

Minimax Rates of Estimation for Optimal Transport Maps between Infinite Dimensional Spaces

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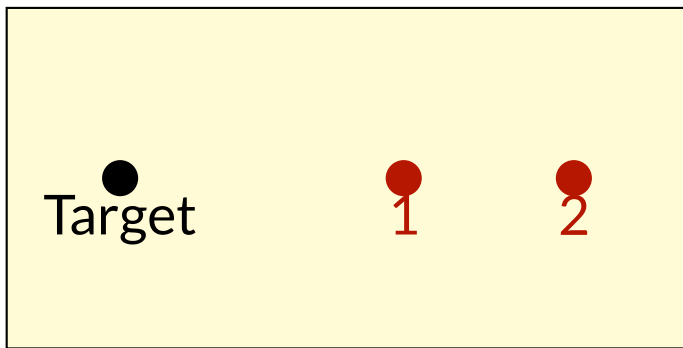
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Overview

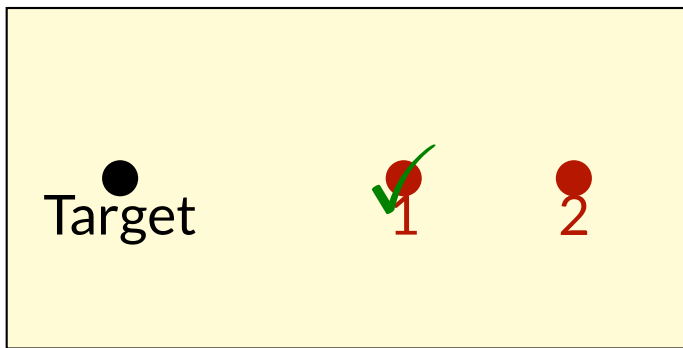
- Introduction to Optimal Transport
- Optimal Transport Map in Finite Dimensions
- Optimal Transport Map in Infinite Dimensions

Motivating Question



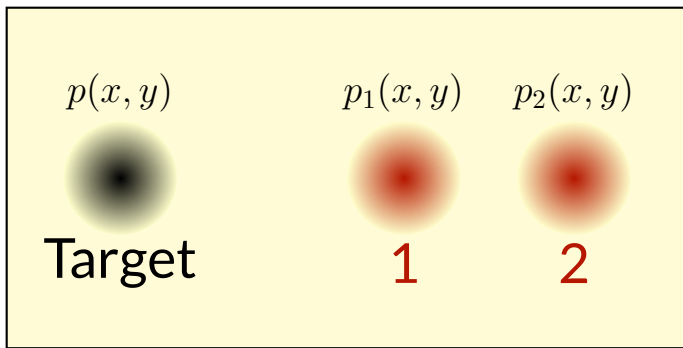
Which is closer, 1 or 2?

Motivating Question



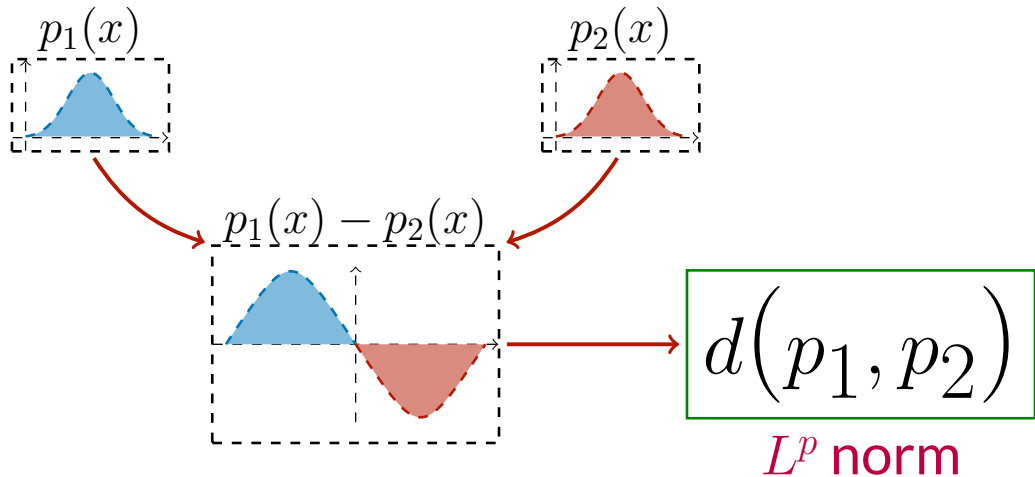
Which is closer, 1 or 2?

Fuzzy Version



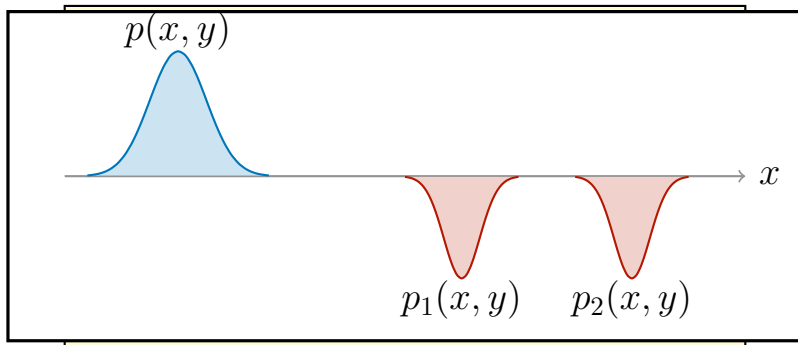
Which is closer, 1 or 2?

