

# Nomenclature

|                                |   |
|--------------------------------|---|
| $\ \cdot\ $                    | Euclidean Norm on $\mathbb{R}^d$          |
| $\langle \cdot, \cdot \rangle$ | Scalar product on $\mathbb{R}^d$          |
| $\mathbb{R}_{\geq 0}$          | Positive real numbers                     |
| $\lambda^d$                    | Lebesgue measure on $\mathbb{R}^d$        |
| $\mathcal{B}^d$                | Borel $\sigma$ -algebra on $\mathbb{R}^d$ |
| $\text{Pot}(\cdot)$            | Power set of a set                        |
| $ \cdot $                      | Cardinality of a set                      |
| $\mathcal{L}(\mu)$             | $\mu$ -integrable functions               |

TODO: Motivation for Optimal Transport & recall some definitions from measure theory

Let  $(X, \mathcal{A})$  be a measurable space and  $\mu, \tilde{\mu}$  two measures on it. We say that  $\mu$  is absolutely continuous with respect to  $\tilde{\mu}$  and write  $\mu \ll \tilde{\mu}$ , if

$$\tilde{\mu}(A) = 0 \Rightarrow \mu(A) = 0 \quad \forall A \in \mathcal{A}.$$

Let  $(X, \mathcal{A}, \mu)$  be a measure space and  $(Y, \mathcal{U})$  a measurable space. For a measurable function  $T : X \rightarrow Y$ , we denote by  $T_{\#}\mu$  the pushforward measure on  $Y$  induced by  $T$ , i.e

$$T_{\#}\mu(B) = \mu(T^{-1}(B)) \quad \forall B \in \mathcal{U}.$$

TODO:

For a given finite set  $S \subset \mathbb{R}^d$ , we want to study the following problem:  
Given two probability spaces  $(\mathbb{R}^d, \mathcal{B}^d, \mu)$  and  $(S, \text{Pot}(S), \nu)$ , we want to minimize

$$\int_{\mathbb{R}^d} \|x - T(x)\|^2 d\mu \tag{0.1}$$

over all measurable maps  $T : \mathbb{R}^d \rightarrow S$ , that satisfy  $T_{\#}\mu = \nu$ .

Recall that as  $(S, \text{Pot}(S), \nu)$  is a finite probability space, we can write  $\nu$  as a finite sum of dirac measures

$$\nu = \sum_{s \in S} \nu_s \delta_s \quad \text{where } \nu_s \in \mathbb{R}_{\geq 0} \text{ and such that } \sum_{s \in S} \nu_s = 1. \tag{0.2}$$

Thus, the problem we are considering consists in finding a measurable map  $T$  that minimizes the functional (0.1) and that fulfills  $\mu(T^{-1}(s)) = \nu_s$  for all  $s \in S$ . For  $s \in S$ , we will call  $\mu(T^{-1}(s))$  the capacity of  $s$ .

TODO: \*\* Prove existence and uniqueness of a solution

As shown by [AHA], finding a measurable map that minimizes the functional (0.1) is equivalent to finding the maximum of a concave function and thus, can be solved

with standard optimization methods. The formulation of this optimization problem is based in two steps. First, we find a minimizer of the functional (0.1) over all measurable functions with same capacities. This optimal solution  $T_W$  is inspired geometrically and constructed using a predefined *weight vector*  $W$ .

The next step will consist in adapting this weight vector, such that the condition  $T_{W\#}\mu = \nu$  is fulfilled.

The motivation behind this approach is inspired geometrically by studying a generalization of *Voronoi diagrams*. For clarity, we recall the definition of this diagrams and review the necessary concepts needed for this approach.

**Definition 0.1** (Voronoi Diagrams). Let  $S \subset \mathbb{R}^d$  be a finite set. We define for every point  $s \in S$

$$\text{reg}(s) := \{x \in \mathbb{R}^d : \|x - s\| \leq \|x - \tilde{s}\| \quad \forall \tilde{s} \in S \setminus \{s\}\}.$$

We call this, the region (or cell) of the point  $s$ . The partition of  $\mathbb{R}^d$  created by the union of the regions of all points is called the Voronoi diagram of  $S$ .

*Remark.* Note that the partition of  $\mathbb{R}^d$  generated by the Voronoi diagram is given by convex regions. Such a partition induces naturally a map  $T : \mathbb{R}^d \rightarrow S$ , which assign each point in  $\mathbb{R}^d$  the corresponding point in  $S$  of the cell where it is located, i.e

$$T(x) = s \quad \Leftrightarrow \quad x \in \text{reg}(s). \quad (0.3)$$

By definition, some points in  $\mathbb{R}^d$  may belong to more than one region. By convention,  $T$  assigns those points an arbitrary one in  $S$  of a region where it is located. We call  $T$ , the from the Voronoi diagram induced assignment.

