The Optimal Transport Problem

Master Thesis

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by

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UAB

Preface

Preface…

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Contents

1

Preliminaries.

Notation

$\mathbb{R}$	Real numbers field.
$\bar{\mathbb{R}}$	$\mathbb{R} \cup \{+\infty\}$. That is $[-\infty, \infty]$
$\mathbb{R}_+$	The set of nonnegative real numbers, that is the interval $[0, \infty)$.
$\bar{\mathbb{R}}_+$	The set of nonnegative extended real numbers, that is the interval $[0, \infty]$
δ_x	The Dirac mass at point x.
$\mathbb{R}^d$	The d-dimensional Euclidean space.
id	Identity map.
$\mathcal{P}(X)$	Space of probabilities on X.
$\mu \ll \nu$	The measure is absolutely continuous with respect to ν.
$\mathbb{1}_\Omega$	Indicator function of a set Ω. If $x \in \Omega$ then $\mathbb{1}_\Omega(x) = 1$. If $x \in \Omega^c$, we have $\mathbb{1}_\Omega(x) = 0$.
$\mu \llcorner A$	A measure μ restricted to a set A.
ω_d	The Measure of the unite ball in $\mathbb{R}^d$.
$\wedge$	The min operator, that is $a \wedge b := \min\{a, b\}$.
$\vee$	The max operator, that is $a \vee b := \max\{a, b\}$.
$\mathrm{D}T(x)$	Jacobian matrix of a map $T(x)$.
$T_\# \mu$	The image measure of μ through the map T.
$f_{\vert\Omega}$	The restriction of a function f to a set Ω.
$\Pi(\mu, \nu)$	The set of transport plans from μ to ν.
$\frac{\delta F}{\delta \rho}$	First variation of $F : \mathcal{P}(X) \to \mathbb{R}$, that is $\frac{\mathrm{d}}{\mathrm{d}\epsilon} F(\rho + \epsilon\chi)\Big\vert_{\epsilon=0} = \int \frac{\delta F}{\delta \rho} \mathrm{d}\chi$
W_p	Wasserstein distance of order p.
$\mathbb{W}_p$	Wasserstein space of order p.
γ_T	The transport plan in $\Pi(\mu, \nu)$ induced by a map T. That is $\gamma_T = (\mathrm{id}, T)_\# \mu$ and $T_\# \mu = \nu$.
$M(T)$	Monge cost of a map T.
$K(\gamma)$	Kantorovich cost of a plan γ.
$\mu \otimes \nu$	The product measure of μ and ν such that $\mu \otimes \nu(A \times B) = \mu(A)\nu(B)$.
$M^{k \times h}$	The set of real matrices with k rows and h columns.
$M^\top$	Transpose of a matrix M.
i.i.d.	Independent and identical probability distributions.
l.s.c.	Lower semicontinuous.

Definitions and important theorems to remember.

We start this chapter reminding the basic definitions in topology and measure theory.

Definition 1.1.

Definition 1.2. *Let X be a Hausdorff space. Let $\mathcal{V}(x_0)$ be a topological basis of X, such that all $V \in \mathcal{V}$*

contains x_0. Let $f : X \to \bar{\mathbb{R}}$ a functional valued in $\bar{\mathbb{R}}$. We define,

$$\liminf_{x \to x_0} f(x) = \sup_{V \in \mathcal{V}(x_0)} \inf_{s \in V} f(s)$$

$$\limsup_{x \to x_0} f(x) = \inf_{V \in \mathcal{V}(x_0)} \sup_{s \in V} f(s)$$

The above definitions can be expressed in terms of sequences of real numbers. Let $(x_n)_{n\in\mathbb{N}}$ be a sequence in X, the above formulation is equivalent to say.

$$\liminf_{n\in\mathbb{N}} x_n := \lim_{n\to\infty} \left(\inf_{m\geq n} x_m \right)$$

Equivalently for $\limsup$*,*

$$\liminf_{n\in\mathbb{N}} x_n := \lim_{n\to\infty} \left(\sup_{m\geq n} x_m \right)$$

Please note that the convergence to some point x_0, $(x_n)_{n\in\mathbb{N}} \to x_0$ is not required in the last definitions.

Definition 1.3 (Lower Semicontinuity)**.** *On a complete metric space X, a function $f : X \to \bar{\mathbb{R}}$ is said to be lower semi-continuous (l.s.c.) if for every sequence $(x_n)_{n\in\mathbb{N}}$ converging to $x \in X$, we have*

$$f(x) \leq \liminf_{n\in\mathbb{N}} f(x_n)$$

Definition 1.4 (Sequentially compact)**.** *A subset K of a metric space X is said to be compact if from any sequence x_n, we can extract a converging subsequence $x_{n_k} \to x \in K$.*

We can see from the above definition that any continuous function is lower-semicontinuous.

