

MATH 8803: Optimal Transport: Theory and Applications

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Contents

1	Introduction	4
1.1	Monge’s Original Formulation of Optimal Transport	4
1.2	The Kantorovich Optimal Transport Problem	5
1.3	Monge VS Kantorovich	7
1.4	Basic questions and examples	8
2	Multi-Marginal Optimal Transport (MMOT)	12

1 Introduction

1.1 Monge's Original Formulation of Optimal Transport

Consider a measure μ , another measure ν , and x, y in the supports of μ and ν respectively, *what is the optimal way of moving x to y ?*

1. Pile and hole

- Pile and hole should have the same volume \rightarrow normalize to 1.
- modern way of thinking about pile and hole: probability measure on some metric space X and Y respectively, $\mu \in \mathcal{P}(X), \nu \in \mathcal{P}(Y)$. It could be point cloud: $\mu = \sum_i \alpha_i \delta_{x_i}$; or continuous densities: $\mu(dx) = f(x)dx$.

2. Transport pile to hole region: Transport described by a map $T : X \rightarrow Y$. Notice that T may be discontinuous. We need T to be measurable.

3. Transport Cost: $c : X \times Y \rightarrow [0, \infty) \cup \{\infty\}$, where $c(x, y)$ represents the cost of moving one unit of mass from x to y (how it is transported does not matter). Implicit Assumption: cost only depends on initial and final. Typical cost: $c(x, y) = |x - y|$; $c(x, y) = |x - y|^2$; $c(x, y) = \frac{1}{|x - y|}$.

4. Filling the hole completely: $\mu(T^{-1}(B)) = \nu(B)$ for every measurable $B \subseteq Y$.

Definition 1.1: Push-Forward Measure

Let $\mu \in \mathcal{X}$ be a probability measure on X , $T : X \rightarrow Y$ be a measurable map between metric space X, Y . Then push-forward (or image) measure of μ under T is the measure $T_{\#}\mu$ on Y defined by $\mu(T^{-1}(B)) = T_{\#}\mu(B)$ for every $B \subseteq Y$ measurable.

A little bit of functional analysis

- $C_b(X)$: the Banach space of bounded continuous function on X endowed with the norm $\|f\|_{\infty} := \sup_{x \in X} |f(x)|$.
- $C_o(X) \subseteq C_b(X)$: closed subspace (w.r.t. $\|\cdot\|_{\infty}$), which is the space of continuous functions vanishing at ∞ : $f \in C_o(X)$ if $f \in C_b(X)$ and for every $\epsilon > 0$, there exists a compact set $K_{\epsilon} \subseteq X$, such that $|f| < \epsilon$ on $X \setminus K_{\epsilon}$.
- $\mathcal{M}(X)$: space of finite signed measures on X . $\lambda \in \mathcal{M}(X)$ if
 - (a) $\lambda(A) \in \mathbb{R}$ for any (Borel) measurable $A \subseteq X$.
 - (b) for every countable disjoint union $A = \cup_{i \in \mathbb{N}} A_i, A_i \cap A_j = \emptyset$ for $i \neq j$, these holds
 - $\sum_{i \in \mathbb{N}} |\lambda(A_i)| < \infty$
 - $\sum_{i \in \mathbb{N}} \lambda(A_i) = \lambda(A)$.

To every $\lambda \in \mathcal{M}(X)$, we can associate a unique non-negative measure $|\lambda| \in \mathcal{M}_+(X)$ via $|\lambda|(A) := \sup \{ \sum_{i \in \mathbb{N}} |\lambda(A_i)| : A = \cup_{i \in \mathbb{N}} A_i, A_i \cap A_j = \emptyset \text{ for } i \neq j \}$, the total variation measure of λ . $\|\lambda\| := |\lambda|(X)$ is a norm on $\mathcal{M}(X)$.

Theorem 1.2: Riesz Representation Theorem

Suppose X is separable, and locally compact. Then $\mathcal{M}(X) \cong [C_o(X)]^*$ (the dual space of $C_o(X)$). That is, every continuous linear functional $L : C_o(X) \rightarrow \mathbb{R}$ is represented in a unique way by an element of $\mathcal{M}(X)$, i.e., there exists a unique measure $\mu_L \in \mathcal{M}(X)$ s.t. $L(\varphi) = \int_X \varphi d\mu_L$.

Remark. Consider a special case of $T_{\#}\mu = \nu$; assume that T is a C^1 -diffeomorphism between X, Y and $X, Y \subseteq \mathbb{R}^d$ open, and that $\mu(dx) = f(x)dx, \nu(dy) = g(y)dy$. Then for any $B \subseteq \mathbb{R}^d$ measurable:

$$(T_{\#}\mu)(B) = \mu(T^{-1}(B)) = \int_{\mathbb{R}^d} \mathbb{1}_{T^{-1}(B)}(x) f(x) dx = \int_{T^{-1}(B)} f(x) dx.$$

Write $y = T(x)$, $dy = |\det DT(x)|dx$, we can write

$$(T_{\#}\mu)(B) = \nu(B) = \int_B g(y)dy = \int_{T^{-1}(B)} g(T(x))|\det DT(x)|dx,$$

which implies $f(x) = g(T(x))|\det DT(x)|$ for almost every $x \in X$ (technically remark: $f \geq \alpha$ for some $\alpha > 0$ on X).

Reminder: $T_{\#}\mu = \nu$ means:

1. $(T_{\#}\mu)(B) = \mu(T^{-1}(B)) = \nu(B)$ for any measurable subset $B \subseteq Y$.
2. $\int_Y \varphi d(T_{\#}\mu) = \int_X \varphi \circ T d\mu = \int_Y \varphi d\nu$, $\forall \varphi \in C_o(Y)$.

A quick remark on the change of variables formula:

$$\int_Y \varphi d(T_{\#}\mu) = \int_X \varphi(T(x))\mu(dx).$$

Definition 1.3: Monge's Optimal Transport Problem

Given $\mu \in \mathcal{P}(X), \nu \in \mathcal{P}(Y)$,

$$\min I[T] = \int_X c(x, T(x))\mu(dx) \quad (\mathcal{M})$$

over all transport maps $T : X \rightarrow Y$ (i.e., all measurable maps from X to Y such that $T_{\#}\mu = \nu$).

Remark. • I is a highly nonlinear functional of T subject to the nonlinear constraint $T_{\#}\mu = \nu$.

