Tutorial on Optimal Transport Theory

With a machine learning touch

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A Geometric Motivation

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

Goal

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

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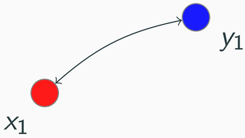
$$\mu = \delta_{x_1}, \qquad \nu = \delta_{y_1}$$



Distance between μ and ν...

$$\text{dist}(x_1, y_1)$$

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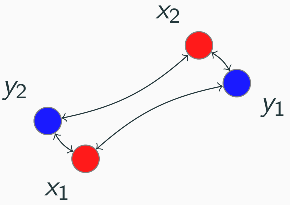

$$\mu = \frac{1}{n}\sum_{i=1}^{n} \delta_{x_i}, \quad \nu = \frac{1}{n}\sum_{j=1}^{n} \delta_{y_j}$$

Distance between μ and ν...

$$\frac{1}{n^2}\sum_{ij} \text{dist}(x_i, y_j)?$$

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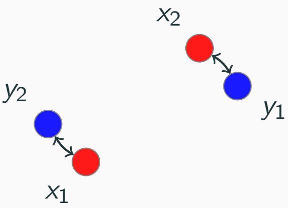

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Distance between μ and ν...

$$\min_{\sigma \text{ perm.}} \frac{1}{n}\sum_{i} \text{dist}(x_i, y_{\sigma(i)})?$$

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

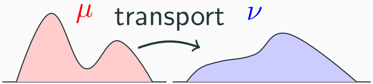
Distance between μ and ν...

?

Origin and Ramifications

Monge Problem (1781)

Move dirt from one configuration to another with least effort



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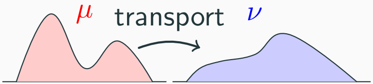
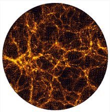
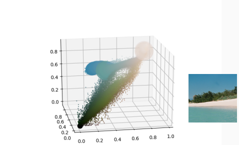


Strong modelization power:

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

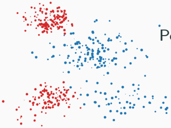
Early universe
(Brenier *et al.* '08)





Color histograms (Delon *et al.*)

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



Point clouds

Part 1: Qualitative Overview

- **classical theory**
- **selection of properties and variants**

Part 2: Algorithms and Approximations

- **entropic regularization**
- **computational aspects**
- **statistical aspects**

Outline

Outline

Main Theoretical Facts

A Glimpse of Applications

Unbalanced Optimal Transport

Differentiability

Computation and Approximation

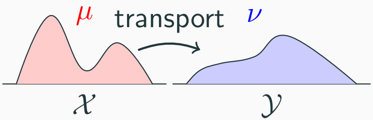
Density Fitting

Losses between Probability Measures

Definition

Ingredients

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



Transport map

Definition (pushforward)

Let $T : \mathcal{X} \to \mathcal{Y}$ be a map. The *pushforward measure* of μ by T is characterized by

$$T_{\#}\mu(B) = \mu(T^{-1}(B)) \quad \text{for all } B \subset \mathcal{Y}.$$

If X is a random variable such that $\mathrm{Law}(X) = \mu$, then

$$\mathrm{Law}(T(X)) = T_{\#}\mu.$$

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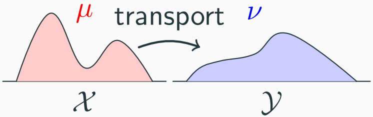


Definition (Monge problem)

$$\inf_{T:\mathcal{X}\to\mathcal{Y}} \left\{ \int_{\mathcal{X}} c(x, T(x))\mathrm{d}\mu(x) \; ; \; T_{\#}\mu = \nu \right\}$$

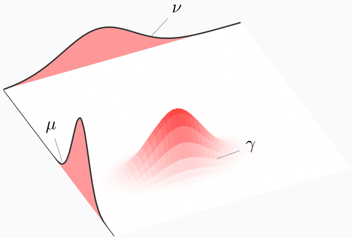
$\rightsquigarrow$ in some cases: no solution, no feasible point...

