Searching for Realizations of Finite Metric Spaces in Tight Spans

Sven Herrmann\textsuperscript{a}, Vincent Moulton\textsuperscript{a,*}, Andreas Spillner\textsuperscript{b}

\textsuperscript{a}School of Computing Sciences, University of East Anglia, Norwich, NR4 7TJ, United Kingdom
\textsuperscript{b}Department of Mathematics and Computer Science, University of Greifswald, Walther-Rathenau-Str. 47, 17487 Greifswald

Abstract

An important problem that commonly arises in areas such as internet traffic-flow analysis, phylogenetics and electrical circuit design, is to find a representation of any given metric $D$ on a finite set by an edge-weighted graph, such that the total edge length of the graph is minimum over all such graphs. Such a graph is called an \textit{optimal realization} and finding such realizations is known to be NP-hard. Recently S. Varone presented a heuristic greedy algorithm for computing optimal realizations. Here we present an alternative heuristic that exploits the relationship between realizations of the metric $D$ and its so-called tight span $T_D$. The tight span $T_D$ is a canonical polytopal complex that can be associated to $D$, and our approach explores parts of $T_D$ for realizations in a way that is similar to the classical simplex algorithm. We also provide computational results illustrating the performance of our approach for different types of metrics, including $l_1$-distances and two-decomposable metrics for which it is provably possible to find optimal realizations in their tight spans.

Keywords: combinatorial optimization, metric, graph, realization, tight span

\*Corresponding author

\textit{Email addresses:} sherrmann@mathematik.tu-darmstadt.de (Sven Herrmann), vincent.moulton@cmp.uea.ac.uk (Vincent Moulton), andreas.spillner@uni-greifswald.de (Andreas Spillner)
1. Introduction

An important problem that commonly arises in areas such as internet traffic-flow analysis (Chung et al., 2001), phylogenetics (Bandelt and Dress, 1992) and electrical circuit design (Hakimi and Yau, 1964), is to realize any given metric $D$ on some finite set $X$ by an edge-weighted graph with $X$ labeling its vertex set, often with the additional requirement that the total edge length of the graph is minimum. This can be useful, for example, for visualizing the metric, or for trying to better understand its structural properties. More formally this optimization problem can be stated as follows. A realization $(G, \omega, \tau)$ of $D$ is a connected graph $G = (V, E)$ with vertex set $V$ and edge set $E$, together with an edge-weighting $\omega : E \rightarrow \mathbb{R}_{>0}$ and a labeling map $\tau : X \rightarrow V$ such that, for all $x, y \in X$, $D(x, y)$ is the length of a shortest path from $\tau(x)$ to $\tau(y)$ in $G$ (cf. Figure 1(a) and (b)). The problem then is to find an optimal realization of $D$, that is, a realization of $D$ that has minimum total edge length over all possible realizations of $D$.

![Figure 1](image-url)

Figure 1: (a) A metric $D$ on $X = \{a, b, c, d, e, f\}$. (b) A realization of $(X, D)$ that is not optimal. Vertices associated with an element of $X$ are drawn as black dots, the remaining vertices are drawn as empty circles. (c),(d) Two optimal realizations of $(X, D)$.

Early work on optimal realizations started with Hakimi and Yau (1964) (see also Varone (2006) for a comprehensive list of references), which focused mainly on special classes of metrics such as, for example, those that admit
an optimal realization where the underlying graph is a tree (so-called treelike metrics). Subsequently it was found that every metric on a finite set has an optimal realization \cite{Dress1984, Imrich1984}, although this need not be unique (cf. Figure 1(c) and (d)), and it was shown that computing an optimal realization is NP-hard \cite{Althofer1988, Winkler1984}. More recently, there has been renewed interest in computational aspects of this problem. For example, in \cite{Hertz2007, Hertz2008} (see also \cite{Dress2010}) a way to break up the problem of computing an optimal realization into subproblems using so-called cut points is presented, and in \cite{Varone2006} a heuristic is presented for computing optimal realizations.

Here we present an alternative heuristic for systematically computing optimal realizations that exploits the relationship between optimal realizations of a metric $D$ and its so-called tight span $T_D$ \cite{Dress1984, Isbell1964}. In brief (see Section 2 for details), $T_D$ is a polytopal complex (essentially a union of polytopes) that can be canonically associated to $D$ which is itself a (non-finite) metric space and into which the metric $D$ can be canonically embedded. Remarkably, in \cite{Dress1984} it is shown that the 1-skeleton $G_D$ of $T_D$ (i.e., the edge-weighted graph formed essentially by taking all of the 0- and 1-dimensional faces of $T_D$) is always a realization of $D$. Moreover, Dress conjectured \cite[(3.20)]{Dress1984} that some optimal realization of $D$ can always be obtained by removing some set of edges from $G_D$.