A generalization of the presented concepts arise when using another distance function for the definition of the regions. One practical way for this, appears by using the *power function with weights*  $W$ .

**Definition 0.2** (Power function). Let  $S \subset \mathbb{R}^d$  be a finite set and  $W : S \rightarrow \mathbb{R}$  a function on  $S$ . The power function with weights  $W$  is defined as

$$\text{pow}_W(x, s) = \|x - s\|^2 - W(s).$$

$W$  is called weight function on  $S$ .

*Remark.* For simplicity of notation we will identify sometimes the weight function  $W : S \rightarrow \mathbb{R}^d$  as a vector in  $\mathbb{R}^{|S|}$ . We call then  $W$ , weight vector on  $S$ .

Similarly as by Voronoi Diagrams, we can define regions on  $\mathbb{R}^d$  by using the power function with weights  $W$ . For a point  $s \in S$  we call

$$\text{reg}_W(s) := \{x \in \mathbb{R}^d : \text{pow}_W(x, s) \leq \text{pow}_W(x, \tilde{s}) \quad \forall \tilde{s} \in S \setminus \{s\}\}$$

the *power region* (or power cell) of  $s$  with weights  $W$ . Power regions also create a partition of  $\mathbb{R}^d$  which is called the *power diagram* of  $S$  with weights  $W$ .

The geometric intuition behind the definition of power diagrams appears by looking the spheres around  $s \in S$  with positive radius

$$\mathbb{S}_{\sqrt{W}}^{d-1}(s) := \{x \in \mathbb{R}^d : \|x - s\| = \sqrt{W(s)}\}$$

when  $W : S \rightarrow \mathbb{R}_{>0}$ . The power function  $\text{pow}(\cdot, s)$  for a fixed  $s \in S$ , returns a negative (resp. positive) value whenever  $x \in \mathbb{R}^d$  is inside (resp. outside) the sphere  $\mathbb{S}_{\sqrt{W}}^{d-1}(s)$  and zero when  $s \in \mathbb{S}_{\sqrt{W}}^{d-1}(s)$ . Thus, increasing (resp. decreasing) the values of the weights  $W(s)$  on each point  $s$  would expand (resp. shrink) the power cells.

*Remark.* Unlike Voronoi diagrams, the power cells of a point  $s \in S$  may not contain the point  $s$  or may be even empty. Nevertheless, the power diagram still partitioned  $\mathbb{R}^d$  in convex polyhedron.

By replacing  $\text{reg}$  with  $\text{reg}_W$  in (0.3) we obtain a map  $T_W : \mathbb{R}^d \rightarrow S$  which depends on  $W$ . Similarly as by Voronoi diagrams, we assign those points who share different cells, an arbitrarily point  $s \in S$  of those shared regions. We call this map, the *power assignment* of  $S$  with weights  $W$ .

Power assignments have a natural optimization property, since by definition it holds

$$(T_W(x) = s \Leftrightarrow x \in \text{reg}_W(s)) \Leftrightarrow T_W(x) = \min_{s \in S} \|x - s\|^2 - W(s) \quad (0.4)$$

for all points  $x \in \mathbb{R}^d$  which doesn't share different regions. In fact, power functions even minimize the functional (0.1) for a fixed predefined weight vector  $W$ . We will prove this in Lemma 0.4. Consequently, the next natural question will deal the choice of the weights  $W$ , s.t it fullfills the condition  $T_{W\#}\mu = \nu$ .

We recall the change of variables theorem from the measure theory.

**Theorem** (change of variables). *Let  $(X, \mathcal{A}, \mu)$  be a measure space,  $(Y, \mathcal{U})$  a measurable space and  $T : X \rightarrow Y$  a measurable function. For a measurable function  $f : Y \rightarrow \mathbb{R}^d$  holds  $f \in \mathcal{L}(T_{\#}\mu) \Leftrightarrow f \circ T \in \mathcal{L}(\mu)$  and when one of this statments is true then*

$$\int_{T^{-1}(B)} f \, dT_{\#}\mu = \int_B f \circ T \, d\mu \quad \text{for all } B \in \mathcal{U}. \quad (0.5)$$