Transport Plans

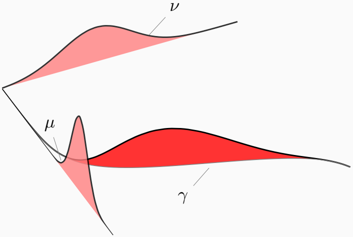
Definition (Set of transport plans)

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

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



Product coupling
$\gamma = \mu \otimes \nu$



Deterministic coupling
$\gamma = (\mathrm{Id} \times T)_\# \mu$

- Generalizes permutations, bistochastic matrices, matchings
- convex, weakly compact

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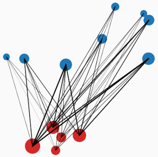

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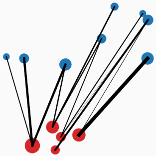

Cycle-free coupling

- Generalizes permutations, bistochastic matrices, matchings
- convex, weakly compact

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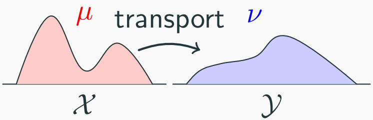
Definition (Optimal transport problem)

$$C(\mu, \nu) := \min_{\gamma \in \Pi(\mu,\nu)} \int_{\mathcal{X} \times \mathcal{Y}} c(x, y) d\gamma(x, y)$$



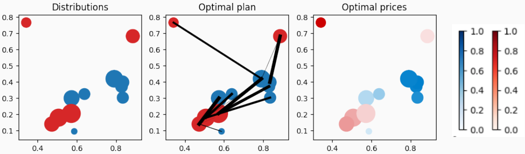
Probabilistic view: $\min_{(X,Y)} \{\mathbb{E}[c(X, Y)] : X \sim \mu \text{ and } Y \sim \nu\}$

Duality

Theorem (Kantorovich duality)

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

Economy: (Primal) centralized vs. (Dual) externalized planification



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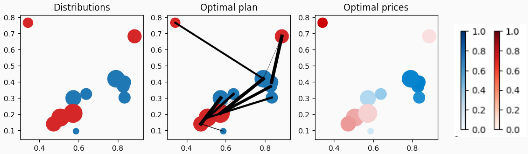


At optimality

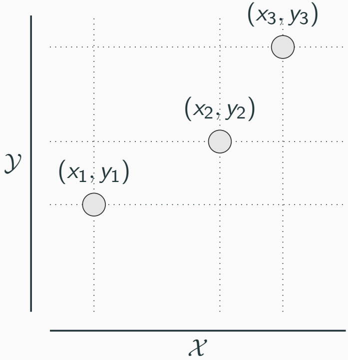
- $\phi(x)+\psi(y) = c(x,y)$ for γ almost every (x,y)
- γ is concentrated on a "c-cyclically monotone" set

Generalizing Convex Analysis Tools (I)

Definition (Cyclical monotonicity)

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

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



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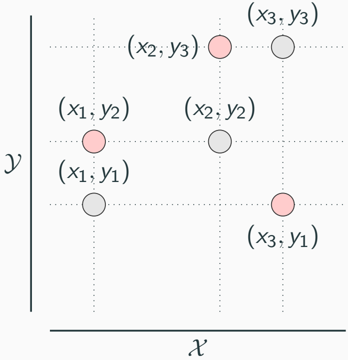


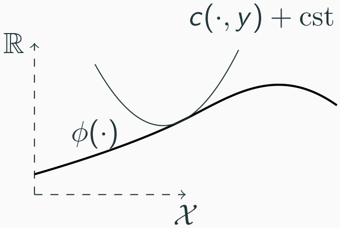
Generalizing Convex Analysis Tools (II)

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

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

Special Cases

- real line ($\mathcal{X} = \mathcal{Y} = \mathbb{R}$)
- distance cost ($c = \text{dist}$)
- quadratic cost ($c = \| \cdot - \cdot \|^2$)

Real Line

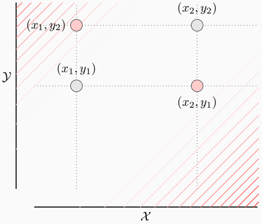
Theorem (Monotone Rearrangement)

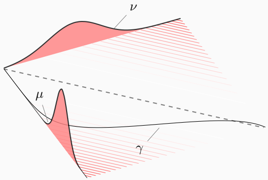
If $\mu, \nu \in \mathcal{P}(\mathbb{R})$ and $c(x, y) = h(y - x)$ with h strictly convex:

- unique optimal transport plan γ^*
- 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. □



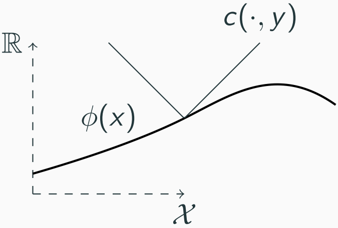


Distance Cost

If $\mathcal{X} = \mathcal{Y}$ and $c(x, y) = \text{dist}(x, y)$

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

$$C(\mu, \nu) = \max_{\phi \text{ 1-Lipschitz}} \left\{ \int_{\mathcal{X}} \phi(x) d(\mu - \nu)(x) \right\} \tag{Dual}$$