Definition 1.5 (Compactness)**.** *A subset K of a metric space X is compact if every open cover of K has a finite subcover.*

Theorem 1.1. *A subset of a metric space is compact if and only if it is sequentially compact.*

Theorem 1.2 (Maxima and Minima)**.** *Let X be a compact metric space and $f : X \to \mathbb{R}$ is continuous, real-valued function. Then f is bounded on X and attains its maximum and minimum. That is, there are x, y belonging to X such that,*

$$f(x) = \inf_{z\in X} f(z) \qquad \text{and} \qquad f(y) = \sup_{z\in X} f(z)$$

Continuity is a strong requirement. Luckily we can assure the existence of a minimizer on lower-semicontinuous functions (or maximizer on upper-semicontinuous). The usual procedure to prove existence of a minimizer is making use of Weierstrass' criterion. We take a minimizing sequence and then we prove that the space in which we are trying to find a minimizer element is compact.

Theorem 1.3 (Weierstrass' criterion for existence of minimizers)**.** *If $f : X \to \bar{\mathbb{R}}$ is lower semi-continuous and X is compact, then there exists $\hat{x} \in X$.*

Proof. Define $l := \inf\{f(x) : x \in X\} \in \bar{\mathbb{R}}$, notice that $l = +\infty$ only if f is identically $+\infty$, then this case is trivial since any point minimizes f. By compactness there exists a minimizing sequence x_n, that is $f(x_n) \to l$. By compactness we can extract a subsequence converging to some $\hat{x}$ such that $\hat{x} \in X$. By lower-semicontinuity of f, we have that $f(\hat{x}) \liminf_n f(x_n) = l$. Since l is the infimum $l \leq f(\hat{x})$. This proves that $l = f(\hat{x}) \in \mathbb{R}$. □

We can apply the above analysis using a notion of upper-semicontinuity and compactness to find the maximum.

Definition 1.6 (Topological Dual)**.** *If X is a normed space, the dual space $X^* = \mathcal{B}(X, \mathbb{R})$. Consists of all linear and bounded functionals mapping from X to $\mathbb{R}$.*

Definition 1.7 (Weak compactness in dual spaces)**.** *A sequence x_n in a Banach space X is said to be weakly converging to x, and we write $x_n \rightharpoonup x$, if for every $\xi \in X^*$. We have $\langle \xi, x_n \rangle \to \langle \xi, x \rangle$. A sequence $\xi_n \in X^*$ is said to be weakly-* converging to ξ, and we write $\xi_n \rightharpoonup \xi$, if for every $x \in X$ we have $\langle \xi_n, x \rangle \to \langle \xi, n \rangle$.*

Theorem 1.4 (Banach-Alaouglu)**.** *If X is separable and ξ_n is a bounded sequence in X^*, then there exists a subsequence ξ_{n_k} weakly converging to some $\xi \in X^*$.*

The Banach-Alaouglu's theorem is a well known result in functional analysis, an equivalent formulation is saying the closed unit ball in X^* is weak-* compact.

Definition 1.8. *A sequence μ_n probability measures over X is said to be tight if for every $\epsilon > 0$, there exists a compact subset $K \subset XS$ such that $\mu_n\,(X \backslash K) < \epsilon$ for every n.*

Definition 1.9 (Tightness)**.** *Let $(\mathcal{X}, \mathcal{T})$ a topological space, and let $\mathcal{A}$ a σ-algebra on $\mathcal{X}$ that contains the topology $\mathcal{T}$. Let M be a collection of measures defined on $\mathcal{A}$. The collection M is called tight if for every $\epsilon > 0$ there is a compact subset K_ϵ of $\mathcal{X}$ such that, for all measures $\mu \in M$ we have,*

$$|\mu|\,(\mathcal{X} \backslash K_\epsilon) < \epsilon$$

Note that $C_0(X) = C_b(X) = C(X)$ if X is compact and both notions of convergence coincide.