While Dress’ conjecture is still open for metrics in general, recently it has been shown to hold for the class of so-called two-decomposable metrics \cite{Herrmann2011, Theorem 1.2}, a class which includes treelike metrics and $l_1$-distances between points in the plane (see Section 3 for more details). In particular, this and Dress’ aforementioned result suggest that it could be useful to consider $G_D$ as a “search space” in which to look for some optimal realization of $D$ (or at least some interesting realization of $D$ which has relatively small total edge length).

Guided by this principle, given an arbitrary finite metric $D$, in Section 4 we propose a heuristic for computing a realization of $D$ that is a subgraph of $G_D$. This heuristic explores parts of $T_D$ in a way similar to the classical simplex algorithm \cite{Dantzig1963}. Moreover, it does not explicitly compute $G_D$, whose vertex set can have cardinality that is exponential in $|X|$ (see e.g. \cite{Herrmann2007} for some explicit bounds). We also show that the heuristic is guaranteed to find optimal realizations for some simple types of metrics.

Since, as mentioned above, the problem of finding optimal realizations is
NP-hard, we assess the performance of our new heuristic using two strategies. First, we consider a special instance of the problem where we take metrics to be $l_1$-distances between points in the plane. In Section 5 we show that finding optimal realizations of such a metric $D$ in $G_D$ is equivalent to the so-called minimum Manhattan network problem (which was also recently shown to be NP-hard (Chin et al., 2009)). This allows us to compare the realizations computed by our heuristic with realizations computed using a mixed integer linear program (MIP) for the minimum Manhattan network problem presented in (Benkert et al., 2006) (see also Knauer and Spillner (2011) for a comprehensive list of references on other approaches for solving this well-studied problem). Second, in Section 6 we describe a mixed integer program (MIP) for computing a minimal subrealization of a realization of some metric, that is, a subrealization with minimum total edge length. This allows us to obtain some impression of how close the realizations computed by our heuristic are to a minimal subrealization of $G_D$ in case $|X|$ is not too large. Moreover, in case the metric is two-decomposable, a minimal subrealization of $G_D$ is (by the aforementioned result) an optimal realization and so we can compare the realizations computed by our new heuristic with optimal ones for this special class of metrics.

Based on these considerations, in Section 7 we present simulations for $l_1$-distances, two-decomposable metrics and random metrics to assess the performance of our heuristic. An implementation of this heuristic is freely available for download at www.uea.ac.uk/cmp/research/cmpbio/CoMRiT/. This includes the algorithm for efficiently computing cut points as described in Dress et al. (2010) and auxiliary programs that allow to generate the MIP description for the minimum Manhattan network problem, as well as for the problem of computing a minimal subrealization so that they can be solved using existing MIP solvers (we used the solver that is part of the GNU linear programming kit (www.gnu.org/software/glpk/) in our experiments). We conclude the paper with a brief discussion of some possible future directions in Section 8.

2. Preliminaries

In this section, we first recall the formal definition of the tight span of a metric, a concept that has been discovered and re-discovered several times in the literature (see e.g. Chrobak and Larmore (1994); Dress (1984); Isbell (1964)). We also recall some facts concerning tight spans and optimal re-
alizations that will be used later on (for more on this see e.g. Dress et al. 2012, Chapter 5)).

2.1. Some tight span theory

A finite metric space is a pair \((X, D)\) consisting of a finite non-empty set \(X\) and a symmetric bivariate map \(D : X \times X \to \mathbb{R}_{\geq 0}\) such that \(D(x, x) = 0\) and \(D(x, z) \leq D(x, y) + D(y, z)\) hold for all \(x, y, z \in X\). A map \(h : X \to X'\) from a metric space \((X, D)\) into a metric space \((X', D')\) is an isometric embedding if \(D'(h(x), h(y)) = D(x, y)\) holds for all \(x, y \in X\).

Now, given any finite metric space \((X, D)\), the tight span \(T_D\) is defined to be the polytopal complex (see e.g. Klee and Kleinschmidt 1999)) that is the union of the bounded faces of the polyhedron

\[
P_D := \{ f \in \mathbb{R}^X : f(x) + f(y) \geq D(x, y) \text{ for all } x, y \in X \}.
\]

Viewed as a subset of \(\mathbb{R}^X\), \(T_D\) can be endowed with the \(l_\infty\)-metric which is defined by

\[
D_\infty(f, g) = \max\{|f(x) - g(x)| : x \in X\}
\]

for all \(f, g \in T_D\) so that \((T_D, D_\infty)\) is also a (non-finite!) metric space. Note that there exists a canonical isometric embedding of \((X, D)\) into \((T_D, D_\infty)\), the so-called Kuratowski embedding (Kuratowski, 1935), that maps every \(x \in X\) to \(k_x : X \to \mathbb{R} : y \mapsto D(x, y)\). Note that the map \(k_x\) is a 1-dimensional face (or vertex) of \(T_D\) for every \(x \in X\) and, therefore, it is contained in the 1-skeleton \(G_D\).

