$ to be the length of a shortest path between u and v defines a metric space $(W, d_{(G,w)})$.

We *suppress* a vertex of degree two in a weighted graph when we remove it and replace its two incident edges by a single edge whose length is equal to the sum of their lengths. Given two weighted graphs (G_1, w_1) and (G_2, w_2) , they are *isomorphic* if there exists an isomorphism between G_1 and G_2 that also preserves the length of each edge; they are *homeomorphic* if there exist two isomorphic weighted graphs (G'_1, w'_1) and (G'_2, w'_2) such that (G'_i, w'_i) ($i = 1, 2$) can be obtained from (G_i, w_i) by suppressing a sequence of degree two vertices.

As mentioned in the introduction, a weighted graph (G, w) with $X \subseteq V(G)$ and $d = d_{(G, w)}$ is called a *realisation* of the metric space (X, d) . The elements in $V(G) \setminus X$ are called *auxiliary vertices* of the realisation, and throughout this paper we will use the convention that all auxiliary vertices of degree two are suppressed.

2.2. Optimal realisations and geodesics. We now recall some well-known observations concerning optimal realisations.

Lemma 2.1 (Lemma 2.1 in [2]). *Let (G, w) be an optimal realisation of a finite metric space (X, d) . Then*

- (1) *For any edge $e \in E(G)$, there exist two elements $x, x' \in X$ such that e belongs to all shortest paths between x and x' .*
- (2) *For any two edges in $E(G)$ that share a common vertex, there exists a shortest path between two elements of X that contains these edges.*

As a consequence we have:

Corollary 2.2. *Let (G, w) be an optimal realisation of a finite metric space (X, d) . Then G is triangle-free.*

Proof. Suppose that we have $v_1, v_2, v_3 \in V(G)$ and edges $e_1 = \{v_1, v_2\}, e_2 = \{v_2, v_3\}, e_3 = \{v_3, v_1\} \in E(G)$. Since e_1 and e_2 share the common vertex v_2 , Lemma 2.1 (2) implies that there exists shortest path in (G, w) containing e_1 and e_2 . In particular, this implies $w(e_1) + w(e_2) \leq w(e_3)$, because otherwise e_1 and e_2 could be replaced by e_3 to get a shorter path. Similarly, we derive $w(e_2) + w(e_3) \leq w(e_1)$ and $w(e_3) + w(e_1) \leq w(e_2)$, a contradiction to the fact that w only takes strictly positive values. ■

As mentioned in the introduction, not all optimal realisations are homeomorphic to subgraphs of the tight-span. However, we will now present some properties of optimal realisations that will guarantee this property. If (G, w) is a weighted graph and $A \subseteq V(G)$, we denote by $\Gamma(G, w; A)$ the set of shortest paths in G connecting elements of A . An optimal realisation (G, w) of a metric space (X, d) is called *path-saturated* if $|\Gamma(G, w; X)| \geq |\Gamma(G', w'; X)|$ holds for all optimal realisations (G', w') of (X, d) . If in addition the number of vertices $V(G)$ is minimal among all path-saturated realisations of (X, d) , then (G, w) is called a *minimal path-saturated realisation* of (X, d) .

Now, if (X, d) is a (not necessarily finite) metric space, a function $\gamma : [0, 1] \rightarrow X$ is called a *geodesic* in (X, d) if for all $a < b < c \in [0, 1]$ one has $d(\gamma(a), \gamma(c)) = d(\gamma(a), \gamma(b)) + d(\gamma(b), \gamma(c))$. Note that this implies that γ is continuous. A map $\psi : X \rightarrow X'$ between two arbitrary metric spaces (X, d) and (X', d') is called *non-expansive*, if $d'(\psi(x_1), \psi(x_2)) \leq d(x_1, x_2)$ for all $x_1, x_2 \in X$. If ψ^{-1} exists and is non-expansive, too, ψ is an *isometry* and (X, d) and (X', d') are said to be *isometric*.

For a weighted graph (G, w) we denote by $\|(G, w)\|$ its *geometric realisation*, that is, the metric space obtained by regarding each edge $e \in E(G)$ as a real interval of length $w(e)$ and gluing them together at the vertices of G (see, e.g., Daverman and Sher [9, p. 547] for details of this construction). For $X \subset V(G)$ a function $\gamma : [0, 1] \rightarrow \|(G, w)\|$ is called an *X-geodesic* if it is a geodesic between two points of X interpreted as points in $\|(G, w)\|$.

The following theorem gives us a way to relate the geometric realisation of an optimal realisation of a metric with its tight-span. The first part is due to Dress [11, Theorem 5], and the second part is given in [25, Proposition 7.1].