Typical Measurement



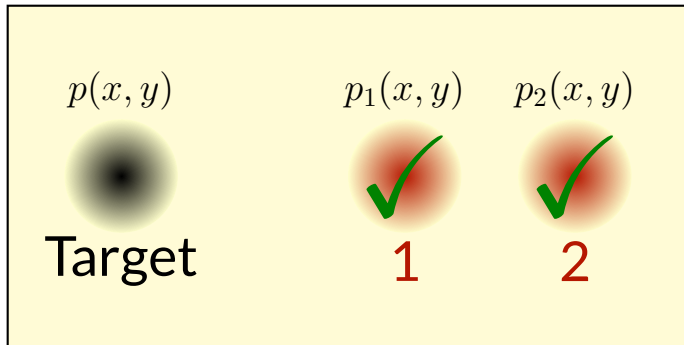
KL divergence

Returning to the Question



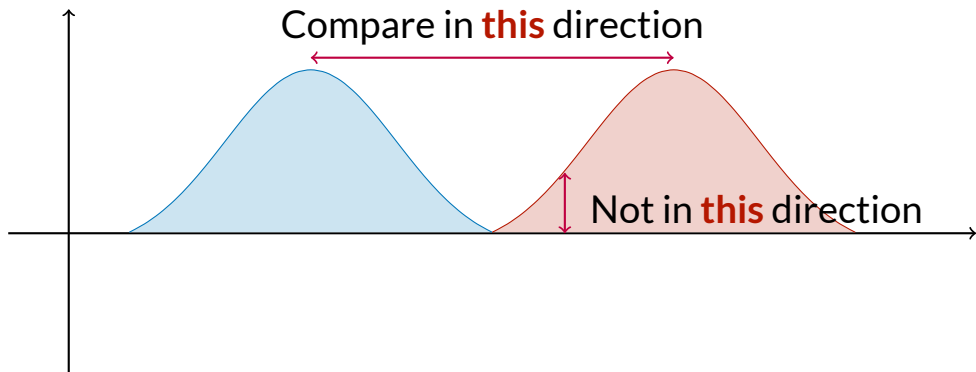
Which is closer, 1 or 2?

Returning to the Question

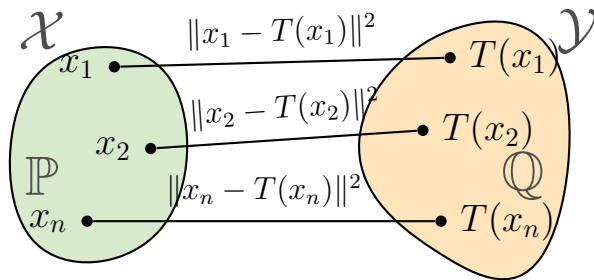


Both have the same distance!

Alternative Idea



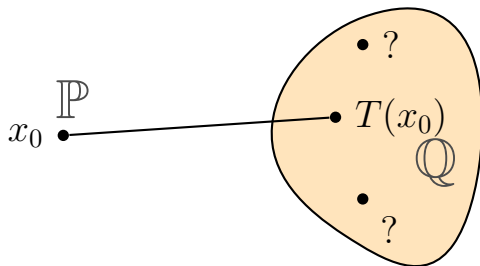
Monge's Formulation



$$T_{\#}\mathbb{P} = \mathbb{Q} \iff X \sim \mathbb{P} \Rightarrow Y \sim \mathbb{Q}.$$

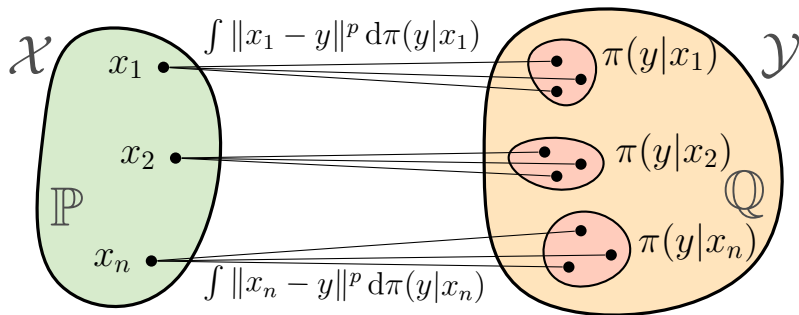
Monge's Formulation

Monge's Formulation might not have a solution!



Example: $d\mathbb{P}(x) = \delta_{x_0}(x) dx$, $d\mathbb{Q}(y) = \frac{1}{2\pi} e^{-y^2/2} dy$.
There's no T such that $T_{\#}\mathbb{P} = \mathbb{Q}$!