Quadratic Cost

Reformulation

- $\mu, \nu \in \mathcal{P}(\mathbb{R}^d)$ 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:

$$\max_{\gamma \in \mathcal{M}_+(\mathcal{X} \times \mathcal{Y})} \left\{ \int_{\mathcal{X} \times \mathcal{Y}} \langle x, y \rangle d\gamma(x, y) : \gamma \in \Pi(\mu, \nu) \right\} \qquad \text{(Primal)}$$

Theorem (Brenier '87)

(i) At optimality, $\operatorname{spt} \gamma \subset \partial \phi$, *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

Whenever the dual potential ϕ is quadratic: transport of covariance

Theorem (Affine transport map)

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

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

- $\mathrm{dist}_b(A, B)^2 = \mathrm{tr}\, A + \mathrm{tr}\, B - 2\,\mathrm{tr}(A^{\frac{1}{2}} B A^{\frac{1}{2}})^{\frac{1}{2}}$ Bures metric on S_+^d
- Transport map $T = A^{-1} \# B$ ($\cdot\#\cdot$ geometric mean).

[Refs]:

Bhatia, Jain, Lim (2017). *On the Bures-Wasserstein distance between positive definite matrices*

Wasserstein distance

Definition

Let $\text{dist} : \mathcal{X} \times \mathcal{X} \to \mathbb{R}$ be a metric. The Wasserstein distance is

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

- W_2 metrizes weak convergence + 2-nd order moments
- if $(\mathcal{X}, \text{dist})$ is a geodesic space, so is $(\mathcal{P}(\mathcal{X}), W_2)$
- similar definition for W_p with $p \geq 1$

Constant speed geodesic for W_2 on $\mathcal{P}(\mathbb{R})$

$$((1-t)\mathrm{Id} + tT)_{\#}\mu$$

Summing up

First Properties

- rich duality with concepts from convex analysis
- rich structure in specific cases

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

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

Outline

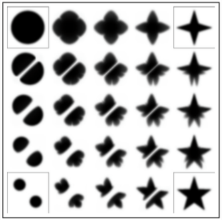
Histogram & shapes processing

Color transfer

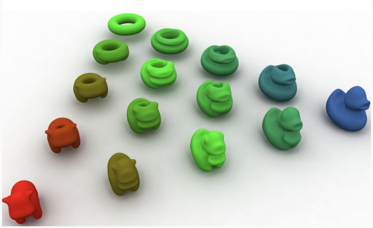
 +  =  or 

color | target | OT | unbalanced OT

Barycenters



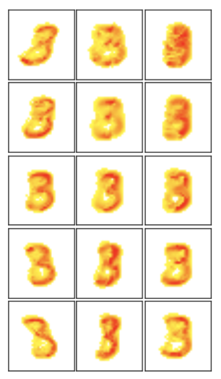
(Benamou et al. '15)



(Solomon et al. '15)

Histograms and shape processing

- compute barycenter $\bar{\mu}$ of a family $(\mu_k)_k$
- transport maps from $\bar{\mu}$ gives a Hilbertian parameterization
- apply your favorite data analysis method!



Three PCs from the MNIST dataset (Seguy and Cuturi, 2015)

[Refs]:
Seguy, Cuturi (2015). *Principal Geodesic Analysis for Probability Measures [...].*
Wang, Slepcev, Basu, Ozolek, Rohde (2012). *A linear optimal transportation framework.*

Loss for regression:

Learn predictor $f_\theta : \mathcal{X} \to \mathcal{Y} := \mathcal{P}(\{1, \dots, k\})$

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

(a) **Flickr user tags**: zoo, run, mark; **our proposals**: running, summer, fun; **baseline proposals**: running, country, lake.

(b) **Flickr user tags**: travel, architecture, tourism; **our proposals**: sky, roof, building; **baseline proposals**: art, sky, beach.

(c) **Flickr user tags**: spring, race, training; **our proposals**: road, bike, trail; **baseline proposals**: dog, surf, bike.

