A tutorial on optimal transport

Part 1: theory, models, properties

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What is optimal transport?

Setting: Probability measures $P(\mathcal{X})$ on a metric space $(\mathcal{X}, d)$.

Motive

Build a metric on $P(\mathcal{X})$ consistent with the geometry of $(\mathcal{X}, d)$.

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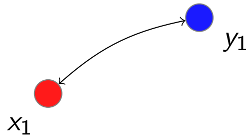

$W(\mu, \nu) = \ldots$

$$d(x_1, y_1)$$

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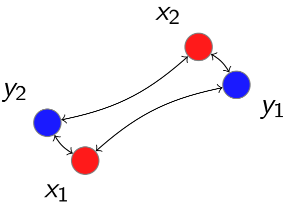

$$\mu = \frac{1}{N}\sum_{i=1}^{N} \delta_{x_i}, \quad \nu = \frac{1}{N}\sum_{j=1}^{N} \delta_{y_j}$$

$W(\mu, \nu) = \dots$

$$\frac{1}{N^2}\sum_{ij} d(x_i, y_j)?$$

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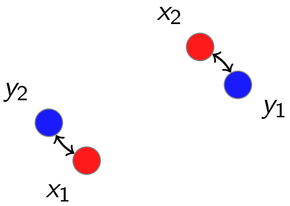

$$\mu = \frac{1}{N}\sum_{i=1}^{N} \delta_{x_i}, \quad \nu = \frac{1}{N}\sum_{j=1}^{N} \delta_{y_j}$$

$W(\mu, \nu) = \dots$

$$\min_{\sigma \in \mathfrak{S}_N} \frac{1}{N} \sum_i d(x_i, y_{\sigma(i)})?$$

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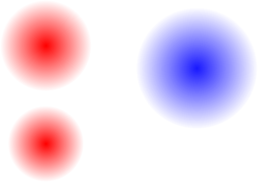
Build a metric on $P(\mathcal{X})$ consistent with the geometry of $(\mathcal{X}, d)$.

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



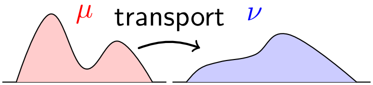
$W(\mu, \nu) = \dots$

?

Origin and ramifications

Monge Problem (1781)

Move dirt from one configuration to another with least effort



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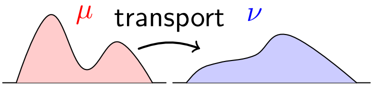
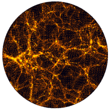


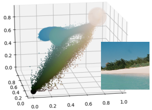
Strong modelization power:

Replace "dirt" by :

- probability distribution, empirical distribution
- weighted undistinguishable particles
- density of a gas, a species, a crowd, cells.

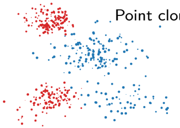
Early universe (Brenier *et al.* '08)





Color histograms (Delon *et al.*)

Crowd motion (Roudneff *et al.*, 12')



Point clouds

Aim of the tutorial

Convey that optimal transport ...
is a *rich* theory, useful as a *theoretical* and *practical* tool;

In part 1: theory

- essentials
- selection of properties and variants;

In part 2: practice

- numerical solvers, entropic regularization
- applications to imaging and machine learning

Outline

Outline

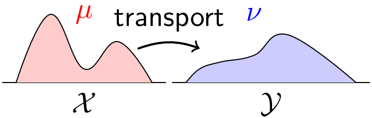
Optimal transport

Ingredients

- Two (complete, separable) metric spaces $\mathcal{X}$ and $\mathcal{Y}$
- Cost function $c : \mathcal{X} \times \mathcal{Y} \to \mathbb{R} \cup \{\infty\}$ (lower bounded, lsc)
- Two probability measures $\mu \in P(\mathcal{X})$ and $\nu \in P(\mathcal{Y})$

Definition (Optimal transport problem)

$$C(\mu, \nu) := \min_{\gamma \in M_+(\mathcal{X}\times\mathcal{Y})} \left\{ \int_{\mathcal{X}\times\mathcal{Y}} c(x,y) d\gamma(x,y) : \pi^x_\# \gamma = \mu, \ \pi^y_\# \gamma = \nu \right\}$$



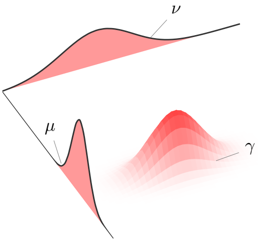
Probabilistic : $\min_{(X,Y)} \{\mathbb{E}[c(X,Y)] : X \sim \mu \text{ and } Y \sim \nu\}$