- Functional relatively simple: depends only locally on T (or its pointwise values)
 - no coupling between different values of T .
 - without constraint could just minimize pointwise, i.e. find minimum $y_{\min}(x)$ of $y \mapsto c(x, y)$ for each x and get $T(x) = y_{\min}(x)$.
- constraint complicated: nonlocal, couples values of T . If we could restrict to smooth diffeomorphisms, problem requires solving highly nonlinear PDE. Also, it is not even clear whether T such that $T_{\#}\mu = \nu$ exists for given μ, ν .

1.2 The Kantorovich Optimal Transport Problem

Comparing to Monge's OT problem, Kantorovich OT problem allows measure splitting, so we are looking for probability measure on $X \times Y$.

- Pile and hole: $\mu \in \mathcal{P}(X), \nu \in \mathcal{P}(Y)$.
- Transport: probability measure $\gamma \in \mathcal{P}(X \times Y)$ (transport plan).

$$\gamma(A \times B) = \int_{A \times B} \gamma(dxdy)$$

is the amount of mass moved from measurable $A \subseteq X$ to measurable $B \subseteq Y$. All the mass of μ has to be transported somewhere, hence, $\gamma(A \times Y) = \mu(A)$ for all $A \subseteq X$ measurable.

- Transport cost: Let $c(x, y)$ be the cost of moving one unit of mass from x to y , then the total cost is

$$\int_{X \times Y} c(x, y)\gamma(dxdy) = c[\gamma].$$

- Filling hole completely: $\gamma(X \times B) = \nu(B)$ for all $B \subseteq Y$ measurable. That is, the amount of mass transported to B has to be the volume of the hole in region B .

Remark. Note that, from above, $\gamma(X \times Y) = \mu(X) = \nu(Y) = 1$, so $\gamma \in \mathcal{P}(X \times Y)$, and $\gamma(A \times Y), \gamma(X \times B)$ defined marginals.

Definition 1.4: Marginals

Let $\gamma \in \mathcal{P}(X \times Y)$.

- *Marginal w.r.t. X* : $M_X \gamma \in \mathcal{P}(X)$ defined via

$$(M_X \gamma)(A) = \gamma(A \times Y) = \int_{A \times Y} \gamma(dxdy), \forall \text{ measurable } A \subseteq X,$$

- *Marginal w.r.t. Y* : $M_Y \gamma \in \mathcal{P}(Y)$ defined via

$$(M_Y \gamma)(B) = \gamma(X \times B) = \int_{X \times B} \gamma(dxdy), \forall \text{ measurable } B \subseteq Y.$$

Remark. Transport plans are probability measures on $X \times Y$ with marginals $M_X \gamma = \mu, M_Y \gamma = \nu, \gamma$ is a *coupling* of the probability measure μ and ν .

Let $\Pi(\mu, \nu)$ be the set of all couplings between μ and ν .

Lemma 1.5

Let $\varphi \in L^1(X, \mu)$ and $\psi \in L^1(Y, \nu)$. Then for any coupling $\gamma \in \Pi(\mu, \nu)$. These hold

$$(M1) \int_{X \times Y} \varphi(x) \gamma(dxdy) = \int_X \varphi(x) (M_X \gamma)(dx) = \int_X \varphi(x) \mu(dx).$$

$$(M2) \int_{X \times Y} \psi(y) \gamma(dxdy) = \int_Y \psi(y) (M_Y \gamma)(dy) = \int_Y \psi(y) \nu(dy).$$

Proof sketch. Any function $\varphi \in L^1(X, \mu)$ can be approximated by simple functions: $\varphi = \lim_{n \rightarrow \infty} \sum_{j=1}^n \alpha_j \mathbb{1}_{A_j}$, for $A_j \subseteq X$ measurable.

$$\begin{aligned} \int_{X \times Y} \varphi(x) \gamma(dxdy) &= \lim_{n \rightarrow \infty} \sum_{j=1}^n \alpha_j \int_{A_j \times Y} \gamma(dxdy) = \lim_{n \rightarrow \infty} \sum_{j=1}^n \alpha_j \mu(A_j) \\ &= \lim_{n \rightarrow \infty} \int_X \sum_{j=1}^n \alpha_j \mathbb{1}_{A_j}(x) \mu(dx) = \int_X \varphi(x) \mu(dx). \end{aligned}$$

□

Definition 1.6: Couplings

Let $\mu \in \mathcal{P}(X), \nu \in \mathcal{P}(Y)$. A probability measure $\gamma \in \mathcal{P}(X \times Y)$ is called *coupling* of μ and ν if $M_X \gamma = \mu, M_Y \gamma = \nu$. The set of all couplings between μ and ν is called $\Pi(\mu, \nu)$.

Definition 1.7: Kantorovich Optimal Transport Problem

Given $\mu \in \mathcal{P}(X), \nu \in \mathcal{P}(Y)$,

$$\min C[\gamma] = \int_{X \times Y} c(x, y) \gamma(dxdy) \quad (\mathcal{K})$$

over all couplings $\gamma \in \Pi(\mu, \nu)$.

Structure of (\mathcal{K}) :

- (1) $\gamma \mapsto C[\gamma]$ linear function.
- (2) $M_X \gamma = \mu, M_Y \gamma = \nu$ linear constraints.
- (3) $\Pi(\mu, \nu)$ is a convex set: if $\gamma_1, \gamma_2 \in \Pi(\mu, \nu)$, $\lambda \in (0, 1)$, then
 - (a) $\lambda\gamma_1 + (1-\lambda)\gamma_2 \in \mathcal{P}(X \times Y)$, since $\lambda\gamma_1(X \times Y) + (1-\lambda)\gamma_2(X \times Y) = 1$, and $\lambda\gamma_1(Z) + (1-\lambda)\gamma_2(Z) \geq 0$ for any $Z \subseteq X \times Y$ measurable.
 - (b) $(\lambda\gamma_1 + (1-\lambda)\gamma_2)(A \times Y) = \lambda\gamma_1(A \times Y) + (1-\lambda)\gamma_2(A \times Y) = \lambda\mu(A) + (1-\lambda)\mu(A) = \mu(A)$; analogously, $(\lambda\gamma_1 + (1-\lambda)\gamma_2)(X \times B) = \nu(B)$, for any $A \subseteq X, B \subseteq Y$ measurable.

