

Combinatorial invariants of finite metric spaces and the Wasserstein arrangement

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Abstract. In 2010, Vershik proposed a new combinatorial invariant of metric spaces given by a class of polytopes that arise in the theory of optimal transport and are called “Wasserstein polytopes” or “Kantorovich–Rubinstein polytopes” in the literature. Answering a question posed by Vershik, we describe the stratification of the metric cone induced by the combinatorial type of these polytopes through a hyperplane arrangement. Moreover, we study its relationships with the stratification by combinatorial type of the injective hull (i.e., the tight span) and, in particular, with certain types of metrics arising in phylogenetic analysis. We also compute enumerative invariants in the case of metrics on up to six points.

Keywords: finite metric spaces, Lipschitz polytopes, hyperplane arrangements

1 Introduction

This article is centered around the study of finite metric spaces through the lens of polytopes and hyperplane arrangements. Finite metric spaces arise in several applied contexts. Let us mention for instance mathematical biology, where finite metrics model genetic dissimilarities between different species [27]. In this setting, a main research direction is to identify suitable classes of metric spaces and study the combinatorics and geometry of the associated subset of the metric cone, e.g., for geometric statistics. This field of research goes back to the study of phylogenetic trees [1, 4], has grown to include more general phylogenetic networks [19] and is presently very active (see e.g., [12, 15, 14]).

One of the combinatorial invariants of metric spaces that are widely used in the aforementioned applications as well as for theoretical considerations is their *injective*

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hull, introduced by Isbell [20] and rediscovered by Dress [13] under the name *tight span*. The stratification of the metric cone by combinatorial type of tight spans is equivalent to the one determined by the subdivisions of the second hypersimplex studied by Sturmfels and Yu [28] and recently by Casabella, Joswig, and Kastner [6].

Motivated by the theory of optimal transport, Vershik described a correspondence between finite metric spaces and a class of symmetric convex polytopes, the so-called *Kantorovich–Rubinstein–Wasserstein (KRW) polytopes* or *fundamental polytopes* [29].

Definition 1.1. The KRW polytope of an n -metric ρ is a polytope in \mathbb{R}^n defined as the convex hull:

$$KRW(\rho) = \text{conv} \left\{ \frac{e_i - e_j}{\rho_{ij}} \mid 1 \leq i, j \leq n \right\},$$

where e_i is the i -th standard basis vector of \mathbb{R}^n . From now on, we abbreviate

$$p_{ij} := \frac{e_i - e_j}{\rho_{ij}} \text{ for } i \neq j.$$

The metric is called *generic* if it is strict and the KRW polytope is simplicial.

If ρ is the n -metric with $\rho_{ij} = 1$ for all $i \neq j$, then $KRW(\rho)$ is the type A_n *root polytope*.

The dual of a KRW polytope is the so-called *Lipschitz polytope* [29]. This is a symmetric *alcoved polytope* [22]; a class of polytopes that recently gained significant attention due to its connections to theoretical physics in the form of positive geometries and polypositroids [23].

The problem of understanding the combinatorial structure (e.g., computing face numbers) of KRW and Lipschitz polytopes is open and significant for applications, see e.g., [3, 7]. In this article, we focus on a related problem that goes back to a question by Vershik.

Problem 1.2 ([29, “General Problem”, §1]). Study and classify finite metric spaces according to the combinatorial properties of their KRW polytopes.

The first progress on this question was achieved by Gordon and Petrov who gave a description of the face poset of KRW polytopes via linear inequalities on the values of the metric [17], see [Section 1.3](#) for further details. This is the starting point for an in-depth study of KRW polytopes using the theory of hyperplane arrangements initiated in this paper.

