Optimal realizations of generic 5-point metrics

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Abstract

Given a metric d on a finite set X, a realization of d is a triple (G, φ, w) consisting of a graph $G = (V, E)$, a labeling $\varphi : X \to V$, and a weighting $w : E \to \mathbb{R}_{>0}$ such that for all $x, y \in X$ the length of any shortest path in G between $\varphi(x)$ and $\varphi(y)$ equals $d(x, y)$. Such a realization is called optimal if $\|G\| := \sum_{e \in E} w(e)$ is minimal amongst all realizations of d. In this paper we will consider optimal realizations of generic 5-point metric spaces. In particular, we show that there is a canonical subdivision $\mathcal{C}$ of the metric fan of 5-point metrics into cones such that (i) every metric d in the interior of a cone $C \in \mathcal{C}$ has a unique optimal realization (G, φ, w), (ii) if d' is also in the interior of C with optimal realization (G', φ', w') then (G, φ) and (G', φ') are isomorphic as labeled graphs, and (iii) any labeled graph that underlies all optimal realizations of the metrics in the interior of some cone $C \in \mathcal{C}$ must belong to one of three isomorphism classes.

1 Introduction

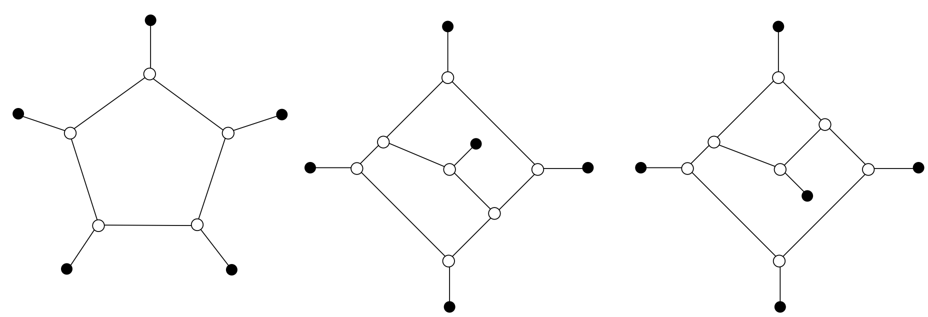
Let (X, d) be a finite metric space, that is, a finite set X, $|X| \geq 2$, together with a metric d (i.e., a symmetric map $d : X \times X \to \mathbb{R}_{\geq 0}$ that vanishes precisely on the diagonal and that satisfies the triangle inequality). To simplify notation, we will also use the notation xy for $d(x, y)$ for $x, y \in X$.

An X-*labeled graph* is a pair $(G = (V, E), \varphi)$ consisting of a graph $G = (V, E)$ and an injective map $\varphi : X \to V$. A *realization* of a metric d on X, (G, φ, w), consists of an X-labeled graph (G, φ) together with a weighting $w : E \to \mathbb{R}_{>0}$ such that for all $x, y \in X$ the length of any shortest path in G between $\varphi(x)$ and $\varphi(y)$ – or an xy-*path* for short – equals xy. Given such a realization, let $\|G\| = \sum_{e \in E} w(e)$ denote the *total edge weight* of G. A realization G of d is called *optimal* if $\|G\|$ is minimal amongst all realizations of d. Note that for any metric d an optimal realization of d always exists [5, 8], but it is not necessarily unique [5, 8], and in general it is NP-hard to compute optimal realizations [1, 13].

In this paper we will consider optimal realizations of 5-point metrics, i.e. metrics d on X for which $|X| = 5$. Note that optimal realizations of metric spaces having 4 or fewer points are well-understood – see e.g. [6]. Before proceeding to state our main results, we first recall that, for $|X| = n$, the cone of all metrics on X, or *metric cone* $C_n \subseteq \mathbb{R}^{\binom{X}{2}}$ [4], has a canonical subdivision into subcones MF_n called the *metric fan* [3, 12]. A metric d in C_n is *generic* if it lies in the interior of a maximum cone in the metric fan. In general, we denote the maximal cone in MF_n containing d by $C(d)$. Note that MF_4 consists of 3 elements [5, 3], MF_5 consists of 102 elements coming in 3 symmetry classes (Types I, II and III) [5, 3], and that MF_6 consists of 194,160 elements coming in 339 symmetry classes [12]. An explicit description of Type I,II and III metrics is presented in Section 2.