$\implies (\mathcal{K})$ is a linear programming problem. *But*: it is in infinite dimensions.
- (4) Existence of couplings is trivial: independent coupling (product measure) $\gamma = \mu \otimes \nu$ defined via $\gamma(A \times B) = \mu(A)\nu(B)$ for every measurable $A \subseteq X, B \subseteq Y$, is a coupling of μ and ν .
- (5) (\mathcal{K}) is higher-dimensional than (\mathcal{M}) in the following sense: consider transport plan given by a density $\tilde{\gamma} : \mathbb{R}^{2d} \rightarrow \mathbb{R}$. Discretize \mathbb{R}^d by ℓ gridpoints then $\tilde{\gamma}$ corresponds to ℓ^2 real numbers. Transport $T : \mathbb{R}^d \rightarrow \mathbb{R}^d$ however only corresponds to ℓd real numbers. e.g. ℓ = number of pixels in a 2D picture, say $\ell = 500 \times 500$, then $\ell d = 500000$, but $\ell^2 = 62.5^9$.

1.3 Monge VS Kantorovich

Kantorovich problem is a relaxation of Monge Problem in the following sense: Monge = restriction of Kantorovich to sparse plan.

$$\gamma_T(dx dy) = \delta_{T(x)}(dy)\mu(dx)$$

for $T : X \rightarrow Y$ measurable such that $T_{\#}\mu = \nu$. For any $\varphi \in C_o(X \times Y)$,

$$\begin{aligned} \int_{X \times Y} \varphi d\gamma_T &= \int_{X \times Y} \varphi(x, y) \gamma_T(dx \times dy) = \int_{X \times Y} \varphi(x, y) \delta_{T(x)}(dy) \mu(dx) = \int_X \varphi(x, T(x)) \mu(dx) \\ &= \int_X \varphi((id, T)(x)) \mu(dx) = \int_X \varphi \circ (id, T) d\mu = \int_{X \times Y} \varphi(x, y) [(id, T)_{\#}\mu](dx \times dy). \end{aligned}$$

In other words, Monge measures that

$$\begin{aligned} \text{supp } \gamma &= \{(x, y) \in X \times Y : \gamma(B_\epsilon(x, y)) > 0 \text{ for every } \epsilon > 0\} \\ &= \cap \{Z \subseteq X \times Y \text{ closed} : \gamma(Z) = 1\} \\ &\subseteq \text{graph } T = \{(x, T(x)) \in X \times Y : x \in X\} \end{aligned}$$

Lemma 1.8

Let $T : X \rightarrow Y$ be measurable such that $T_{\#}\mu = \nu$. Then

- (i) $C[\gamma_T] = I[T]$.
- (ii) $\gamma_T \in \Pi(\mu, \nu)$
- (iii) $(\mathcal{K}) \leq (\mathcal{M})$.

Proof. (i) $C[\gamma_T] = \int_{X \times Y} c(x, y) \gamma_T(dx \times dy) = \int_{X \times Y} c(x, y) ((id, T)_{\#}\mu)(dx dy) = \int_X c(x, T(x)) \mu(dx) = I[T]$.

(ii) Let $A \subseteq X$, $B \subseteq Y$ measurable. Then

$$\begin{aligned}
 (M_X \gamma_T)(A) &= \gamma_T(A \times Y) = \int_{A \times Y} d\gamma_T = \int_X \mathbb{1}_{A \times Y}(x, y) \underbrace{\gamma_T(dx \times dy)}_{((id, T)_\# \mu)(dx dy)} \\
 &= \int_X \underbrace{\mathbb{1}_{A \times Y}(x, T(x))}_{\mathbb{1}_A(x)} \mu(dx) \\
 &= \int_A d\mu = \mu(A) \\
 (M_Y \gamma_T)(B) &= \int_X \underbrace{\mathbb{1}_{X \times B}(x, T(x))}_{\mathbb{1}_B(T(x))} \mu(dx) = \int_Y \mathbb{1}_B(y) (T_\# \mu)(dy) \\
 &= \int_B d\nu = \nu(B)
 \end{aligned}$$

(iii) By (i) and (ii),

$$(\mathcal{M}) = \inf_{T: X \rightarrow Y \text{ measurable}, T_\# \mu = \nu} I[T] = \inf_{T: X \rightarrow Y \text{ measurable}, T_\# \mu = \nu} C[\gamma_T] \geq \inf_{\gamma \in \Pi(\mu, \nu)} C[\gamma] = (\mathcal{K}),$$

by $\gamma_T \in \Pi(\mu, \nu)$. □

1.4 Basic questions and examples

1. Existence Do optimal plans/maps exist? For optimal plans, yes, under reasonable assumptions on c , \inf in (\mathcal{K}) is \min . For optimal maps:

Example 1.1. Let $X = Y = \mathbb{R}^d$, $\mu = \delta_a$, $a \in \mathbb{R}^d$, $\nu = \frac{1}{2}(\delta_b + \delta_c)$ for $b \neq c \in \mathbb{R}^d$. Let $T : \mathbb{R}^d \rightarrow \mathbb{R}^d$ be measurable for all $A \subseteq \mathbb{R}^d$ open.

$$(T_\# \delta_a)(A) = \delta_a(T^{-1}(A)) = \begin{cases} 1 & \text{if } a \in T^{-1}(A) \\ 0 & \text{otherwise} \end{cases} = \delta_{T(a)}(A).$$

i.e. $T_\# \delta_a = \delta_{T(a)}$, so I cannot map the mass to two different points so $T_\# \mu = \nu$ is only possible if $b = c$.

The class of all transport plans $\Pi(\mu, \nu)$ consist of a single measure

$$\Pi(\mu, \nu) = \left\{ \mu \otimes \nu = \frac{1}{2} (\delta_a \otimes \delta_b + \delta_a \otimes \delta_c) \right\}.$$

Indeed, note that

$$\begin{aligned}
 &\gamma(\underbrace{\mathbb{R}^{2d} \setminus \{(a, b), (a, c)\}}_{=(\mathbb{R}^d \setminus \{a\} \times \mathbb{R}^d) \cup (\mathbb{R}^d \times \mathbb{R}^d \setminus \{b, c\})}) \\
 &\leq \gamma((\mathbb{R}^d \setminus \{a\} \times \mathbb{R}^d)) + \gamma((\mathbb{R}^d \times \mathbb{R}^d \setminus \{b, c\})) = \mu(\mathbb{R}^d \setminus \{a\}) + \nu(\mathbb{R}^d \setminus \{b, c\}) \\
 &= \delta_a(\mathbb{R}^d \setminus \{a\}) + \frac{1}{2}(\delta_b + \delta_c)(\mathbb{R}^d \setminus \{b, c\}) = 0.
 \end{aligned}$$

For any $\gamma \in \Pi(\mu, \nu)$,

\implies Any $\gamma \in \Pi(\mu, \nu)$ is supported on the points (a, b) and (a, c) .