Predict probability over tags from an image (Frogner et al. 2015)

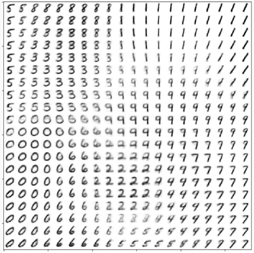
[Refs]:
Frogner, Zhang, Mobahi, Araya, Poggio (2015). *Learning with a Wasserstein loss.*

Machine learning

Loss for density fitting:
Given $\mu \in \mathcal{P}(\mathcal{X})$, $\nu \in \mathcal{P}(\mathcal{Y})$,
learn map $f_\theta : \mathcal{X} \to \mathcal{Y}$

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

$\Rightarrow$ more in part II.



Generating figure from MNIST (Genevay et al. 2018)

[Refs]:
Genevay, Peyré, Cuturi (2017). *Learning Generative Models with Sinkhorn Divergences.*

Often needed

- differentiability properties
- unbalanced optimal transport

Outline

Unbalanced OT

Optimal Transport has an intrinsic constraint:

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

What if $\mu(\mathcal{X}) \neq \nu(\mathcal{Y})$?

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Unbalanced Optimal Transport

- often comes up in applications
- normalization is generally a poor choice
- are there approaches that stand out?

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Optimal Transport has an intrinsic constraint:

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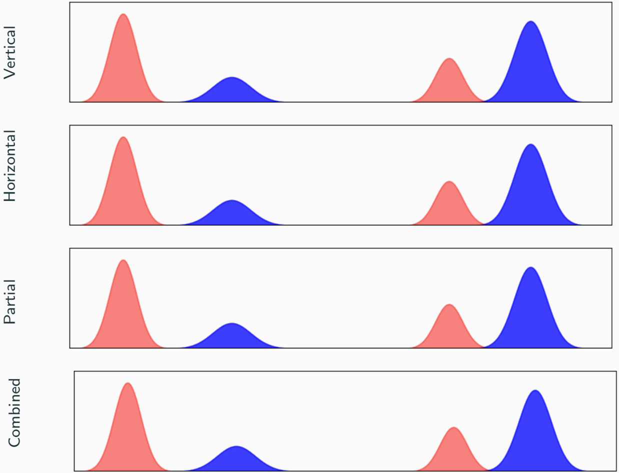
Strategy

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

Vertical/Horizontal



Optimal Partial Transport

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

Variational Problem

Choose $0 < m \leq \min\{\mu(\mathcal{X}), \nu(\mathcal{Y})\}$ and solve

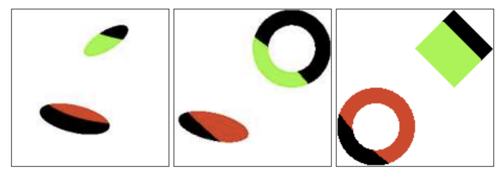
$$\min_{\gamma \in \mathcal{M}_+(\mathbb{R}^{2d})} \int c(x,y) d\gamma(x,y)$$

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

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

$$\gamma(\mathcal{X} \times \mathcal{Y}) = m$$

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



Optimal partial transport in 2D (Benamou et al. 2015)

[Refs]:
Benamou, Carlier, Cuturi, Nenna, Peyré (2015) *Iterative Bregman Projections for Regularized Transportation Problems*

Wasserstein Fisher-Rao a.k.a. Hellinger-Kantorovich

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

Definition

The natural generalization of W_2 to this setting is

$$\widehat{W_2^2}(\mu, \nu) = \min_{\gamma \in \mathcal{M}_+(\mathcal{X} \times \mathcal{Y})} \mathrm{KL}(\pi^x_\# \gamma | \mu) + \mathrm{KL}(\pi^y_\# \gamma | \nu) + \int c_\ell(x, y) d\gamma(x, y)$$

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

where KL is the Kullback-Leibler divergence, defined if $\mu_1 \ll \mu_2$ as

$$\mathrm{KL}(\mu_1 | \mu_2) = \int \log\left(\frac{d\mu_1}{d\mu_2}\right) \mathrm{d}\mu_1 - \mu_1(\mathcal{X}) + \mu_2(\mathcal{X})$$

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

Main properties

- geodesic space, Riemannian-like structure
- growth and displacement intertwined
- various explicit formulations: lifted problem, dynamic problem

[Refs]:
Liero, Mielke, Savaré (2015). *Optimal Entropy-Transport Problems and a New Hellinger–Kantorovich Distance [...]*
Kondratyev, Monsaingeon, Vorotnikov (2015). *A New Optimal Transport Distance on the Space of [...] Measures.*
Chizat, Peyré, Schmitzer, Vialard (2015). *An Interpolating Distance between Optimal Transport and Fisher-Rao.*