Later we will use the fact that the tight span can be viewed as a hull of the given metric space similar to the convex hull associated to a set of points in Euclidean space. To make this more precise, define a map \(h : X \to X'\) from a metric space \((X, D)\) into a metric space \((X', D')\) to be non-expansive if \(D'(h(x), h(y)) \leq D(x, y)\) holds for all \(x, y \in X\), and a metric space \((X', D')\) to be injective if for every metric space \((X, D)\) and every subset \(Y \subseteq X\) any non-expansive map of the subspace \((Y, D|_Y)\) into \((X', D')\) can be extended to a non-expansive map of \((X, D)\) into \((X', D')\). The tight span satisfies the following universal property (Dress, 1984; Isbell, 1964):

**Lemma 1.** Any isometric embedding of a metric space \((X, D)\) into an injective metric space \((X', D')\) can be extended to an isometric embedding of \((T_D, D_\infty)\) into \((X', D')\).
2.2. Tight spans and optimal realizations

We now present a key relationship between realizations and tight spans that was first discovered by A. Dress. Let \((X, D)\) be an arbitrary finite metric space. Defining the map \(\omega_D\) by putting \(\omega_D(\{u, v\}) = D_\infty(u, v)\) for all edges \(\{u, v\}\) of \(G_D\) and the map \(\tau_D\) by putting \(\tau_D(x) = k_x\), it is shown in [Dress, 1984, Theorem 5] that \((G_D = (V, E_D), \omega_D, \tau_D)\) is a realization of \((X, D)\) (see also Dress et al. (2012, Theorem 5.15)). Moreover, in Dress (1984) it is shown that, for any optimal realization \((G = (V, E, \omega, \tau))\) of \((X, D)\), there exists a map \(h : V \rightarrow T_D\) such that, for any \(x \in X\), \(h(\tau(x)) = k_x\) and, for any edge \(\{u, v\} \in E\), \(\omega(\{u, v\}) = D_\infty(h(u), h(v))\) hold. While this suggests that every optimal realization \((G = (V, E, \omega, \tau))\) of \((X, D)\) is “contained” in \(T_D\), it was shown by Althöfer (1988) that it might not be isomorphic to any sub-realization of \((G_D = (V_D, E_D), \omega_D, \tau_D)\). Still, as mentioned in the introduction, it is not known whether or not there always exists some optimal realization of \((X, D)\) that is a sub-realization of \((G_D = (V_D, E_D), \omega_D, \tau_D)\).

3. Two-decomposable metrics

In this section we shall consider a special class of finite metrics \(D\), the two-decomposable metrics, for which it is known that \(G_D\) always contains a subrealization that is an optimal realization of \(D\). As mentioned in the introduction, these metrics are of interest as we can in principle compute optimal realizations for them exactly and thus measure the accuracy of our heuristic for computing realizations for small metric spaces.

We first need to recall some relevant concepts. A split \(S\) of a finite set \(X\) is a bipartition \(\{A, B\}\) of \(X\) into two non-empty subsets \(A\) and \(B\), also denoted by \(A|B\). For any \(x \in X\), that set in \(S\) that contains \(x\) is denoted by \(S(x)\) and the other set by \(\overline{S}(x)\). Two splits \(A|B\) and \(A'|B'\) of \(X\) are compatible if at least one of the intersections \(A \cap A'\), \(A \cap B'\), \(B \cap A'\) and \(B \cap B'\) is empty. Otherwise the two splits are incompatible. A set \(\Sigma\) of splits of \(X\) is called a split system (on \(X\)). A split system \(\Sigma\) is two-compatible if there is no subset \(\Sigma' \subseteq \Sigma\) with \(|\Sigma'| = 3\) and any two distinct splits in \(\Sigma'\) are incompatible.

Now, for any split \(S\) of \(X\), define the metric \(D_S\) on \(X\) putting, for all \(x, y \in X\), \(D_S(x, y) = 0\) if \(S(x) = S(y)\) holds and \(D(x, y) = 1\) otherwise. A metric \(D\) on \(X\) is two-decomposable if there exists a two-compatible split system \(\Sigma\) on \(X\) and a weighting \(\lambda : \Sigma \rightarrow \mathbb{R}_{>0}\) with \(D = \sum_{S \in \Sigma} \lambda(S) \cdot D_S\). We
Figure 2: (a) The tight span $T_D$ of the metric $D$ in Figure 1(a). It consists of four maximal 2-dimensional faces surrounding the vertex $k_c$, and three maximal 1-dimensional faces all of which have a vertex in common (and which form the “fork” in the figure). (b) The 1-skeleton $G_D$ of $T_D$. (c) A weighted two-compatible split system that induces $D$.

We illustrate this theorem in Figure 2. More specifically, the metric $D$ in Figure 1(a) is two-decomposable, and its tight span is depicted in Figure 2(a). The realization $G_D$ is pictured in Figure 2(b), and a two-compatible split system associated to $D$ is given in Figure 2(c). Note that both of the optimal realizations for $D$ given in Figure 2(c) and (d) can be obtained from $G_D$ by removing precisely two edges.