$\implies \gamma = \lambda \delta_{(a, b)} + (1 - \lambda) \delta_{(a, c)} = \lambda \delta_a \otimes \delta_b + (1 - \lambda) \delta_a \otimes \delta_c$, for some $\lambda \in [0, 1]$.

Since $M_Y \gamma = \lambda \delta_b + (1 - \lambda) \delta_c$, $\nu = M_Y \gamma$ implies that $\lambda = \frac{1}{2}$.

2. Monge VS Kantorovich: discussed above.

3. Uniqueness Are minimizers unique? If not, can we characterize the set of minimizers?

Example 1.2. Consider $X = Y = \mathbb{R}^2$, $a = (-1, 0)$, $b = (1, 0)$, $a' = (0, -1)$, $b' = (0, 1)$; $\mu = \frac{1}{2}(\delta_a + \delta_b)$, $\nu = \frac{1}{2}(\delta_{a'} + \delta_{b'})$.

a) Consider Monge problem with quadratic distance cost

$$\inf_{T \in \mathcal{T}(\mu, \nu)} \int_{\mathbb{R}^2} |T(x) - x|^2 \mu(dx),$$

where $\mathcal{T}(\mu, \nu)$ is the set of push-forward maps, has two minimizers, defined on the support of μ :

$$T^{(1)}(a) = a', T^{(1)}(b) = b'; \quad T^{(2)}(a) = b', T^{(2)}(b) = a'.$$

Indeed, $\mathcal{T}(\mu, \nu) = \{T^{(1)}, T^{(2)}\}$, and

$$\begin{aligned} \int_{\mathbb{R}^2} |T^{(1)}(x) - x|^2 \mu(dx) &= \frac{1}{2} \left(|T^{(1)}(a) - a|^2 + |T^{(1)}(b) - b|^2 \right) \\ &= \frac{1}{2} (|a' - a|^2 + |b' - b|^2) = \frac{1}{2} (2 + 2) = 2. \\ \int_{\mathbb{R}^2} |T^{(2)}(x) - x|^2 \mu(dx) &= \frac{1}{2} \left(|T^{(2)}(a) - a|^2 + |T^{(2)}(b) - b|^2 \right) \\ &= \frac{1}{2} (|b' - a|^2 + |a' - b|^2) = \frac{1}{2} (2 + 2) = 2. \end{aligned}$$

b) Non-uniqueness in Kantorovich is even bigger:

$$\begin{aligned} \Pi(\mu, \nu) &= \{ \text{convex combinations of } \gamma_{T^{(1)}} \text{ and } \gamma_{T^{(2)}} \} \\ &= \left\{ \frac{1}{2} [(1 - \lambda)\delta_a \otimes \delta_{a'} + \lambda\delta_a \otimes \delta_{b'} + \lambda\delta_b \otimes \delta_{a'} + (1 - \lambda)\delta_b \otimes \delta_{b'}] : \lambda \in [0, 1] \right\} \end{aligned}$$

4. Exact solutions

Example 1.3. Optimality of translation Let $X = Y = \mathbb{R}^d$, μ be a compactly supported probability measure on \mathbb{R}^d , and $\nu = (\tau_a)_\# \mu$, $\tau_a : \mathbb{R}^d \rightarrow \mathbb{R}^d$ translation by $a \in \mathbb{R}^d$, where $\tau_a(x) = x + a$. e.g., $\mu(dx) = f(x)dx$, then $\nu(dy) = g(y)dy$ with $g(y) = f(y - a)$ for all $y \in \mathbb{R}^d$.

$$\min I[T] = \int_{\mathbb{R}^d} |T(x) - x|^p \mu(dx), \quad 1 < p < \infty$$

over $\mathcal{T}(\mu, \nu)$.

- Best to move each piece of mass by some distance?
- or better to move right side of pile to left side of hole (shorter distance) and make up for it by moving left side of pile to right side of hole (longer distance)?

The answer lies in *convexity* of the cost in displacement $T(x) - x$.

Definition 1.9

$\Phi : \mathbb{R}^d \rightarrow \mathbb{R} \cup \{\infty\}$ convex if

$$\Phi((1 - t)z + tz') \leq (1 - t)\Phi(z) + t\Phi(z')$$

for all $z \neq z' \in \mathbb{R}^d$, $t \in (0, 1)$. It is strictly convex if the inequality is always strict.

Theorem 1.10: Jensen's Inequality

$\Phi : \mathbb{R}^d \rightarrow \mathbb{R}$ convex and continuous. If μ is a probability measure on \mathbb{R}^d and $v : \mathbb{R}^d \rightarrow \mathbb{R}^d$ integrable w.r.t. μ , then

$$\Phi \left(\int_{\mathbb{R}^d} u d\mu \right) \leq \int_{\mathbb{R}^d} \Phi(u) d\mu.$$

If Φ is strictly convex, inequality is strict, unless $u(x) = \bar{u} \in \mathbb{R}^d$ for μ -almost-everywhere x .