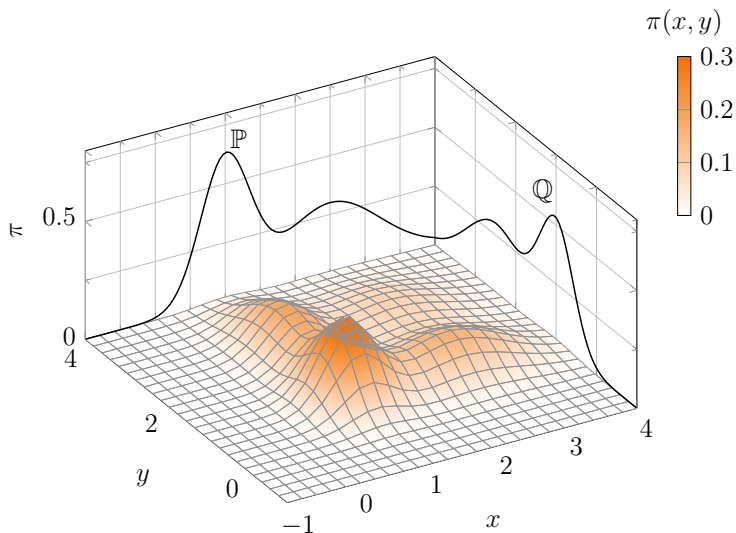
Wasserstein- p Distance



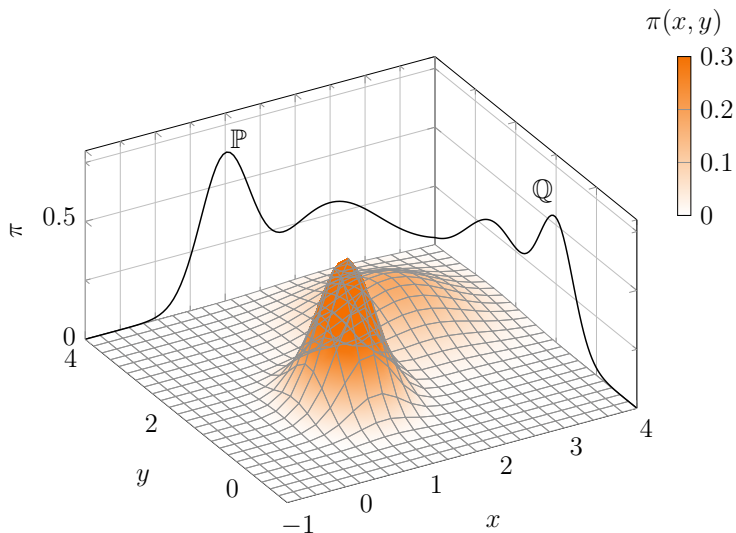
$$W_p^p(\mathbb{P}, \mathbb{Q}) = \inf_{\pi} \int_{\mathcal{X} \times \mathcal{Y}} \|x - y\|^p d\pi(x, y)$$

s.t. π is a **coupling** (i.e. marginals $\mathbb{P}$ on $\mathcal{X}$ and $\mathbb{Q}$ on $\mathcal{Y}$).

Example of Couplings



Example of Couplings



Kantorovich Problem

Primal form

$$\inf_{\pi} \int_{\mathcal{X} \times \mathcal{Y}} \|\mathbf{x} - \mathbf{y}\|^2 d\pi(x, y)$$

s.t. π is a coupling of $\mathbb{P}$ and $\mathbb{Q}$

Dual form

$$\sup_{\mathbf{f} \in L^1(\mathbb{P}), \mathbf{g} \in L^1(\mathbb{Q})} \int_{\mathcal{X}} \mathbf{f} d\mathbb{P} + \int_{\mathcal{Y}} \mathbf{g} d\mathbb{Q}$$

s.t. $\mathbf{f}(x) + \mathbf{g}(y) \leq \|\mathbf{x} - \mathbf{y}\|^2, \forall (x, y) \in \mathcal{X} \times \mathcal{Y}$

Easier to optimize: Real-valued functions instead of coupling.

Primal and Dual Form Solutions

Let $\mathbf{c} = \|\mathbf{x} - \mathbf{y}\|^2$.

$$\begin{aligned} & \inf_{\pi \text{ coupling}} \int \mathbf{c} \, d\pi(x, y) \\ &= \sup_{\mathbf{f}, \mathbf{g}} \left[\inf_{\pi \text{ positive}} \int \mathbf{c} - \mathbf{f}(x) - \mathbf{g}(y) \, d\pi(x, y) \right] + \int \mathbf{f} \, d\mathbb{P} + \int \mathbf{g} \, d\mathbb{Q} \\ & \quad = -\infty \text{ if } \mathbf{c} - \mathbf{f}(x) - \mathbf{g}(y) < 0 \text{ for some } x, y \end{aligned}$$

Complementary Slackness

If $(\pi_0, \mathbf{f}_0, \mathbf{g}_0)$ is a solution:

$$\pi_0(x^*, y^*) > 0 \iff \mathbf{f}_0(x^*) + \mathbf{g}_0(y^*) = \|\mathbf{x}^* - \mathbf{y}^*\|^2$$

Solving the Dual Form

Dual form

$$\sup_{f \in L^1(\mathbb{P}), g \in L^1(\mathbb{Q})} \int_{\mathcal{X}} f \, d\mathbb{P} + \int_{\mathcal{Y}} g \, d\mathbb{Q}$$

$$\text{s.t. } f(x) + g(y) \leq \|x - y\|^2, \forall (x, y) \in \mathcal{X} \times \mathcal{Y}$$

For any $(x^*, y^*) \in \text{Supp}(\pi_0)$,

$$f_0(x^*) + g_0(y^*) = \|x^* - y^*\|^2 \Rightarrow x^* \text{ maximizes } \|x - y^*\|^2 - f_0(x)$$

$$(\text{assume } f_0 \text{ is differentiable}) \Rightarrow x^* \text{ solves } \nabla \|x - y^*\|^2 = \nabla f_0(x)$$

$$\Rightarrow y^* = x^* - \frac{1}{2} \nabla f_0(x^*).$$

Existence and Unique of Transport Map

Brenier's theorem

Let $\mathbb{P}$ be absolutely continuous wrt the Lebesgue measure and both $\mathbb{P}$ and $\mathbb{Q}$ have finite second moments. Then, there exists a unique optimal transport map $T_0 : \mathcal{X} \rightarrow \mathcal{Y}$, defined by:

$$T_0(x) = x - \frac{1}{2} \nabla f_0(x) = \nabla \underbrace{\left(\frac{1}{2} \|x\|^2 - \frac{1}{2} f_0(x) \right)}_{\varphi_0(x)}.$$

for some differentiable function f_0 . In addition, φ_0 is convex.