Theorem 2.3. *Let (G, w) be an optimal realisation of a finite metric space (X, d) . Then there exists a non-expansive map ψ from $\|(G, w)\|$ to $(T(d), d_\infty)$ such that $\psi(x) = \kappa(x)$ for all $x \in X$. If, in addition, (G, w) is path-saturated, then ψ is injective.*

2.3. Splits and total-decomposability. A *split* $S = \{A, B\}$ of a set X is a bipartition of X , that is $A \cup B = X$ and $A \cap B = \emptyset$. A *weighted split system* (\mathcal{S}, α) on X is a pair consisting of a set \mathcal{S} of splits of X , and a weight function $\alpha : \mathcal{S} \rightarrow \mathbb{R}_{>0}$. For all $x, y \in X$, we set $\mathcal{S}(x, y) = \{\{A, B\} \in \mathcal{S} \mid x \in A, y \in B \text{ or } x \in B, y \in A\}$ and define

$$d_{(\mathcal{S}, \alpha)}(x, y) = \sum_{S \in \mathcal{S}(x, y)} \alpha(S).$$

If $\mathcal{S}(x, y) \neq \emptyset$ for all distinct $x, y \in X$, the pair $(X, d_{(\mathcal{S}, \alpha)})$ becomes a finite metric space.

Two splits $\{A, B\}$ and $\{A', B'\}$ of X are called *incompatible* if none of the four intersections $A \cap A'$, $A \cap B'$, $B \cap A'$ and $B \cap B'$ is empty. A weighted split system (\mathcal{S}, α) is called (1) *two-compatible* if \mathcal{S} does not contain three pairwise incompatible splits, (2) *weakly compatible* if for any three splits S_1, S_2, S_3 in \mathcal{S} , there exist $A_i \in S_i$, for each $i \in \{1, 2, 3\}$, such that $A_1 \cap A_2 \cap A_3 = \emptyset$, and (3) *octahedral-free* if there exists no partition $X = X_1 \sqcup \dots \sqcup X_6$ of X into six non-empty subsets X_i , $1 \leq i \leq 6$, such that each one of the following four splits:

$$\begin{aligned} S_1 &= \{X_1 \sqcup X_2 \sqcup X_3, X_4 \sqcup X_5 \sqcup X_6\}, & S_2 &= \{X_2 \sqcup X_3 \sqcup X_4, X_5 \sqcup X_6 \sqcup X_1\}, \\ S_3 &= \{X_3 \sqcup X_4 \sqcup X_5, X_6 \sqcup X_1 \sqcup X_2\}, & S_4 &= \{X_1 \sqcup X_3 \sqcup X_5, X_2 \sqcup X_4 \sqcup X_6\} \end{aligned}$$

belongs to \mathcal{S} . Note that it is easily seen that two-compatible split systems are octahedral-free.

It can be shown (cf. [14]) that a metric space (X, d) is totally-decomposable if and only if there exists a weakly compatible weighted split system (\mathcal{S}, α) on X such that $d = d_{(\mathcal{S}, \alpha)}$. Furthermore, if (X, d) is totally-decomposable, then d has dimension at most two if and only if (\mathcal{S}, α) is two-compatible (cf. [14]). From now on we will call two-dimensional, totally-decomposable metric spaces *two-decomposable*.

2.4. Polytopal complexes. We now recall some definitions about polytopes (see [30] for further details). A *polyhedron* P is the intersection of a finite collection of halfspaces in a real vector space \mathbb{V} , and a *polytope* is a bounded polyhedron. For any linear functional $L : \mathbb{V} \rightarrow \mathbb{R}$ the set $F = \{x \in P \mid L(x) = \max_{y \in P} L(y)\}$ is called a *face* of P , as is the empty set. The zero- and one-dimensional faces are called *vertices* and *edges* of P and they naturally gives rise to a *graph* of the polyhedron. A *cell complex* (or *polytopal complex*) P is a finite collection of polytopes (called *cells*) such that each face of a member of P is itself a member of P , and the intersection of two members of P is a face of each. We denote the set of vertices of P by $V(P)$. Two cell complexes P, P' are *isomorphic* if there exists a bijection π (called *cell-complex isomorphism*) between them such that for all $F, F' \in P$ the cell F is a face of F' if and only if $\pi(F)$ is a face of $\pi(F')$. Examples of cell complexes include the set of all faces of a polytope or the set of all bounded faces of a polyhedron.

For a finite metric space (X, d) , the set $P(d)$ defined in the introduction is obviously a polyhedron and it can be easily observed that $T(d)$ is the union of bounded faces of $P(d)$ (cf. [11]) and hence naturally carries the structure of a cell complex $\mathbb{T}(d)$.