Now, suppose $(G = (V, E), \varphi : X \to V)$ and $(G' = (V', E'), \varphi' : X \to V')$ are X-labeled graphs. We say that these graphs are in the same *class* if there is a graph isomorphism $\Phi : V \to V'$ of G and G' such that $\varphi' = \varphi \circ \Phi$. In this paper we shall prove the following:

Theorem 1. *Suppose that (G, φ, w) is an optimal realization of some generic metric $d \in C_5$. Then (G, φ) must be in one of the three classes (a)–(c) pictured in Figure 1. Moreover, if d is in the interior of a Type I or Type II cone, then (G, φ) must be in class (a) or class (b), respectively, whereas if d is in the interior of a Type III cone then (G, φ) can be either in class (b) or in class (c).*



(a) (b) (c)

Figure 1: Three classes of X-labeled graphs for $|X| = 5$. For each graph $G = (V, E)$, the set of black vertices V_B denotes the set of vertices that must be labeled by elements of X.

Now, given an X-labeled graph (G, φ), we let $O(G, \varphi) \subseteq C_n$ denote the set of metrics $d \in C_n$ for which there is some $w : E \to \mathbb{R}_{>0}$ such that (G, φ, w)

is an optimal realization of d. Note that the set $O(G, \varphi)$ is not necessarily convex. For example, if $X = \{x, y, u, v, w\}$ and

$$d_1 = 2\delta_{yu} + \delta_{yw} + 3\delta_{xu} + 2\delta_{xv} + d'$$
$$d_2 = 3\delta_{yu} + 2\delta_{yv} + 2\delta_{xu} + \delta_{xw} + d'$$

(see Section 2 for notation) then it can be checked using our results below that d_1 and d_2 are both generic metrics of Type III with the same X-labeled graph (G, φ) underlying each of their optimal realizations, whilst $(d_1 + d_2)/2$ is a generic metric of Type II whose underlying X-labeled graph is not isomorphic to (G, φ).

Even so, we will also show that the sets $O(G, \varphi)$ still induce a subdivision of MF_5 into cones:

Theorem 2. *Suppose that C is a cone in MF_5.*

- *If C is of Type I and $G = (V, E)$ is the graph in Figure 1 (a), then there is a labeling $\varphi : X \to V_B$ such that $O(G, \varphi) = C$.*
- *If C is of Type II and $G = (V, E)$ is the graph in Figure 1 (a), then there exist distinct labelings $\varphi_1, \varphi_2 : X \to V_B$ such that both $C \cap O(G, \varphi_1)$ and $C \cap O(G, \varphi_2)$ are cones, and the union of these two cones is C.*
- *If C is of Type III and $G = (V, E)$, $G' = (V', E')$ are the graphs in Figure 1 (b),(c), respectively, then there exist distinct labelings $\varphi_1, \varphi_2 : X \to V_B$, and $\varphi_3 : X \to V'_B$, such that $C \cap O(G, \varphi_i)$ is a cone for $i = 1, 2, 3$, and the union of these three cones is C.*

The rest of this paper is organised as follows. In Section 2 we recall the description of the three types of generic metrics given in [5]. In Section 3 we prove three propositions, Propositions 1, 2, 3, concerning optimal realizations of Type I, II and III metrics, respectively, from which Theorems 1 and 2 follow immediately. We conclude in Section 4 with a discussion of our results and some possible future directions for study.

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2 Generic 5-point metrics

As mentioned in the introduction, there are three types of generic 5-point metrics [3, 5]. In this section we recall the description of these types given in [5] (see also [2]).