c -transform

To simplify the dual problem, we define the c -transform:

$$f^c(y) = \inf_x \|x - y\|^2 - f(x).$$

Plugging $g = f^c$ in the dual problem:

Kantorovich's Semi-Dual Problem

$$\sup_{f \in L^1(\mathbb{P})} \int_{\mathcal{X}} f \, d\mathbb{P} + \int_{\mathcal{Y}} f^c \, d\mathbb{Q}.$$

(f_0, g_0) solves dual problem $\implies f_0$ solves semi-dual problem

Relating back to T_0

Plugging $f(x) = \|x\|^2 - 2\varphi(x)$ in the Kantorovich's problem:

Brenier's Semi-Dual Problem

$$\inf_{\varphi \in L^1(\mathbb{P})} \int_{\mathcal{X}} \varphi \, d\mathbb{P} + \int_{\mathcal{Y}} \varphi^* \, d\mathbb{Q},$$

where φ^* is the convex conjugate of φ :

$$\varphi^*(y) = \sup_x \langle x, y \rangle - \varphi(x).$$

φ_0 solves Brenier problem $\implies \nabla \varphi_0$ is the transport map.

Summary of Semi-Dual Problems

Brenier's Problem

$$\inf_{\varphi \in L^1(\mathbb{P})} \int_{\mathcal{X}} \varphi \, d\mathbb{P} + \int_{\mathcal{Y}} \varphi^* \, d\mathbb{Q}$$



φ_0

Brenier potential

Kantorovich's Problem

$$\sup_{f \in L^1(\mathbb{P})} \int_{\mathcal{X}} f \, d\mathbb{P} + \int_{\mathcal{Y}} f^c \, d\mathbb{Q}.$$



f_0

Kantorovich potential

$f_0(x) = \|x\|^2 - 2\varphi_0(x)$

←-----→

Estimation

Assume Brenier's assumptions hold $\implies T_0$ exists

Goal: Estimate T_0 from data:

$$X_1, \dots, X_n \sim \mathbb{P} \text{ and } Y_1, \dots, Y_n \sim \mathbb{Q}$$



Plug-In Estimator

$$\hat{\varphi}_n = \operatorname{argmin}_{\varphi \in \mathcal{F}} \frac{1}{n} \sum_{i=1}^n \varphi(X_i) + \frac{1}{n} \sum_{j=1}^n \varphi^*(Y_j).$$

$$\hat{T}_n = \nabla \hat{\varphi}_n$$

over some function class $\mathcal{F}$.

Minimax Problem

Setup: Assume that T_0 lies in some function class $\mathcal{F}_0$.

Minimax Risk

$$R_n(\mathcal{F}_0) = \inf_{T_n} \sup_{T_0 \in \mathcal{F}_0} \int \|T_n(x) - T_0(x)\|^2 d\mathbb{P}(x)$$

The **estimator** that minimizes the **worst-case estimation error**.

Minimax Lower Bound: Euclidean Case

Minimax Lower Bound [Hütter and Rigollet, 2021]

If $\alpha > 1$, $\Omega \subset \mathbb{R}^d$ _{bounded} and the true transport map lies in:

$$\mathcal{F} = \{T \in C^\alpha(\Omega), M^{-1} \prec \nabla T \prec M, \\ T = \nabla \varphi \text{ for some differentiable convex } \varphi : \Omega \rightarrow \mathbb{R}\},$$

then the following bound holds:

Rate improves with smoothness

$$R_n(\mathcal{F}) \gtrsim n^{-\frac{2\alpha}{2\alpha-2+d}}$$

Curse of dimensionality

Optimal Estimators

Which estimator $\hat{T}_n$ achieves the minimax rate?

Target Error Rate

$$\int \|\hat{T}_n(x) - T_0(x)\|^2 d\mathbb{P}(x) \approx n^{-\frac{2\alpha}{2\alpha-2+d}}.$$

Plug-In Estimator

$$\hat{\varphi}_n = \operatorname{argmin}_{\varphi \in \mathcal{F}} \frac{1}{n} \sum_{i=1}^n \varphi(X_i) + \frac{1}{n} \sum_{j=1}^n \varphi^*(Y_j).$$
$$\hat{T}_n = \nabla \hat{\varphi}_n,$$

is minimax optimal when:

- $\mathcal{F} = \{\text{finite wavelet series, must be strongly convex}\}$
[Hütter and Rigollet, 2021]
- $\mathcal{F} = \{\text{finite wavelet series}\}$ or $\{\text{ReQU neural networks}\}$
[Divol et al., 2025]

Estimators from smoothed densities

Estimate densities $\hat{p}_n(x)$ and $\hat{q}_n(y)$ using kernel or wavelets.

Let $\hat{\mathbb{P}}_n$ and $\hat{\mathbb{Q}}_n$ be distributions w/ densities $\hat{p}_n(x)$ and $\hat{q}_n(y)$.

$$\hat{T}_n = \operatorname{argmin}_{T_{\#} \hat{\mathbb{P}}_n = \hat{\mathbb{Q}}_n} \int \|T(x) - x\|^2 d\hat{\mathbb{P}}_n.$$

$\hat{T}_n$ is minimax optimal for both kernel and wavelet estimators [Manole et al., 2021].