Couplings

Definition (Set of couplings)

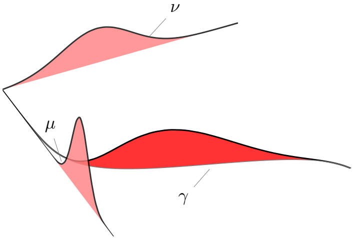
Positive measures on $\mathcal{X} \times \mathcal{Y}$ with specified marginals :

$$\Pi(\mu,\nu) := \left\{\gamma \in M_+(\mathcal{X}\times\mathcal{Y}) : \pi^x_\# \gamma = \mu,\ \pi^y_\# \gamma = \nu\right\}$$



Product coupling

$\gamma = \mu \otimes \nu$



Deterministic coupling

$\gamma = (Id \times T)_\# \mu$

Generalizes: permutations, discrete matchings

Properties: convex, weakly compact

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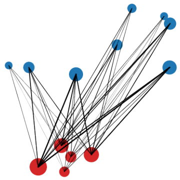

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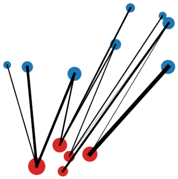

Cycle-free coupling

Generalizes: permutations, discrete matchings

Properties: convex, weakly compact

Duality

Theorem (Kantorovich duality)

$$\min_{\gamma \in M_+(\mathcal{X}\times\mathcal{Y})} \left\{ \int_{\mathcal{X}\times\mathcal{Y}} c(x,y) d\gamma(x,y) : \pi^x_\# \gamma = \mu,\ \pi^y_\# \gamma = \nu \right\} \qquad \text{(P)}$$

$$=$$

$$\max_{\substack{\phi \in L^1(\mu) \\ \psi \in L^1(\nu)}} \left\{ \int_{\mathcal{X}} \phi(x) d\mu(x) + \int_{\mathcal{Y}} \psi(y) d\nu(y) : \phi(x) + \psi(y) \leq c(x,y) \right\} \qquad \text{(D)}$$

Interpretation: (P) centralized planification, (D) externalized

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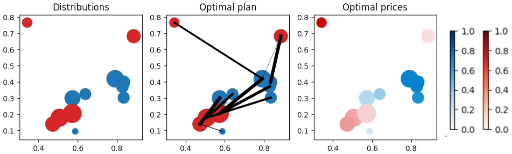


At optimality

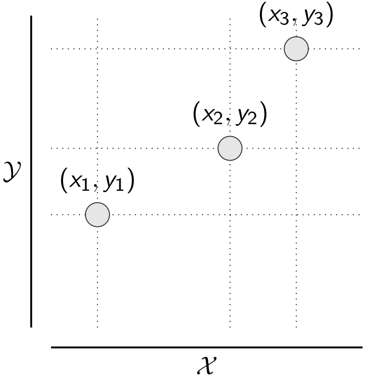
- $\phi(x) + \psi(y) = c(x,y)$ for γ almost every (x,y)
- γ is concentrated on a c-cyclically monotone set

Tools from convex analysis

Definition (Cyclical monotonicity)

$\Gamma \subset \mathcal{X} \times \mathcal{Y}$ is c-cyclical monotone iff for all $(x_i, y_i)_{i=1}^n \in \Gamma^n$

$$\sum_{i=1}^n c(x_i, y_i) \leq \sum_{i=1}^n c(x_i, y_{\sigma(i)}) \text{ for all permutation } \sigma \in \mathfrak{S}_n.$$



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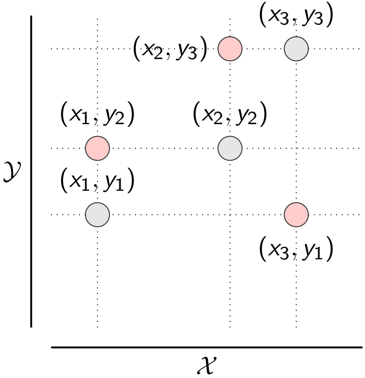


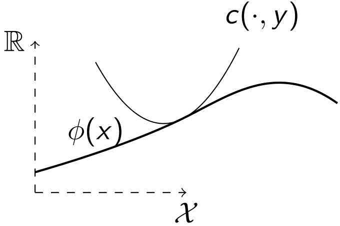
Tools from convex analysis

Definition (c-conjugacy)

For $\mathcal{X} = \mathcal{Y}$ and $c : \mathcal{X}^2 \to \mathbb{R}$ symmetric :

$$\phi^c(y) := \inf_{x \in \mathcal{X}} c(x, y) - \phi(x)$$

A function ϕ is *c-concave* iff there exists ψ such that $\phi = \psi^c$.