Let us prove (using convexity) that uniform transition, $T = \tau_a$ is the best:

Step 1 Introduce centers of mass of μ and ν ,

$$R_\mu = \int_{\mathbb{R}^d} x \mu(dx), R_\nu = \int_{\mathbb{R}^d} y \nu(dy),$$

$$\text{then } R_\nu = \int_{\mathbb{R}^d} y((\tau_a)_\# \mu) dy = \int_{\mathbb{R}^d} \tau_a(x) \mu(dx) = \int_{\mathbb{R}^d} x \mu(dx) + \int_{\mathbb{R}^d} a \mu(dx) = R_\mu + a.$$

Step 2 Average displacement of any $T \in \mathcal{J}(\mu, \nu)$

$$\int_{\mathbb{R}^d} (T(x) - x) \mu(dx) = \underbrace{\int_{\mathbb{R}^d} T(x) \mu(dx)}_{\int_{\mathbb{R}^d} y d(T_\# \mu)(y) = R_\nu} - \underbrace{\int_{\mathbb{R}^d} x \mu(dx)}_{R_\mu} = R_\nu - R_\mu = a$$

Step 3 Strict convexity of $\Phi_p : \mathbb{R}^d \rightarrow \mathbb{R}, z \rightarrow |z|^p$ for $1 < p < \infty$. By Jensen's inequality:

$$\begin{aligned} I[T] &= \int_{\mathbb{R}^d} |T(x) - x|^p \mu(dx) = \int_{\mathbb{R}^d} \Phi_p(T(x) - x) \mu(dx) \\ &\geq \Phi \left(\underbrace{\int_{\mathbb{R}^d} (T(x) - x) \mu(dx)}_a \right) = \Phi_p(a) = |a|^p \end{aligned}$$

for every $T \in \mathcal{J}(\mu, \nu)$.

- $T = \tau_a$ achieves equality by $\tau_a(x) - x = x + a - x = a$, so $I[\tau_a] = \int_{\mathbb{R}^d} |a|^p \mu(dx) = |a|^p$.
- Φ_p is strictly convex for $p > 1$: so equality holds if and only if $T(x) - x$ is a constant μ -a.e., which implies that $T = \tau_a$ is a unique minimizer.

Example 1.4 (Book Shifting (Gangbo-McCann 1996)). Consider $\mu(dx) = \frac{4}{3} \mathbb{1}_{[0, \frac{3}{4}]}(x) dx$ and $\nu(dx) = \frac{4}{3} \mathbb{1}_{[\frac{1}{4}, 1]}(y) dy$. Consider the problem

$$\inf \int_{[0,1]} |T(x) - x| \mu(dx)$$

where define $\Phi_1(x) := |x|$. Since Φ_1 is convex, a solution is given by $T_1(x) = x + \frac{1}{4}$ for $x \in [0, \frac{3}{4}]$, which is minimal. Its transportation cost is $\frac{3}{4} * \frac{4}{3} * \frac{1}{4} = \frac{1}{4}$. Consider another shift:

$$T_2(x) = \begin{cases} x + \frac{3}{4}, & \text{if } x \in [0, \frac{1}{4}] \\ x, & \text{otherwise.} \end{cases}$$

The transport cost is $\frac{4}{3} \int_{[0, \frac{1}{4}]} \frac{3}{4} dx + \frac{4}{3} \int_{[\frac{1}{4}, \frac{3}{4}]} 0 = \frac{1}{4}$, so T_2 is also minimal. Notice Φ_1 is convex but not strictly.

Example 1.5 (A dam and two ditches). We now consider a problem where Monge's problem has an optimal value but the inf is not attained.

Let $X = Y = \mathbb{R}^2$, and let $\mu(dx) = dx_2|_{x_1=0, x_2 \in [0,1]}$, $\nu(dy) = \frac{1}{2} dy_2|_{y_1=-1, y_2 \in [0,1]} + \frac{1}{2} dy_2|_{y_1=1, y_2 \in [0,1]}$. The goal is

$$\min I[T] = \int_{\mathbb{R}^2} |T(x) - x|^2 \mu(dx) \text{ among all } T \in \mathcal{J}(\mu, \nu).$$

- $|T(x) - x| \geq d(\text{supp } \mu, \text{supp } \nu) = 1$ for all $x \in \text{supp } \mu$ and for all $T \in \mathcal{J}(\mu, \nu)$, which implies that $I[T] \geq \int_{\mathbb{R}^2} 1 \mu(dx) = 1$.
- Now we show $\inf_{T \in \mathcal{J}(\mu, \nu)} I[T] = 1$. Split up the dam into even number of segments of length $\epsilon > 0$ and consider the transport map T_ϵ depicted on the left. The maximal displacement of any point in the support is ϵ . Hence

$$|T_\epsilon(x) - x| \leq \sqrt{1 + \epsilon^2} \implies I(T_\epsilon) = \int_{\mathbb{R}^2} |T_\epsilon(x) - x|^2 \mu(dx) \leq 1 + \epsilon^2.$$

Since ϵ can be chosen arbitrarily, $\inf I = 1$.

Claim. No $T \in \mathcal{J}(\mu, \nu)$ achieves $I[T] = 1$.

Proof. Assume there exists $T \in \mathcal{J}(\mu, \nu)$ such that $I(T) = 1$. This means $T(x) \in \text{supp } \nu$ for μ -a.e. x ; $|T(x) - x| = 1$ for μ -a.e. x . Hence, $T(0, x_2) = (\pm 1, x_2)$ for every Lebesgue-a.e. $x_2 \in [0, 1]$. Set $\Omega_+ := \{x_2 \in [0, 1] : [T(0, x_2)]_1 = 1\}$ and $\Omega_- := \{x_2 \in [0, 1] : [T(0, x_2)]_1 = -1\}$. Then

$$T_{\#}\mu = dx_2|_{x_1=-1, x_2 \in \Omega_-} + dx_2|_{x_1=1, x_2 \in \Omega_+} \neq \nu$$

so $T \notin \mathcal{J}(\mu, \nu)$. Hence $\inf_{T \in \mathcal{J}(\mu, \nu)} I[T]$ is not attained. \square

Everything holds if change $|T(x) - x|^2$ to $|T(x) - x|^p, p > 0$.

Problem: minimizing sequence T_ϵ exhibits faster and faster oscillations as $\epsilon \downarrow 0$. Hence, T_ϵ converges weakly, but not strongly in any $L^p(\mathbb{R}^2; \mu)$,

$$T_\epsilon(0, x_k) \xrightarrow[L^p]{\epsilon \downarrow 0} T_0(0, x_2) = \begin{pmatrix} 0 \\ x_2 \end{pmatrix}, \quad \forall p > 1, \text{ but } T_0 \notin \mathcal{J}(\mu, \nu).$$

- Corresponding Kantorovich ProblemL

$$\inf_{\gamma \in \Pi(\mu, \nu)} \int_{\mathbb{R}^2 \times \mathbb{R}^2} |y - x|^2 \gamma(dxdy)$$

has simple explicit solution. Let $\gamma(dxdy) = \delta_0(x_1) \mathbb{1}_{[0,1]}(x_2) dx_2 \cdot \frac{\delta_1(y_1) + \delta_{-1}(y_1)}{2} \delta_{x_2}(y_2)$, which splits half of the mass to the left ditch and another half to the right one. It is not hard to see that the objective value of this γ is 1.