1.1 The main results

We now summarize the main contributions of this article:

1. In [Section 2](#) we introduce a *Wasserstein arrangement* whose cells correspond to the combinatorial types of KRW polytopes. This arrangement builds upon the Gordon–Petrov description of the faces of KRW polytopes and could be of independent interest.
2. Using the computer algebra system OSCAR [9] together with the Julia package `CountingChambers.jl` [5] and the software TOPCOM [25] we obtain an enumeration of the combinatorial types of KRW polytopes of generic metrics on $n = 4, 5, 6$ points. This is displayed in [Table 1](#), where the number of combinatorial types of generic KRW polytopes – i.e., the number of chambers of the Wasserstein arrangement – is shown in the column titled “Labeled”. The column “Unlabeled” shows the number of combinatorial types up to combinatorial isomorphisms, which is the number of chambers of the Wasserstein arrangement modulo the natural action of the symmetric group S_n via coordinate permutation.

n	Unlabeled	Labeled
3	1	1
4	1	6
5	12	882
6	25,224	

Table 1: Combinatorial types of KRW polytopes of generic n -metrics.

3. We clarify the relation between KRW polytopes and tight spans in [Section 3](#) by providing examples of five-point metrics with isomorphic tight spans and combinatorially different KRW polytopes and vice versa. Hence, the two fan structures of the metric fan induced by the tight spans or the KRW polytopes are not refinements of each other.
4. We derive formulae for the number of faces of the KRW polytopes of non-generic strict metrics in [Section 4](#).

Remark 1.3. This extended abstract corresponds to an article that is published as preprint on the arXiv [10].

1.2 The metric cone

We begin by defining finite metric spaces and setting up some terminology.

Definition 1.4. An n -metric is a real symmetric $n \times n$ matrix ρ with entries ρ_{ij} for $1 \leq i, j \leq n$ satisfying

1. $\rho_{ii} = 0$ for all $1 \leq i \leq n$,
2. $\rho_{ij} > 0$ for all $1 \leq i \neq j \leq n$ and
3. $\rho_{ij} + \rho_{jk} \geq \rho_{ik}$ for all $1 \leq i, j, k \leq n$.

The metric ρ is called *strict* if $\rho_{ij} + \rho_{jk} > \rho_{ik}$ for all $j \in [n] \setminus \{i, k\}$.

Every n -metric ρ is given as a symmetric $n \times n$ matrix with zero diagonal, thus it is determined by the $\binom{n}{2}$ values ρ_{ij} with $i < j$.

Definition 1.5. Consider the vector space $\mathbb{R}^{\binom{n}{2}}$ with coordinates $x_{\{i,j\}}$ indexed by pairs of elements of $[n]$. The *metric cone* on n elements is the subset $\mathbf{M}_n \subseteq \mathbb{R}^{\binom{n}{2}}$ defined by

$$x_{\{i,j\}} > 0, \quad x_{\{i,j\}} + x_{\{j,k\}} \geq x_{\{i,k\}}, \quad \text{for all pairwise distinct } i, j, k \in [n].$$

We denote by $\overline{\mathbf{M}}_n$ the (topological) closure of \mathbf{M}_n .

Remark 1.6. The space $\overline{\mathbf{M}}_n$ is a polyhedral cone. It contains points that do not correspond to metrics but rather to pseudometrics (where $\rho_{ij} = 0$ can be allowed). The set of all strict metrics on n elements is the interior of \mathbf{M}_n .

1.3 Admissible graphs and strict metrics

Let ρ be an n -metric and F any face of the polytope $KRW(\rho)$. We associate with the face F a directed graph $G(F)$ on the vertex set $[n]$ which contains the edge (i, j) if the point p_{ij} lies on F . Following [17], the collection of graphs of the form $G(F)$ is called *the combinatorial structure* of $KRW(\rho)$.

Theorem 1.7 ([17, Theorem 3]). *Let ρ be an n -metric and $G = ([n], E)$ be a directed graph with the set of vertices $[n]$. The following are equivalent:*

1. *There exists a facet F of the polytope $KRW(\rho)$ containing every vertex p_{ij} for $(i, j) \in E$.*
2. *For any array of directed edges $(x_i, y_i), 1 \leq i \leq k$ of G with all x_i pairwise distinct and all y_i pairwise distinct:*

$$\sum_{i=1}^k \rho_{x_i y_i} \leq \sum_{i=1}^k \rho_{x_i y_{i+1}}, \quad (1.8)$$

where $y_{k+1} = y_1$.

Definition 1.9. A directed graph G on the vertex set $[n]$ is called *admissible* for an n -metric ρ if it satisfies one of the two equivalent conditions of Equation (1.7).

