

Regularized Optimal Transport is Ground Cost Adversarial

MokaMeeting

May 11, 2022

FRANÇOIS-PIERRE PATY

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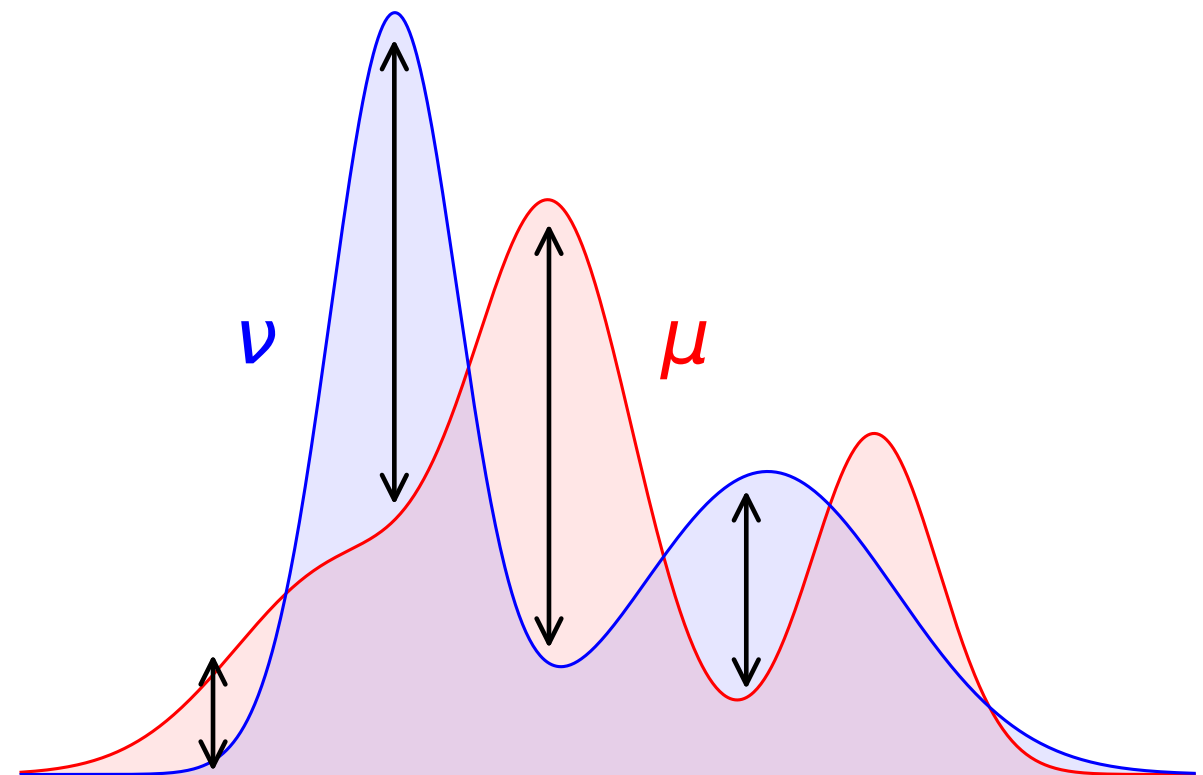
*Based on a joint work with **Marco Cuturi***

COMPARING DISTRIBUTIONS

1. Vertical comparison

Look at the difference, or the ratio of the densities

e.g. *Total Variation distance*,
Kullback Leibler divergence, etc.