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- on $\mathbb{R}^n$, for $c(x,y) = x \cdot y$: ψ c-concave $\Leftrightarrow$ ψ concave;
- for all ϕ, $\phi^{ccc} = \phi^c$;
- consequence :

$$C(\mu,\nu) = \max_{\phi \text{ } c\text{-concave}} \left\{ \int_{\mathcal{X}} \phi(x) d\mu(x) + \int_{\mathcal{Y}} \phi^c(y) d\nu(y) \right\} \qquad \text{(D)}$$

Special cases

- real line
- distance cost
- quadratic cost

The real line

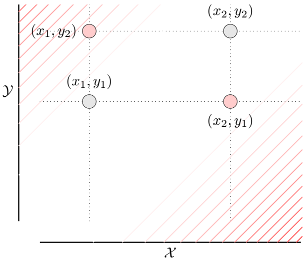
Theorem

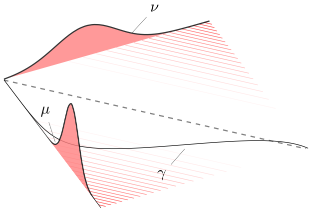
If $(\mu, \nu) \in P(\mathbb{R})^2$ and $c(x, y) = h(y - x)$ with h strictly convex

- unique optimal coupling γ^* : the *monotone rearrangement*
- denoting $F^{[-1]}$ the quantile functions:

$$C(\mu, \nu) = \int_0^1 h(F_\mu^{[-1]}(s) - F_\nu^{[-1]}(s))ds$$

Proof. Here, c-cyclically monotone $\Leftrightarrow$ increasing graph. $\square$



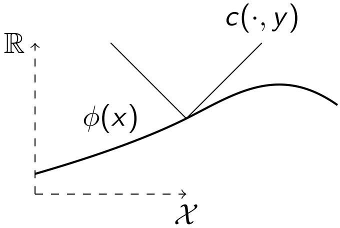


Distance cost

If $c(x,y) = d(x,y)$ with d distance

- ϕ c-concave $\Leftrightarrow$ ϕ 1-Lipschitz
- $\phi^c(y) = \inf_x d(x,y) - \phi(x) = -\phi(y)$
- consequence :

$$C(\mu,\nu) = \max_{\phi \text{ 1-Lipschitz}} \left\{ \int_{\mathcal{X}} \phi(x) d(\mu-\nu)(x) \right\} := \|\mu-\nu\|_K \qquad \text{(D)}$$



Quadratic cost

Context & reformulation

- $(\mu, \nu) \in P(\mathbb{R}^n)^2$ with finite moments of order 2
- cost $c(x, y) := \frac{1}{2}|y - x|^2$
- note that $c(x, y) = (|x|^2 + |y|^2)/2 - x \cdot y$, thus solve:

$$\max_{\gamma \in M_+(\mathcal{X}\times\mathcal{Y})} \left\{ \int_{\mathcal{X}\times\mathcal{Y}} (x \cdot y) d\gamma(x, y) : \gamma \in \Pi(\mu, \nu) \right\} \qquad \text{(P)}$$

Theorem (Brenier)

(i) At optimality, $\operatorname{supp}\gamma \subset \partial\phi$*, where* $\phi : \mathbb{R}^n \to \mathbb{R}$ *convexe.*
(ii) If μ *has a density,* $T = \nabla\phi$ *is the unique optimal map.*

Proof. (i) $\phi(x) + \phi^*(y) = x \cdot y$, γ-a.e (ii) $\nabla\phi$ defined $\mathcal{L}$-a.e.

Transport of covariance

Case of a quadratic dual potential ϕ

Theorem (Affine transport map)

Let $c(x, y) = \frac{1}{2}|y - x|^2$ on $\mathbb{R}^n$ and let $A, B \in S^n_+$. It holds

$$\min_{\substack{\mathrm{cov}(\mu)=A \\ \mathrm{cov}(\nu)=B}} C(\mu, \nu) = d_b(A, B)^2$$

where d_b is the Bures (geodesic) metric on S^n_+.