Lemma 1.10. *If ρ be a strict metric, the condition in Equation (1.7).(2) can only be satisfied if $x_1, \dots, x_k, y_1, \dots, y_k$ are pairwise distinct.*

We close this section with a characterization of generic metric spaces (in the sense of Equation (1.1)).

Theorem 1.11 ([17, Theorem 5]). *A strict n -metric ρ is generic if and only if for arbitrary $2k$ distinct points $x_1, \dots, x_k, y_1, \dots, y_k$ in $[n]$ the minimum of the terms*

$$\sum_{i=1}^k \rho_{x_i, y_{\pi(i)}}$$

is attained by a unique permutation $\pi \in S_k$.

2 The Wasserstein arrangement and the Wasserstein fan

We now define an arrangement of hyperplanes whose faces encode the combinatorial structures of KRW polytopes.

Definition 2.1 (Wasserstein arrangement). Let n be a positive integer. We define a hyperplane arrangement in $\mathbb{R}^{\binom{n}{2}}$ as follows. Given $1 < k$ and k -tuples $\mathbf{a} = (a_1, \dots, a_k)$, $\mathbf{b} = (b_1, \dots, b_k)$ with $a_i, b_i \in [n]$ for all $i = 1, \dots, k$, define a hyperplane

$$H_{\mathbf{a}, \mathbf{b}} := \left\{ x \in \mathbb{R}^{\binom{n}{2}} \mid \sum_{i=1}^k x_{\{a_i, b_i\}} = \sum_{i=1}^k x_{\{a_i, b_{i+1}\}} \right\} \quad \text{where } b_{k+1} = b_1.$$

The “positive side” of $H_{\mathbf{a}, \mathbf{b}}$ is

$$H_{\mathbf{a}, \mathbf{b}}^+ := \left\{ x \in \mathbb{R}^{\binom{n}{2}} \mid \sum_{i=1, \dots, k} x_{\{a_i, b_i\}} \leq \sum_{i=1, \dots, k} x_{\{a_i, b_{i+1}\}} \right\}.$$

The Wasserstein arrangement is then the set of hyperplanes

$$\mathcal{W}_n := \left\{ H_{\mathbf{a}, \mathbf{b}} \mid \begin{array}{l} 1 < k \leq n, \mathbf{a}, \mathbf{b} \in [n]^k \\ a_1, \dots, a_k, b_1, \dots, b_k \text{ mutually distinct} \end{array} \right\}.$$

The hyperplanes $H_{\mathbf{a}, \mathbf{b}}$ in \mathcal{W}_n were already mentioned as “exceptional planes” in the proof of Theorem 7 in [17].

Remark 2.2. In the case $k = 2$, the tuple (a_1, a_2) forms the same hyperplane when combined with either of the tuples (b_1, b_2) or (b_2, b_1) . In order for the notion of positive side to be well-defined, we establish the convention that we choose the tuple starting with $\min\{b_1, b_2\}$.

Definition 2.3 (Wasserstein fan). Let \mathcal{F}_n denote the fan determined by the intersections of the Wasserstein arrangement \mathcal{W}_n with the metric cone \mathbf{M}_n . We call \mathcal{F}_n the *Wasserstein fan*. Moreover, write $\overline{\mathcal{F}}_n$ for the (polyhedral) fan of pseudometrics, defined by the intersections of \mathcal{W}_n with the cone $\overline{\mathbf{M}}_n$.

Remark 2.4. The arrangement \mathcal{W}_n and the fan \mathcal{F}_n have the same number of i -cells for any i . In particular, we can count the number of maximal cells of the fan \mathcal{F}_n by counting the number of chambers of the arrangement \mathcal{W}_n .

Remark 2.5. Each hyperplane $H_{\mathbf{a},\mathbf{b}}$ corresponds to a cycle $C_{H_{\mathbf{a},\mathbf{b}}}$ of the complete graph K_n determined by the sequence of vertices $a_1, b_1, a_2, b_2, \dots, a_n, b_n$.

Proposition 2.6. *The arrangement \mathcal{W}_n consists of*

$$|\mathcal{W}_n| = \frac{1}{2} \sum_{k=2}^{\lfloor \frac{n}{2} \rfloor} \binom{n}{2k} (2k-1)!$$

many hyperplanes.