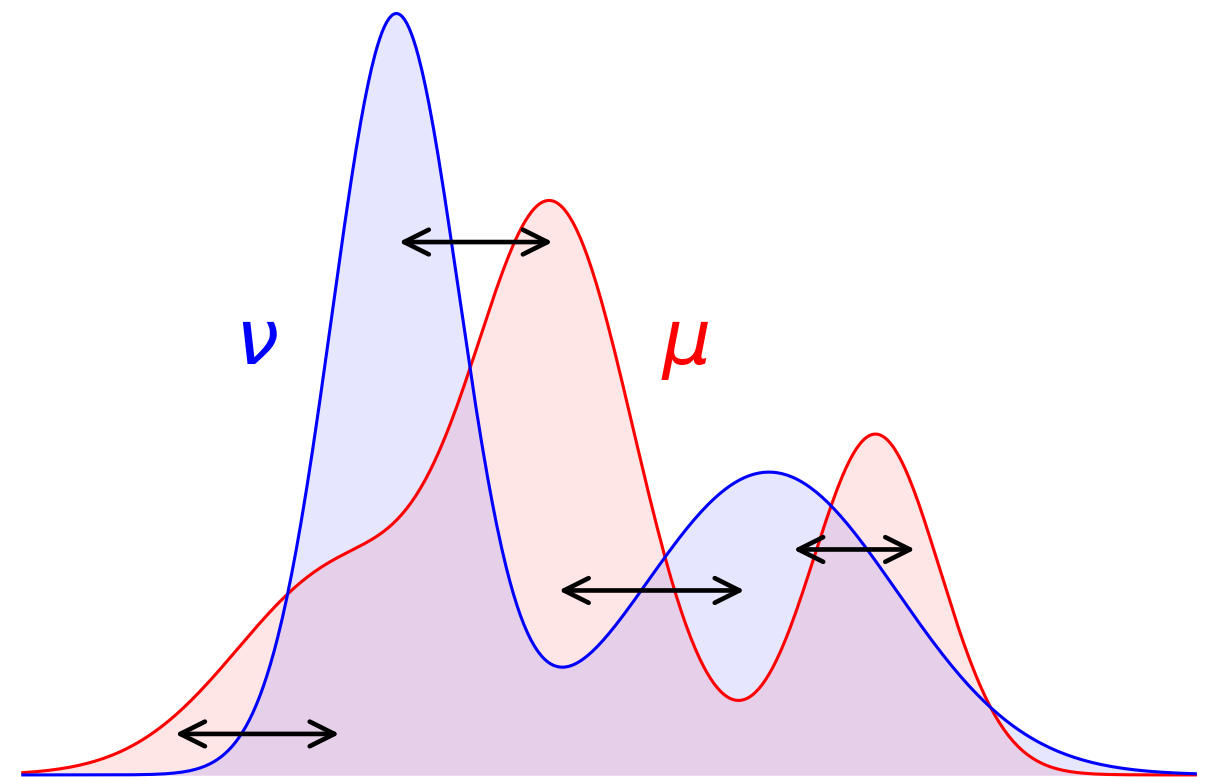


COMPARING DISTRIBUTIONS

2. Horizontal comparison aka Optimal Transport

Move the mass across the
ground space

! Need for a notion of
displacement cost on the
ground space





OPTIMAL TRANSPORT

Leonid Kantorovich

OPTIMAL TRANSPORT

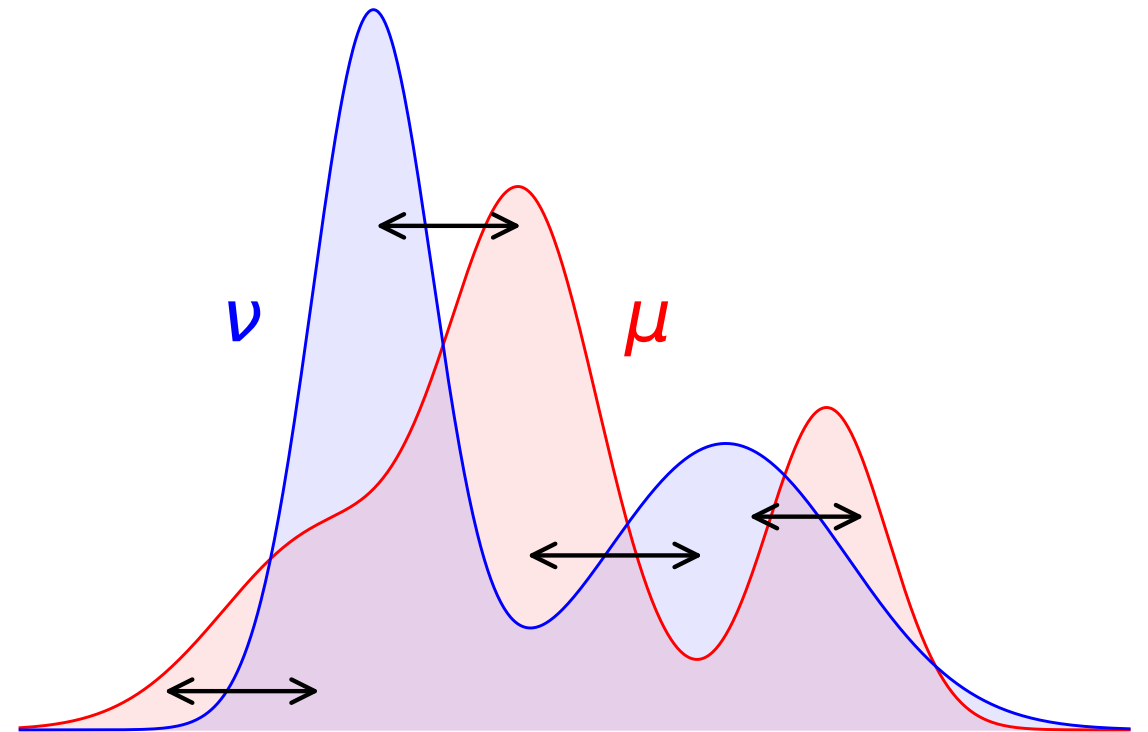
Data:

Two distributions μ and ν over \mathbb{R}^d

Parameter:

A (continuous) cost function

$$c : \mathbb{R}^d \times \mathbb{R}^d \rightarrow \mathbb{R}$$



OPTIMAL TRANSPORT

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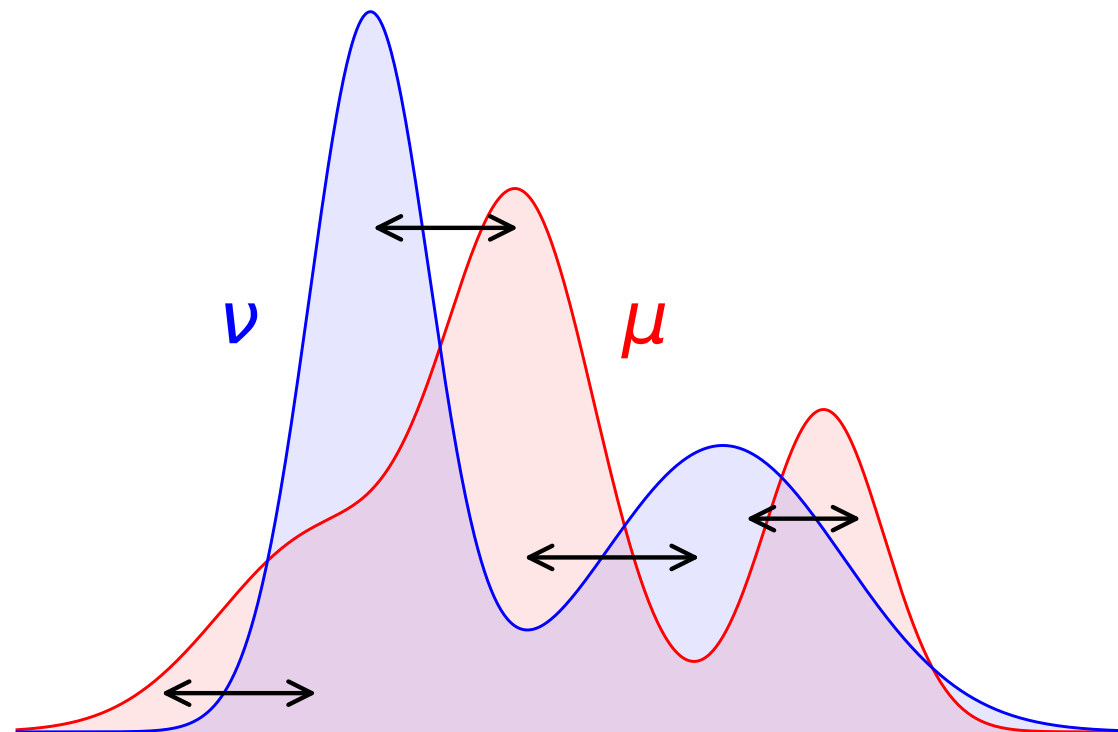
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Definition of Optimal Transport (OT):



OPTIMAL TRANSPORT

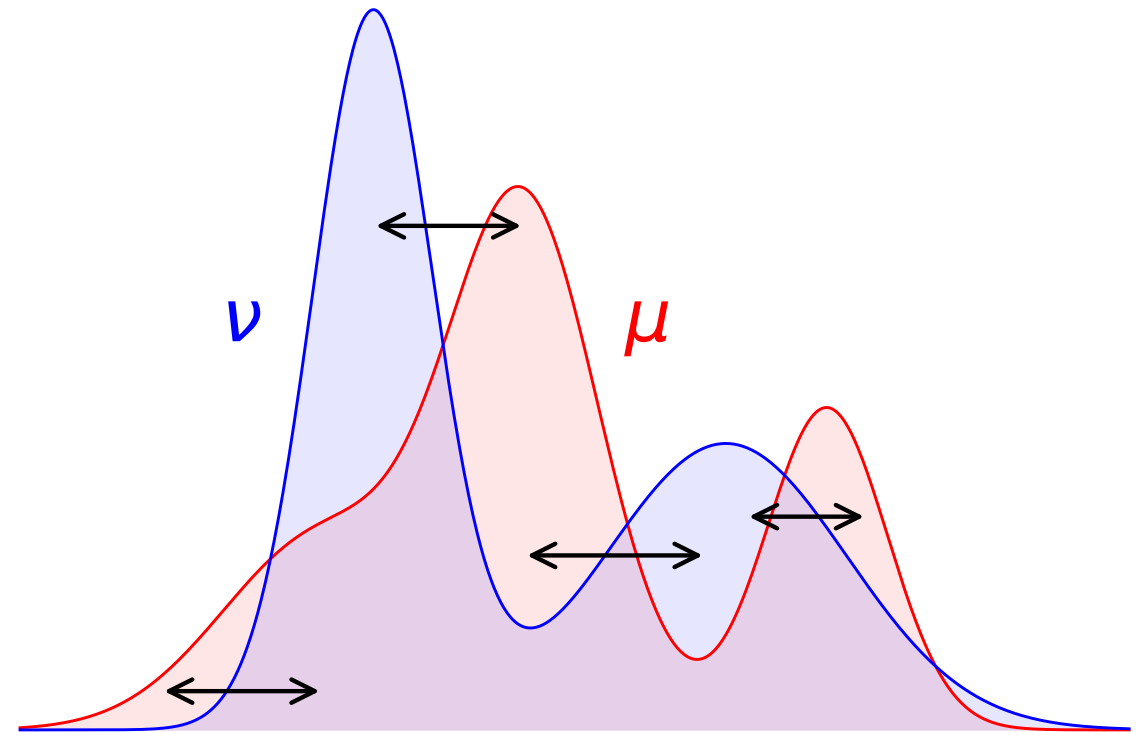
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Definition of Optimal Transport (OT):