- $d_b(A, B)^2 = \operatorname{tr} A + \operatorname{tr} B - 2 \operatorname{tr}(A^{\frac{1}{2}} B A^{\frac{1}{2}})^{\frac{1}{2}}$
- Transport map $T = A^{-1} \# B$ ($\cdot\#\cdot$ geometric mean).
- see, e.g. (Bhatia et al. '17)

Wasserstein distance

Theorem

Let $d : \mathcal{X} \times \mathcal{X} \to \mathbb{R}$ be a metric. The function

$$W_2(\mu,\nu) := \left\{ \min_{\gamma \in M_+(\mathcal{X}^2)} \int_{X^2} d(x,y)^2 d\gamma(x,y) : \gamma \in \Pi(\mu,\nu) \right\}^{\frac{1}{2}}$$

defines a metric on $P(\mathcal{X})$.

- W_2 metrizes weak convergence + 2-nd order moments;
- if $(\mathcal{X}, d)$ is a geodesic space, so is $(P(\mathcal{X}), W_2)$.

Figure: A constant speed geodesic for W_2 on $P(\mathbb{R}^2)$

Geodesics in $\mathbb{R}^n$

Consider μ, ν probability measures on $\mathbb{R}^n$.

Variational characterization of geodesics (Benamou-Brenier)

$$W_2^2(\mu,\nu) = \min_{(\rho_t, v_t)_{t\in[0,1]}} \int_0^1 \left(\int_{\mathbb{R}^n} |v_t(x)|^2 d\rho_t(x) \right) dt$$
$$\text{s.t. } \partial_t \rho_t = -\mathrm{div}\,(\rho_t v_t)$$
$$\text{and } (\rho_0, \rho_1) = (\mu, \nu)$$

Consequences

- minimizers are geodesics;
- convex in variables $(\rho, v\rho)$;
- W_2 is similar to a Riemannian metric.

Summing up

Properties of OT

- rich duality, with concepts from convex analysis
- real line, distance cost, quadratic cost

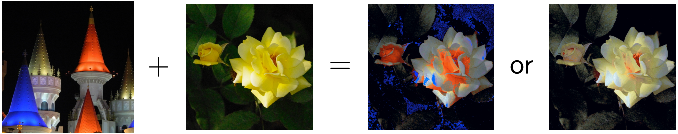
Properties of the distance W_2 on $\mathbb{R}^n$

- optimal plans supported on $\partial\phi$ with $\phi : \mathbb{R}^n \to \mathbb{R}$ convex;
- the space $(P(\mathbb{R}^n), W_2)$ is a complete geodesic space;
- some explicit cases (real line, linear maps).

Outline

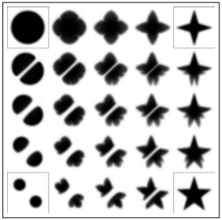
Histogram & shapes processing

Color transfer



color + target = OT or unbalanced OT

Barycenters



(Benamou et al'15)

and much more

- PCA (Seguy, Cuturi'15)
- regression (Bonneel et al'16)

Wasserstein gradient flows

Objective: characterize certain evolution EDP as *gradient flows* of some functional $F : P(\mathbb{R}^n) \to \mathbb{R}$ in the Wasserstein space:

$$\partial_t \mu_t + \mathrm{div}(\mu_t v_t) = 0 \quad \text{with} \quad v_t = \nabla F'(\mu_t).$$

Interest

- theoretical: existence, uniqueness, convergence...
- numerical: intrinsic mass conservation and positivity

Crowd motions
(Roudneff-Chupin et al.'14)

Statistical learning

- *W_p loss for regression* (Frogner et al.'15):
  Learn predictor $f_\theta : X \to Y := P(\{1, \dots, k\})$

$$\min_{\theta \in \mathbb{R}^d} \mathbb{E}_{(X,Y)\sim\mu} \left[W_2^2(f_\theta(X), Y) \right].$$

- *W_p loss for generative models*:
  Given $\mu \in P(\mathcal{X})$, $\nu \in P(\mathcal{Y})$, learn map $f_\theta : X \to Y$

$$\min_{\theta \in \mathbb{R}^d} W_2^2((f_\theta)_\# \mu, \nu)$$

- Barycenters for multiscale learning (Srivastava et al'17), transfer learning (Courty et al'17), convergence of Langevin MC (Dalalyan'17)...

And much more...

- *applied analysis* :
  incompressible flows (Euler), sticky particules
- *metric geometry* :
  Ricci curvature, perimetric inequalities
- *mathematical physics* :
  density functional theory, Schröedinger bridge
- *mathematical economy* :
  matching problems, principal agent, MFG, finance (martingale transport)...