We now prove two simple but useful facts concerning the relationship between $l_1$-distances between points in the plane, two-decomposable metrics and treelike metrics. For a point $p \in \mathbb{R}^2$ we denote by $x(p)$ and $y(p)$ the $x$- and $y$-coordinate of $p$, respectively, and the $l_1$-distance between two points $p, q \in \mathbb{R}^2$ by $D_1(p, q) = |x(p) - x(q)| + |y(p) - y(q)|$. Then we have:

**Lemma 3.** Let $P$ be a finite non-empty set of points in $\mathbb{R}^2$. Then the metric $D_1|_P$ is
(i) two-decomposable.

(ii) the sum of two treelike metrics.

Proof. (i) Let $\Sigma_v$ be the set of those splits $A|B$ of $P$ for which there exists a real number $r$ such that $A = \{ p \in P : x(p) < r \}$ and $B = \{ p \in P : x(p) > r \}$. Similarly, let $\Sigma_h$ be the set of those splits $A|B$ of $P$ for which there exists a real number $r$ such that $A = \{ p \in P : y(p) < r \}$ and $B = \{ p \in P : y(p) > r \}$. For every $S \in \Sigma_v$, put $\alpha(S) = \min \{ x(b) - x(a) : a \in A, b \in B \}$ and, for every $S \in \Sigma_h$ put $\beta(S) = \min \{ y(b) - y(a) : a \in A, b \in B \}$. Note that any two splits in $\Sigma_v$ as well as any two splits in $\Sigma_h$ are compatible. Hence, the split system $\Sigma := \Sigma_v \cup \Sigma_h$ is two-compatible.

Now, define, for any split $S$ in $\Sigma$, the weight

$$\lambda(S) = \begin{cases} 
\alpha(S), & \text{if } S \in \Sigma_v \setminus \Sigma_h, \\
\beta(S), & \text{if } S \in \Sigma_h \setminus \Sigma_v, \\
\alpha(S) + \beta(S), & \text{if } S \in \Sigma_h \cap \Sigma_v.
\end{cases}$$

It is not hard to check that $D_1|_P = \sum_{S \in \Sigma} \lambda(S) \cdot D_S$ holds, implying that $D_1|_P$ is indeed two-decomposable.

(ii) Continuing to use the notation introduced in the proof of (i), note that we have $D_1|_P = D_v + D_h$ with $D_v = \sum_{S \in \Sigma_v} \alpha(S) \cdot D_S$ and $D_h = \sum_{S \in \Sigma_h} \beta(S) \cdot D_S$. Therefore, it remains to note that $D_v$ and $D_h$ are treelike in view of the fact that a metric space $(D', X')$ is treelike if there exists a system $\Sigma'$ of pairwise compatible splits of $X'$ and a map $\lambda : \Sigma' \to \mathbb{R}_{>0}$ with $D' = \sum_{S \in \Sigma'} \lambda(S) \cdot D_S$ (Buneman, 1971).

4. Computing a realization in the tight span

In this section we shall present our algorithm for computing realizations using the tight span. We also prove that it is guaranteed to work for some special types of metrics. Given a finite metric space $(X, D)$, the basic idea of our algorithm is to select, for each pair $\{x, y\}$ of distinct elements in $X$, a shortest path from $k_x$ to $k_y$ in $G_D$. The union of these paths is then a realization of $(X, D)$. This is summarized in the form of pseudo-code in Algorithm 1.

Pseudocode for the function find_path is presented in Algorithm 2. This function essentially computes, for any vertex $u$ of $G_D$ and any $x \in X$, a shortest path from $u$ to $k_x$ in $G_D$. To avoid computing the whole graph...
Algorithm 1: The basic algorithm.

**Input:** A finite metric space \((X, D)\)

**Output:** A realization of \((X, D)\)

1. Initialize the graph \(G = (V, E)\) with \(V = \{k_x : x \in X\}\), \(E = \emptyset\);
2. Form a list \(L\) of all pairs \(\{x, y\} \in (X^2)\);
3. foreach \(\{x, y\} \in L\) do
   
   4. find_path\((D, k_x, y, G)\);
   
   /* Adds, if necessary, edges of \(G_D\) to \(G\) so that, after the call, \(G\) contains a path of length \(D(x, y)\) from \(k_x\) to \(k_y\). */
4. end
5. return \((G = (V, E), \omega_D|_E, \tau_D)\)

Algorithm 2: Compute a path using the existing partial realization.