*Proof.* Measure theory, e.g p.191 [J.E] □

*Remark 0.3.* Note that as the power region of a point  $s \in S \subset \mathbb{R}^d$  is even an empty set or a convex polyhedra, it is measurable with respect to the Lebesgue measure  $\lambda^d$  on  $\mathbb{R}^d$ . Denoting by  $\overset{\circ}{B}$  the interior of a set  $B$  with respect to the standard topology, it holds

$$\lambda^d(\text{reg}(s)) = \lambda^d(\overset{\circ}{\text{reg}}(s)).$$

For a Probabilty space  $(\mathbb{R}^d, \mathcal{B}^d, \mu)$  s.t  $\mu \ll \lambda^d$ , holds then

$$\mu(\text{reg}(s)) = \mu(\overset{\circ}{\text{reg}}(s)) \quad \text{and} \quad \sum_{s \in S} \mu(\text{reg}(s)) = 1.$$

**Lemma 0.4.** *Let  $(\mathbb{R}^d, \mathcal{B}, \mu)$  be a Probabilty space, s.t  $\mu \ll \lambda^d$ . Let  $S$  be a finite subset of  $\mathbb{R}^d$  with weights  $W$  and  $\zeta : S \rightarrow \mathbb{R}_{\geq 0}$  be a function on  $S$ . Then, the power assignment  $T_W$  minimizes*

$$\int_{\mathbb{R}^d} \|x - T(x)\|^2 \, d\mu$$

over all measurable maps  $T : \mathbb{R}^d \rightarrow S$  with capacities  $\mu(T^{-1}(s)) = \zeta(s)$  for all  $s \in S$ .

*Proof.* Using the minimality condition (0.4) of power assignments, it holds

$$\text{pow}_W(x, T_W(x)) \leq \text{pow}_W(x, s)$$

for all  $s \in S$ . Consequently,  $T_W$  minimizes

$$\int_{\mathbb{R}^d} \text{pow}_W(x, T(x)) \, d\mu = \int_{\mathbb{R}^d} \|x - T(x)\|^2 \, d\mu - \int_{\mathbb{R}^d} \omega(T(x)) \, d\mu$$

over all measurable maps  $T : \mathbb{R}^d \rightarrow S$ . Using the fact that  $\mathbb{R}^d = \bigcup_{s \in S} \text{reg}(s)$  in combination with remark 0.3, it holds

$$\begin{aligned} \int_{\mathbb{R}^d} \omega(T(x)) \, d\mu &= \sum_{s \in S} \int_{\text{reg}(s)} W(T(x)) \, d\mu \\ &\stackrel{(0.5)}{=} \sum_{s \in S} \int_s W \, dT_{\#}\mu \\ &= \sum_{s \in S} \mu(T^{-1}(s)) W(s) \\ &= \sum_{s \in S} \zeta(s) W(s) \end{aligned}$$

which is constant for a fixed  $\zeta$  and  $W$ . □

The natural question to handle next, is how to chose  $W$ , s.t the condition  $T_{W\#}\mu = \nu$  holds. As we will show below, this question can be equivalently formulated as finding the maximum of a concave function. In order to achive this, we first recall the original setting of our original problem and introduce some definitions.

Let  $(\mathbb{R}^d, \mathcal{B}, \mu)$  and  $(S, \text{Pot}(S), \nu)$  be two proabilty spaces s.t  $\mu \ll \lambda^d$ . As in (0.2), we write  $\nu = \sum_{s \in S} \nu_s \delta_s$  as a finite sum of dirac measures.

For  $\mathcal{F} := \{f : \mathbb{R}^d \rightarrow S : f \text{ is measurable}\}$ , define

$$L : \mathcal{F} \times \mathbb{R}^{|S|} \rightarrow \mathbb{R}, \quad (T, W) \mapsto \int_{\mathbb{R}^d} \text{pow}_W(x, T(x)) \, d\mu.$$