2.5. The Buneman complex. The Buneman complex is a cell complex that can be associated to any weighted split system, and that has proven useful in, for example, understanding the structure of the tight-span of a totally-decomposable metric [15]. It is defined as follows. Given a weighted split system (\mathcal{S}, α) on X we define its *support* to be the set $\text{supp}(\alpha) := \{A \subseteq X \mid \text{there exists } S \in \mathcal{S} \text{ with } A \in S\}$. Consider the polytope (which is a hypercube)

$$H(\mathcal{S}, \alpha) := \left\{ \mu \in \mathbb{R}_{\geq 0}^{\text{supp}(\alpha)} \mid \mu(A) + \mu(B) = \alpha(S) \text{ for all } S \in \mathcal{S} \right\}.$$

Its subset

$$B(\mathcal{S}, \alpha) := \{ \mu \in H(\alpha) \mid \mu(A) \neq 0 \neq \mu(B) \text{ and } A \cup B = X \Rightarrow A \cap B = \emptyset \}$$

carries the structure of a cell complex and is the *Buneman complex* $\mathbb{B}(\mathcal{S}, \alpha)$ of (\mathcal{S}, α) . Obviously, the set of vertices of $H(\mathcal{S}, \alpha)$ consists of those $\mu \in H(\mathcal{S}, \alpha)$ with $\mu(A) \in \{0, \alpha(\{A, X \setminus A\})\}$ for all $A \in \text{supp}(\alpha)$. It is easily seen that the set $V(B(\mathcal{S}, \alpha))$ of vertices of $B(\mathcal{S}, \alpha)$ consists of the $\mu \in B(\mathcal{S}, \alpha)$ with this property.

Setting

$$d_1(\mu, \nu) := \frac{1}{2} \sum_{A \in \text{supp}(\alpha)} |\mu(A) \setminus \nu(A)|$$

for all $\mu, \nu \in B(\mathcal{S}, \alpha)$, we obtain a metric space $(B(\mathcal{S}, \alpha), d_1)$ and the map $\Phi : X \rightarrow B(\mathcal{S}, \alpha)$ defined via

$$(1) \quad \Phi(x)(A) := \begin{cases} \alpha(\{A, X \setminus A\}) & \text{if } x \in A; \\ 0 & \text{else,} \end{cases}$$

for any $x \in X$ and $A \in \text{supp}(\alpha)$ is an isometric embedding from $(X, d_{(\mathcal{S}, \alpha)})$ to $(B(\mathcal{S}, \alpha), d_1)$.

There exists a natural map $\Lambda : \mathbb{R}^{\text{supp}(\alpha)} \rightarrow \mathbb{R}^X, \mu \mapsto f_\mu$ where

$$f_\mu(x) = \sum_{A \in \text{supp}(\alpha)} \mu(A) \quad \text{for all } x \in X.$$

It is easily seen that $\Lambda(\Phi(x)) = \kappa(x)$ for all $x \in X$. Depending on properties of the split system (\mathcal{S}, α) , this map takes elements from $H(\mathcal{S}, \alpha)$ to elements of $P(d_{(\mathcal{S}, \alpha)})$ or even from $B(\mathcal{S}, \alpha)$ to elements of $T(d_{(\mathcal{S}, \alpha)})$; see [15, 12, 13] for details. In case (\mathcal{S}, α) is weakly compatible and octahedral-free the following holds:

Theorem 2.4 (Theorem 3.1 in [15]). *If (\mathcal{S}, α) is a weakly compatible, octahedral-free weighted split system on X , then the map $\Lambda|_{B(\mathcal{S}, \alpha)}$ is a bijection onto $T(d_{(\mathcal{S}, \alpha)})$ that induces a cell-complex isomorphism $\Lambda' : \mathbb{B}(\mathcal{S}, \alpha) \rightarrow \mathbb{T}(d_{(\mathcal{S}, \alpha)})$.*

Recall that if \mathcal{S} is two-compatible, then it is weakly compatible and octahedral-free. In fact, in the two-compatible case we know even more about the relation between $B(\mathcal{S}, \alpha)$ and $T(d_{(\mathcal{S}, \alpha)})$.

Theorem 2.5. *Suppose that (\mathcal{S}, α) is a two-compatible weighted split system on X . Then the following hold:*

- (1) *The cell complex $\mathbb{B}(\mathcal{S}, \alpha)$ is at most two-dimensional and all two dimensional cells are quadrangles.*
- (2) *The map $\Lambda|_{B(\mathcal{S}, \alpha)} : B(\mathcal{S}, \alpha) \rightarrow T(d_{(\mathcal{S}, \alpha)})$ is an isometry of the metric spaces $(B(\mathcal{S}, \alpha), d_1)$ and $(T(d_{(\mathcal{S}, \alpha)}), d_\infty)$.*

Proof. (1) By [14, Lemma 2.1], the dimension of $B(\mathcal{S}, \alpha)$ is bounded by two if (\mathcal{S}, α) is two-compatible. Corollary 7.3 in [20] states that for weakly compatible split systems (\mathcal{S}, α) all cells in $\mathbb{T}(d_{(\mathcal{S}, \alpha)})$ are isomorphic to either hypercubes or rhombic dodecahedra. Hence (1) follows from Theorem 2.4.

