

Regularized Optimal Transport is Ground Cost Adversarial

MokaMeeting

May 11, 2022

FRANÇOIS-PIERRE PATY
francoispierrepaty.github.io

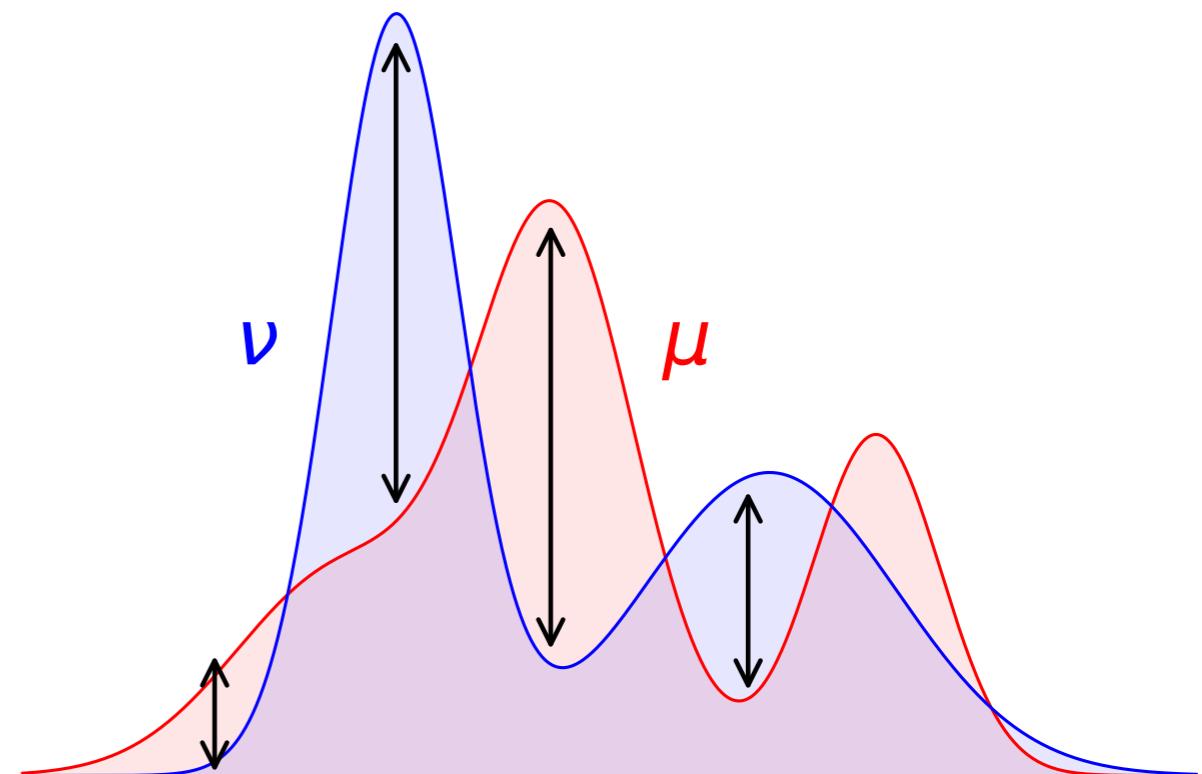
*Based on a joint work with **Marco Cuturi***