Outline

Vertical Perturbations

Reminder

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

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

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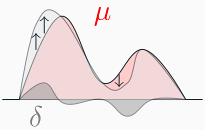

Perturbed marginal: $\mu + \epsilon\delta$

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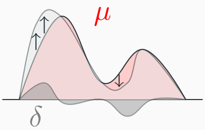

Perturbed marginal: $\mu + \epsilon\delta$

Vertical (linear) derivative

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

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

Horizontal Perturbations

Reminder

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

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

Horizontal Perturbations

Reminder

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

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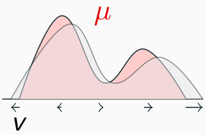

Perturbed cost: $c(x + \epsilon v(x), y) \approx c(x, y) + \epsilon \nabla_x c(x, y) \cdot v(x)$

Horizontal Perturbations

Reminder

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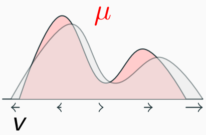


Perturbed cost: $c(x+\epsilon v(x), y) \approx c(x,y) + \epsilon \nabla_x c(x,y) \cdot v(x)$

Horizontal (Wasserstein) perturbation

Let $v : \mathbb{R}^d \to \mathbb{R}^d$ a curl free map. If optimal γ unique,

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

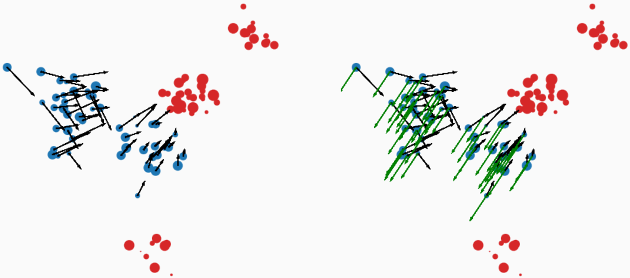
Special case of W_2

Setting: quadratic cost on $\mathbb{R}^d$, $v : \mathbb{R}^d \to \mathbb{R}^d$ a curl free map.

Differentiability of W_2

If unique optimal transport plan γ, then

$$\frac{d}{d\epsilon}\frac{1}{2}W_2^2((\mathrm{id}+\epsilon v)_{\#}\mu,\nu)|_{\epsilon=0} = \int_{(\mathbb{R}^d)^2}(x-y)\cdot v(x)d\gamma(x,y)$$



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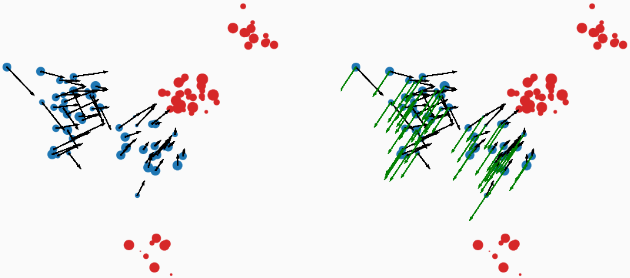


Next section: regularized W_2, always differentiable.

Outline

Main Theoretical Facts

A Glimpse of Applications

Unbalanced Optimal Transport

Differentiability

Computation and Approximation

Density Fitting

Losses between Probability Measures

Discrete Optimal Transport

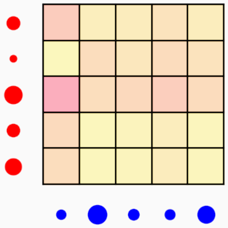
Discrete Setting

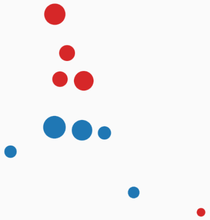
- Discrete measures $\mu = \sum_{i=1}^{n} p_i \delta_{x_i}$, $\nu = \sum_{j=1}^{n} q_j \delta_{y_i}$.
- Cost matrix $C_{i,j} = c(x_i, y_j)$

Linear Program

$$\min_{\gamma \in \mathcal{S}(p,q)} \sum_{i,j} C_{i,j} \gamma_{i,j}$$

where $\mathcal{S}(p,q) = \{\gamma \in \mathbb{R}_+^{n \times m} \; ; \; p_i = \sum_j \gamma_{i,j} \text{ and } q_j = \sum_i \gamma_{i,j}\}$.