**Function:** find_path\((D, u, x, G)\)

1. Initialize \(v = u\);
2. if \(u\) is a vertex of \(G\) then
   
   3. Put \(M\) the set of vertices of \(G\) such that there is a path of length \(D_\infty(u, v)\) from \(u\) to \(v\) in \(G\) and \(D_\infty(u, x) = D_\infty(u, v) + D_\infty(v, x)\);
   
   4. Put \(v\) to be a vertex in \(M\) with \(D_\infty(v, x)\) minimum;
5. end
6. else
7. Add \(u\) to \(G\);
8. end
9. if \(v\) equals \(k_x\) then
10. return ;
11. end
12. Make a simplex step from \(v\) to arrive at vertex \(w\);
13. Add the edge \(\{v, w\}\) to \(G\);
14. find_path\((D, w, x, G)\);

\(G_D\), it constructs such a path edge by edge employing the polyhedron \(P_D\) as follows. It computes in polynomial time from the description of \(P_D\) all vertices \(v\) of \(G_D\) that are adjacent to \(u\) in \(G_D\). Among these vertices, one with \(D_\infty(u, k_x) = D_\infty(u, v) + D_\infty(v, k_x)\) that minimizes \(D_\infty(v, k_x)\) is selected.
We refer to this as a simplex step from $u$ that arrives at vertex $v$, since this is similar to one step in Dantzig’s well-known simplex algorithm (Dantzig, 1963).

To make use of the fact that certain edges of $G_D$ might have been added to $G$ in previous rounds of the foreach-loop in Algorithm 1, the function find_path first explores whether the current graph $G$ already contains edges that can serve as the initial part of a suitable path from $u$ to $k_x$. One would expect that the choice of the order in which pairs are processed in the foreach-loop has some impact on how many edges can be re-used in subsequent rounds. We found that ordering the pairs according to increasing distances between them tends to work well in practice. Then, in particular, for any elements $x, y, z \in X$ with $D(x, y) + D(y, z) = D(x, z)$, no edges will be added when processing the pair $\{x, z\}$.

Note that our algorithm is guaranteed to output an optimal realization for any treelike metric and any metric that corresponds to the shortest path distances between the pairs of vertices of a graph that is a cycle. The former follows from the fact that, for any treelike metric, $G_D$ is a tree (Dress, 1984), and the latter is an immediate consequence of the fact that we process the pairs of elements in $X$ according to increasing distances between them. Moreover, using the decomposition of metric realizations according to Hertz and Varone (2007, 2008) as a preprocessing step, it follows that an optimal realization can be obtained for a given metric $D$ if the decomposition of $D$ yields only sub-instances for which our algorithm outputs an optimal realization. In particular, it follows that our algorithm produces optimal realizations for all inputs given in the appendix of Varone (2006).

5. Minimum Manhattan networks and optimal realizations

In this section, using properties of the tight span, we give a concise proof of the fact that the problem of computing a minimum Manhattan network is nothing other than the problem of computing an optimal realization for a special class of finite metric spaces (see also Eppstein (2011) for related work). This allows us to directly compare our heuristic for computing realizations with some existing algorithms for computing minimum Manhattan networks. Note that this fact seems to have not been pointed out before in the literature and has some interesting consequences for the computational complexity of constructing an optimal realization which we shall also point out.
To state the main result of this section, we first introduce some more notation. A Manhattan network \((G = (V, E), \omega)\) consists of a finite graph \(G\) whose vertex set \(V \subseteq \mathbb{R}^2\) is a set of points in the plane and a map \(\omega\) that assigns to each edge \(\{p, q\} \in E\) as its length \(D_1(p, q)\) between the points \(p\) and \(q\). Note that, for every edge \(\{p, q\} \in E\), the straight line segment \(\overline{p, q}\) with endpoints \(p\) and \(q\) is either horizontal or vertical and, for any two distinct edges \(e_1 = \{p_1, q_1\}\) and \(e_2 = \{p_2, q_2\}\) in \(E\), the straight line segments \(\overline{p_1, q_1}\) and \(\overline{p_2, q_2}\) do not cross, that is, \(\overline{p_1, q_1} \cap \overline{p_2, q_2} \subseteq e_1 \cap e_2\) holds.

For any path \(p\) from \(p\) to \(q\) in \(G\), \(\ell(p)\) denotes the length of \(p\), and \(p\) is monotone if \(D_1(p, q) = \ell(p)\) holds.

Now, given a finite set of points \(P \subseteq \mathbb{R}^2\), a Manhattan network for \(P\) is a Manhattan network \((G = (V, E), \omega)\) with \(P \subseteq V\) such that for any two distinct \(p, q \in P\) there exists a monotone path from \(p\) to \(q\) in \(G\). Such a network is called minimum if its total length is minimum among all Manhattan networks for \(P\) (cf. Figure 3). The minimum Manhattan network problem has been studied by several researchers over the last few years (for a comprehensive list of references for this problem see e.g. Knauer and Spillner [2011]). We have the following relationship between minimum Manhattan networks and optimal realizations:

**Theorem 4.** Let \(P\) be a finite non-empty set of points in \(\mathbb{R}^2\). Then, for any minimum Manhattan network \((G = (V, E), \omega)\) for \(P\), \((G = (V, E), \omega, id_P)\) is an optimal realization of \((P, D_1|_P)\), where \(id_P\) is the identity map on \(P\).