COMPARING DISTRIBUTIONS

1. Vertical comparison

Look at the difference, or
the ratio of the densities

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

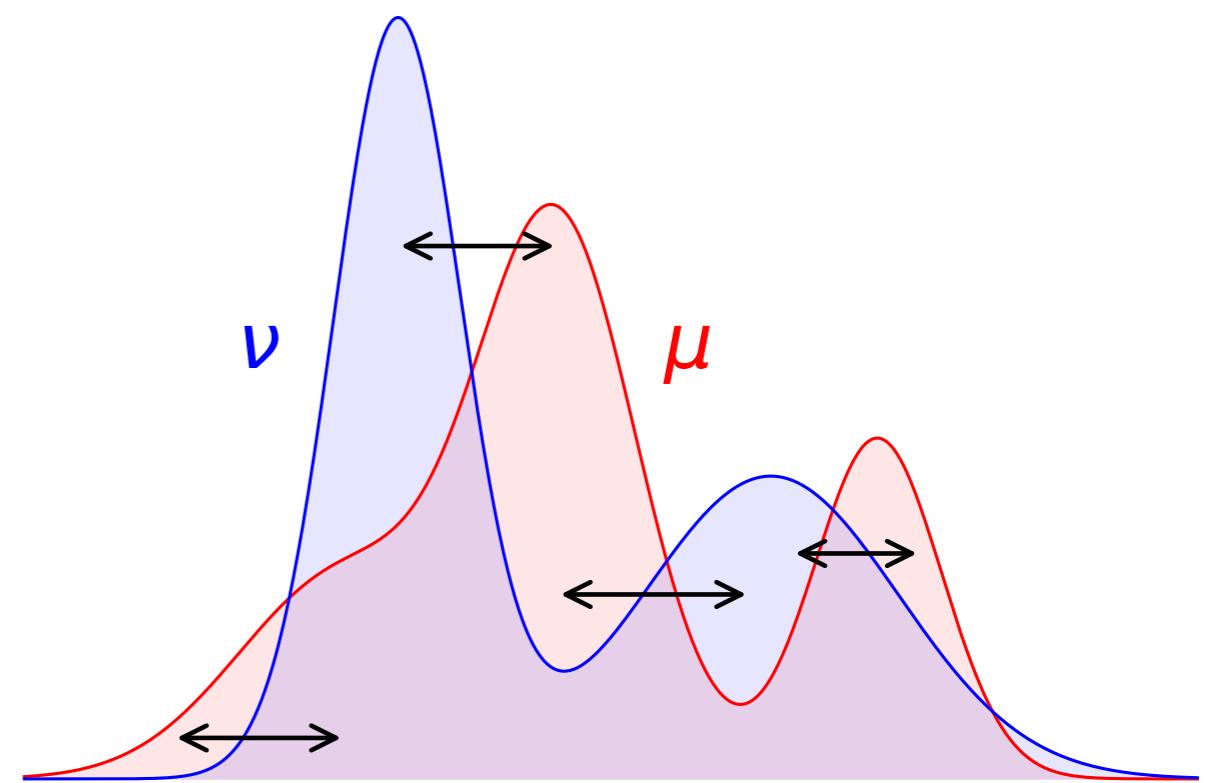


COMPARING DISTRIBUTIONS

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

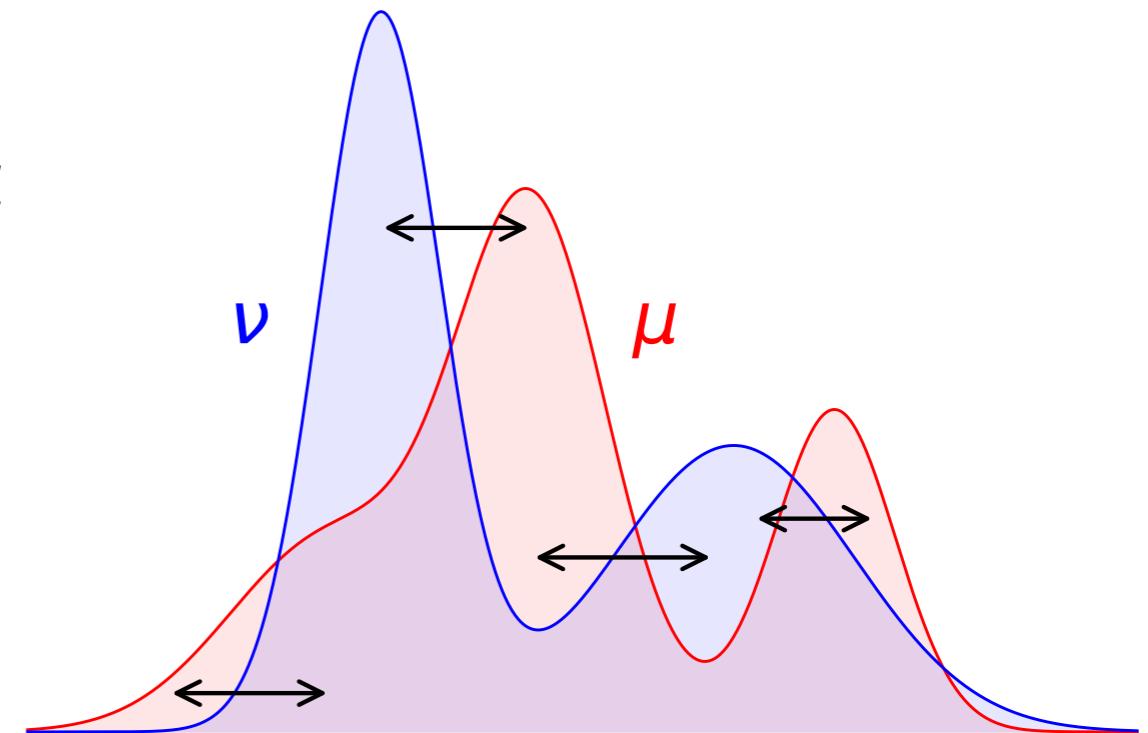
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Two distributions μ and ν over \mathbb{R}^d