The proof of this proposition uses the aforementioned cycle characterization of the hyperplanes.

The next proposition relates the combinatorial structure of KRW polytopes with the face structure of the Wasserstein fan.

Proposition 2.7. *Let $n \geq 2$ be an integer and consider two n -metrics $\rho^{(1)}, \rho^{(2)}$. The following two statements are equivalent:*

1. *The metrics $\rho^{(1)}, \rho^{(2)}$ are in the open part of one cone σ of the Wasserstein fan \mathcal{F}_n .*
2. *The combinatorial structures of the polytopes $KRW(\rho^{(1)})$ and $KRW(\rho^{(2)})$ are the same, i.e., both polytopes have the same set of admissible directed graphs.*

3 Relationship to tight spans and injective hulls

We now want to relate the stratification of the metric cone by combinatorial type of KRW polytopes with the one in terms of the combinatorial type of a well-known polyhedral complex associated to metric spaces: the *injective hull* defined by Isbell [20] and rediscovered by Dress [13] with the name *tight span*. We start by outlining the construction and some key facts, and refer to [24] for a more detailed account and for a thorough analysis of the structure of injective hulls of general metric spaces.

Given an n -metric ρ we consider the (unbounded) polyhedron

$$P(\rho) := \{x \in \mathbb{R}^n \mid x_i + x_j \geq \rho_{ij} \text{ for all } i, j \in [n]\}.$$

Definition 3.1 ([24, §3], [13, Theorem 3.(v)]). The injective hull, or tight span $E(\rho)$ of ρ is the set of coordinate-wise minimal elements of $P(\rho)$.

Now recall the *second hypersimplex* $\Delta_{2,n} := \text{conv}\{e_i + e_j \mid i, j \in [n], i \neq j\} \subseteq \mathbb{R}^n$. Following, e.g., [18], every n -metric ρ defines a lift of $\Delta_{2,n}$:

$$L(\rho) := \text{conv}\{(e_i + e_j, \rho_{ij}) \mid i, j \in [n], i \neq j\} + \mathbb{R}_{\geq 0} e_{n+1} \subseteq \mathbb{R}^{n+1}.$$

The projection of the bounded faces of $L(\rho)$ onto \mathbb{R}^n defines the regular subdivision $\Delta_{2,n}(\rho)$. As was shown by Herrmann and Joswig [18], there is a linear equivalence between $P(\rho)$ and the polar dual of the polyhedron $L(\rho)$ that induces a combinatorial isomorphism between the face poset of $E(\rho)$ and the face poset of $\Delta_{2,n}(\rho)$.

Thus, the combinatorial type of the tight span of an n -metric ρ is dual to that of the induced regular subdivision of the second hypersimplex. In particular, the subdivision of the metric cone by combinatorial type of tight spans coincides with the intersection of the metric cone and the secondary fan of $\Delta_{2,n}$, the latter being a well-studied object in its own right (see, e.g., [8]).

Theorem 3.2. *The fan \mathcal{F}_n is neither a coarsening nor a refinement of the subdivision of the metric cone induced by secondary fan of $\Delta_{2,n}$ for $n \geq 5$.*

3.1 Split decomposition

We now turn to the class of totally split-decomposable spaces, as introduced by Dress and studied by Bandelt and Dress [2].

Definition 3.3. Let ρ be a symmetric function on a set X and let $A, B \subseteq X$. Define the *isolation index* $\alpha_{A,B}^\rho$ as

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

where $uv = \rho(u, v)$.

Remark 3.4. As noted in [2], $\alpha_{A,B}^\rho \geq 0$, $\alpha_{A,B}^\rho = 0$ whenever $A \cap B \neq \emptyset$. Moreover, if ρ is a metric and both A and B have at least 2 elements, then $\alpha_{A,B}^\rho = \alpha_{\{a, a'\}, \{b, b'\}}^\rho$ for some points $a, a' \in A$, $b, b' \in B$ with $a \neq a'$, $b \neq b'$.

In the following, when writing expressions such as $\alpha_{\{a, a'\}, \{b, b'\}}^\rho$ we will assume that a, a', b, b' are pairwise distinct points.