2 Multi-Marginal Optimal Transport (MMOT)

Goal: Find multivariate probability measure $\gamma \in \mathcal{P}(X_1 \times \cdots \times X_N)$. Given $N \in \mathbb{N}$, $N \geq 2$,

$$\min \int_{X_1 \times \cdots \times X_N} c(x_1, \dots, x_N) \gamma(dx_1, \dots, dx_N) =: c[\gamma] \quad (\text{MMOT})$$

subject to constraint of given multivariate marginals $\gamma \in \Pi(\mu_1, \dots, \mu_N)$, given measures $\mu_i \in \mathcal{P}(X_i)$, where X_i are locally compact, separable, metric space and complete.

Definition 2.1: Marginal and Couplings

$\gamma \in \mathcal{P}(X_1 \times \cdots \times X_N)$ has marginals μ_1, \dots, μ_N with $\mu_i \in \mathcal{P}(X_i)$ if and only if $(M_{X_i} \gamma)(A_i) = \gamma(X_1 \times \cdots \times X_{i-1} \times A_i \times X_{i+1} \times \cdots \times X_N) = \mu_i(A_i)$ for any μ_i measurable $A_i \subseteq X_i$ for every $i \in \{1, \dots, N\}$. Equivalently,

$$\int_{X_1 \times \cdots \times X_N} \varphi_i(x_i) \gamma(dx_1, \dots, dx_N) = \int_{X_i} \varphi_i d\mu_i, \quad \forall \varphi_i \in C_o(X_i), i \in \{1, \dots, N\}.$$

Denote the set of all couplings as $\Pi(\mu_1, \dots, \mu_N) := \{\gamma \in \mathcal{P}(X_1 \times \cdots \times X_N) : M_{X_i} \gamma = \mu_i, \forall i = 1, \dots, N\}$.

Lemma 2.2

(MMOT) is a linear programming problem.

- 1) $\gamma \mapsto c(\gamma)$ is a linear map.
- 2) $\Pi(\mu_1, \dots, \mu_N)$ is a convex subset of space of finite signed measure on $X_1 \times \cdots \times X_N$.

Remark. When $N = 2$, (MMOT) is equivalent to (K). $\Pi(\mu_1, \dots, \mu_N) \neq \emptyset$ since $\mu_1 \otimes \cdots \otimes \mu_N \in \Pi(\mu_1, \dots, \mu_N)$.

Theorem 2.3

Let $c : \mathbb{R}^{d_1} \times \cdots \times \mathbb{R}^{d_N} \rightarrow \mathbb{R} \cup \{\infty\}$ be lower semi-continuous (l.s.c.) and bounded from below. Then for any $\mu_i \in \mathcal{P}(\mathbb{R}^{d_i})$, $i = 1, \dots, N$, (MMOT) has a minimizer.

Remark. Lower semi-continuous (sequential): Let X be a vector space with some notion of convergence. A functional $f : X \rightarrow \mathbb{R} \cup \{\infty\}$ is called (sequentially) lower semi-continuous (with respect to the given notion of convergence) if for any $x \in X$ and for any $\{x_j\}_{j \in \mathbb{N}} \subseteq X$ such that $x_j \xrightarrow{j \rightarrow \infty} x$, we have $f(x) \leq \liminf_{j \rightarrow \infty} f(x_j)$.

Proof. Direct method of the calculus of variations.

1. Assume that $c[\gamma] = \int_{X_1 \times \cdots \times X_N} c d\gamma < \infty$ for at least one $\gamma \in \Pi(\mu_1, \dots, \mu_N)$ (otherwise every coupling is a minimizer with cost ∞). Since c is bounded from below, say $c \geq \alpha$ for some $\alpha \in \mathbb{R}$, then

$$c[\gamma] = \int_{X_1 \times \cdots \times X_N} c d\gamma \geq \alpha \gamma(X_1 \times \cdots \times X_N) = \alpha > -\infty \implies \inf_{\gamma \in \Pi(X_1 \times \cdots \times X_N)} c[\gamma] \in \mathbb{R}.$$

2. Let $\{\gamma_k\}_{k \in \mathbb{N}} \subseteq \Pi(\mu_1, \dots, \mu_N)$ be a minimizing sequence (exists by 1), i.e. $c[\gamma_k] \xrightarrow{k \rightarrow \infty} \inf_{\gamma \in \Pi(\mu_1, \dots, \mu_N)} c[\gamma]$.

3. Notions of convergence for measures

- Signed Measure: $\mathcal{M}(X) = \{\mu - \nu : \mu, \nu \text{ non-negative Borel measures of finite mass}\}$. whose norm is defined as $\|\lambda\|_\pi = |\lambda|(X)$, $|\lambda|(A) := \sup\{\sum_{i \in \mathbb{N}} |\lambda(A_i)| : A = \cup_{i \in \mathbb{N}} A_i, A_i \cap A_j = \emptyset, \forall i \neq j\}$.
- Riesz Representation Theorem:

$$\mathcal{M}(\mathbb{R}^d) \cong [C_o(\mathbb{R}^d)]^* \cong [C_c(\mathbb{R}^d)]^*$$

where $C_o(\mathbb{R}^d) = \overline{C_c(\mathbb{R}^d)}^{\|\cdot\|_\infty}$, where $C_o(\mathbb{R}^d)$ is the set of continuous function vanishing at ∞ on \mathbb{R}^d , and $C_c(\mathbb{R}^d)$ is the set of compactly supported continuous function on \mathbb{R}^d .

- weak-* convergence: $\mu_n \xrightarrow{*} \mu$ as $n \rightarrow \infty$ if and only if $\mu_n(\varphi) \xrightarrow{n \rightarrow \infty} \mu(\varphi)$, i.e.,

$$\int \varphi d\mu_n \xrightarrow{n \rightarrow \infty} \int \varphi d\mu, \forall \varphi \in C_o(\mathbb{R}^d).$$

□

Theorem 2.4: (Sequentia) Banach-Alaoglo

Let $X (C_o(\mathbb{R}^d))$ be a normed vector space, $X^* (\mathcal{M}(\mathbb{R}^d))$ be its dual. If X is separable, then every bounded sequence in X^* possesses a weakly-* convergence subsequence.