Parameter:

A (continuous) cost function

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



OPTIMAL TRANSPORT

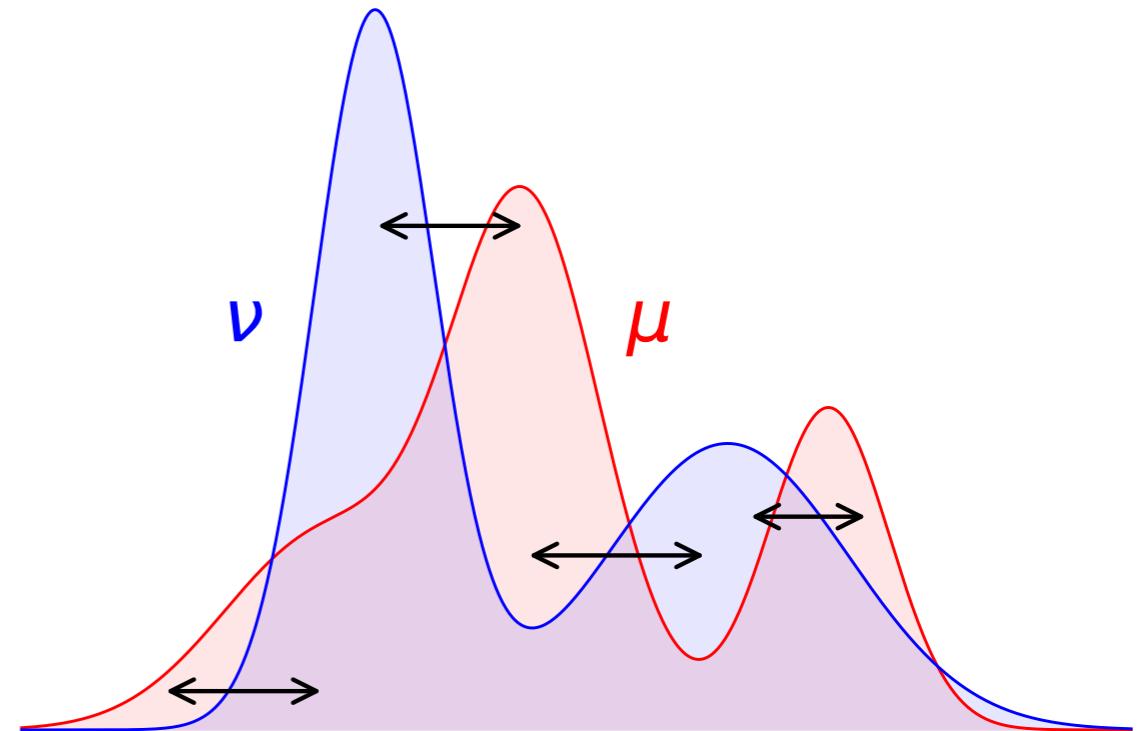
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Definition of Optimal Transport (OT):