(2) This follows from (1) in connection with the equivalence of (i) and (vi) in [14, Theorem 1.1 (c)]. ■

3. EMBEDDINGS IN THE TIGHT-SPAN AND THE BUNEMAN COMPLEX

We have seen in the introduction that any metric space (X, d) can be embedded into its tight-span and that $d(x, y) = d_\infty(x, y) = d_{(G_d, w_\infty)}(x, y)$ holds for all $x, y \in X$. A key in the proof of our main theorem will be the following observation, which shows that for two-decomposable metrics the latter equality holds for general vertices of the tight-span.

Proposition 3.1. *Let (X, d) be a two-decomposable metric space. Then for any two elements $f, g \in V(T(d))$, we have $d_\infty(f, g) = d_{(G_d, w_\infty)}(f, g)$.*

Proof. For any geodesic $\gamma : [0, 1] \rightarrow T(d)$ denote by $\Omega(\gamma)$ the set of all cells C in $\mathbb{T}(d)$ with dimension greater or equal to two such that their intersection with γ is not contained in the union of the vertices and edges of $\mathbb{T}(d)$. By Theorem 2.5 (1), all elements of $\Omega(\gamma)$ are quadrangles. It now suffices to show that for any distinct $f, g \in V(T(d))$ there exists a geodesic γ between f and g with $\Omega(\gamma) = \emptyset$.

Suppose that is not the case and let γ be a geodesic between f and g such that the set $\Omega(\gamma)$ has minimal cardinality among all those geodesics. For any $C \in \Omega(\gamma)$, denote the minimal (resp. maximal) element $t \in [0, 1]$ with $\gamma(t) \in C$ by t_C^- (resp. t_C^+). Since γ is a geodesic, $\gamma(t) \in C$ holds if and only if $t \in [t_C^-, t_C^+]$.

Let $C \in \Omega(\gamma)$ be the first two-dimensional cell met by γ , that is, the one with minimal t_C^- . Clearly, $\gamma(t_C^-) \in V(T(d))$ and, since C is a quadrangle, there exists a geodesic segment γ' between $\gamma(t_C^-)$ and $\gamma(t_C^+)$ using only the boundary edges of C . This allows us to construct a geodesic γ^* between f and g with $|\Omega(\gamma^*)| = |\Omega(\gamma)| - 1$, a contradiction. \blacksquare

The following example shows that Proposition 3.1 is not true for totally-decomposable metrics of dimension greater or equal to three.

Example 3.2. Let $X = \{1, 2, \dots, 6\}$, and

$$\mathcal{S} = \left\{ \{1, 2, 3\}, \{4, 5, 6\}, \{2, 3, 4\}, \{5, 6, 1\}, \{3, 4, 5\}, \{6, 1, 2\} \right\}.$$

It is easily seen that \mathcal{S} is weakly compatible and hence the metric $d_{(\mathcal{S}, \alpha)}$ is totally-decomposable for any weight function $\alpha : \mathcal{S} \rightarrow \mathbb{R}_{>0}$. The tight-span of $d_{(\mathcal{S}, \alpha)}$ is three-dimensional: It is a cuboid whose edge-lengths are the values of α and six of its vertices correspond to the elements of X . If α assigns 1 to each split, we have a cube with edge-length 1 and the two remaining vertices have coordinates $u = (1, 2, 1, 2, 1, 2)$ and $v = (2, 1, 2, 1, 2, 1)$. So $d_\infty(u, v) = 1$ but $d_{(G_d, w_\infty)}(u, v) = 3$.

We now start to investigate embeddings of optimal realisations into the Buneman complex given by Theorem 2.3 and show that they have the following useful property (where Φ is the map defined in Equation 1):

Theorem 3.3. *Let (\mathcal{S}, α) be a weighted split system on X and (G, w) a minimal path-saturated optimal realisation of $(X, d_{(\mathcal{S}, \alpha)})$. Then for any non-expansive map $\psi : \|(G, w)\| \rightarrow B(\mathcal{S}, \alpha)$ with $\psi(x) = \Phi(x)$ for all $x \in X$ we have $\psi(V(G)) \subseteq V(B(\mathcal{S}, \alpha))$.*

We shall prove this theorem at the end of the next section. However, first we will introduce and investigate the notions of split-flow digraphs and split potentials.

4. SPLIT-FLOW DIGRAPHS AND SPLIT POTENTIALS

We begin with some presenting some notation for digraphs. A *directed graph* (or *digraph* for short) $D = (V, \mathcal{A})$ is a pair consisting of a set V of vertices and a subset $\mathcal{A} \subseteq V \times V$, whose elements are called the *arcs* of D . A sequence v_0, v_1, \dots, v_k of vertices of D is called a *directed path* (from v_0 to v_k) in D if $(v_{i-1}, v_i) \in \mathcal{A}$ holds for all $i = 1, \dots, k$. A *strong connected component* in D is a maximal subset C of V such that for all distinct $u, v \in C$ there exists a directed path from u to v . Obviously, the set of strong connected components forms a partition of V .