**Proof.** By definition, any Manhattan network for \(P\) is, up to adding the map \(id_P\), a realization of \((P, D_1|_P)\). Hence, it suffices to show that there exists a Manhattan network for \(P\) whose total length is at most the total length of some optimal realization of \((P, D_1|_P)\).
Consider an optimal realization \((G = (V, E), \omega, \tau)\) of \((P, D_1|_P)\) such that there exists an injective map \(h : V \rightarrow T_{D_1|_P}\) with \(w(\{u, v\}) = D_{\infty}(h(u), h(v))\) for all edges \(\{u, v\} \in E\) and \(h(\tau(p)) = k_p\) for all \(p \in P\). By Lemma 3 and Theorem 2 such an optimal realization always exists.

Now, since the metric space \((\mathbb{R}^2, D_1)\) is injective (see e.g. Catusse et al. (2011)), it follows that for every finite set \(P\) of points in \(\mathbb{R}^2\) there exists an isometric embedding of \((T_{D_1|_P}, D_{\infty})\) into \((\mathbb{R}^2, D_1)\) that maps every \(k_p, p \in P, to p\). Therefore, there exists an injective map \(g : V \rightarrow \mathbb{R}^2\) with \(w(\{u, v\}) = D_1(g(u), g(v))\) for all edges \(\{u, v\} \in E\) and \(g(\tau(p)) = p\) for all \(p \in P\). To obtain a Manhattan network for \(P\), start with the points in \(g(V)\) and then add, step by step, for every \(\{u, v\} \in E\), edges to obtain a monotone path from \(g(u)\) to \(g(v)\). Note that in the resulting Manhattan network \(\mathcal{N}\) the length of a shortest path between \(g(u)\) and \(g(v)\) can be at most the length of a shortest path between \(u\) and \(v\) in \(G\) for all \(u, v \in V\). This implies that there is a monotone path from \(p\) to \(q\) in \(\mathcal{N}\) for all \(p, q \in P\). Hence, \(\mathcal{N}\) is indeed a Manhattan network for \(P\). Finally, the total length of \(\mathcal{N}\) is, by construction, not larger than the total length of \(G\), as required.

Before concluding this section, we point out some interesting implications of the last result:

**Corollary 5.** Computing an optimal realization of a finite metric space \((X, D)\) is NP-hard even if

(i) \(D\) is two-decomposable, or

(ii) \(D\) is the sum of two treelike metrics on \(X\).

**Proof.** In Chin et al. (2009) it is shown that computing (even just the total edge length of) a minimum Manhattan network is NP-hard. In view of Theorem 4 this implies that computing an optimal realization of \((P, D_1|_P)\) for a given point set \(P\) is NP-hard. By Lemma 3(i) the metric \(D_1|_P\) is two-decomposable. This establishes (i). Alternatively, this also follows from the NP-hardness proof in Althöfer (1988): It can be checked that the metric that arises from applying the reduction is always two-decomposable.

In Lemma 3(ii) it was shown that \(D_1|_P\) is even the sum of two treelike metrics on \(P\). This establishes (ii). □
6. Finding minimal subrealizations

In a similar spirit to finding optimal realizations, there is a whole family of so-called inverse shortest path problems (see e.g. Cui and Hochbaum (2010) and the references therein), where a minimum cost editing of a given graph is sought so that the shortest path distances between certain pairs of vertices equal given distances for those pairs. The problem of finding a minimal subrealization mentioned in the introduction can be viewed as yet another variant of this theme and we will briefly collect some facts about it in this section.

First note that, in view of the fact that the problem of computing a minimum Manhattan network is NP-hard (Chin et al., 2009) and the fact that there is always a minimum Manhattan network that is contained in the grid induced by the given point set (see e.g. Benkert et al. (2006)), we have:

**Proposition 6.** The problem of computing a minimal sub-realization of a given realization \((G, \omega, \tau)\) is NP-hard even if \(G\) is a two-dimensional grid graph.

Next note that, following a similar approach to the one used in Benkert et al. (2006) for computing a minimum Manhattan network, one can phrase the problem of computing a minimal subrealization as a MIP. For the convenience of the reader, we include below the description of the MIP that we used for benchmarking in the computational experiments and that yields, for any given realization \((G = (V, E), \omega, \tau)\) of a finite metric space \((X, D)\), a subgraph \(G' = (V', E')\) of \(G\) with minimum total edge length such that \((G', \omega|_{E'}, \tau)\) is also a realization of \((X, D)\):

- For every edge \(\{u, v\} \in E\), we introduce two directed edges \((u, v)\) from \(u\) to \(v\) and \((v, u)\) from \(v\) to \(u\). Let \(E\) denote the set of these directed edges.

- For every edge \(\{u, v\} \in E\), we have a binary variable \(x_{\{u,v\}}\) indicating whether or not \(\{u, v\}\) is an edge of \(G'\).

- For any two distinct elements \(x, y \in X\), we send one unit of flow from \(\tau(x)\) to \(\tau(y)\) that ensures that there is at least one path from \(x\) to \(y\) of length \(D(x, y)\) in \(G'\). To describe this flow, we introduce, for every directed edge \((u, v) \in E\), a real-valued variable \(f_{(u,v)}\).
• For any two distinct elements \( x, y \in X \), the variables must satisfy the following constraints:

1. \( x_{\{u,v\}} \geq f_{(u,v)}(x,y) \geq 0 \) and \( x_{\{u,v\}} \geq f_{(v,u)}(x,y) \geq 0 \) for all \( \{u,v\} \in E \).