Remark. Let $\{x_n\}_{n \in \mathbb{N}} \subseteq \mathbb{R}^d$ such that $|x_n| \rightarrow \infty$. Then $\delta_{x_n} \xrightarrow{*} 0$. For all $\varphi \in C_o(\mathbb{R}^d) : \int_{\mathbb{R}^d} \varphi d\delta_{x_n} = \varphi(x_n) \xrightarrow{n \rightarrow \infty} 0$. That is, indeed, we do not capture how the δ_{x_n} behaves when x_n goes to ∞ .

Definition: Narrow convergence

Narrow convergence (probabilist: weak convergence): $\mu_n \rightarrow \mu$ narrowly as $n \rightarrow \infty$ if and only if

$$\int_{\mathbb{R}^d} \varphi d\mu_n \rightarrow \int_{\mathbb{R}^d} \varphi d\mu, \forall \varphi \in C_b(\mathbb{R}^d)$$

where $C_b(\mathbb{R}^d)$ is the set of bounded continuous function on \mathbb{R}^d . In particular, if $\mu_n \rightarrow \mu$ narrowly as $n \rightarrow \infty$, then (pick $\varphi \equiv 1$), $\mu_n(\mathbb{R}^d) \rightarrow \mu(\mathbb{R}^d)$ (Notice that we might have this for weak-* convergence as $\varphi \equiv 1$ does not vanish at ∞).

Theorem 2.5: Prokhorov

For a set $K \subseteq \mathcal{M}_+(\mathbb{R}^d)$ the following are equivalent:

1. K is bounded and tight, i.e. $\sup_{\mu \in K} \mu(\mathbb{R}^d \setminus \overline{B}_R) \xrightarrow{R \rightarrow \infty} 0$. This could be understood as the mass outside any large ball uniformly small for all measure on K .
2. K is relatively sequentially compact with respect to narrow convergence, i.e., every sequence in K has a narrowly convergent subsequence.

Proof. Assume K is bounded and tight and let $\{\mu_j\}_{j \in \mathbb{N}}$ be a sequence in K .

- K bounded, and by THM 2.4 and the fact that $C_o(\mathbb{R}^d)$ is separable, there exists a subsequence $\{\mu_{j_k}\}_{k \in \mathbb{N}} \subseteq K$ such that $\mu_{j_k} \xrightarrow{*} \mu \in \mathcal{M}(\mathbb{R}^d)$.

Note that $\mu \in \mathcal{M}_+(\mathbb{R}^d)$: to see this, let $B \subseteq \mathbb{R}^d$ be compact, and approximate $\mathbb{1}(B)$ by continuous functions: Define $\varphi_B^\epsilon := (1 - \epsilon^{-1}d(x, B))_+$, where $d(x, B) = \inf_{y \in B} |x - y|$, and $B^\epsilon := \{x \in \mathbb{R}^d : d(x, B) \leq \epsilon\}$. Then

1. For $\epsilon_1 < \epsilon_2$, $B^{\epsilon_1} \subseteq B^{\epsilon_2}$, and $B = \bigcap_{n \in \mathbb{N}} B^{1/n}$.
2. $\mathbb{1}_B \leq \varphi_B^\epsilon \leq \mathbb{1}_{B^\epsilon}$.
3. φ_B^ϵ continuous with $|\varphi_B^\epsilon(x) - \varphi_B^\epsilon(y)| \leq \epsilon^{-1}|x - y|$.

Hence

$$\mu(B^\epsilon) = \int \mathbb{1}_{B^\epsilon} d\mu \geq \int \varphi_B^\epsilon d\mu \geq \lim_{k \rightarrow \infty} \int \varphi_B^\epsilon d\mu_{j_k} \geq \limsup_{k \rightarrow \infty} \int \mathbb{1}_B d\mu_{j_k} = \limsup_{k \rightarrow \infty} \mu_{j_k}(B) \geq 0.$$

Note that

$$\mu(B) \stackrel{1}{=} \mu(\bigcap_{n \in \mathbb{N}} B^{1/n}) \stackrel{(*)}{=} \lim_{n \rightarrow \infty} \mu(B^{1/n}) \geq 0$$

so $\mu \in \mathcal{M}_+(\mathbb{R}^d)$.

(*) continuity: since μ finite (signed) measure, we can write

$$\begin{aligned}
 \mu(B^*) - \mu(\cap_{n \in \mathbb{N}} B^{1/n}) &= \mu(B^1 \setminus \cap_{n \in \mathbb{N}} B^{1/n}) = \mu(\cup_{n \in \mathbb{N}} (B^1 \setminus B^{1/n})) \\
 &= \mu\left(\dot{\cup}_{n \in \mathbb{N}} (B^1 \setminus B^{1/(n+1)}) \setminus (B^1 \setminus B^{1/n})\right) \\
 &= \sum_{n \in \mathbb{N}} \mu\left((B^1 \setminus B^{1/(n+1)}) \setminus (B^1 \setminus B^{1/n})\right) \\
 &= \lim_{N \rightarrow \infty} \sum_{n=1}^{N-1} \mu\left((B^1 \setminus B^{1/(n+1)}) \setminus (B^1 \setminus B^{1/n})\right) \\
 &= \lim_{N \rightarrow \infty} \mu\left(\cup_{n=1}^{N-1} (B^1 \setminus B^{1/(n+1)}) \setminus (B^1 \setminus B^{1/N})\right) \\
 &= \lim_{N \rightarrow \infty} \mu(B^1 \setminus B^{1/N}) = \mu(B^1) - \lim_{N \rightarrow \infty} \mu(B^{1/N})
 \end{aligned}$$

where the limit exists because $|\mu|(\mathbb{R}^d) < \infty$.

More generally, we have

Theorem: Portmanteau theorem

Let $\{\mu_n\} \subseteq \mathcal{P}(\mathbb{R}^d)$. Then the following are equivalent:

1. $\mu_n \rightarrow \mu$ narrowly.
2. $\limsup_{n \rightarrow \infty} \mu_n(F) \leq \mu(F)$ for all F closed.
3. $\mu(O) \leq \liminf_{n \rightarrow \infty} \mu_n(O)$ for all O open.
4. $\mu_n(A) \rightarrow \mu(A)$ for all A measurable such that $\mu(\partial A) = 0$, where ∂A is the boundary of A .