$$c(x, y) d\pi(x, y)$$

OPTIMAL TRANSPORT

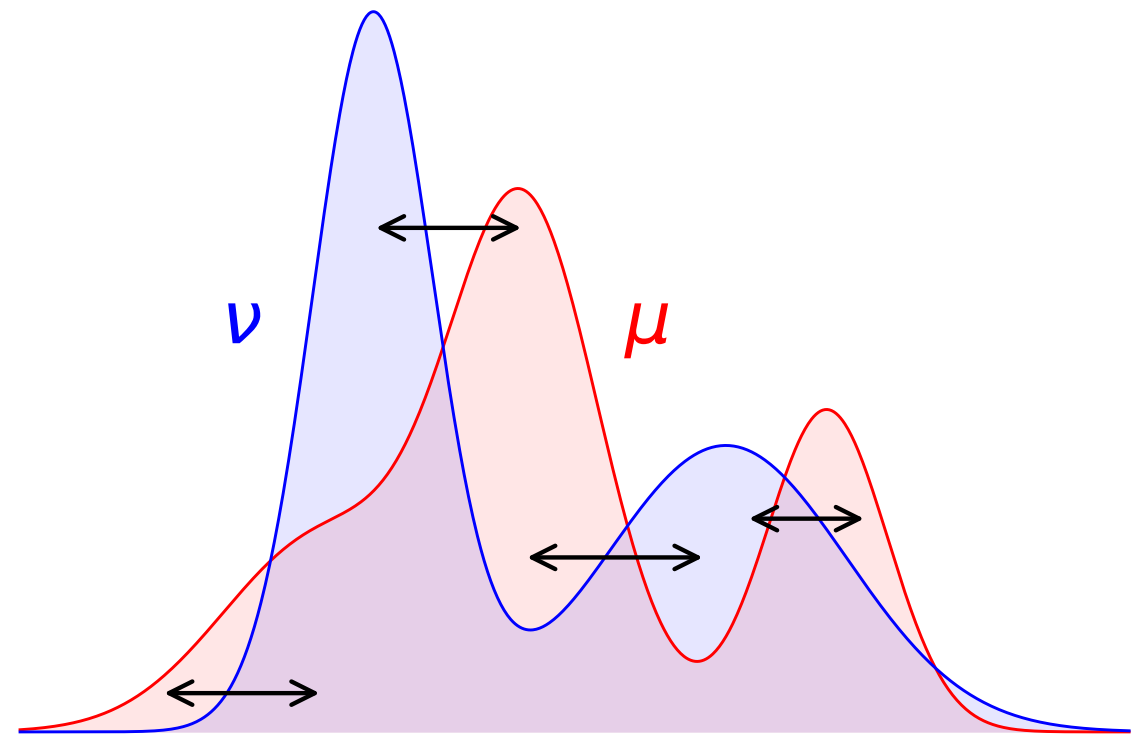
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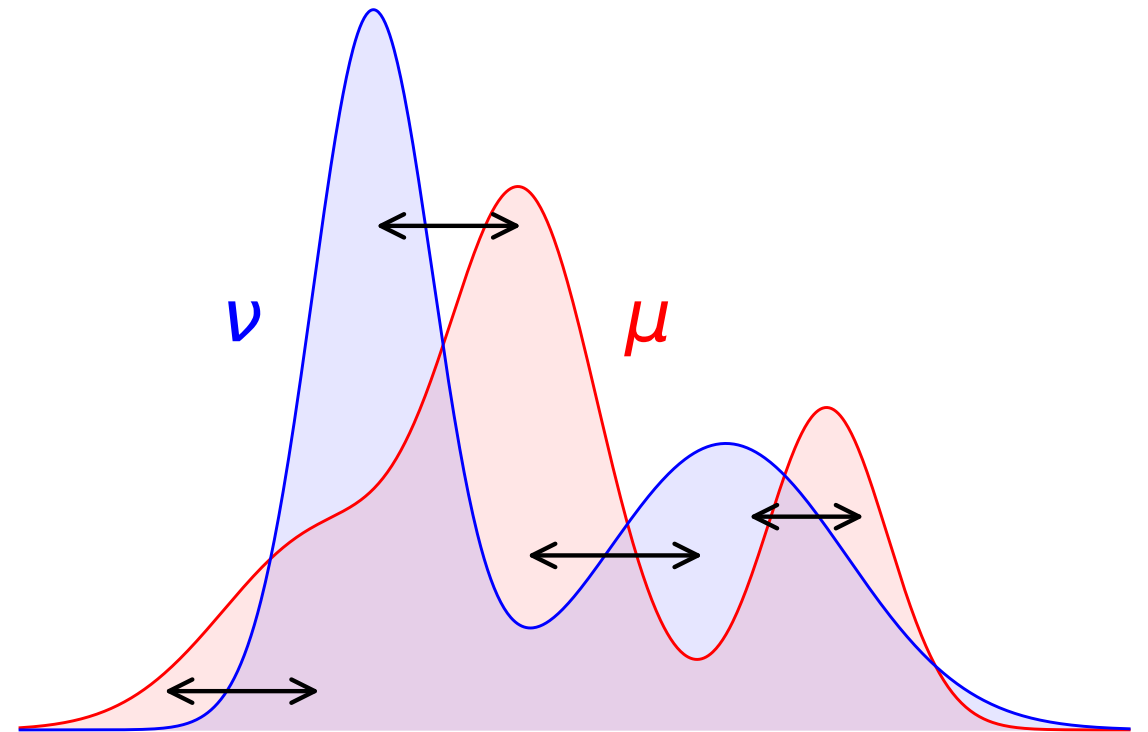
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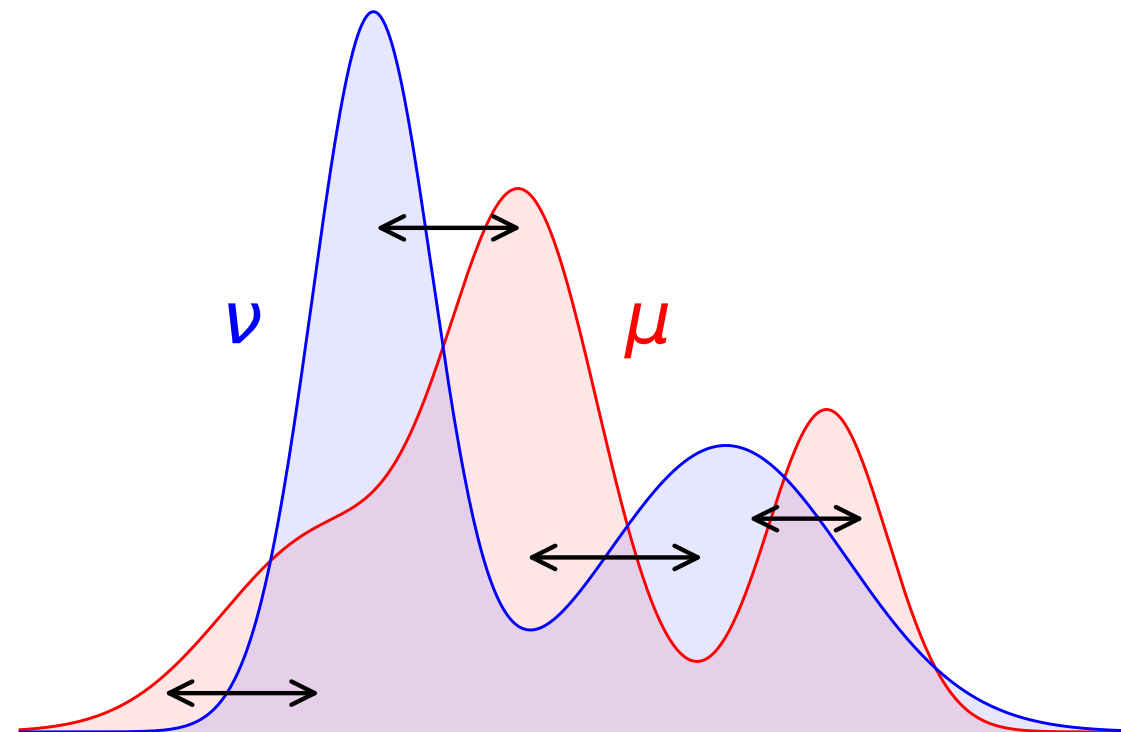
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Definition of Optimal Transport (OT):