Define a *split* $S = A|B$ of X to be a bipartition of X into two nonempty subsets A and B, and to any such split associate the *split (pseudo-)metric* $\delta_{A|B}$, defined by

$$\delta_{A|B}(x,y) = \begin{cases} 0 & \text{if } x,y \in A \text{ or } x,y \in B \\ 1 & \text{else.} \end{cases}$$

Given a metric d on X and a split $A|B$ of X, define the *isolation index* $\alpha^d_{A|B} = \alpha_{A|B}$ to be the quantity

$$\alpha_{A|B} := \frac{1}{2} \min_{a,a' \in A, b,b' \in B} (\max\{ab + a'b', a'b + ab', aa' + bb'\} - aa' - bb')$$

(cf. also [2]). To simplify notation, split metrics and isolation indices will also be subscripted by the smallest part of the split.

Now, a generic metric d on a 5-point set X is of

(Type I) if there is some labeling $\{x_0, x_1, x_2, x_3, x_4\}$ of X such that

$$d = \sum_{i=0}^{4} \alpha_{x_i}\delta_{x_i} + \sum_{i=0}^{4} \alpha_{x_i,x_{i+1}}\delta_{x_i,x_{i+1}},$$

where indices are taken modulo 5, and all isolation indices are positive;

(Type II) if there is some labeling $\{x, y, u, v, w\}$ of X such that

$$d = \sum_{z \in X} \alpha_z\delta_z + \alpha_{xu}\delta_{xu} + \alpha_{xv}\delta_{xv} + \alpha_{uy}\delta_{uy} + \alpha_{vy}\delta_{vy} + \gamma d',$$

where d' is the metric

$$d'(a,b) = \begin{cases} 0 & \text{if } a = b, \\ 2 & \text{if } \{a,b\} \in \{\{x,y\},\{u,v\},\{u,w\},\{v,w\}\}, \\ 1 & \text{else,} \end{cases}$$

and all isolation indices are positive;

(Type III) if there is a labeling $\{x, y, u, v, w\}$ of X such that

$$d = \sum_{z \in X} \alpha_z \delta_z + \alpha_{xu}\delta_{xu} + \alpha_{xv}\delta_{xv} + \alpha_{wy}\delta_{wy} + \alpha_{vy}\delta_{vy} + \gamma d',$$

where d' is as for Type II metrics and all isolation indices are again positive.

3 Optimal realizations of generic 5-point metrics

In this section we will prove our main results. Before we begin, we first make some observations concerning realizations.

First, we define a *pendant-free* metric to be a metric d on X for which $\alpha_x = 0$ for all splits $\{x\}|X \setminus \{x\}$ of X, $x \in X$. Note that given any metric d on X, any optimal realization of d may be obtained by finding any optimal realization (G, φ, w) of the pendant-free metric

$$d - \sum_{x \in X} \alpha_x \delta_x,$$

and then, for each $x \in X$, attaching a new edge e to the vertex $\varphi(x)$ in G, labeling the end vertex of e with degree 1 with x instead, and assigning weight α_x to e (see e.g. [8, Corollary 5.4]).

Second, we shall make use of the following result concerning realizations that is presented in [8, Lemma 3.1].

Lemma 1. *Suppose that (X, d) is a metric space, and that x, y, z, u, v are distinct elements of X.*

(i) If $xy + yz = xz$, then y is the only common point of any xy-path and any yz-path in any realization of d.

(ii) If $xy + uv < \max\{xu + yv, xv + yu\}$, then every xy-path is disjoint from any uv-path in any realization of d.

Third, we recall that for d a metric on X, the *UG graph* of d, $G = (X, E, w)$ is the weighted graph with vertex set X, edge set E consisting of those $\{x, y\} \in \binom{X}{2}$, for which there is no $z \neq x, y$ with $xz + zy = xy$, and weighting given by putting $w(\{x,y\}) = xy$. Note that in general the UG graph of d is a realization of d; in [10, Theorem 1] a characterization is presented for when the UG graph is actually an optimal realization (see also [8, Theorem 3.2]).