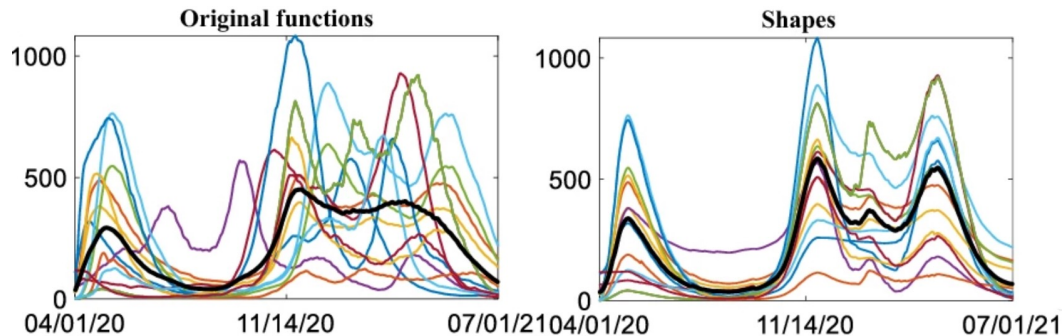
Extending to Infinite Dimensions

Optimal transport from $X \in [0, 1]^\infty$ to $Y \in [0, 1]^\infty$.

Why?

- We could gain some insight into combatting the curse of dimensionality.
- Application to functional data analysis:
 - We can view function $f \in L^2([0, 1])$ as infinite sequence $(a_1, a_2, \dots)$ via Fourier or Wavelet transform.
 - Example: Matching time series between two individuals.

Time series alignment



Hospitalization rates (per million) for 16 European countries from April 1, '20, to July 1, '21.
[Wu et al., 2023]

Optimal Transport in Infinite Dimensions

Let $\mathcal{H}$ be a separable Hilbert space with basis $\{e_i\}_{i=1}^{\infty} \subset \mathcal{H}$.

Definition

A Borel-measurable set $E \subset \mathcal{H}$ is a **Gaussian null set** if $\mu(E) = 0$ for any Gaussian measure¹ μ on $\mathcal{H}$.

¹(measure of variables of the form $a + \sum_{i=1}^{\infty} X_i e_i$ where $X_i \sim N(0, 1)$.)

Optimal Transport in Infinite Dimensions

Brenier's Theorem on $\mathcal{H}$ [Ambrosio et al., 2005]

Let $\mathbb{P}, \mathbb{Q}$ be prob. measures with supports $\Omega_{\mathbb{P}}, \Omega_{\mathbb{Q}} \subset \mathcal{H}$.

Assume $\mathbb{P}$ is zero on all Gaussian null sets, $\mathbb{Q}$ has a bounded support, and both $\mathbb{P}$ and $\mathbb{Q}$ have finite second moments.

Then, there exists a unique transport map:

$$T_0 : \Omega_{\mathbb{P}} \rightarrow \Omega_{\mathbb{Q}},$$

and a convex function $\varphi_0 \in L^1(\mathbb{P})$ such that $\nabla \varphi_0 = T_0$.

Minimax Lower Bound for C^2 Functions

Theorem (Informal) [Ponnoprat and Imaizumi, 2025]

There is a subset $\Omega \subset [0, 1]^\infty$ such that, if the transport map T_0 lies in:

$$\mathcal{F} \subset \{T = \nabla \varphi \mid \varphi \in C^2(\Omega)\},$$

then the following bound holds:

$$\sum_{i=1}^{\infty} |\partial_i \varphi| + \sum_{i,j=1}^{\infty} |\partial_i \partial_j \varphi| \leq B$$

$$R_n(\mathcal{F}) \gtrsim \frac{1}{\log n}.$$

Very slow rate!

New Function Space for φ_0

Let $\mathbb{Z}_0^\infty = \{(\mathbf{l}_1, \mathbf{l}_2, \dots) \mid \mathbf{l}_i \in \mathbb{Z}, \mathbf{l}_i = 0 \text{ for all but finitely many } i\}$

Fact: Any function $\varphi \in L^2([0, 1]^\infty)$ can be approximated by Fourier series:

$$f(\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3, \dots) \approx \sum_{\mathbf{l} \in \mathbb{Z}_0^\infty} f_{\mathbf{l}} \psi_{\mathbf{l}_1}(\mathbf{x}_1) \psi_{\mathbf{l}_2}(\mathbf{x}_2) \psi_{\mathbf{l}_3}(\mathbf{x}_3) \cdots ,$$

where $f_{\mathbf{l}} \in \mathbb{R}$ and

$$\psi_{\mathbf{l}_i}(\mathbf{x}_i) = \begin{cases} \sqrt{2} \cos(2\pi |\mathbf{l}_i| \mathbf{x}_i), & \mathbf{l}_i < 0 \\ \sqrt{2} \sin(2\pi |\mathbf{l}_i| \mathbf{x}_i), & \mathbf{l}_i > 0 \\ 1, & \mathbf{l}_i = 0. \end{cases}$$

Grouping Frequencies

Let's denote

$$\psi_{\mathbf{l}}(\mathbf{x}) = \psi_{l_1}(\mathbf{x}_1)\psi_{l_2}(\mathbf{x}_2)\psi_{l_3}(\mathbf{x}_3)\cdots.$$

For each $\mathbf{s} = (s_1, s_2, \dots) \in \mathbb{N}^\infty$, we gather all terms between two consecutive **dyadic frequencies**: 2^{s_i-1} and 2^{s_i} :

$$\delta_{\mathbf{s}}(f) = \sum_{\mathbf{l} \in \mathbb{Z}_0^\infty: 2^{s_i-1} \leq |l_i| < 2^{s_i}} f_{\mathbf{l}} \psi_{\mathbf{l}}.$$

Function Space for T_0

- We want to characterize the **Brenier potential** φ_0 by Fourier series.
- However, φ_0 has to be convex! There is no nice way to describe convexity in terms of Fourier coefficients.
- So we use the Fourier series for the **Kantorovich potential** f_0 instead.