2. \( \sum_{\{u,v\} \in E} (f_{(u,v)}(x,y) - f_{(v,u)}(x,y)) = 0 \) for all \( v \in V \setminus \{\tau(x), \tau(y)\} \).

3. \( \sum_{\{u,v\} \in E} (f_{(u,v)}(x,y) - f_{(v,u)}(x,y)) = -1 \) for \( v = \tau(x) \).

4. \( \sum_{\{u,v\} \in E} (f_{(u,v)}(x,y) - f_{(v,u)}(x,y)) = 1 \) for \( v = \tau(y) \).

5. \( \sum_{\{u,v\} \in E} w(\{u,v\}) \cdot (f_{(u,v)}(x,y) + f_{(v,u)}(x,y)) \leq D_G(\tau(x), \tau(y)) \).

• The objective function is

\[
\sum_{\{u,v\} \in E} w(\{u,v\}) \cdot x_{\{u,v\}} \rightarrow \min.
\]

In practice, we found that the size of the MIP can often be reduced considerably by only introducing the variable \( f_{(u,v)}(x,y) \) for those edges \( \{u,v\} \in E \) that actually lie on some shortest path from \( \tau(x) \) to \( \tau(y) \) in \( G \).

7. Computational Experiments

To perform computational experiments, we have implemented the algorithm described in Section 4 in C++ as an extension to the mathematical software system polymake [Gawrilow and Joswig, 2000]. In this implementation, we apply, as a preprocessing step, the decomposition of a given instance by cut points.

The experiments are designed to give an impression of the range of inputs that can be attacked by our algorithm in terms of size and also how close the realization produced by our algorithm is to an optimal realization. For each size \( n \) of the ground set of the metric space, 100 randomly generated inputs were considered and we present the mean run-time \( t \) of our algorithm (including the preprocessing) and the mean ratio \( r_{sg} \) between the length of the realization produced by our algorithm and a minimal sub-realization of \((G_D, \omega_D, \tau_D)\) (if available). The variance of these values was usually quite low and is omitted.

In the tables below, \( t_{TS} \) denotes the time to compute the whole tight span (if the size if the tight span admitted to compute it using polymake), \( t_{solve} \)
Table 1: Results of the computational experiments for instances of the minimum Manhattan network problem.

denotes the time needed to solve the MIP described in Section 6 using the solver glpksol from the GNU linear programming kit, and \( r_{TS} \) denotes the ratio of the length of the realization produced by our algorithm to the total edge length of the whole 1-skeleton of the tight span. A \( * \) indicates that the corresponding value could not be obtained because the 1-skeleton of the tight span was too large or at least too large to solve the resulting MIP. All run-times were taken on a Intel(R) Core(TM)2 Quad CPU 2.66GHz machine running CentOx 5.6 using only one core.

7.1. Manhattan networks

Inputs were generated by choosing \( n \) random points on an integer \( 10^6 \times 10^6 \) grid. In addition to the MIP described in Section 6 we also used the MIP presented in Benkert et al. (2006) to compute an optimal realization for each input point set. The run time \( t_{man} \) for solving this alternative MIP using glpksol is also given in Table 1. As can be seen, for all instances, our realizations are usually within a factor of \( \frac{3}{2} \) of the optimum. Note that there exist several polynomial time algorithms that guarantee to produce a realization whose length is within a constant factor of the optimum — currently, for the best known algorithms, the factor is 2 (Chepoi et al., 2008; Guo et al., 2008; Nouioua, 2005).
Recall that, in case the metric \( D \) is two-decomposable, we know that there exists an optimal realization that is a sub-realization of \((G_D, \omega_D, \tau_D)\) (see Section 3). Hence, \( r_{sg} \) is actually the ratio between the length of the realization produced by our algorithm and the length of an optimal realization.

We tested two types of two-decomposable metrics (cf. Table 2):

- **Metrics that are the sum of two treelike metrics**: We choose two random binary trees with \( n \) leaves, took the set of these leaves as the ground set of the metric space and assigned uniformly distributed lengths (between 1 and \( 10^6 \)) to the edges of the trees. Then we formed the sum of the two treelike metrics realized by the binary trees.