OPTIMAL TRANSPORT

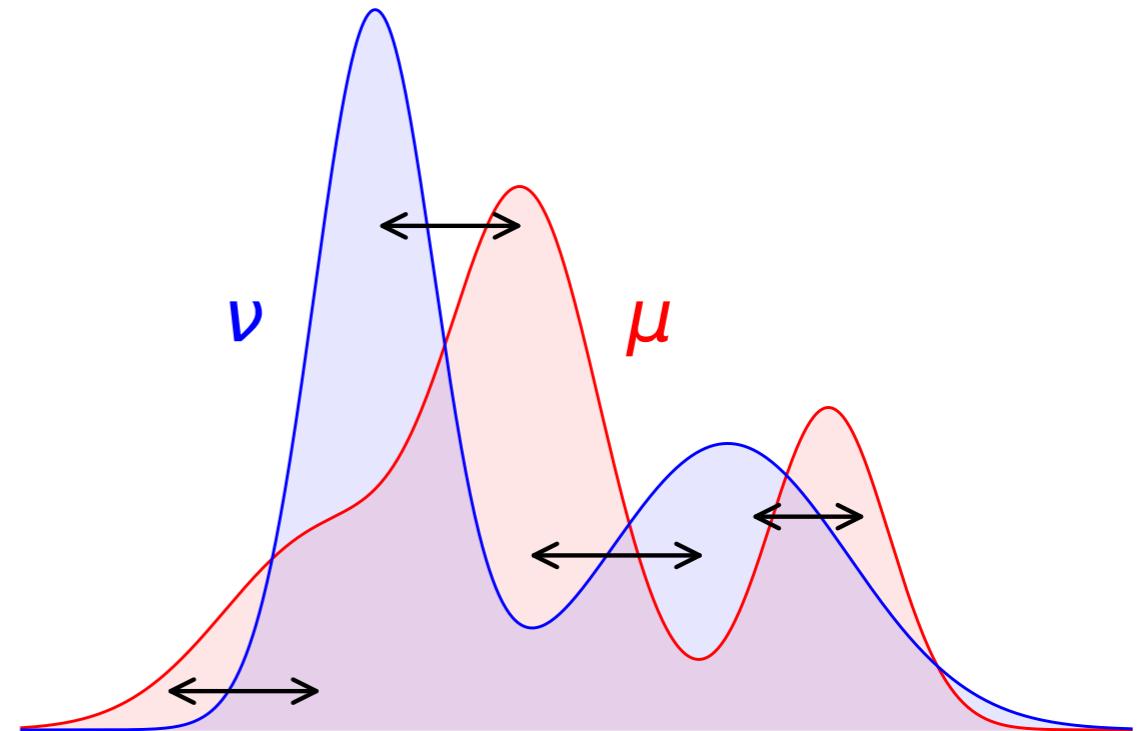
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$$c(\mathbf{x}, \mathbf{y}) d\pi(\mathbf{x}, \mathbf{y})$$