$$\mathcal{T}_c(\mu, \nu) = \inf_{\pi} \iint c(x, y) d\pi(x, y)$$

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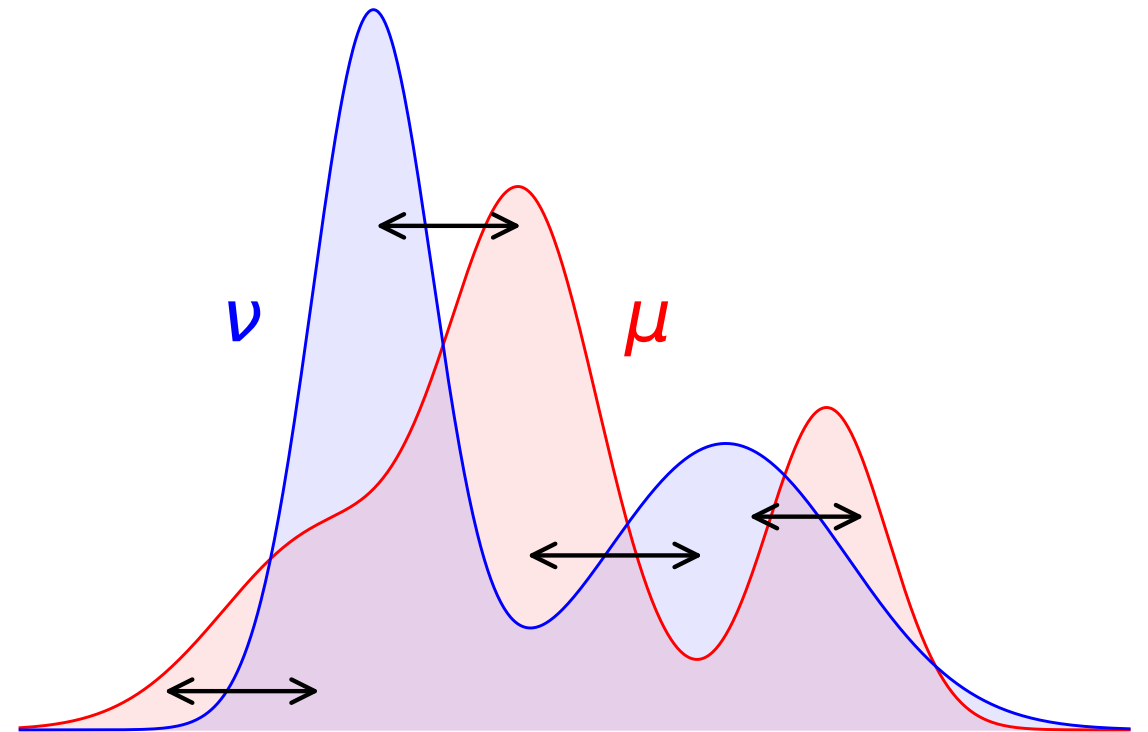
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Definition of Optimal Transport (OT):

$$\mathcal{T}_c(\mu, \nu) = \inf_{\pi} \iint c(x, y) d\pi(x, y)$$

over all π such that

$$\begin{cases} \int d\pi(x, y) = d\mu(x) \quad \forall x \\ \int d\pi(x, y) = d\nu(y) \quad \forall y \end{cases}$$

OPTIMAL TRANSPORT

Two main questions in practice

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1. How to choose the ground cost c in a way that makes sense for the data distributions μ and ν ?