A bipartition $A \uplus B = [n]$ is called a ρ -split if $\alpha_{A,B}^\rho > 0$. A symmetric function ρ which does not admit any ρ -splits is called *split-prime*.

Theorem 3.5. *[[2, Theorem 2 and Corollary 2]] Every symmetric function $\rho : X \times X \rightarrow \mathbb{R}$ on a finite set X can be expressed as*

$$\rho = \rho_0 + \sum \alpha_{A,B}^\rho \cdot \delta_{A,B}$$

with ρ_0 split-prime. The metric ρ_0 is uniquely determined.

Definition 3.6. A metric ρ is called *totally split-decomposable* if it can be written as a positively weighted sum of split metrics. Equivalently, $\rho_0 = 0$ in the above expression.

The following is a criterion for checking whether a metric is totally split-decomposable:

Theorem 3.7 ([2, Theorem 6]). *Let $\rho : X \times X \rightarrow \mathbb{R}$ be a symmetric function with zero diagonal. The following conditions are equivalent:*

1. ρ is a totally split-decomposable metric.
2. For all $t, u, v, w, x \in X$ it holds that $\alpha_{\{t,u\},\{v,w\}} \leq \alpha_{\{t,x\},\{v,w\}} + \alpha_{\{t,u\},\{v,x\}}$.

Remark 3.8. From Equation (3.7) it is clear that all metrics on 4 points are split-decomposable. For $|X| \geq 5$ we can ask the question whether two metrics in the same cone of the Wasserstein arrangement are either both split-decomposable or both not split-decomposable. The next example answers this question in the negative.

Example 3.9. Consider the two metrics (ρ_1, ρ_2) on five points given by the following matrices:

$$\rho_1 = \begin{pmatrix} 0 & 125 & 48 & 149 & 84 \\ 125 & 0 & 149 & 48 & 99 \\ 48 & 149 & 0 & 125 & 77 \\ 149 & 48 & 125 & 0 & 92 \\ 84 & 99 & 77 & 92 & 0 \end{pmatrix}, \quad \rho_2 = \begin{pmatrix} 0 & 7447 & 4316 & 10083 & 5584 \\ 7447 & 0 & 10083 & 4316 & 5199 \\ 4316 & 10083 & 0 & 7447 & 7560 \\ 10083 & 4316 & 7447 & 0 & 6179 \\ 5584 & 5199 & 7560 & 6179 & 0 \end{pmatrix}.$$

These metrics lie in the same cone of the Wasserstein arrangement \mathcal{W}_5 , and therefore the associated KRW polytopes have the same combinatorial structure.

The metric ρ_1 is split-decomposable but for the metric ρ_2 we find

$$\alpha_{\{5,2\},\{1,3\}}^{\rho_2} > \alpha_{\{2,4\},\{1,3\}}^{\rho_2} + \alpha_{\{5,2\},\{1,4\}}^{\rho_2}.$$

By Equation (3.7), this certifies that ρ_2 is not split-decomposable, which in turn implies that the split-decomposable metrics do not form a subfan of the Wasserstein fan.

Example 3.10. Consider the following two 4-metrics.

$$\rho_1 := \begin{pmatrix} 0 & 3 & 3 & 4 \\ 3 & 0 & 4 & 3 \\ 3 & 4 & 0 & 3 \\ 4 & 3 & 3 & 0 \end{pmatrix} \quad \rho_2 := \begin{pmatrix} 0 & 4 & 3 & 5 \\ 4 & 0 & 5 & 3 \\ 3 & 5 & 0 & 4 \\ 5 & 3 & 4 & 0 \end{pmatrix}$$

These metrics have combinatorially isomorphic tight spans, but non-isomorphic KRW polytopes. The polytopes are not combinatorially isomorphic as $KRW(d_1)$ has two square faces whereas $KRW(d_2)$ is simplicial.

4 The f -vector in the strict case

In this section, we recall results for the number of faces of KRW-polytopes in dimensions 0 and 1 and give a formula for the number of 2-dimensional faces.

The starting point of this section is the following result by Gordon and Petrov. Recall from Equation (1.1) the definition of a generic metric.