3.1 Metrics of Type I

Proposition 1. *Suppose that d is a pendant-free, 5-point metric on the set $X = \{x_0, x_1, x_2, x_3, x_4\}$ with*

$$d = \sum_{i=0}^{4} \alpha_{x_i x_{i+1}} \delta_{x_i x_{i+1}},$$

where indices are taken $\mod 5$*, and all isolation indices are greater than zero. Then d has a unique optimal realization as given in Figure 2(a). In particular, if d' is a Type I generic metric on X of the form $d' = d + \sum_{x \in X} \alpha_x$, then every metric in the interior of the cone $C(d)$ has unique optimal realization that can be obtained by adding appropriately weighted pendant-edges to Figure 2(a).*

Proof: The set of all metrics d as in the statement of the theorem is precisely the interior of the cone that is defined by the equations $d(x_i, x_{i+1}) + d(x_{i+1}, x_{i+2}) = d(x_i, x_{i+2}) \pmod 5$ for all $i \in \{1, \ldots, 5\}$, and where the triangle inequality is strict for any other triplet in X. In particular, the UG graph of any element in this cone is the graph pictured in Figure 2 (b), where each edge $\{x_i, x_{i+1}\}$ is given weight $d(x_i, x_{i+1}) = \alpha_{x_{i-1}x_i} + \alpha_{x_{i+1}x_{i+2}}$. It follows by [10, Theorem 1] that d has the unique optimal realization given in Figure 2 (a). ∎

3.2 Metrics of Type II

Proposition 2. *Suppose that d is a pendant-free, 5-point metric on the set $X = \{x, y, u, v, w\}$ with*

$$d = \alpha_{xu}\delta_{xu} + \alpha_{xv}\delta_{xv} + \alpha_{uy}\delta_{uy} + \alpha_{vy}\delta_{vy} + \gamma d'$$

(see Section 2), and all isolation indices greater than zero.

(i) If $\alpha_{xv}+\alpha_{uy} > \alpha_{xu}+\alpha_{vy}$, then d has the unique optimal realization given in Figure 2 (c) with vertices p and q labeled by u and v, respectively.

(ii) If $\alpha_{xu}+\alpha_{vy} > \alpha_{xv}+\alpha_{uy}$ then d has the unique optimal realization given in Figure 2 (c) with vertices p and q labeled by v and u, respectively.

In particular, if d' is a Type II generic metric on X of the form $d' = d + \sum_{x\in X} \alpha_x$, then the cone $C(d)$ can be subdivided into two cones such that every metric in the interior of each of these subcones has a unique optimal realization that can be obtained by adding appropriately weighted pendant-edges to precisely one of the two optimal realizations given in (i) or (ii).

Proof: The set of metrics d of the form given in the statement of the proposition is a cone that is defined by the equalities $xy = xw + wy$, $xy = xu + uy$, $xy = xv + vy$, $uv = ux + xv$, and $uv = uy + vy$, and where the triangle inequality is strict for any other triplet in X. In particular, the UG graph of d is as in Figure 2(d).

Note that combining the last four of these equalities implies that $xu = vy$ and $xv = uy$, which in turn implies $xy = uv$. Note also that if, for any $p, q, r \in X$, we define

$$F_q(p, r) := \frac{1}{2}(pq + qr - pr), \tag{1}$$

then using the definition of isolation indices it is straight-forward to check that $\alpha_{xu} = F_x(v, w)$, $\alpha_{xv} = F_x(u, w)$, $\alpha_{uy} = F_y(v, w)$, and $\alpha_{vy} = F_y(u, w)$.

Now, to determine an optimal realization of d we shall consider how the shortest paths in any realization G of d may intersect. Using Lemma 1 it is straight-forward to check that, for all $a \neq b \in \{u, v, w\}$, no xa-path in G intersects any by-path. Indeed, for any $a \in \{u, v, w\}$,

$$\max\{xy+ab, xb+ay\} = \max\{xa+ay+ab, xb+ay\} = xa+ay+ab > xa+by,$$

and so any xa-path and by-path are disjoint. Moreover, since $xa + ay = xy$ for all $a \in u, v, w$, an xa-path and an ay-path in G can only intersect at a by Lemma 1. In addition, since $xu + xv = uv$, an xu-path and an xv-path in G can only intersect at x, and similarly an uy-path and vy-path can only intersect at y. So in view of the above equalties, it follows that G must contain a subgraph that is homeomorphic (i.e. isomorphic up to replacing vertices of degree 2 by edges) to the 4-cycle x, u, y, v with weights $xu = vy$ and $xv = uy$. Call this subgraph H.