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Two main questions in practice

1. How to choose the ground cost c in a way that makes sense for the data distributions μ and ν ?
2. How to compute/approximate the OT cost $\mathcal{T}_c(\mu, \nu)$, at least when the measures are discrete (i.e. are finite sums of Dirac masses) in a scalable way?

A portrait of Gaspard Monge, a French mathematician and engineer. He is depicted from the waist up, wearing a dark blue coat with ornate gold embroidery on the collar and cuffs. A white cravat is visible at his neck. He has white hair and is looking slightly to the right. The background is dark and indistinct.

GROUND COST

Gaspard Monge

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$$c(x, y) = \|x - y\|^p \quad \text{where } p \geq 1$$

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But does it make sense when the ground space is high-dimensional



But does it make sense when the data lives on a low-dimensional manifold



GROUND COST

Idea: Find a ground cost c that is adversarial, *i.e.* that best separates the two distributions by maximizing the OT cost

$$\max_{c \in \mathcal{C}} \mathcal{J}_c(\mu, \nu) \quad \text{where } \mathcal{C} \text{ is a convex class of functions}$$

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$$\max_c \mathcal{I}_c(\mu, \nu) - f(c) \quad \text{for some convex } f$$

$$f(c) = \begin{cases} 0 & \text{if } c \in \mathcal{C} \\ +\infty & \text{if } c \notin \mathcal{C} \end{cases}$$

GROUND COST

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- Links with the Robust Optimization literature
- Links with the matchings literature in Economics
- Initially proposed by Genevay *et al.* in 2017 to learn generative models
- When \mathcal{C} is the set of Mahalanobis distances, it defines the Subspace Robust Wasserstein distances (ICML 2019, cf. in a few slides)

IN ECONOMICS

Data: Two probability distributions μ and ν representing two groups of people (e.g. men and women), and a matching between them π_0 (e.g. marriage/dating data)

Problem: Explain/understand the observed matching π_0

Method: Assume π_0 is optimal for a certain ground-cost c_\star , which we can then interpret. We just have to solve:

$$\sup_c \mathcal{T}_c(\mu, \nu) - \int c d\pi_0$$

In practice, economists assume that

$$c_\star \in \{d_\Omega^2 : (x, y) \mapsto (x - y)^\top \Omega (x - y) \mid \Omega \succeq 0, \|\Omega\| \leq 1\}$$

and seek Ω , i.e. rather solve

$$\sup_c \mathcal{T}_c(\mu, \nu) - \int c d\pi_0 - R^*(c)$$



REGULARIZATION

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2. How to compute/approximate the OT cost $\mathcal{T}_c(\mu, \nu)$?

1. This is a Linear Program $\longrightarrow \mathcal{O}(n^3)$ complexity
2. Entropic regularization $\longrightarrow \mathcal{O}(n^2)$ Sinkhorn algorithm, GPU-friendly, differentiable...

$$\inf_{\pi} \iint c(x, y) d\pi(x, y) + \varepsilon R(\pi)$$

where $R(\pi) = \text{KL}(\pi || \mu \otimes \nu)$

Other regularizations have been proposed: e.g. quadratic, group-lasso, capacity constraints, with different algorithms and effects on the OT plan / value

REGULARIZATION

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How can we interpret the effect of the regularization ?

TWO VIEWS OF THE SAME PHENOMENON



GROUND-COST ADVERSARIAL TRANSPORT

$$\max_{\mathcal{C}} \mathcal{I}_{\mathcal{C}}(\mu, \nu) - f(\mathcal{C})$$


GROUND-COST ADVERSARIAL TRANSPORT

$$\max_{\mathcal{C}} \mathcal{T}_{\mathcal{C}}(\mu, \nu) - f(\mathcal{C}) = \max_{\mathcal{C}} \min_{\pi \in \Pi(\mu, \nu)} \int \mathcal{C} d\pi - f(\mathcal{C})$$

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$$\max_{\underline{c}} \mathcal{T}_{\underline{c}}(\mu, \nu) - f(\underline{c}) = \max_{\underline{c}} \min_{\pi \in \Pi(\mu, \nu)} \int \underline{c} d\pi - f(\underline{c})$$

Sion's minimax
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$$\max_{\mathbf{c}} \mathcal{T}_{\mathbf{c}}(\boldsymbol{\mu}, \boldsymbol{\nu}) - f(\mathbf{c}) = \max_{\mathbf{c}} \min_{\pi \in \Pi(\boldsymbol{\mu}, \boldsymbol{\nu})} \int \mathbf{c} d\pi - f(\mathbf{c})$$

Sion's minimax theorem

$$= \min_{\pi \in \Pi(\boldsymbol{\mu}, \boldsymbol{\nu})} \max_{\mathbf{c}} \int \mathbf{c} d\pi - f(\mathbf{c})$$