•

Claim. $\int \varphi d\mu_{j_k} \rightarrow \int \varphi d\mu$ for all $\varphi \in C_b(\mathbb{R}^d)$, i.e., $\mu_{j_k} \rightarrow \mu$ narrowly as $k \rightarrow \infty$.

Truncation argument: fix $\varphi \in C_b(\mathbb{R}^d)$ and define the cutoff function ξ_R via

$$\xi_R(x) = \begin{cases} 1, & \text{if } |x| \leq R, \\ 1 - (|x| - R), & \text{if } R < |x| \leq R + 1, \\ 0, & \text{otherwise.} \end{cases}$$

Then

$$\int_{\mathbb{R}^d} \varphi d\mu_{j_k} - \int_{\mathbb{R}^d} \varphi d\mu = \underbrace{\int_{\mathbb{R}^d} \xi_R \varphi d(\mu_{j_k} - \mu)}_{\rightarrow 0 \text{ by weak-* convergence}} + \underbrace{\int_{\mathbb{R}^d} (\varphi - \varphi \xi_R) d\mu_{j_k}}_{=: T_R^{(j_k)}} + \underbrace{\int_{\mathbb{R}^d} (\xi_R \varphi - \varphi) d\mu}_{=: T_R}.$$

Note that by tightness

$$\begin{aligned}
 |T_R^{(j_k)}| &\leq \|\varphi\|_\infty \int_{\mathbb{R}^d \setminus \bar{B}_R} d\mu_{j_k} = \|\varphi\|_\infty \mu_{j_k}(\mathbb{R}^d \setminus \bar{B}_R) =: \alpha_R \xrightarrow{R \rightarrow \infty} 0 \\
 |T_R| &\leq \|\varphi\|_\infty \int_{\mathbb{R}^d \setminus \bar{B}_R} d\mu =: \beta_R \xrightarrow{R \rightarrow \infty} 0
 \end{aligned}$$

Thus, $\lim_{j \rightarrow \infty} \left| \int \varphi d\mu_{j_k} - \int \varphi d\mu \right| \leq \alpha_R + \beta_R$ for all $R > 0$. Letting $R \rightarrow \infty$ proves the narrow convergence.

□

Proposition 2.6

The set of couplings $\Pi(\mu_1, \dots, \mu_N) \subseteq \mathcal{M}_+(\mathbb{R}^d)$ is

- (a) Bounded and tight
- (b) closed under narrow convergence.

Proof. (a) Being bounded is clear since they are probability measures.

Tightness: using marginal conditions: since $\mu_i(\mathbb{R}^d) = 1, \forall i = 1, \dots, N$, we can find, for every $\epsilon > 0$, a closed ball \bar{B}_i such that $\mu(\mathbb{R}^{d_i} \setminus \bar{B}_i) < \epsilon/N$. Note that $\mathbb{R}^d \setminus (\bar{B}_1 \times \dots \times \bar{B}_N) = \cup_{i=1}^N \{x = (x_1, \dots, x_N) : x_i \in \mathbb{R}^{d_i} \setminus \bar{B}_i\}$, then for $\gamma \in \Pi(\mu_1, \dots, \mu_N)$, we have

$$\gamma(\mathbb{R}^d \setminus \bar{B}_1 \times \dots \times \bar{B}_N) \leq \sum_{i=1}^N \gamma(\{x : x_i \in \mathbb{R}^{d_i} \setminus \bar{B}_i\}) = \sum_{i=1}^N \mu_i(\mathbb{R}^{d_i} \setminus \bar{B}_i) < \epsilon.$$

- (b) Let $\gamma_j \rightarrow \gamma$ narrowly, $\{\gamma_j\}_{j \in \mathbb{N}} \subseteq \Pi(\mu_1, \dots, \mu_N)$. Want to show that $\gamma \in \Pi(\mu_1, \dots, \mu_N)$. Take $\varphi_i \in C_o(\mathbb{R}^{d_i})$ and set $\Phi_i(x_1, \dots, x_N) = \varphi_i(x_i) = \varphi_i(x_i)$. Then $\Phi \in C_b(\mathbb{R}^d)$ (Not in $C_o(\mathbb{R}^d)$ necessarily) and by narrow convergence

$$\int \varphi_i d\mu_i = \int \Phi_i d\gamma_j \xrightarrow{\text{narrow convergence}} \int \Phi_i d\gamma = \int_{\mathbb{R}^{d_i}} \varphi d(M_{X_i}\gamma), \forall i = 1, \dots, N$$

So $M_{X_i}\gamma = \mu$ for each i , we are done. □

Corollary 2.7

Our minimizing sequence $\{\gamma_j\}_{j \in \mathbb{N}} \subseteq \Pi(\mu_1, \dots, \mu_N)$, (s.t. $c(\gamma_j) \rightarrow \inf_{\gamma \in \Pi} c[\gamma]$) has narrowly convergent subsequence $\{\gamma_{j_k}\}_{k \in \mathbb{N}} \subseteq \Pi(\mu_1, \dots, \mu_N)$ s.t. $\gamma_{j_k} \xrightarrow{k \rightarrow \infty} \gamma \in \mathcal{M}_+(\mathbb{R}^d)$ narrowly. Since $\Pi(\mu_1, \dots, \mu_N)$ is closed under narrow convergence, it follows that $\gamma \in \Pi(\mu_1, \dots, \mu_N)$.

Question: Is γ the minimizer we are looking for? I.e., do we have

$$c[\gamma] = c[\text{narrow } \lim_{k \rightarrow \infty} \gamma_{j_k}] \leq \liminf_{k \rightarrow \infty} c[\gamma_{j_k}] = \inf_{\gamma \in \Pi} c[\gamma]?$$

Yes if we have lower semi-continuous of c with respect to narrow convergence.

Proposition 2.8

Let $f : \mathbb{R}^d \rightarrow \mathbb{R} \cup \{\infty\}$ be lower semi-continuous and bounded from below. Then the functional $F : \mathcal{M}_+(\mathbb{R}^d) \rightarrow \mathbb{R} \cup \{\infty\}$, $F[\mu] := \int_{\mathbb{R}^d} f d\mu$ is lower semi-continuous on $\mathcal{M}_+(\mathbb{R}^d)$ with respect to narrow convergence. I.e., if $\mu_j \rightarrow \mu$ narrowly, then $F[\mu] \leq \liminf_{j \rightarrow \infty} F[\mu_j]$.