This map has important properties, which we will show and then transfer them to the concave function of our reformulated problem. For a map  $T \in \mathcal{F}$ , let

$$\zeta_T : S \rightarrow \mathbb{R}, \quad s \mapsto \mu(T^{-1}(s))$$

be the vector of capacities induced by  $T$  and

$$Q : \mathcal{F} \rightarrow \mathbb{R}, \quad T \mapsto \int_{\mathbb{R}^d} \|x - T(x)\|^2 \, d\mu$$

be the functional that we want to study. As shown in Lemma 0.4, it holds

$$L(T, W) = Q(T) - \langle \zeta_T, W \rangle.$$

And hence,  $L_T := L(T, \cdot)$  defines a linear function on  $\mathbb{R}^{|S|}$  for a fixed  $T \in \mathcal{F}$ . Recall that for a given  $W \in \mathbb{R}^{|S|}$  and a power assignment  $T_W$ , holds  $\text{pow}_W(x, T_W(x)) \leq \text{pow}_W(x, s)$  for all  $s \in S$ . Consequently, for a fixed  $W \in \mathbb{R}^d$  holds

$$T_W(W) = \arg \min_{T \in \mathcal{F}} L(T, W). \quad (0.6)$$

We claim that

$$f : \mathbb{R}^{|S|} \rightarrow \mathbb{R}^d, \quad W \mapsto L(T_W, W) = L_{T_W}(W)$$

is concave.

*Proof.* Let  $\alpha \in [0, 1]$  and  $W_1, W_2 \in \mathbb{R}^{|S|}$ , then

$$\begin{aligned} f(\alpha W_1 + (1 - \alpha)W_2) &= L_{T_{\alpha W_1 + (1 - \alpha)W_2}}(\alpha W_1 + (1 - \alpha)W_2) \\ &= L_{T_{\alpha W_1 + (1 - \alpha)W_2}}(\alpha W_1) + L_{T_{\alpha W_1 + (1 - \alpha)W_2}}((1 - \alpha)W_2) \\ &\stackrel{(0.6)}{\geq} L_{T_{\alpha W_1}}(\alpha W_1) + L_{T_{(1 - \alpha)W_2}}((1 - \alpha)W_2) \\ &= \alpha L_{T_{\alpha W_1}}(W_1) + (1 - \alpha) L_{T_{(1 - \alpha)W_2}}(W_2) \\ &\stackrel{(0.6)}{\geq} \alpha L_{T_{W_1}}(W_1) + (1 - \alpha) L_{T_{W_2}}(W_2) = \alpha f(W_1) + (1 - \alpha) f(W_2) \end{aligned}$$

□

TODO: Prove formally that f is smooth

$f$  is smooth and the gradient of  $f$  at  $W$  is given by  $\nabla f(W) = -\zeta_{T_W}$ . Recall that because of Lemma 0.4, to solve our problem (0.1) we need to find a weight vector  $W^*$  s.t  $T_{W^*}(\mu) = \nu$ . In other words, it should hold  $\mu(T_{W^*}^{-1}(s)) = \nu_s$  for all  $s \in S$ . Consider now the function

$$H : \mathbb{R}^{|S|} \rightarrow \mathbb{R}, \quad W \mapsto f(W) + \langle \nu, W \rangle = \langle \nu - \zeta_{T_W}, W \rangle + Q(T_W).$$

This function is concave and differentiable as a sum of concave differentiable functions, it holds  $\nabla H(W) = \nu - \zeta_{T_W}$  and hence

$$T_{W\#} \mu(s) = \mu(T_W^{-1}(s)) = \nu_s \quad \forall s \in S \quad \Leftrightarrow \quad \zeta_{T_W} = \nu \quad \Leftrightarrow \quad \nabla H(W) = 0.$$

Thus finding a solution of the problem (0.1) is equivalent to finding a maximum of the concave function  $H$ . For this function holds

$$\begin{aligned} \frac{\partial H}{\partial W}(s) &= \frac{\partial f(W)}{\partial W}(s) + \frac{\partial \langle \nu, W \rangle}{\partial W}(s) \\ &= -\mu(T_W^{-1}(s)) + W(s) \\ &= -\mu(\text{reg}(s)) + W(s). \end{aligned}$$

This optimization problem has a probabilistic interpretation. If we realize  $X$  as a random variable of distribution  $\mu$ , i.e  $X \sim \mu$ . Then, defining

$$h_W^\nu(x) := \min_{s \in S} \|x - s\|^2 - W(s) + \langle W, \nu \rangle = \|x - T_W(x)\|^2 - W(s) + \langle W, \nu \rangle,$$

it holds

$$\begin{aligned} \mathbb{E}[h_W^\nu(X)] &= \int_{\mathbb{R}^d} \min_{s \in S} \|X - s\|^2 - W(s) \, d\mu + \int_{\mathbb{R}^d} \langle W, \nu \rangle \, d\mu \\ &= \int_{\mathbb{R}^d} \|x - T_W(X)\|^2 - W(s) \, d\mu + \langle W, \nu \rangle = H(W). \end{aligned}$$

Thus, our problem consists in minimizing the expectation of  $h_W^\nu(X)$ .