- **Metrics resulting from random two-compatible split systems**: We generated random two-compatible split systems of size \( 2n \) by generating random splits and adding them to an initially empty system if it remains two-compatible after adding the split. The metric considered in the experiment is the metric induced by the resulting split system where we again assigned uniformly distributed weights to the splits.

| \( n \) | \( t \) | \( t_{TS} \) | \( t_{solve} \) | \( r_{sg} \) | \( r_{TS} \) |
|---|---|---|---|---|---|
| 5  | 0.46 | 0.01 | 0.43 | 1.02 | 0.95 |
| 10 | 1.46 | 0.07 | 2.05 | 1.10 | 0.77 |
| 15 | 3.00 | 3.49 | 6.83 | 1.16 | 0.70 |
| 20 | 5.44 | 225.32 | 43.73 | 1.19 | 0.66 |
| 25 | 9.18 | 13174.89 | 314.37 | 1.22 | 0.63 |
| 30 | 12.87 | * | * | * | * |
| 35 | 24.13 | * | * | * | * |
| 40 | 38.62 | * | * | * | * |
| 45 | 75.90 | * | * | * | * |
| 50 | 114.40 | * | * | * | * |
| 55 | 169.91 | * | * | * | * |
| 60 | 250.89 | * | * | * | * |
| 65 | 363.25 | * | * | * | * |
| 70 | 506.94 | * | * | * | * |
| 75 | 587.90 | * | * | * | * |
| 80 | 844.98 | * | * | * | * |
| 85 | 1090.04 | * | * | * | * |
| 90 | 1319.21 | * | * | * | * |
| 95 | 2143.58 | * | * | * | * |

Table 2: Results of the computational experiments for metrics that are the sum of two treelike metrics (left) and general two-decomposable metrics (right).

**7.2. Two-decomposable metrics**

Recall that, in case the metric \( D \) is two-decomposable, we know that there exists an optimal realization that is a sub-realization of \((G_D, \omega_D, \tau_D)\) (see Section 3). Hence, \( r_{sg} \) is actually the ratio between the length of the realization produced by our algorithm and the length of an optimal realization. We tested two types of two-decomposable metrics (cf. Table 2):

- **Metrics that are the sum of two treelike metrics**: We choose two random binary trees with \( n \) leaves, took the set of these leaves as the ground set of the metric space and assigned uniformly distributed lengths (between 1 and \( 10^6 \)) to the edges of the trees. Then we formed the sum of the two treelike metrics realized by the binary trees.

- **Metrics resulting from random two-compatible split systems**: We generated random two-compatible split systems of size \( 2n \) by generating random splits and adding them to an initially empty system if it remains two-compatible after adding the split. The metric considered in the experiment is the metric induced by the resulting split system where we again assigned uniformly distributed weights to the splits.
7.3. Random metrics

Finally, we generated random metrics on \( n \) points by choosing each pair-wise distance uniformly between \( 10^6 \) and \( 2 \cdot 10^6 \). The results are presented in Table 3. Note that in this experiment it is not known whether \((G_D, \omega_D, \tau_D)\) contains an optimal realization of the given metric as a sub-realization. Therefore, the value \( r_{sg} \) is only a lower bound on the ratio between the length of the realization produced by our algorithm and the length of an optimal realization.

| \( n \) | \( t \) | \( t_{TS} \) | \( l_{solve} \) | \( r_{sg} \) | \( r_{TS} \) |
|---|---|---|---|---|---|
| 5  | 0.48 | 0.01 | 0.53 | 1.04 | 0.90 |
| 6  | 0.72 | 0.01 | 1.80 | 1.06 | 0.74 |
| 7  | 0.88 | 0.02 | 3.46 | 1.10 | 0.56 |
| 8  | 1.35 | 0.04 | 10.12 | 1.15 | 0.39 |
| 9  | 1.31 | 0.12 | 758.07 | 1.20 | 0.26 |
| 10 | 1.32 | 0.35 | 33652.08 | 1.21 | 0.18 |
| 15 | 3.52 | 300.29 | * | * | 0.01 |
| 25 | 15.97 | * | * | * | * |
| 30 | 40.47 | * | * | * | * |
| 35 | 84.81 | * | * | * | * |
| 40 | 181.73 | * | * | * | * |
| 45 | 330.98 | * | * | * | * |
| 50 | 545.36 | * | * | * | * |
| 55 | 749.25 | * | * | * | * |
| 60 | 1204.18 | * | * | * | * |
| 65 | 2081.53 | * | * | * | * |

Table 3: Results of the computational experiments for general metrics.

8. Discussion

Our experiments indicate that, for most of the inputs considered, the length of the realization produced by our algorithm is within a factor of \( \frac{3}{2} \) of the length of a shortest sub-realization of \((G_D, \omega_D, \tau_D)\) or even within a factor of \( \frac{3}{2} \) of the length of an optimal realization. It could be interesting to investigate whether our algorithm (or a suitable variant of it) yields a constant-factor approximation algorithm, at least for certain classes of metrics such as, for example, two-decomposable metrics.

We also see that our algorithm can produce realizations for metric spaces with up to 50 elements, even in the case of general random metrics. Note also that all computations are done with arbitrary precision rationals/integers, to ensure combinatorial accuracy. Using floating point numbers instead (which
would make sense at least for the general random metrics, that is, generic metrics) could further speed up the computations.

In future work it could also be interesting to try and develop an exact, exponential time algorithm for computing an optimal realization of any metric space. This would be helpful for benchmarking heuristics but would also allow to check Dress’ conjecture for more examples. We expect that this could at least give some interesting further insights into the structure of the problem.

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