Given a realisation (G, w) of a finite metric space (X, d) and $A \subseteq X$, the *split-flow digraph* $D(G, w; A)$ is the digraph with vertex set $V(G)$ and arc set

$$\begin{aligned} \mathcal{A} := & \{(u, v), (v, u) \in V \times V \mid \text{there exists } x, y \in A \text{ or } x, y \in X \setminus A \\ & \text{such that } \{u, v\} \text{ belongs to a shortest path from } x \text{ to } y \text{ in } (G, w)\} \\ & \cup \{(u, v) \in V \times V \mid \text{there exists } x \in A \text{ and } y \in X \setminus A \\ & \text{such that } \{u, v\} \text{ belongs to a shortest path from } x \text{ to } y \text{ in } (G, w)\}. \end{aligned}$$

If (G, w) is an optimal realisation, Lemma 2.1 implies that for each $\{u, v\} \in E(G)$ we have $(u, v) \in \mathcal{A}$ or $(v, u) \in \mathcal{A}$ and both hold if and only if $\{u, v\}$ belongs to a shortest path between two elements of A or between two elements of $X \setminus A$. Furthermore, this implies that there exist strong connected components C_A and $C_{X \setminus A}$ such that $A \subseteq C_A$ and $X \setminus A \subseteq C_{X \setminus A}$. (Note that C_A and $C_{X \setminus A}$ might be equal.) For the case of minimal path-saturated optimal realisations, we will now see that these are the only strong connected components of $D(G, w; A)$.



FIGURE 1. An example of split-flow digraphs: the picture on the left is (G, w) , an optimal realisation of the metric in [2]; the picture on the right is $D(G, w; A)$, the split-flow digraph for (G, w) and $A = \{a, b, c\}$.

Proposition 4.1. *Let (G, w) be a minimal path-saturated optimal realisation of a metric space (X, d) and $A \subseteq X$. Then the number of strong connected components of the split-flow digraph $D(G, w; A)$ is either one or two.*

Proof. Let $D := (V, \mathcal{A}) := D(G, w; A)$. To establish the proposition, it suffices to show that there can not exist a strong component of D that is distinct from both C_A and $C_{X \setminus A}$. Suppose that there exists such a strong connected component W and define the map $\delta : E(G) \rightarrow \mathbb{R}$ as

$$\delta(\{u, v\}) := \begin{cases} +1, & \text{if } (u, v) \in \mathcal{A} \text{ with } u \in V \setminus W, v \in W, \\ -1, & \text{if } (u, v) \in \mathcal{A} \text{ with } u \in W, v \in V \setminus W, \\ 0, & \text{otherwise.} \end{cases}$$

So for any $e \in E(G)$ we have $\delta(e) = +1$ (resp. $\delta(e) = -1$) if e induces an arc in D that is *entering* (resp. *leaving*) W . By exchanging A and $X \setminus A$ if necessary, we can assume that the difference N of arcs entering W and arcs leaving W is non-negative. Since W is a strong connected component, for all $u \in V \setminus W$ and $v \in W$ with $\{u, v\} \in E(G)$, we have either $(u, v) \in \mathcal{A}$ or $(v, u) \in \mathcal{A}$, but not both. Therefore the above map δ is well defined.

Define $t := \min\{w(e) \mid e \in E(G) \text{ and } \delta(e) = -1\}$. For any $\epsilon \in (0, t)$, the map $w_\epsilon : E(G) \rightarrow \mathbb{R}_{>0}$ defined as

$$w_\epsilon(e) := w(e) + \epsilon\delta(e)$$

is a weight function on $E(G)$, and hence (G, w_ϵ) is a weighted graph. Now let $P \in \Gamma(G, w; X)$ be a shortest path in (G, w) . Since $X \cap W = \emptyset$, the number of edges in P entering W equals the number of edges in P leaving W , so we have $w(P) = w_\epsilon(P)$. This implies

$$d_{(G, w_\epsilon)}(x, y) \leq d_{(G, w)}(x, y) = d(x, y) \text{ for all } x, y \in X.$$

Since there are only finitely many paths in G , we can choose $\epsilon_0 > 0$ in such a way there does not exist a $P \in \Gamma(G, w_{\epsilon_0}; X)$ that was not in $\Gamma(G, w; X)$, hence (G, w_{ϵ_0}) is a realisation of (X, d) . Moreover, we have $l(G, w_{\epsilon_0}) = l(G, w) - \epsilon_0 N$, which, since (G, w) is optimal, implies $N = 0$ and that (G, w_{ϵ_0}) is optimal, too.