Function Space for T_0

Specify the **direction-wise smoothness levels**:

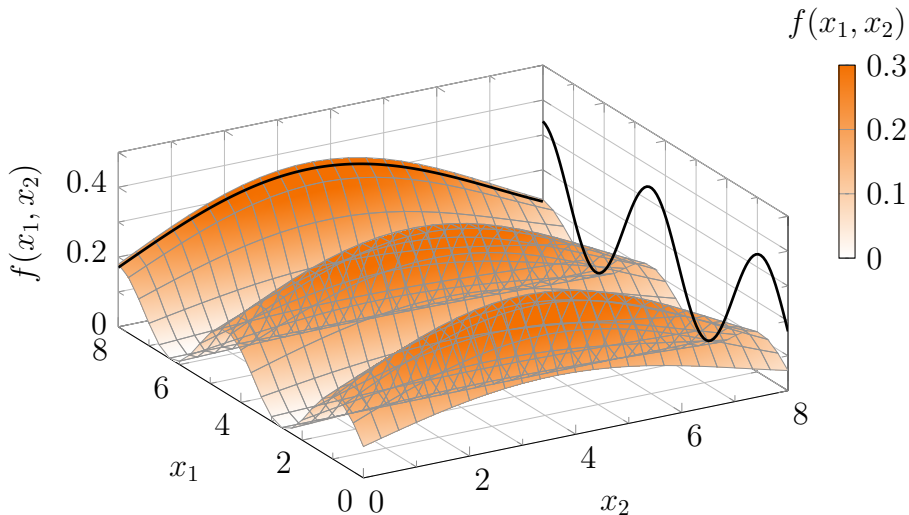
$$\mathbf{a} = (a_1, a_2, \dots)$$

Characterize smoothness of **Kantorovich potential** f_0 by the decay of each $\delta_s(\mathbf{f})$:

must be small for large s_i and a_i

$$\mathcal{F}_{\mathbf{a}} = \left\{ T = \nabla \left(\frac{1}{2} \|\cdot\|^2 - \frac{1}{2} \mathbf{f} \right) \mid \underbrace{\sum_{s \in \mathbb{N}_0^\infty} 2^{2 \sum_i a_i s_i} \|\delta_s(\mathbf{f})\|_{L^2}^2}_{\|\mathbf{f}\|_{H\mathbf{a}}} \leq 1 \right\}.$$

For example, $\mathbf{a} = (1, 2, \infty, \infty, \dots)$ represents $\mathbf{f} : [0, 1]^2 \rightarrow \mathbb{R}$ that is twice as smooth along x_2 compared to x_1 .



Minimax Lower Bound

Theorem [Ponnoprath and Imaizumi, 2025]

Suppose that $\mathbb{P}$ and $\mathbb{Q}$ satisfy all the assumptions of the Brenier's Theorem, and that $\mathbf{a}_1 \leq \mathbf{a}_2 \leq \dots$

The minimax lower bound of learning an optimal transport map from $\mathcal{F}_{\mathbf{a}}$ is:

$$R_n(\mathcal{F}_{\mathbf{a}}) \gtrsim n^{-\frac{2\mathbf{a}_1}{2\mathbf{a}_1+1}}.$$

Our Proposed Estimator

Specify a positive integer J , and then solve:

Plug-In Estimator

$$\hat{\varphi}_{n,\mathbf{a},J} = \operatorname{argmin}_{\varphi \in \mathcal{F}_{\mathbf{a},J}} \frac{1}{n} \sum_{i=1}^n \varphi(X_i) + \frac{1}{n} \sum_{j=1}^n \varphi^*(Y_j).$$

$$\hat{T}_{n,\mathbf{a},J} = \nabla \hat{\varphi}_{n,\mathbf{a},J}$$

$$\mathcal{F}_{\mathbf{a},J} = \left\{ \varphi = \frac{1}{2} \|\cdot\|^2 - \frac{1}{2} \mathbf{f} \mid \mathbf{f} = \sum_{|l_i| \lesssim 2^{J/a_i}} f_l \psi_l, \|\mathbf{f}\|_{H^{\mathbf{a}}} \leq 1 \right\}$$

Optimality of the Plug-In Estimator

Theorem [Ponnoprat and Imaizumi, 2025]

Suppose that $\mathbb{P}$ and $\mathbb{Q}$ satisfy all the assumptions of the Bre-
nier's Theorem, $\mathbf{a}_1 \leq \mathbf{a}_2 \leq \dots$, and $\mathbf{a}_i \approx i^q$ for some $q > 0$.

Let $\mathbf{J} \approx \log n$.