Theorem 4.1 ([17, Theorem 1]). *Let $X, |X| = n + 1$ be a metric space with generic metric ρ . Then for $0 \leq m \leq n$, the number of $(n - m)$ -dimensional faces of the Lipschitz polytope of ρ is*

$$\binom{n + m}{m, m, n - m}.$$

The strict, non generic case is somewhat more complicated, but general formulae for faces of dimension 0 and 1 can be stated by using the graphic characterization of the faces.

Corollary 4.2 ([17, Corollary 1.(2)]). *Let ρ be a strict metric, then $f_0(KRW(\rho)) = n \cdot (n + 1)$.*

For $k \in \mathbb{N}$, denote by

$$\mathcal{W}_n^k := \left\{ H_{a,b} \mid \begin{array}{l} a, b \in [n]^k \\ a_1, \dots, a_k, b_1, \dots, b_k \text{ mutually distinct} \end{array} \right\}$$

the set of hyperplanes in \mathcal{W}_n corresponding to cycles of length $2k$ in K_n .

Definition 4.3. Let ρ be a strict metric on l points and define $X_\rho := \bigcap_{\substack{H \in \mathcal{W}_l \\ \rho \in H}} H$ and $r_k(\rho) :=$

$$|\{H \in \mathcal{W}_l^k \mid X_\rho \subseteq H\}|.$$

Lemma 4.4. *Let ρ be a strict metric which is not contained in any hyperplane of \mathcal{W}_l^2 . Then for each quadruple x_1, y_1, x_2, y_2 of vertices, if the edge set $\{(x_1, y_1), (x_2, y_2)\}$ is admissible, it is face-defining.*

With this, we can obtain the following general statement.

Proposition 4.5. *Let ρ be a strict metric on $l = n + 1$ points. Then*

$$f_1(KRW(\rho)) = \binom{n + 2}{2, 2, n - 2} - 2 \cdot r_2(\rho).$$

Note that the multinomial coefficient is the number of faces in the generic case, where X_ρ is the empty intersection.

5 Explicit computations

In this section, we explicitly study the KRW polytopes of metrics on 4, 5, and 6 points. We published an accompanying data set of one generic metric of each combinatorial type of these sizes on Zenodo [11].

5.1 The case $n = 4$.

There is only one generic KRW polytope up to symmetry.

In this case, the arrangement agrees with the braid arrangement \mathcal{A}_3 up to the lineality space and thus has 6 chambers.

There are three different types of strict, not generic metrics, two of which have the same f -vector, but different combinatorial type. The f -vector only depends on the rank of the intersection of the corresponding hyperplanes while their tight spans differ.

5.2 The case $n = 5$.

The characteristic polynomial of the Wasserstein arrangement \mathcal{W}_5 is $\chi_{\mathcal{W}_5}(t) = t^{10} - 15t^9 + 90t^8 - 260t^7 + 350t^6 - 166t^5$ which does not factor over the integers. Thus by Zaslavsky's theorem, the arrangement \mathcal{W}_5 has 882 chambers which agrees with the number of maximal cones of the fan \mathcal{F}_5 [30]. There are 12 generic KRW polytopes up to symmetry with f -vector (20 90 140 70) that are pairwise not isomorphic.

Moreover, there are 65 combinatorial types of strict but not generic KRW polytopes. We computed these using the `polymake` [16] hyperplane arrangement package [21] by enumerating all cells of the Wasserstein arrangement.

The symmetric group S_5 acts on the chambers by coordinate permutation.

Two chambers yield combinatorially equivalent polytopes if and only if there is $\sigma \in S_5$ mapping one chamber to the other.

5.3 The case $n = 6$.

For 6-point metrics, \mathcal{W}_6 is an arrangement in \mathbb{R}^{15} with a 6-dimensional lineality space consisting of 105 hyperplanes, see Equation (2.6).

The generic KRW polytopes correspond exactly to certain regular triangulations of RP_n^0 , the (full) root polytope together with the origin. Jörg Rambau computed all symmetric regular triangulations of RP_6^0 up to symmetry using the latest version of his software TOPCOM [26]. There are exactly 25,224 such triangulations.

Theorem 5.1. *There are 25,224 generic KRW polytopes up to symmetry (action of S_6) that are pairwise not isomorphic.*

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