Now put

$$\epsilon' := \sup\{\epsilon \in (0, t) \mid (G, w_\epsilon) \text{ is a realisation of } (X, d)\}.$$

We distinguish two cases:

Case 1: $\epsilon' < t$. Our arguments above imply that $(G, w_{\epsilon'})$ is an optimal realisation of (X, d) . Let $\epsilon > \epsilon'$. Then the weighted graph (G, w_ϵ) is not a realisation of (X, d) , so there exists a path P connecting $x, y \in X$ with $w_\epsilon(P) < d(x, y)$. Since $w_{\bar{\epsilon}}(P) \geq d(x, y)$ for all $\bar{\epsilon} < \epsilon'$ and $w_t(P)$ is a continuous function in t , we get $w_{\epsilon'} = d(x, y)$. Obviously, by the construction of w_ϵ , we have $P \notin \Gamma(G, w; X)$. Since $P \in \Gamma(G, w_{\epsilon'}; X)$ this is a contradiction to the fact that (G, w) is path-saturated.

Case 2: $\epsilon' = t$. Let

$$M := \{\{u, v\} \in E(G) \mid w(\{u, v\}) = t \text{ and } (u, v) \in \mathcal{A} \text{ leaves } W\}.$$

We will first show that no two edges in M share a common vertex. Suppose M contains $e_1 = \{u, v\}$ and $e_2 = \{v, u'\}$ for some $u, v, u' \in V(G)$. We may assume $v \in W$ and $u, u' \in V \setminus W$, as the other case (i.e., $u, u' \in W$ and $v \in V \setminus W$) is similar. By Lemma 2.1 (2), this implies that e_1 and e_2 are contained in a shortest path between two elements of X . By the construction of D , this is a contradiction to the assumption that W is a strong connected component.

Now let G' be the graph obtained from G by *contracting* all edges in M . That is, for every edge $e = \{u, v\}$ in M , where $u \in W$, we add an edge $\{u', v\}$ for all $u' \neq v$ that is adjacent to u , and delete u and all edges incident to it. Since G is triangle-free by Corollary 2.2 and all edges in M are disjoint, the graph G' is well-defined. We define the weight function $w' : E(G') \rightarrow \mathbb{R}_{>0}$ by setting $w'(e) = w(e) + t\delta(e)$ if $e \in E(G)$ and $w'(e) = w(e^*) + t\delta(e^*)$ otherwise, where $e^* = \{u', u\}$ for the unique vertex u in G so that $\{u, v\} \in M$.

Since contracting length-zero edges does not change any path lengths, (G', w') is an optimal realisation of (X, d) . Now it remains to show $|\Gamma(G', w'; X)| \geq |\Gamma(G, w; X)|$, because this implies (G', w') is a path-saturated optimal realisation of (X, d) with $|V(G')| < |V(G)|$, a contradiction as required.

To this end, let $P_1, P_2 \in \Gamma(G, w; X)$ and $P'_1, P'_2 \in \Gamma(G', w'; X)$ be the paths obtained by contracting all its edges contained in M . If $P'_1 = P'_2$, then there exists some edge $e = \{u, v\} \in M$ such that e is contained in exactly one path among P_1, P_2 , say P_1 . Switching the role of u and v if necessarily, we have $(u, v) \in \mathcal{A}$. Let s be the other vertex in P that is adjacent to u . Since no edges in M share a common vertex, we have $\{s, u\} \notin M$ and hence $\{s, v\} \in P'_1 = P'_2$. Again using the fact that no two edges in M share a common vertex, we get $\{s, v\} \in P_2$ and so $\{u, v\}, \{s, v\}, \{s, u\} \in E(G)$, contradicting Corollary 2.2. ■

Remark 4.2. It would be interesting to know whether the following statement is true: Let (\mathcal{S}, α) be a weighted weakly-compatible split system on a set X , (G, w) a minimal path-saturated optimal realisation of (X, d) and $A \in \text{supp}(\alpha)$ (i.e., $\{A, X \setminus A\}$ is a d -split). Then the number of strong connected components of the split-flow digraph $D(G, \alpha; A)$ is exactly two.

Let (G, w) be a realisation of (X, d) . A map $\lambda : ||(G, w)|| \rightarrow [0, 1]$ is called a *split potential* on $|| (G, w) ||$ if

- (1) $\lambda(x) \in \{0, 1\}$ for all $x \in X$, and
- (2) $\lambda \circ \gamma : [0, 1] \rightarrow [0, 1]$ is monotonic for all X -geodesics $\gamma : [0, 1] \rightarrow ||(G, w)||$.

Lemma 4.3. *Let (G, w) be a minimal path-saturated optimal realisation of (X, d) and λ a split potential on $|| (G, w) ||$. Then $\lambda(v) \in \{0, 1\}$ holds for all $v \in V(G)$.*

Proof. Let A be the set of all $x \in X$ that are mapped to 0 by λ and let $D = (V, \mathcal{A})$ be the split-flow digraph $D(G, w; A)$.

We will now show that $(u, v) \in \mathcal{A}$ implies that $\lambda(u) \leq \lambda(v)$. This implies that λ restricted to any strong connected component of D is a constant, and the lemma then follows from Proposition 4.1.