In particular, the only remaining paths in G which can intersect are an xw-path and an xa-path for some $a \in \{u, v\}$, and similarly a yw-path and an ya-path. However, note that the total length of the maximum possible intersection of any xa-path and xw-path is $F_x(a, w)$, since we cannot have a path in G joining a and w that has length less than aw. Thus G must have total edge weight at least

$$xu+xw+xv+uy+wy+vy-\max\{F_x(u,w), F_x(v,w)\}-\max\{F_y(u,w), F_y(v,w)\}. \tag{2}$$

In particular, if G has this total weight, then it must be an optimal realization.

We now construct an optimal realization of d by adding an xw-path and a yw-path to H. If these two paths intersect paths in H with a common endpoint, say the xw-path intersects the xu-path in H and the yw-path intersects the uy-path, then the resulting graph does not contain a wv-path, and vice versa if we interchange the roles of u and v. So, in the first case, to obtain a graph which realizes d we would have to add a wv-path, which we can assume intersects $\{x, v\}$ or $\{v, y\}$ (since otherwise the total weight would be higher). So we have added an xw-path and a wy-path which intersect opposing edges of the 4-cycle H. But adding these two paths and letting their intersection with H be maximal is sufficient to realize the metric d, and hence any optimal realization must be of this form.

Hence two cases remain: if $F_x(u, w) + F_y(v, w) > F_x(v, w) + F_y(u, w)$, or equivalently $\alpha_{xv} + \alpha_{uy} > \alpha_{xu} + \alpha_{vy}$, then it follows that $xu + vy > xv + uy$ and the xw-path intersects the xu-path, while the wy-path intersects the vy-path. Hence we obtain a necessarily unique optimal realization of d as in (i). If instead $F_x(v, w) + F_y(u, w) > F_x(u, w) + F_y(v, w)$, then we obtain a unique optimal realization of d is as in (ii). ∎

3.3 Metrics of Type III

Proposition 3. *Suppose that d is a pendant-free, 5-point metric on the set $X = \{x, y, u, v, w\}$ of X with*

$$d = \alpha_{xu}\delta_{xu} + \alpha_{xv}\delta_{xv} + \alpha_{wy}\delta_{wy} + \alpha_{vy}\delta_{vy} + \gamma d',$$

(see Section 2), all isolation indices greater than zero, and the numbers $\alpha := \alpha_{xv} + \alpha_{wy}$, $\beta := \alpha_{xu} + \alpha_{vy}$, distinct.

(i) If $\alpha_{xv} + \alpha_{vy} > \max\{\alpha, \beta\}$*, then* d *has the unique optimal realization given in Figure 2 (e).*

(ii) If $\alpha_{xv} + \alpha_{vy} < \max\{\alpha, \beta\}$*, and* α *or* β *is the largest of the two numbers, then* d *has the unique optimal realization given in Figure 2 (f) with vertices* p, q, r *labeled by* w, u, v *or* v, w, u*, respectively.*

In particular, if d' *is a Type III generic metric on* X *of the form* $d' = d + \sum_{x \in X} \alpha_x$*, then the cone* $C(d)$ *can be subdivided into three cones such that every metric in the interior of each of these subcones has a unique optimal realization that can be obtained by adding appropriately weighted pendant-edges to precisely one of the three optimal realizations given in (i) or (ii).*

Proof: The set of metrics d of the form given in the statement of the proposition is a cone that is defined by the equalities $xy = xw + wy$, $xy = xu + uy$, $xy = xv + vy$, $uv = ux + xv$, and $wv = wy + yv$, and where the triangle inequality is strict for any other triplet in X. In particular, the UG graph of d is given by Figure 2 (g).

Note that, with $F_p(q, r)$ as defined in (1), $\alpha_{xu} = F_x(v, w)$, $\alpha_{xv} = F_x(u, w)$, $\alpha_{wy} = F_y(u, v)$, and $\alpha_{vy} = F_y(u, w)$.

Now, considering intersections of shortest paths, in any realization G of d, no xa-path and by-path where $a, b \in \{u, v, w\}$ can intersect other than at shared endpoints, as in the proof of Proposition 2. Moreover, xu-paths and xv-paths in G can intersect only at x, and wy-paths and yv-paths only at y.