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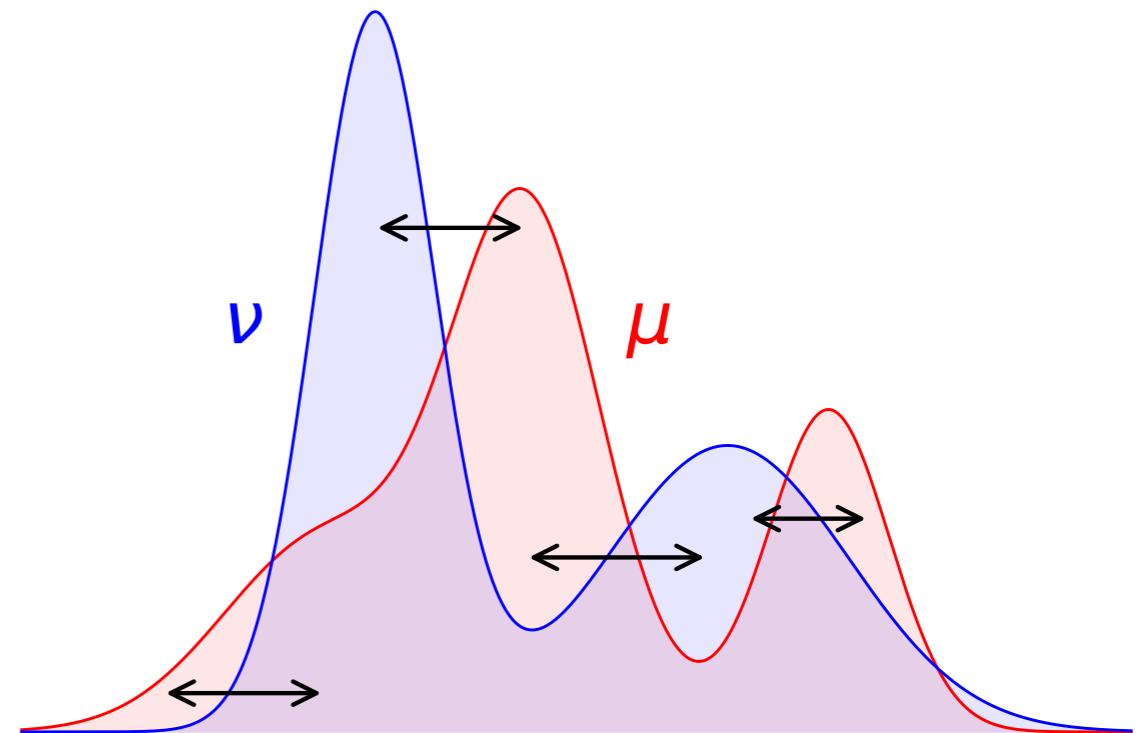
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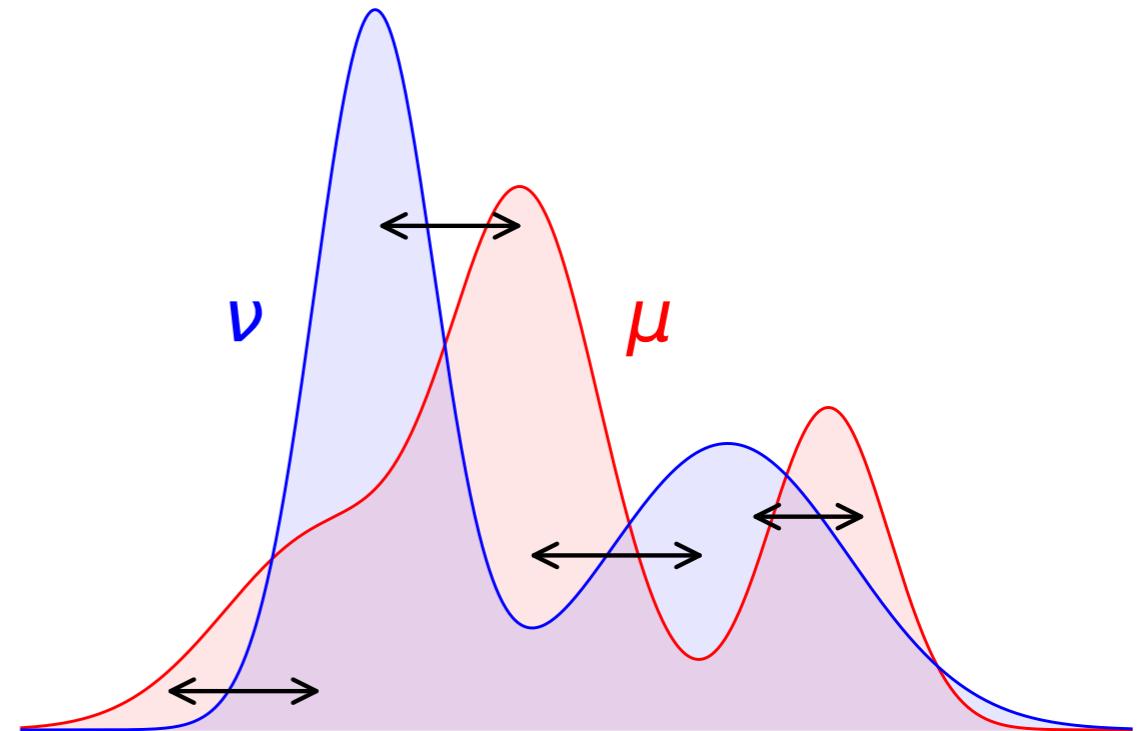
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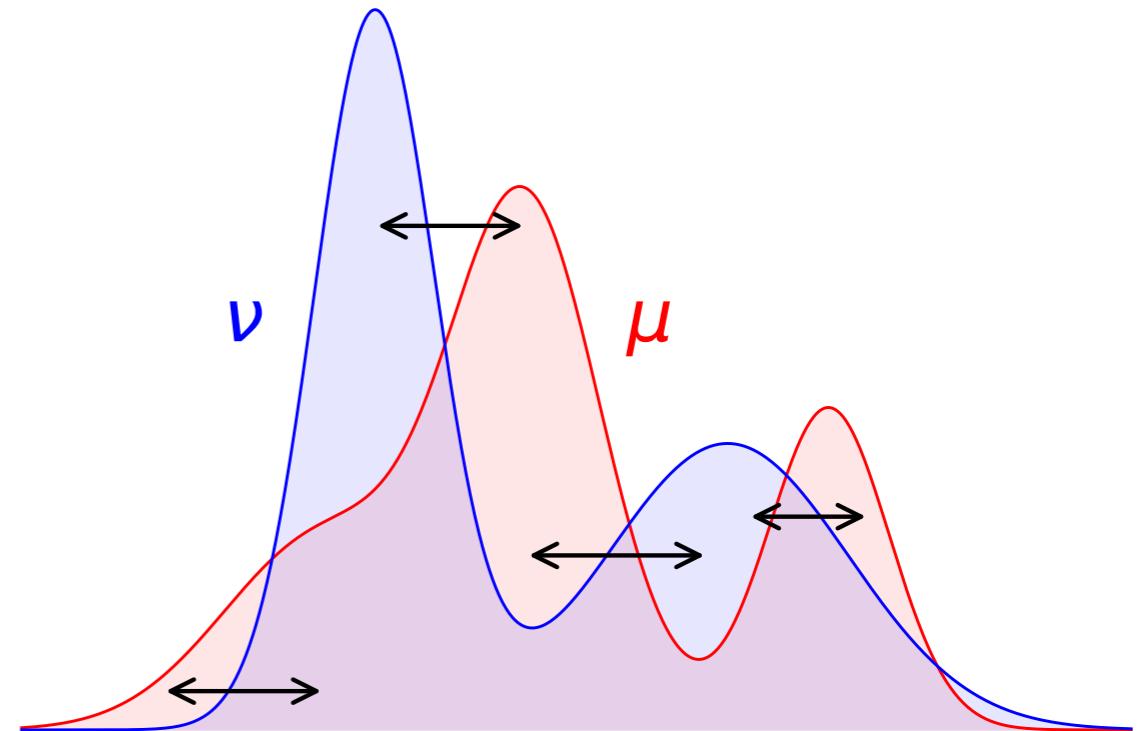