So let $(u, v) \in \mathcal{A}$. If $u \in A$ or $v \in X \setminus A$, then $\lambda(u) \leq \lambda(v)$ obviously holds. Otherwise, there exists $x, y \in X$ and a shortest path P in (G, w) from x to y such that $\{u, v\}$ is an edge in P and either $x \in A$ or $y \in X \setminus A$. Here we shall consider the case $x \in A$ since the other one is similar. The path P induces an X -geodesic γ between x and y that passes first through u and then through v . Since $\lambda \circ \gamma$ is monotonic and $\lambda(\gamma(0)) = \lambda(x) = 0 < 1 = \lambda(y) = \lambda(\gamma(1))$, we get $\lambda(u) \leq \lambda(v)$, as required. \blacksquare

We now present a specific way to define split potentials using the Buneman complex, which will allow us to prove Theorem 3.3.

Let (\mathcal{S}, α) be a weighted split system on X . For any $A \in \text{supp}(\alpha)$, define the map $\lambda_A : B(\mathcal{S}, \alpha) \rightarrow [0, 1]$ by putting

$$\lambda_A(\mu) := \frac{\mu(A)}{\alpha(\{A, X \setminus A\})} \quad \text{for all } \mu \in B(\mathcal{S}, \alpha).$$

Lemma 4.4. *Let (\mathcal{S}, α) be a weighted split system on X , $A \in \text{supp}(\alpha)$ and (G, w) a realisation of $(X, d_{(\alpha, \mathcal{S})})$. Then for any non-expansive map $\psi : \|(G, w)\| \rightarrow B(\mathcal{S}, \alpha)$ with $\psi(x) = \Phi(x)$ for all $x \in X$, the function $\lambda_A \circ \psi$ is a split potential on $\|(G, w)\|$.*

Proof. Let $\gamma : [0, 1] \rightarrow \|(G, w)\|$ be an X -geodesic in $\|(G, w)\|$ and set $\lambda'_A := \lambda_A \circ \psi \circ \gamma$. Since $\psi(x) = \Phi(x)$, we have $(\lambda_A \circ \psi)(x) \in \{0, 1\}$ for all $x \in X$, so it remains to show that λ'_A is monotonic.

Since ψ is non-expansive, the map $\psi \circ \gamma : [0, 1] \rightarrow B(\mathcal{S}, \alpha)$ is a geodesic in $(B(\mathcal{S}, \alpha), d_1)$. Therefore, for any $0 \leq t_1 < t_2 < t_3 \leq 1$, we have

$$d_1(\nu_1, \nu_3) = d_1(\nu_1, \nu_2) + d_1(\nu_2, \nu_3),$$

where $\nu_i := \psi \circ \gamma(t_i)$ for $i = 1, 2, 3$. By the definition of the metric d_1 , this gives us

$$\sum_{B \in \text{supp}(\alpha)} |\nu_1(B) - \nu_3(B)| = \sum_{B \in \text{supp}(\alpha)} (|\nu_1(B) - \nu_2(B)| + |\nu_2(B) - \nu_3(B)|).$$

Since, by definition, for all $B \in \text{supp}(\alpha)$, we have

$$|\nu_1(B) - \nu_3(B)| \leq |\nu_1(B) - \nu_2(B)| + |\nu_2(B) - \nu_3(B)|,$$

this implies that

$$|\nu_1(A) - \nu_3(A)| = |\nu_1(A) - \nu_2(A)| + |\nu_2(A) - \nu_3(A)|$$

and hence

$$(\nu_1(A) - \nu_2(A)) \cdot (\nu_2(A) - \nu_3(A)) \geq 0.$$

Since, for $i = 1, 2, 3$, we have $\nu_i(A) = \alpha(\{A, X \setminus A\})\lambda_A(\nu_i)$, this implies

$$(\lambda'_A(t_1) - \lambda'_A(t_2)) \cdot (\lambda'_A(t_2) - \lambda'_A(t_3)) \geq 0,$$

hence λ'_A is monotonic. \blacksquare

Proof of Theorem 3.3. Lemmas 4.3 and 4.4 show that for all $A \in \text{supp}(\alpha)$ and $v \in V(G)$ we have $\lambda_A(\psi(v)) \in \{0, 1\}$. However, by the definition of the map λ_A , we have $\lambda_A(\mu) \in \{0, 1\}$ if and only if $\mu(A) \in \{0, \alpha(\{A, X \setminus A\})\}$ for all $\mu \in B(\mathcal{S}, \alpha)$. So $\psi(v)$ is a vertex of $B(\mathcal{S}, \alpha)$. \blacksquare

5. PROOF OF THEOREM 5.1

We are now ready to prove the main result of this paper, from which Theorem 1.2 follows immediately:

Theorem 5.1. *Let (X, d) be a totally-decomposable finite metric space with dimension two and (G, w) a minimal path-saturated optimal realisation of (X, d) . Then (G, w) is homeomorphic to a subgraph of (G_d, w_∞) .*