Then, the estimator $\hat{T}_{n,\mathbf{a},\mathbf{J}}$ satisfies the following bound:

$$\int \|\hat{T}_{n,\mathbf{a},\mathbf{J}}(x) - T_0(x)\|^2 d\mathbb{P}(x) \lesssim n^{-\frac{2\mathbf{a}_1}{2\mathbf{a}_1+1}}.$$

Impracticality of Plug-In Estimator

$$\begin{aligned} \hat{\varphi}_{n,\mathbf{a},\mathbf{J}} &= \operatorname{argmin}_{\varphi} \frac{1}{n} \sum_{i=1}^n \varphi(X_i) + \frac{1}{n} \sum_{j=1}^n \varphi^*(Y_j), \\ \text{s.t. } \varphi &= \frac{1}{2} \|\cdot\|^2 - \frac{1}{2} \mathbf{f}, \quad \mathbf{f} = \sum_{|l_i| \lesssim 2^{\mathbf{J}/\mathbf{a}_i}} f_l \psi_l, \quad \|\mathbf{f}\|_{H^{\mathbf{a}}} \leq 1. \end{aligned}$$

Ignoring the φ^* term, this is a constraint linear program over the coefficients f_l .

However, the number of the coefficients is exponential in the number of dimensions, making it impractical.

Neural Network Estimator

Instead, we consider the following function class for f :

$$\mathcal{F}(W, L, R, B) = \{\text{neural networks with width} \leq W, \text{\#layers} \leq L \\ \text{\#parameters} \leq R, \text{values of parameters} \leq B\}$$

Neural Network Estimator

$$\hat{\varphi}_{n,WLRB} = \underset{\varphi}{\operatorname{argmin}} \frac{1}{n} \sum_{i=1}^n \varphi(X_i) + \frac{1}{n} \sum_{j=1}^n \varphi^*(Y_j),$$

$$\text{s.t. } \varphi = \frac{1}{2} \|\cdot\|^2 - \frac{1}{2} f, \quad f \in \mathcal{F}(W, L, R, B).$$

$$\hat{T}_{n,WLRB} = \nabla \hat{\varphi}_{\alpha,WLRB}.$$

Optimality of the Neural Estimator

Theorem [Ponnoprat and Imaizumi, 2025]

Suppose that $\mathbb{P}$ and $\mathbb{Q}$ satisfy all the assumptions of the Bre-
nier's Theorem, $\mathbf{a}_1 \leq \mathbf{a}_2 \leq \dots$, and $\mathbf{a}_i \approx i^{\mathbf{q}}$ for some $\mathbf{q} > 0$.

Let $\mathbf{J} \approx \log n$. Then, there are some W, L, R, B depending on
 $\mathbf{J}, \mathbf{a}_1$ and $\mathbf{q}$ such that $\hat{T}_{n,WLRB}$ satisfies the following bound:

$$\int \|\hat{T}_{n,WLRB}(x) - T_0(x)\|^2 d\mathbb{P}(x) \lesssim n^{-\frac{2\mathbf{a}_1}{2\mathbf{a}_1+1}}.$$

Computational Aspects

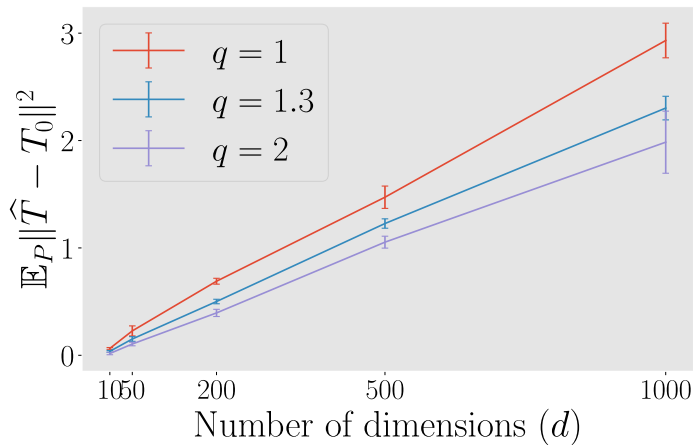
- Still, these estimators are computationally expensive due to the convex conjugate: $\varphi^*(y) = \sup_x \langle x, y \rangle - \varphi(x)$.
- Solution #1: Use another neural network to model φ^* “Amortization” [Amos, 2023].
- Solution #2: Use separate networks to model the potential and the transport map [Korotin et al., 2023]:

$$\sup_{\textcolor{red}{f}} \inf_{\textcolor{blue}{T}} \left\{ \frac{1}{n} \sum_{i=1}^n \|X_i - \textcolor{blue}{T}(X_i)\|^2 - \textcolor{red}{f}(\textcolor{blue}{T}(X_i)) + \frac{1}{n} \sum_{i=1}^n \textcolor{red}{f}(X_i) \right\}.$$

Experiment 1: No Curse of Dimensionality

$$(T_0(x))_i = x_i - \frac{1}{\kappa(i)} |x_i - 0.5|^{\kappa(i)}, \kappa(i) \approx i^{0.1q}. \text{ Fix } n = 100.$$

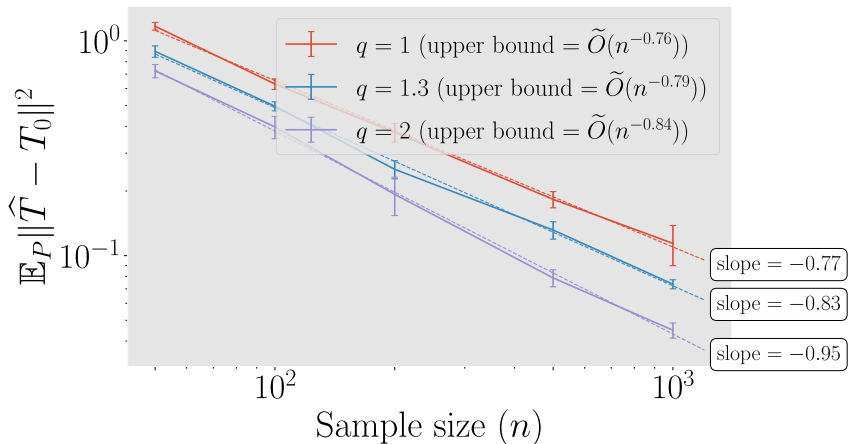
$$\hat{\varphi}_n = \frac{1}{2} \|\cdot\|^2 - \frac{1}{2} \hat{f}_n \longleftarrow \text{CNN with two convolutional layers.}$$