Theorem 1.5 (Prokhorov)**.** *Suppose that μ_n is a tight sequence of probability measures over a Polish space $\mathcal{X}$. Then there exists $\mu \in \mathcal{P}(X)$ and a subsequence μ_{n_k} such that $\mu_{n_k} \rightharpoonup \mu$, in duality with $C_b(X)$. Conversely, every sequence $\mu_{n_k} \rightharpoonup \mu$ is tight.*

Definition 1.10. *Let $F : X \to \bar{\mathbb{R}}$ be a given functional bounded from below on a metric space X. Let $\mathcal{G}$ be the set of lower semicontinuous functions $G : X \to \bar{\mathbb{R}}$, such that $G \leq F$. We call a relaxation the supremum of $\mathcal{G}$. This functional does exist since the supremum of an arbitrary family of lower semicontinuous functions is also lower semicontinuous. It is possible to have a representation formula as follows:*

$$\bar{F}(x) = \inf\left\{\liminf_{n \in \mathbb{N}} F(x_n) : \; x_n \to x\right\}. \tag{1.1}$$

As consequence of this definition we see that $F \geq \bar{F}$ implies $\inf F \geq \inf \bar{F}$. Let $l = \inf F$ then $F \geq l$. A constant function is lower semicontinuous. Therefore, $\bar{F} \geq l$ and $\inf \bar{F} \geq \inf F$. Implying that the infimum of both F and its regularization $\bar{F}$ coincide, i.e. $\inf \bar{F} = \inf F$.

Definition 1.11. *A measure over a set Ω is atomless if $\forall x \in \Omega$, we have $\mu(\{x\}) = 0$.*

Definition 1.12 (Proper convex function)**.** *Let $f : X \to \bar{\mathbb{R}}$, a function taking values in the extended real number line. We call it proper convex function if $\exists x \in X$ such that*

$$f(x) < \infty$$

And $\forall x \in X$,

$$f(x) > -\infty \tag{1.2}$$

2

Basics in Convex Analysis.

Proposition 2.1. *Let $f : X \to \bar{\mathbb{R}}$ be a convex and lower-semicontinuous function. Assume that there exists $x_0 \in X$ such that $f(x_0) = -\infty$. Then f is nowhere finite on X.*

Theorem 2.1. *If f_α is an arbitrary family of lower semi-continuous functions on X, then $f = \sup_\alpha f_\alpha$ is also lower-semicontinuous.*

Definition 2.1 (Convex conjugate function)**.** *Let X be a Banach space, let $f : X \to \bar{\mathbb{R}}$ be a functional over X. We call the convex conjugate to the function $f^* : X^* \to \bar{\mathbb{R}}$, defined as*

$$f^*(x^*) = \sup_{x\in X}\{\langle x^*, x\rangle - f(x)\}$$

Proposition 2.2. *The convex conjugate $f^* : X^* \to \bar{\mathbb{R}}$ of a function $f : X \to \bar{\mathbb{R}}$ is convex.*

Proof. Let x^*, y^* elements of the dual space X^*, and $t \in [0,1]$,

$$\begin{aligned}
f^*\left(tx^* + (1-t)y^*\right) &= \sup_{x\in X}\{\langle tx^* + (1-t)y^*, x\rangle - f(x)\}\\
&= \sup_{x\in X}\{\langle tx^* + (1-t)y^*, x\rangle - tf(x) - (1-t)f(x)\}\\
&= \sup_{x\in X}\{t\langle x^*, x\rangle + (1-t)\langle y^*, x\rangle - tf(x) - (1-t)f(x)\}\\
&\leq \sup_{x,y\in X}\{t\langle x^*, x\rangle + (1-t)\langle y^*, y\rangle - tf(x) - (1-t)f(y)\}\\
&= t\sup_{x\in X}\{\langle x^*, x\rangle - f(x)\} + (1-t)t\sup_{y\in X}\{\langle y^*, y\rangle - f(y)\}\\
&= tf^*(x^*) + (1-t)f^*(y^*).
\end{aligned}$$

Therefore f^* is convex regardless the convexity of f. □

Theorem 2.2. *A function $f : \mathbb{R}^d \to \bar{\mathbb{R}}$ is convex and lower-semicontinuous if and only if $f^{**} = f$.*

Lemma 2.1 (Convex envelope theorem)**.** *Let X be a reflexive Banach Space. Then the convex conjugate function f^* is the maximum convex functional below f (also called convex envelope), i.e. if ϱ is convex functional and $\varrho(x) \leq f(x)$, $\forall x \in X$. Then, $f^{**}(x) \leq f(x)$, and $\varrho(x) \leq f^{**}(u)$, $\forall x \in U$. In particular $f^{**} = f$ if and only if J is convex.*