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Recurring needs :

- differential properties
- unbalanced OT

Outline

Vertical perturbations

Reminder

Optimal transport between $\mu, \nu \in P(\mathbb{R}^n)$ with cost c:

$$C(\mu,\nu) = \sup_{(\varphi,\psi) \text{ admissible}} \int_{\mathbb{R}^n} \varphi \, d\mu + \int_{\mathbb{R}^n} \psi \, d\nu$$

Vertical perturbations

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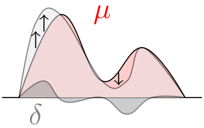

Perturbed marginal: $\mu + \epsilon\delta$

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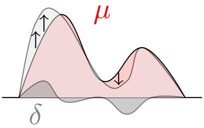

Perturbed marginal: $\mu + \epsilon\delta$

Vertical perturbation

Let δ a signed measure with $\int \delta = 0$. If optimal φ unique,

$$\frac{d}{d\epsilon} C(\mu + \epsilon\delta, \nu)|_{\epsilon=0} = \int_{\mathbb{R}^n} \varphi \, d\delta$$

If φ nonunique (up to a constant) $\Rightarrow$ subdifferential.

Horizontal perturbations

Reminder

Optimal transport between $\mu, \nu \in P(\mathbb{R}^n)$ with cost c:

$$C(\mu,\nu) = \inf_{\gamma \text{ admissible}} \int_{(\mathbb{R}^n)^2} c(x,y)\, d\gamma(x,y)$$

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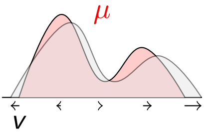

Perturbed cost: $c(x+\epsilon v(x), y) \approx c(x,y) + \epsilon \nabla_x c(x,y) \cdot v(x)$

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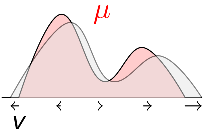

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Horizontal perturbation

Let $v : \mathbb{R}^n \to \mathbb{R}^n$ a velocity field. If optimal γ unique,

$$\frac{d}{d\epsilon} C((\mathrm{id} + \epsilon v)_{\#}\mu, \nu)|_{\epsilon=0} = \int_{(\mathbb{R}^n)^2} \nabla_x c(x,y) \cdot v(x) d\gamma(x).$$

Corresponds to the vertical perturbation $\partial_\epsilon \mu = -\mathrm{div}(v\mu)$

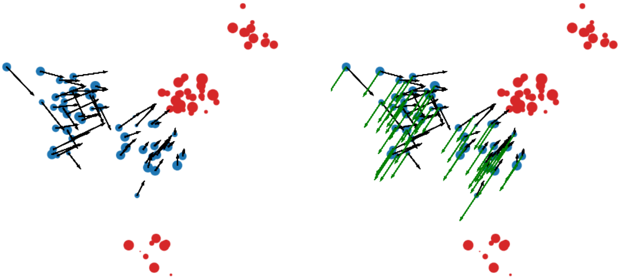
Special case of W_2

Setting: quadratic cost on $\mathbb{R}^n$, $v : \mathbb{R}^n \to \mathbb{R}^n$ velocity field.

Differentiability of W_2

If unique optimal transport plan γ, then

$$\frac{d}{d\epsilon} W_2^2((\mathrm{id} + \epsilon v)_{\#}\mu, \nu)|_{\epsilon=0} = \int_{(\mathbb{R}^n)^2} 2(y-x)\cdot v(x)d\gamma(x,y)$$



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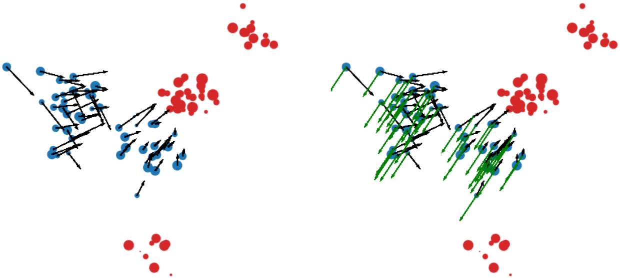

Next talk: regularized W_2, always differentiable.

Euclidean Gradient

Goal: defining the gradient though metric quantities only.