Hence there are four remaining possible intersections of shortest paths in G: An xw-path can intersect either an xu-path, for a maximum distance of $F_x(u, w)$, or an xv-path for a maximum distance of $F_x(v, w)$. Similarly a uy-path can intersect either a vy-path for a maximum distance of $F_y(u, v)$, or a wy-path for a maximum distance of $F_y(u, w)$.

Combining the two possible intersections at x with the two possibilities at y in all four possible ways, and noting that if the xv and xw-paths intersect at x and uy and vy-paths intersect at y then we do not have a realization of d (otherwise there would be no uw-path since $uw < ua + aw$ for all $a \in \{x, y, v\}$), it follows that G must be one of the (necessarily unique) optimal realizations as in (i) or (ii). ∎

4 Discussion

Note that in the statement of Proposition 2 the interior of the cone $C(d')$ intersects the two subcones in a set of metrics that satisfy $\alpha_{xv} + \alpha_{uy} = \alpha_{xu} + \alpha_{vy}$, and that every metric in this intersection has precisely the two optimal realizations given in (i) and (ii). Similarly, in Proposition 3 intersections of the subcones can yield metrics having more that one optimal realization; in case $\alpha_{xv} + \alpha_{vy} = \alpha > \beta$ or $\alpha_{xv} + \alpha_{vy} < \alpha = \beta$ then we obtain metrics with two optimal realizations, and if $\alpha_{xv} + \alpha_{vy} = \alpha = \beta$ we obtain metrics with three optimal realizations.

It is not difficult to show (using e.g. results in [9]) that any pendant-free, 5-point metric must have a UG graph that is isomorphic to one of the graphs in Figure 2 (b), (d), (g), or to $K_{2,3}$. Interestingly, in case a 5-point metric d has UG graph $K_{2,3}$, it can be shown that d must lie in the boundary of a Type III cone, and that it has two possible optimal realizations (those in Figure 2(f) with vertices p, q, r labeled by w, u, v or w, v, u). In particular, it follows that there are non-generic metrics having optimal realizations whose underlying X-labeled graphs are contained one of the classes pictured in Figure 1.

The description of Type I, II and III metrics given in Section 2 is directly related to the structure of the *tight-span* of a metric. For a metric space (X, d), the tight-span $T(X, d)$ is the polytopal complex consisting of the bounded faces of the polyhedral complex

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

(see e.g. [5, 7]). In this context, it is worth noting that our 5-point analysis also sheds some light on h-optimal realizations of 5-point metrics as we now explain.

An *h-optimal realization* of d is a realization of d that can derived directly from the tight-span $T(X, d)$, and that has the attractive property that it is essentially unique [5] (see also [6]). In [1, p.117] Althöfer posed the following question concerning h-optimal realizations: If (G, φ) is an X-labeled graph, then can the optimal realizations of d corresponding to the extremal elements of $O(G, \varphi)$ be obtained by deleting some edges from the h-optimal realization of d? In Figure 2 we illustrate the 1-skeleton of the tight span of the generic Type I, II, III metrics, and the corresponding h-optimal realizations, with the optimal realizations embedded. In particular, it can be seen that the answer to Althöfer's question is "yes" for generic metrics on 5-points, and, in fact, this is also the case for any 5-point metric (see [11] for details). Note that for general metrics the answer to Althöfer's question is "no" [10].

In general, we expect that understanding optimal realizations on metric spaces with more than 5-points will be quite difficult (e.g. MF_6 consists of 194,160 elements coming in 339 types [12]). Even so, we note that it can be shown that there are only finitely many possible classes of X-labeled graphs underlying all possible optimal realizations of n-point metrics, $n \geq 2$. In view of this fact, it would be interesting to know whether some subset of these classes induces a subdivision of MF_n into subcones for $n \geq 6$, as we have found to be the case for MF_5.