Definition 2.2 (Legendre Transform)**.** *Let $f : \mathbb{R}^d \to \bar{\mathbb{R}}$ be a convex function, we call the Legendre transform f^**

$$f^*(y) = \sup_{x\in\mathbb{R}^d}\{x\cdot y - f(x)\}$$

Corollary 2.1. *A function $f : \mathbb{R}^d \to \bar{\mathbb{R}}$ is convex and l.s.c. if and only if $f^{**} = f$.*

Definition 2.3 (Subdifferential)**.** *Given a proper convex function $f : X \to (-\infty, \infty]$, the subdifferential of such a function is the mapping $\partial f : X \to X^*$ defined by,*

$$\partial f(x) = \{x^* \in X^*; f(x) - f(y) \leq \langle x^*, x - y\rangle, \ \forall y \in X\}$$

Theorem 2.3 (Geometrical version of Hahn-Banach Theorem)**.** *Let M be a vector subspace of the topological vector space X. Suppose K is a non-empty convex open subset of X with $K \cap M = \emptyset$. Then there is a closed hyperplane $N \in X$ containing M with $K \cap N = \emptyset$.*

Theorem 2.4. *The epigraph of a convex and lower semicontinuous function is a closed convex set in $\mathbb{R}^d \times \mathbb{R}$, and can be written as the intersection of the half-spaces which contain it.*

3

Linear Programming

Interior Methods

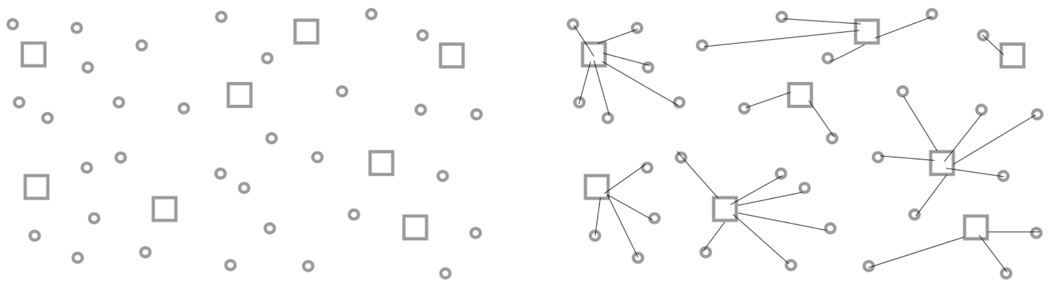
4

Optimal Transport Theory

To introduce the optimal transport problem please imagine we are asked by a consortium of factories to design a plan for distributing their products among its many costumers in such a way that the transportation costs are minimal.

We can start the approach of this problem considering the costumers as members of the set X and the factories as members of a set Y. We want to know which factory $y \in Y$ is going to supply a costumer $x \in X$, i.e. $y = T(x) \in Y$. Therefore, we can estimate the transportation cost $c(x, T(x))$ of supplying a costumer x with a factory $y = T(x)$. We see that our problem is reduced to find an assigning map from the set of costumers to the set of factories in such a way that the total cost $C(X, Y) = \sum_{x \in X} c(x, T(x))$ is minimal.

Figure 4.1: Illustration of the problem of Factories supplying Costumers.



(a) Factories represented by squares. Costumers represented by circles.

(b) Factories represented by squares. Costumers represented by circles. Assignation of a factory to a costumer represented by a line.

Gaspard Monge was a French mathematician who introduced for the first time the optimal transport problem as *déblais et remblais* in 1781. Monge was interested in finding a map that distributes an amount of sand or soil extracted from the earth or a mine distributed according to a density f, onto a new construction whose density of mass is characterized by a density g, in such a way the average displacement is minimal. In order to give a more precise idea of the problem, we make use of modern mathematical language and notation to state it as follows: Given two densities of mass f and g, Monge was interested in finding a map $T : \mathbb{R}^3 \to \mathbb{R}^3$ pushing the one onto the other,

$$\int_A g(y)\mathrm{dy} = \int_{T^{-1}(A)} f(x)\mathrm{dx} \tag{4.1}$$

For any Borel subset $A \subset \mathbb{R}^3$. And the transport also should minimize the quantity,

$$\int_{\mathbb{R}^3} \left| x - T(x) \right| f(x)\mathrm{dx}$$

We need to mention that given the context for which the problem was formulated, originally it was bind to $\mathbb{R}^3$ or $\mathbb{R}^2$ but we can consider the general case in $\mathbb{R}^d$. Notice that the problem requires a notion of measure. Then we find convenient to consider the measures μ on $X \subset \mathbb{R}^d$ and ν on $Y \subset \mathbb{R}^d$ induced by the densities f and g respectively. Therefore, we need to search for the optimum in the set of measurables maps $T : X \to Y$ such that the condition (4.1) is translated to,