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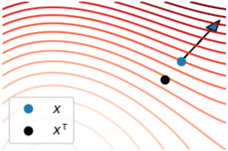
Proximal operator

Let $F : \mathbb{R}^n \to \mathbb{R}$ a (semiconvex) function. The proximal operator assigns to each $x \in \mathbb{R}^n$

$$x^\tau := \arg\min_{y \in \mathbb{R}^n} \frac{|x-y|^2}{2\tau} + F(y)$$

Definition (Euclidean gradient)

$$\mathrm{grad} F(x) := \lim_{\tau \to 0} (x - x^\tau)/\tau \in \mathbb{R}^n$$



Wasserstein Gradient

Proximal map: let $F : P(\mathbb{R}^n) \to \mathbb{R}$ a functional, $\mu \in P^{ac}(\mathbb{R}^n)$.

$$\mu^\tau = \arg \min_{\nu \in P(\mathbb{R}^n)} \frac{W_2^2(\mu, \nu)}{2\tau} + F(\nu)$$

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Fondamental exemple: with $F(\mu) = \int \mu \log(d\mu/d\mathscr{L})$, one has

$$\mathrm{grad}\, F(\mu) = \Delta\mu.$$

Outline

Unbalanced OT

OT comes with an intrisic constraint:

$$\mu(\mathcal{X}) = \nu(\mathcal{Y})$$

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- normalization is generally a poor choice
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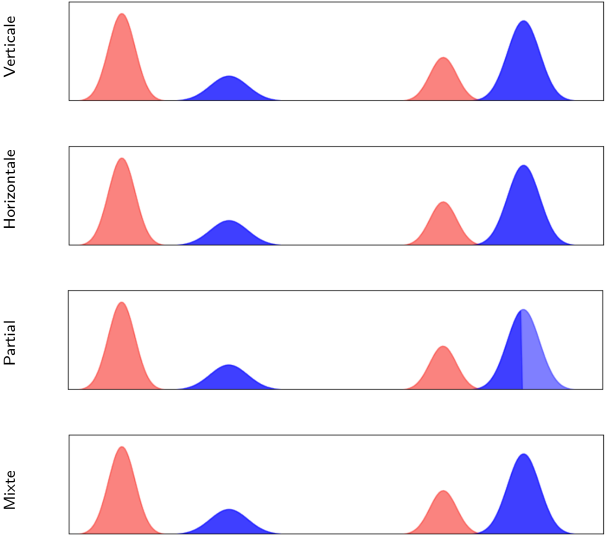
Strategy

- preserve key properties of optimal transport
- combine two geometries:
  horizontal (transport) and *vertical* (linear)

Vertical/Horizontal



Optimal partial transport

Setting: $\mu \in M_+(\mathcal{X})$ and $\nu \in M_+(\mathcal{Y})$ nonnegative measures.

Variational problem

Choose $0 < m \leq \min\{\mu(\mathbb{R}^n), \nu(\mathbb{R}^n)\}$ and solve

$$\min_{\gamma} \int c(x,y) d\gamma(x,y)$$

$$\text{subject to} \quad \pi^x_\# \gamma \leq \mu$$

$$\pi^y_\# \gamma \leq \nu$$

$$\gamma(\mathbb{R}^n \times \mathbb{R}^n) = m$$

- simple modification of the OT problem
- "equivalent" formulations: dynamic, entropy-transport
- alternatively, add a sink/source reachable at a certain cost

Wasserstein Fisher-Rao

Setting: $\mu \in M_+(\mathcal{X})$ and $\nu \in M_+(\mathcal{Y})$ nonnegative measures.

Definition

The natural generalization of W_2 to this setting is

$$\widehat{W}_2^2(\mu,\nu) = \min_{\gamma \in M_+(\mathcal{X}\times\mathcal{Y})} KL(\pi^x_\# \gamma|\mu) + KL(\pi^y_\# \gamma|\nu) + \int c_\ell(x,y) d\gamma(x,y)$$

where $c_\ell(x,y) = -\log\cos^2(\min\{|y-x|, \pi/2\})$.

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Main properties

- geodesic space, Riemannian-like structure
- growth and displacement intertwined
- various explicit formulations: lifted problem, dynamic problem with velocity and *rate of growth*...

References: (Liero et al'15), (Monsaingeon et al'15), (Chizat et al'15), my PhD thesis.

End of part 1

In part 1: theory

- essentials
- selection of properties and variants;

In part 2: practice

- numerical solvers, entropic regularization
- applications to imaging and machine learning

Reference textbooks

- Santambrogio, *OT for applied mathematicians*
- Villani, *OT, Old and New*
- Ambrosio, Gigli, Savaré, *Gradient flows in metric spaces and in the space of probability measures*
- Peyré and Cuturi, *Computational OT* (upcoming)