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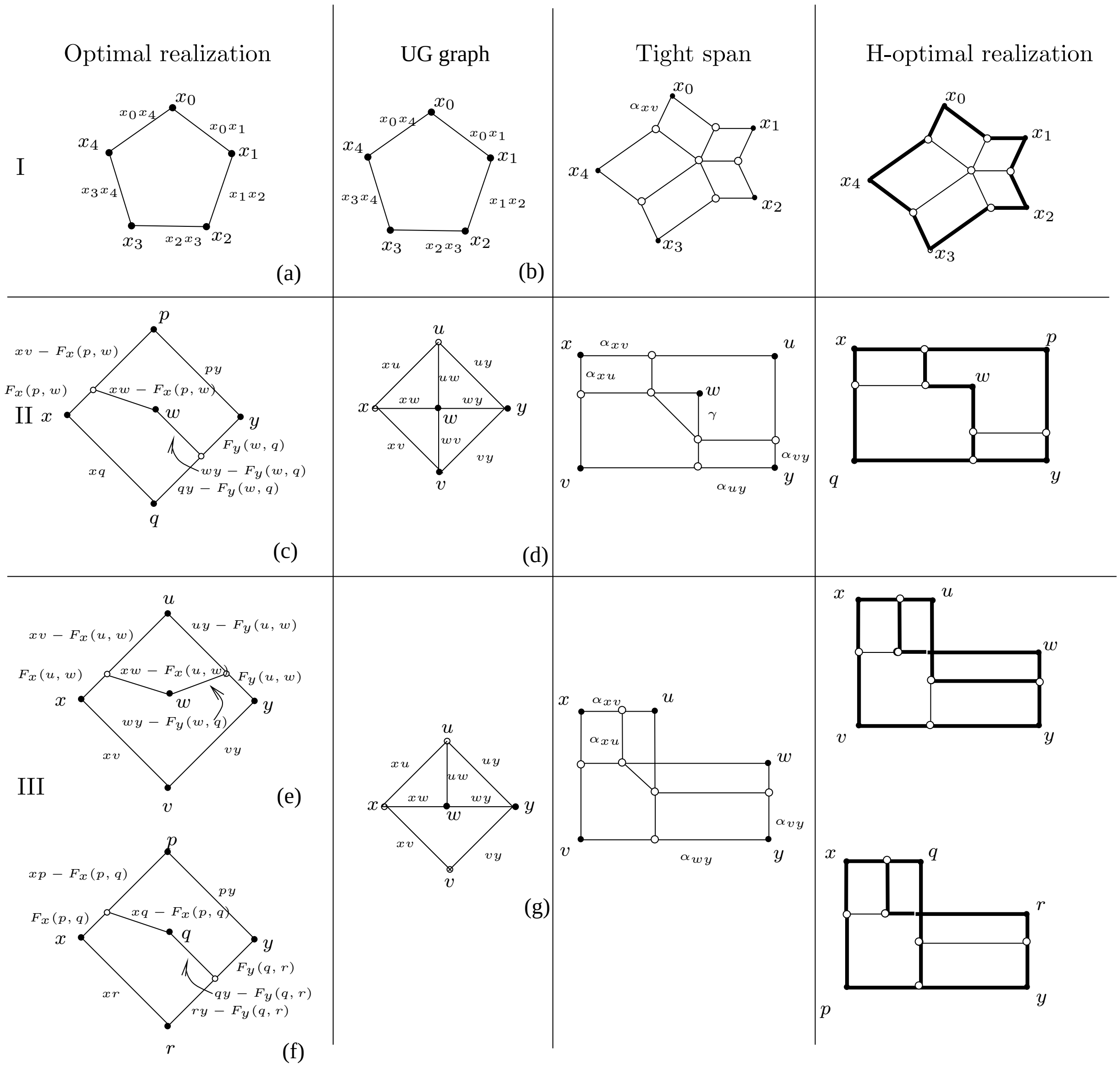

Figure 2: Optimal realizations, UG graphs, tight-spans and h-optimal realizations of pendant-free 5-point metrics. For the optimal realization in (c) there are two possible labelings; either $(p, q) = (u, v)$ or $(p, q) = (v, u)$. Similarly, for the optimal realization in (f) the triple (p, q, r) can be labeled by either (w, u, v) or (v, w, u). See Section 4 for more details concerning tight-spans and h-optimal realizations.