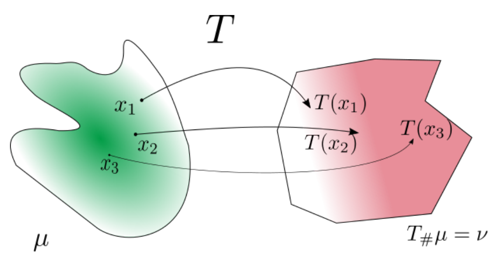
$$(T_{\#}\mu)(A) = \mu(T^{-1}(A)) \tag{4.2}$$

for every measurable set A. In other words, we need $T_{\#}\mu = \nu$. In the Euclidean frameworks if we assume f, g and T regular enough and T also injective, this equality implies,

$$g(T(x)) \det(\mathrm{D}T(x)) = f(x) \tag{4.3}$$

The equation (**??**) is nonlinear in T making difficult the analysis of the Monge Problem. Especially

Figure 4.2



Problem 1. *Given two probability measures $\mu \in \mathcal{P}(X)$ and $\nu \in \mathcal{P}(Y)$ and a cost function $c : X \times Y \to \{0, +\infty\}$, the Monge's problem consists in finding a map $T : X \to Y$*

$$\inf\left\{M(T) := \int_X c(x, T(x))\mathrm{d}\mu(x) : \quad T_{\#}\mu = \nu\right\} \tag{MP}$$

Definition 4.1. *The space of Borel probability measures on $\mathcal{X}$ is denoted by $\mathcal{P}(\mathcal{X})$. The weak topology on $\mathcal{P}(\mathcal{X})$ is induced by convergence against bounded continuous test functions on $\mathcal{X}$, that is $C_b(\mathcal{X})$.*

Definition 4.2 (Coupling)**.** *Let $(\mathcal{X}, \mu)$ and $(\mathcal{Y}, \nu)$ be two probability spaces. Coupling μ and ν means constructing two random variables X and Y on some probability space $(\Omega, \mathcal{P})$ such that $\mathrm{law}(X) = \mu$, $\mathrm{law}(Y) = \nu$. The couple (X, Y) is called a coupling of (μ, ν).*

Theorem 4.1. *Let $(\mathcal{X}_i, \mu_i)$, $i = 1, 2, 3$, be Polish probability spaces. If (X_1, X_2) is a coupling of (μ_1, μ_2) and $(\mathcal{Y}_2, Y_3)$ is a coupling of (μ_2, μ_3), then it is possible to construct a triple of random variables (Z_1, Z_2, Z_3) such that (Z_1, Z_2) has the same law as (X_1, X_2) and (Z_2, Z_3) has the same law as (Y_2, Y_3).*

Problem 2. *Given $\mu \in \mathcal{P}(X)$, $\nu \in \mathcal{P}(Y)$, and $c : X \times Y \to [0, +\infty]$, we consider the problem*

$$\inf\left\{K(\gamma) := \int_{X\times Y} c\mathrm{d}\gamma : \gamma \in \Pi(\mu, \nu)\right\} \tag{KP}$$

where $\Pi(\mu, \nu)$ is the set of transport plans.

Kantorovich formulation as relaxation

Theorem 4.2. *Let X and Y be compact metric spaces, $\mu \in \mathcal{P}(X)$, $\nu \in \mathcal{P}$ and $c : X \times Y \to \mathbb{R}$ a continuous function. Then* (KP) *admits a solution.*

Cyclical Monotonicity.

Definition 4.3. *Let X, Y be arbitrary sets, and $c : X \times Y \to (-\infty, \infty]$ be a cost function. A subset $\Gamma \subset X \times Y$ is said to be c-cyclically monotone if, for any $N \in \mathbb{N}$, and any family of points $(x_1, y_1), (x_2, y_2), \dots (x_N, y_N)$ of Γ, the inequality*

$$\sum_{i=1}^{N} c(x_i, y_i) \leq \sum_{i=1}^{N} c(x_i, y_{i+1})$$

considering $N + 1 = 1$.

5

Computational Optimal Transport

Linear Programming Formulation.

Simplex Method Algorithm.

Sinkhorn-Knopp Algorithm.

Simulated Annealing.

Continuous Formulation.

6

Applications

Nash Equilibrium.
Track of a Dynamic.
Domain Adaptation.
Isoperimetric Inequality.
Barycenter of a Fourier Power Spectrum.

Bibliography