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Take $f(\mathbf{c}) = \varepsilon R^* \left(\frac{\mathbf{c} - \mathbf{c}_0}{\varepsilon} \right)$ where R is convex:

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$$f^*(\pi) = \sup_{\underline{c}} \int \underline{c} d\pi - \varepsilon R^* \left(\frac{\underline{c} - c_0}{\varepsilon} \right) = \sup_d \int (c_0 + \varepsilon d) d\pi - \varepsilon R^*(d)$$

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$$\begin{aligned} &\inf_{\pi \in \Pi(\mu, \nu)} \iint c_0(x, y) d\pi(x, y) + \varepsilon R(\pi) \\ &= \sup_{\underline{c}} \mathcal{T}_{\underline{c}}(\mu, \nu) - \varepsilon R^* \left(\frac{\underline{c} - c_0}{\varepsilon} \right) \end{aligned}$$

GROUND COST ROBUSTNESS \Leftrightarrow REGULARIZATION

Theorem: Regularized OT is ground cost adversarial in the following sense

$$\begin{aligned} \inf_{\pi \in \Pi(\mu, \nu)} \iint c_0(x, y) d\pi(x, y) + \varepsilon R(\pi) \\ = \sup_c \mathcal{J}_c(\mu, \nu) - \varepsilon R^* \left(\frac{c - c_0}{\varepsilon} \right) \end{aligned}$$

where R is a convex regularizer

and R^* is the convex conjugate of R :

$$R^*(c) = \sup_{\pi} \int c d\pi - R(\pi)$$

EXAMPLES: ENTROPIC OT

$$\min_{\pi \in \Pi(\mu, \nu)} \int c_0 d\pi + \varepsilon \text{KL}(\pi \parallel \mu \otimes \nu)$$

EXAMPLES: ENTROPIC OT

$$\begin{aligned} & \min_{\pi \in \Pi(\mu, \nu)} \int c_0 d\pi + \varepsilon \text{KL}(\pi \| \mu \otimes \nu) \\ &= \sup_c \mathcal{T}_c(\mu, \nu) - \varepsilon \int \exp\left(\frac{c - c_0}{\varepsilon}\right) d\mu \otimes \nu + \varepsilon \end{aligned}$$

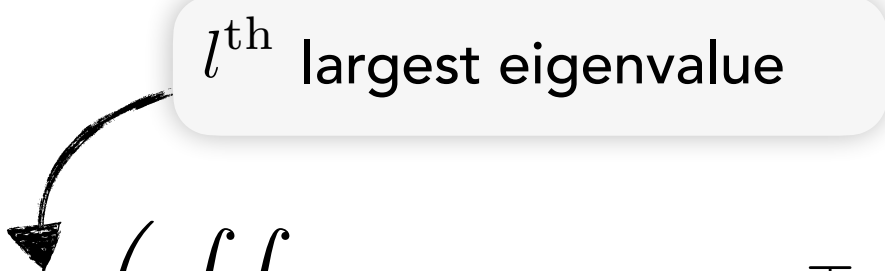
EXAMPLES: SUBSPACE ROBUST WASSERSTEIN

$$\mathcal{S}_k^2(\mu, \nu) = \min_{\pi \in \Pi(\mu, \nu)} \sum_{l=1}^k \lambda_l \left(\iint (\boldsymbol{x} - \boldsymbol{y})(\boldsymbol{x} - \boldsymbol{y})^\top d\pi(\boldsymbol{x}, \boldsymbol{y}) \right)$$

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l^{th} largest eigenvalue



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 &= \max_{\substack{0 \preceq \Omega \preceq I \\ \text{trace}(\Omega) = k}} \mathcal{I}_{d_\Omega^2}(\mu, \nu)
 \end{aligned}$$

l^{th} largest eigenvalue

EXAMPLES: SUBSPACE ROBUST WASSERSTEIN

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λ_l l^{th} largest eigenvalue

$$= \max_{\substack{0 \preceq \Omega \preceq I \\ \text{trace}(\Omega) = k}} \mathcal{T}_{d_\Omega^2}(\mu, \nu)$$

Where $d_\Omega^2(x, y) = (x - y)^\top \Omega (x - y)$ is the squared Mahalanobis distance

EXAMPLES: IN ECONOMICS

$$\sup_{\mathcal{C}} \mathcal{T}_{\mathcal{C}}(\mu, \nu) - \int \mathcal{C} d\pi_0 - R^*(\mathcal{C})$$

EXAMPLES: IN ECONOMICS

$$R^*(c) = \iota \left(\exists \Omega \succeq 0, \|\Omega\| \leq 1, c = d_\Omega^2 \right)$$

$$\sup_c \mathcal{T}_c(\mu, \nu) - \int c d\pi_0 - R^*(c)$$

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EXAMPLES: IN ECONOMICS

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Is the adversarial cost c_\star an interesting
dissimilarity measure on the ground space



A SMALL DETOUR: DUALITY

$$\min_{\pi \in \Pi(\mu, \nu)} f(\pi) = \max_{\underline{c}} \mathcal{T}_{\underline{c}}(\mu, \nu) - f^*(\underline{c})$$