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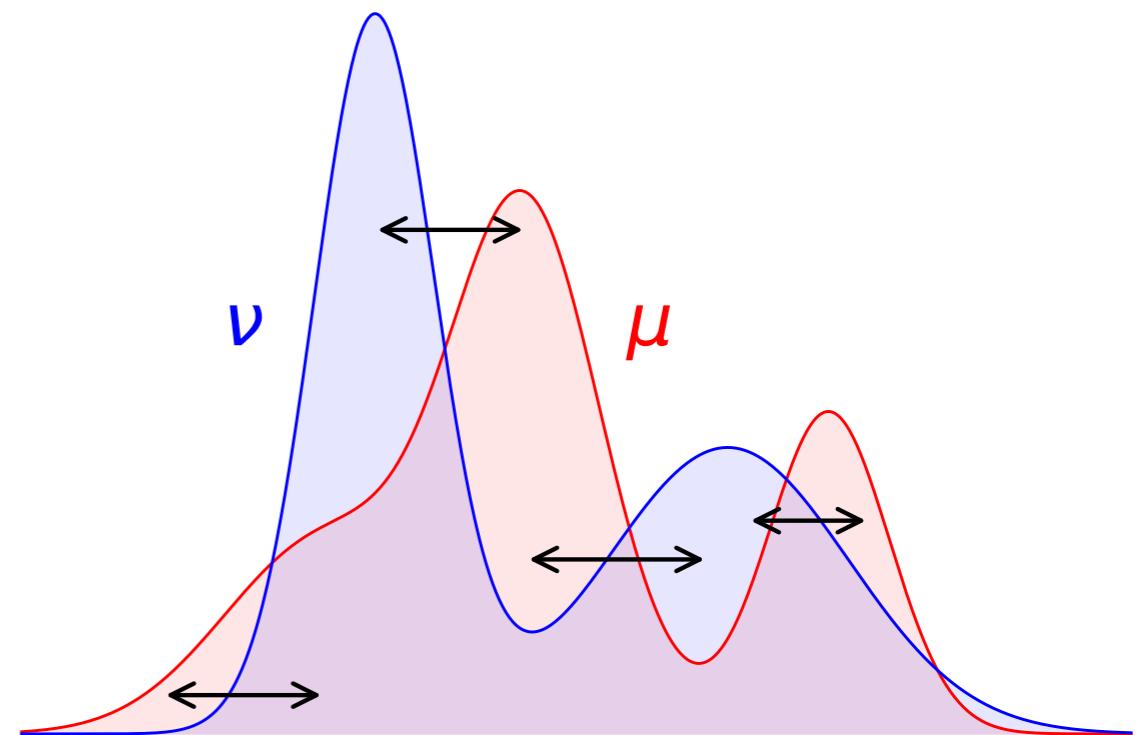
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over all π such that $\left\{ \begin{array}{l} \int d\pi(x, y) = d\mu(x) \quad \forall x \\ \int d\pi(x, y) = d\nu(y) \quad \forall y \end{array} \right.$

