

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
λ^d	Lebesgue measure on \mathbb{R}^d
\mathcal{B}^d	Borel σ -algebra on \mathbb{R}^d
$\text{Pot}(\cdot)$	Power set of a set
$ \cdot $	Cardinality of a set
$\mathcal{L}(\mu)$	μ -integrable functions

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

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

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

and denote this by $\mu \ll \tilde{\mu}$. Let (X, \mathcal{A}, μ) 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 $T : \mathbb{R}^d \rightarrow S$ satisfying $T_{\#}\mu = \nu$.

Recall that as $(S, \text{Pot}(S), \nu)$ is a finite probability space, we can write ν 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 translates to finding a measurable map T that minimizes the functional in (0.1) and such that we have $\mu(T^{-1}(s)) = \nu_s$ for all $s \in S$. For any $s \in S$, we will call $\mu(T^{-1}(s))$ the capacity of s .

TODO: ** Prove existence and uniqueness of a solution

As shown in [AHA], finding a measurable map that minimizes the above functional 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 done in two steps. First, we find a minimizer over all measurable functions with the 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 these 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 by the Voronoi diagram induced assignment.

A generalization of the presented concepts arise when using another distance function for the definition of the regions. One application of this, amounts to using the *power function with weights* W which we now define.

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

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

We call W the *weight function* on S .

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

As in the case of 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 becomes clear by looking at spheres around $s \in S$ with positive radius

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

whenever $W : S \rightarrow \mathbb{R}_{>0}$. 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 even may be empty. Nevertheless, the power diagram still partitions \mathbb{R}^d in a convex polyhedron.

By replacing reg with reg_W in (0.3) we obtain a map $T_W : \mathbb{R}^d \rightarrow S$ depending on the weight vector W . Similarly as with Voronoi diagrams, we assign those points sharing 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 don'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. As a consequence, the natural question which remains to be clarified is how to fix a choice of the weight vector W , such that 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}, μ) be a measure space, (Y, \mathcal{U}) a measurable space and $T : X \rightarrow Y$ a measurable function. For a measurable function $f : Y \rightarrow \mathbb{R}^d$ we have $f \in \mathcal{L}(T_{\#}\mu) \Leftrightarrow f \circ T \in \mathcal{L}(\mu)$ and when one of this statements 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 either an empty set or a convex polyhedra, it is measurable with respect to the Lebesgue measure λ^d on \mathbb{R}^d . Denoting by $\overset{\circ}{B}$ the interior of a set $B \in \mathcal{B}$ with respect to the standard topology, it holds

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

For a probability space $(\mathbb{R}^d, \mathcal{B}^d, \mu)$ such that $\mu \ll \lambda^d$, we have 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 probability space, such that $\mu \ll \lambda^d$. 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 $\mathbb{R}^d = \bigcup_{s \in S} \text{reg}(s)$ together with remark 0.3, we obtain

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

which is constant for a fixed ζ and W . □

The natural question to handle next, is how to choose W , such that 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 achieve 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 probability spaces such that $\mu \ll \lambda^d$. As in Equation (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 , we have

$\text{pow}_W(x, T_W(x)) \leq \text{pow}_W(x, s)$ for all $s \in S$. Consequently, for a fixed $W \in \mathbb{R}^d$ we must have

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

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^* satisfying $T_{W^*}(\mu) = \nu$. 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. Furthermore we have $\nabla H(W) = \nu - \zeta_{T_W}$ and hence also

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

Thus we see that finding a solution of our original problem is in deed equivalent to

finding a maximum of the concave function H . We can compute

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

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

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

we have

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

In other words, our problem can be stated as minimizing the expected value of $h_W^\nu(X)$.