Experiment 2: Error Rate

$$(T_0(x))_i = x_i - \frac{1}{\kappa(i)} |x_i - 0.5|^{\kappa(i)}, \kappa(i) \approx i^{0.1q}. \text{ Fix } d = 200.$$

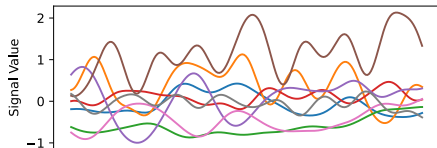
$$\hat{\varphi}_n = \frac{1}{2} \|\cdot\|^2 - \frac{1}{2} \hat{f}_n \leftarrow \text{CNN with two convolutional layers.}$$



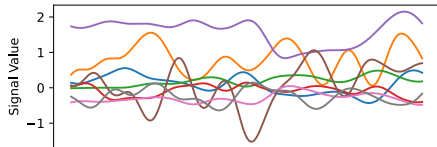
Application: Domain Adaptation

Subject 1

Session 1, Label: 0

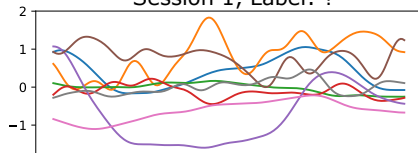


Session 2, Label: 1

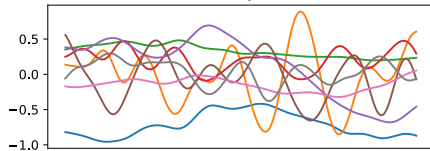


Subject 2

Session 1, Label: ?

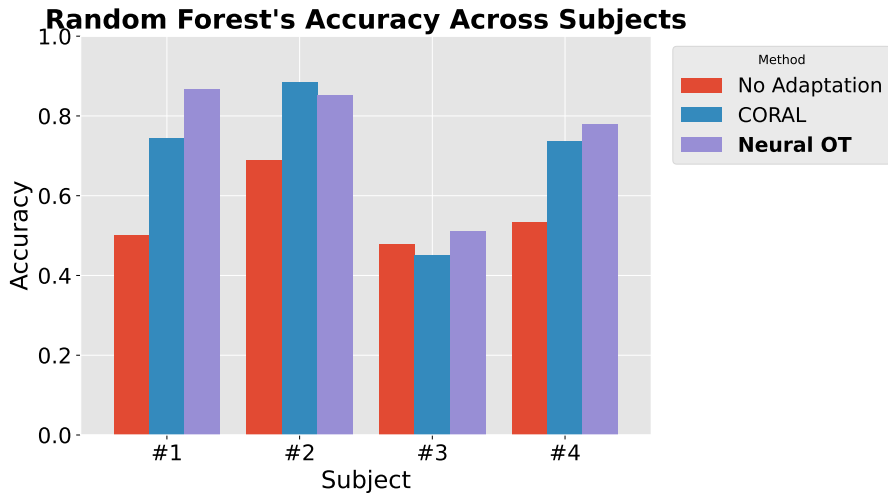


Session 2, Label: ?



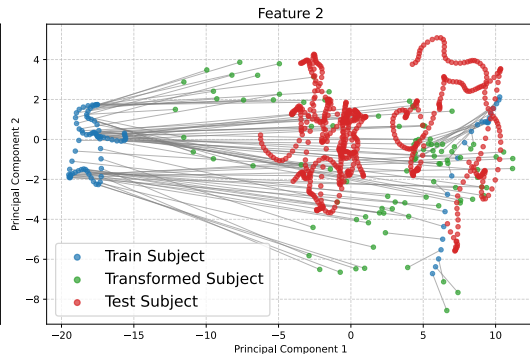
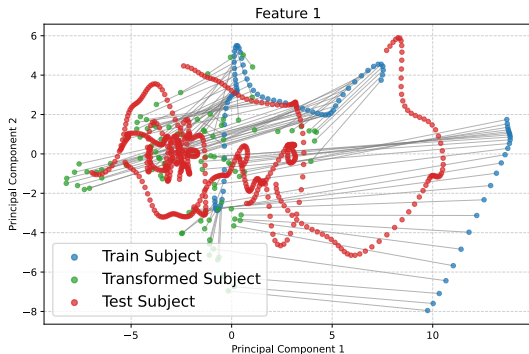
Mental workload data [Huang et al., 2021]. Label: 0 = Normal, 1 = Intense.

Result



Result of adapting 8 training subjects to 4 test subjects.

Functional PCA of the Transports



Conclusion

- We study the problem of optimal transport (OT) map estimation. Existing results suffer from the curse of dimensionality.
- We introduce a way to characterize the smoothness of OT maps on infinite-dimensional spaces that leads to a polynomial error rate.

Challenges

- Main challenge #1: Relaxing the assumptions.
- Main challenge #2: Finding Computational tractable algorithm with theoretical guarantees.

arXiv link: <https://arxiv.org/abs/2505.13570>

Thank you!

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Gradient flows: in metric spaces and in the space of probability measures.
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