OPTIMAL TRANSPORT

Two main questions in practice

OPTIMAL TRANSPORT

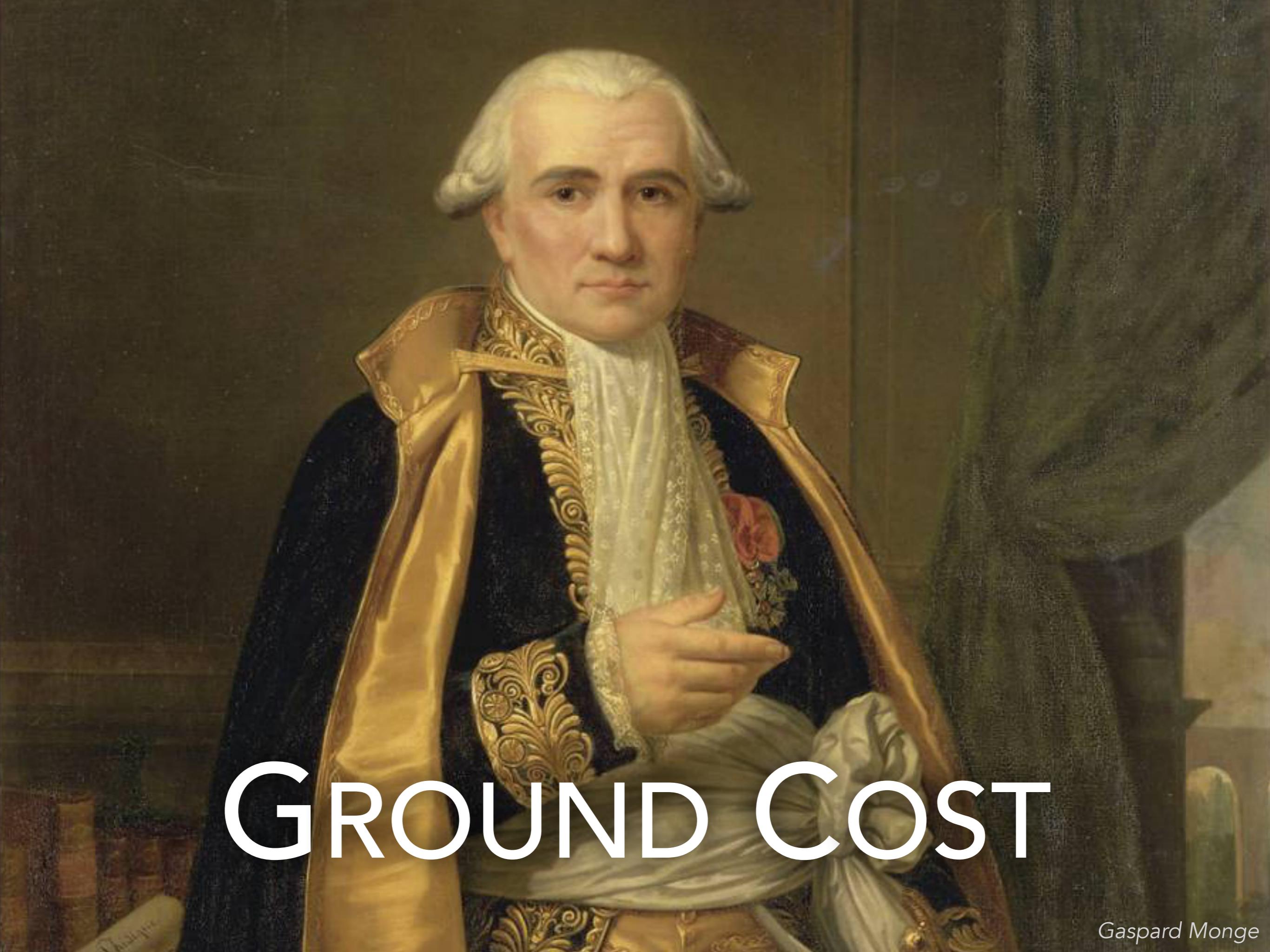
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OPTIMAL TRANSPORT