A SMALL DETOUR: DUALITY

$$\begin{aligned}\min_{\pi \in \Pi(\mu, \nu)} f(\pi) &= \max_{\underline{c}} \mathcal{T}_{\underline{c}}(\mu, \nu) - f^*(\underline{c}) \\ &= \sup_{\underline{c}} \max_{\phi \oplus \psi \leq \underline{c}} \int \phi d\mu + \int \psi d\nu - f^*(\underline{c})\end{aligned}$$

A SMALL DETOUR: DUALITY

$$\begin{aligned}\min_{\pi \in \Pi(\mu, \nu)} f(\pi) &= \max_{\mathbf{c}} \mathcal{T}_{\mathbf{c}}(\mu, \nu) - f^*(\mathbf{c}) \\ &= \sup_{\mathbf{c}} \max_{\phi \oplus \psi \leq \mathbf{c}} \int \phi d\mu + \int \psi d\nu - f^*(\mathbf{c}) \\ &= \sup_{\mathbf{c}} \max_{\phi, \psi} \int \phi d\mu + \int \psi d\nu - f^*(\mathbf{c}) - \iota(\phi \oplus \psi \leq \mathbf{c})\end{aligned}$$

A SMALL DETOUR: DUALITY

$$\begin{aligned}
 \min_{\pi \in \Pi(\mu, \nu)} f(\pi) &= \max_{\mathbf{c}} \mathcal{T}_{\mathbf{c}}(\mu, \nu) - f^*(\mathbf{c}) \\
 &= \sup_{\mathbf{c}} \max_{\phi \oplus \psi \leq \mathbf{c}} \int \phi d\mu + \int \psi d\nu - f^*(\mathbf{c}) \\
 &= \sup_{\mathbf{c}} \max_{\phi, \psi} \int \phi d\mu + \int \psi d\nu - f^*(\mathbf{c}) - \iota(\phi \oplus \psi \leq \mathbf{c}) \\
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If e.g. f^* is increasing, $\inf_{\mathbf{c} \geq \phi \oplus \psi} f^*(\mathbf{c}) = f^*(\phi \oplus \psi)$ hence:

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If e.g. f^* is increasing, $\inf_{\mathbf{c} \geq \phi \oplus \psi} f^*(\mathbf{c}) = f^*(\phi \oplus \psi)$ hence:

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CHARACTERIZATION OF THE GROUND-COST

Duality

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CHARACTERIZATION OF THE GROUND-COST

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$$\begin{aligned} \min_{\pi \in \Pi(\mu, \nu)} f(\pi) &= \max_{\phi, \psi} \int \phi d\mu + \int \psi d\nu - f^*(\phi \oplus \psi) \\ &= \max_{\phi, \psi} \mathcal{T}_{\phi \oplus \psi}(\mu, \nu) - f^*(\phi \oplus \psi) \end{aligned}$$

CHARACTERIZATION OF THE GROUND-COST

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$$\begin{aligned} \min_{\pi \in \Pi(\mu, \nu)} f(\pi) &= \max_{\phi, \psi} \int \phi d\mu + \int \psi d\nu - f^*(\phi \oplus \psi) \\ &= \max_{\phi, \psi} \mathcal{T}_{\phi \oplus \psi}(\mu, \nu) - f^*(\phi \oplus \psi) \\ &\leq \max_{c} \mathcal{T}_c(\mu, \nu) - f^*(c) \end{aligned}$$

CHARACTERIZATION OF THE GROUND-COST

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$$\min_{\pi \in \Pi(\mu, \nu)} f(\pi) = \max_{\phi, \psi} \int \phi d\mu + \int \psi d\nu - f^*(\phi \oplus \psi)$$

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Main result

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Duality

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Main result

$$= \min_{\pi \in \Pi(\mu, \nu)} f(\pi)$$

CHARACTERIZATION OF THE GROUND-COST

Duality

$$\begin{aligned} \min_{\pi \in \Pi(\mu, \nu)} f(\pi) &= \max_{\phi, \psi} \int \phi d\mu + \int \psi d\nu - f^*(\phi \oplus \psi) \\ &= \max_{\phi, \psi} \mathcal{T}_{\phi \oplus \psi}(\mu, \nu) - f^*(\phi \oplus \psi) \\ &\leq \max_c \mathcal{T}_c(\mu, \nu) - f^*(c) \\ \text{Main result} \quad &= \min_{\pi \in \Pi(\mu, \nu)} f(\pi) \end{aligned}$$

So the inequality is an equality and there exists a separable cost function that is an optimal adversarial ground-cost

CHARACTERIZATION OF THE GROUND-COST

Is the adversarial cost c_* an interesting
dissimilarity measure on the ground space



Short answer: In a sense, no.

CHARACTERIZATION OF THE GROUND-COST

Is the adversarial cost c_\star an interesting dissimilarity measure on the ground space



Short answer: In a sense, no.

Theorem: Under some technical assumption on R (verified for the entropic or quadratic regularizations), there exists functions ϕ and ψ such that

$$c : (x, y) \mapsto \phi(x) + \psi(y)$$

is an optimal adversarial cost, i.e. is solution to

$$\sup_c \mathcal{J}_c(\mu, \nu) - \varepsilon R^* \left(\frac{c - c_0}{\varepsilon} \right)$$

WHAT I COULD NOT TALK ABOUT

- Restriction to nonnegative adversarial costs $\sup_{c \geq 0} \dots$
- Extension to several measures

Thank you

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