Proof. Let (\mathcal{S}, α) be a weighted split system on X such that $d = d_{(\mathcal{S}, \alpha)}$. Recall that κ and Φ denote the embeddings of X in the tight-span and Buneman complex, respectively. By Theorem 2.5 (2), we have an isometry Λ from $B(\mathcal{S}, \alpha)$ to $T(d)$ such that $\Lambda(\Phi(x)) = \kappa(x)$ for all $x \in X$. Furthermore, by Theorem 2.3, there exists a non-expansive injection ψ from $\|(G, w)\|$ to $T(d)$ satisfying $\psi(x) = \kappa(x)$ for all $x \in X$. This implies that the map $\psi' := \Lambda^{-1} \circ \psi$ is a non-expansive map from $\|(G, w)\|$ to $B(\mathcal{S}, \alpha)$ with $\psi'(x) = \Phi(x)$ for all $x \in X$. By Theorem 3.3 we have $\psi'(V) \subseteq V(B(\mathcal{S}, \alpha))$, and hence $\Lambda(\psi'(V)) = \psi(V) \subseteq V(T(d)) = V(G_d)$.

To simplify the notation in the remainder of the proof, we set $\tilde{u} := \psi(u)$ for all $u \in V(G)$. Now, for each edge $\{u, v\} \in E(G)$, fix a shortest path $P(\tilde{u}, \tilde{v})$ in G_d between \tilde{u} and \tilde{v} and let $\mathcal{P} := \{P(\tilde{u}, \tilde{v}) \mid \{u, v\} \in E(G)\}$. We now define a subgraph (G^*, w^*) of (G_d, w_∞) by setting

$$\begin{aligned} V(G^*) &:= \{u \in V(G_d) \mid u \text{ is contained in some path } P \in \mathcal{P}\}, \\ E(G^*) &:= \{\{u, v\} \in E(G_d) \mid u \text{ and } v \text{ are adjacent in some path } P \in \mathcal{P}\} \end{aligned}$$

and $w^* = w_\infty|_{E(G^*)}$.

Since, by Proposition 3.1,

$$(2) \quad w_\infty(P(\tilde{u}, \tilde{v})) = d_\infty(\tilde{u}, \tilde{v}) = d_{(G, w)}(u, v),$$

and (G_d, w_∞) and (G, w) are both realisations of (X, d) , for all $x, y \in X$, we get

$$d(x, y) = d_{(G_d, w_\infty)}(x, y) \leq d_{(G^*, w^*)}(x, y) \leq d_{(G, w)}(x, y) = d(x, y).$$

Hence (G^*, w^*) is a realisation of (X, d) . Furthermore, since, by construction, $l(G^*, w^*) \leq \sum_{P \in \mathcal{P}} w_\infty(P)$, Equation (2) yields $l(G^*, w^*) \leq l(G, w)$, so (G^*, w^*) is optimal.

To finish the proof of the theorem, we will show that there exists a subgraph of (G', w') that is homeomorphic to (G, w) . Suppose first that for any two paths $P_1 = P(\tilde{u}_1, \tilde{v}_1)$ and $P_2 = P(\tilde{u}_2, \tilde{v}_2)$ in \mathcal{P} with vertex sets V_1, V_2 , respectively, we have

$$(3) \quad V_1 \cap V_2 \subseteq \{\tilde{u}_1, \tilde{v}_1\} \cap \{\tilde{u}_2, \tilde{v}_2\}.$$

Then the weighted graph (G', w') obtained from (G^*, w^*) by suppressing all vertices with degree two in $V(G^*) \setminus \psi(V)$ is isomorphic to (G, w) . That is, (G, w) is homeomorphic to (G^*, w^*) , a subgraph of (G_d, w_∞) , as desired. So it remains to show that Inclusion (3) always holds.

First, since (G^*, w^*) is an optimal realisation, we must have $|V(P_1) \cap V(P_2)| < 2$ because otherwise G' would contain an edge e such that for any pair $x, y \in X$, e is not contained in some shortest path between \tilde{x} and \tilde{y} contradicting Lemma 2.1. So suppose there exists $f \in (V_1 \cap V_2) \setminus (\{\tilde{u}_1, \tilde{v}_1\} \cap \{\tilde{u}_2, \tilde{v}_2\})$. For $i = 1, 2$, let f_i be a vertex in P_i that is adjacent to f . Since (G', w') is isomorphic to an optimal realisation, Lemma 2.1 implies that there exists a path P' in $\Gamma(G', w'; \psi(X))$ that contains the edges $\{f, f_1\}$ and $\{f, f_2\}$. Since $P' \notin \Gamma(G, w; X)$, we have $|\Gamma(G', w'; \psi(X))| > |\Gamma(G, w; X)|$, a contradiction to the assumption that (G, w) is path-saturated. ■

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