Two main questions in practice

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

A portrait painting of Gaspard Monge, a French mathematician and engineer. He is shown from the waist up, wearing a dark blue velvet jacket over a white cravat and a patterned waistcoat. His right hand rests on a large, open book or manuscript on a table in front of him. He has powdered white hair and is looking slightly to his left.

GROUND COST

Gaspard Monge

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$$c(x, y) = \|x - y\|^p \quad \text{where} \quad p \geq 1$$
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But does it make
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But does it make sense
when the data lives on a
low-dimensional manifold



GROUND COST

Idea: Find a ground cost \mathcal{C} that is adversarial, i.e. that best separates the two distributions by maximizing the OT cost

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

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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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$$\max_{\mathcal{C}} \mathcal{I}_{\mathcal{C}}(\mu, \nu) - f(\mathcal{C}) \quad \text{for some convex } f$$

- 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:

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

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

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

REGULARIZATION



Alessio Figalli

REGULARIZATION

2. How to compute/approximate the OT cost $\mathcal{I}_{\textcolor{green}{c}}(\mu, \nu)$?
1. This is a Linear Program $\rightarrow \mathcal{O}(n^3)$ complexity
2. Entropic regularization $\rightarrow \mathcal{O}(n^2)$ Sinkhorn algorithm, GPU-friendly, differentiable...

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

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



Cédric Villani

GROUND-COST ADVERSARIAL TRANSPORT

$$\max_{\textcolor{violet}{c}} \mathcal{T}_{\textcolor{violet}{c}}(\mu,\nu) - f(\textcolor{violet}{c})$$

GROUND-COST ADVERSARIAL TRANSPORT

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

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$$= \sup_{\mathbf{c}} \mathcal{T}_{\mathbf{c}}(\boldsymbol{\mu}, \boldsymbol{\nu}) - \varepsilon R^* \left(\frac{\mathbf{c} - \mathbf{c}_0}{\varepsilon} \right)$$

GROUND COST ROBUSTNESS \Leftrightarrow REGULARIZATION

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

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

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

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

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

EXAMPLES: SUBSPACE ROBUST WASSERSTEIN

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

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lth largest eigenvalue



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lth largest eigenvalue

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

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

EXAMPLES: IN ECONOMICS

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

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

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

EXAMPLES: IN ECONOMICS

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

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EXAMPLES: IN ECONOMICS

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

?

A SMALL DETOUR: DUALITY

$$\min_{\pi \in \Pi(\mu, \nu)} f(\pi) = \max_c \mathcal{I}_c(\mu, \nu) - f^*(c)$$

A SMALL DETOUR: DUALITY

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

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A SMALL DETOUR: DUALITY

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

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

A SMALL DETOUR: DUALITY

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

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

CHARACTERIZATION OF THE GROUND-COST

Duality

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

CHARACTERIZATION OF THE GROUND-COST

Duality

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

CHARACTERIZATION OF THE GROUND-COST

Duality

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

CHARACTERIZATION OF THE GROUND-COST

Duality

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

Main result



CHARACTERIZATION OF THE GROUND-COST

Duality

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

CHARACTERIZATION OF THE GROUND-COST

Duality

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

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_* 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

$$c : (\textcolor{red}{x}, \textcolor{blue}{y}) \mapsto \phi(\textcolor{red}{x}) + \psi(\textcolor{blue}{y})$$

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

$$\sup_{\textcolor{green}{c}} \mathcal{I}_{\textcolor{green}{c}}(\mu, \nu) - \varepsilon R^* \left(\frac{\textcolor{green}{c} - c_0}{\epsilon} \right)$$

WHAT I COULD NOT TALK ABOUT

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

Thank you

francoispierrepaly.github.io