Discrete Optimal Transport

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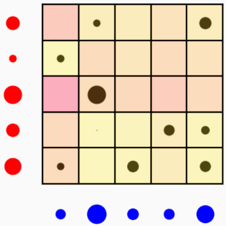
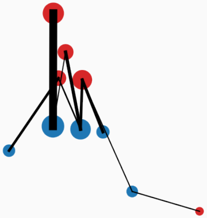


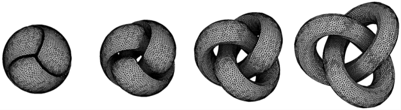


Exact solvers

Algorithm	Setting	Complexity
Network simplex	–	$\tilde{O}(n^3)$
Hungarian	bistochastic	$O(n^3)$
Auction	$C_{i,j}$ integers	$O(n^3)$

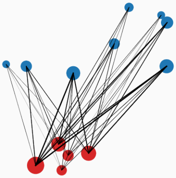
Efficient methods in $\mathbb{R}^2$ or $\mathbb{R}^3$

- semi-discrete solver based on Laguerre cells
- minimizing Benamou-Brenier functional (finite elements)
- resolution of Monge-Ampère equation (finite elements)

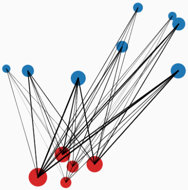


(Levy, 15')

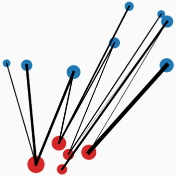
Approximate Solver



Product coupling

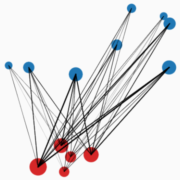


$0 < \beta^{-1} < \infty$

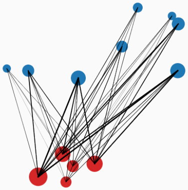


Optimal coupling

Approximate Solver



Product coupling



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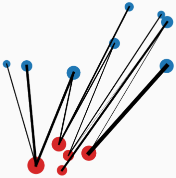
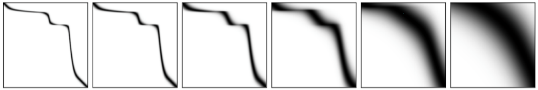


Optimal coupling

Entropic regularization (Cuturi '13)

$$\min_{\gamma \in \mathcal{S}(p,q)} \sum_{i,j} C_{i,j}\gamma_{i,j} + \beta^{-1}\,\mathrm{KL}(\gamma, \mu \otimes \nu)$$

where $\mathrm{KL}(a, b) = \sum_i a_i(\log(a_i/b_i) - 1)$.



Optimal transport plan as β decreases (Nenna et al. '15)

Sinkhorn's algorithm

Proposition (Optimality Condition)

Define the kernel $K_{i,j} = \exp(-\beta \cdot C_{i,j})$. There exists $a, b \in \mathbb{R}_+^n$ such that at optimality:

$$\gamma^*_{i,j} = a_i K_{i,j} b_j$$

Sinkhorn's algorithm

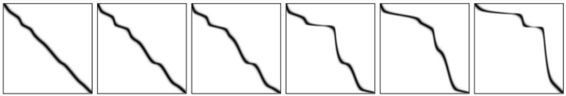
Proposition (Optimality Condition)

Define the kernel $K_{i,j} = \exp(-\beta \cdot C_{i,j})$. There exists $a, b \in \mathbb{R}^n_+$ such that at optimality:

$$\gamma^*_{i,j} = a_i K_{i,j} b_j$$

Sinkhorn's Algorithm

1. initialize $b = (1, \dots, 1)$ and repeat until convergence
   1.1 $a \leftarrow p \oslash (Kb)$ **[rescale rows]**
   1.2 $b \leftarrow q \oslash (K^T a)$ **[rescale columns]**
2. return $\gamma^*_{i,j} = a_i K_{i,j} b_j$.



Evolution of $(a_i K_{i,j} b_j)_{i,j}$, in (Benamou et al. 2015)

Complexity Results

One iteration

- matrix/vector product in $O(n^2)$ (sometimes better)
- highly parallelizable on GPUs

Solving entropy-regularized OT

- Linear convergence of a, b in *Hilbert metric*
- ϵ-accurate solution in $O(n^2 \log(1/\epsilon))$
- stochastic algorithms (see later), accelerations

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- matrix/vector product in $O(n^2)$ (sometimes better)
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Solving entropy-regularized OT

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- ϵ-accurate solution in $O(n^2 \log(1/\epsilon))$
- stochastic algorithms (see later), accelerations

Solving OT

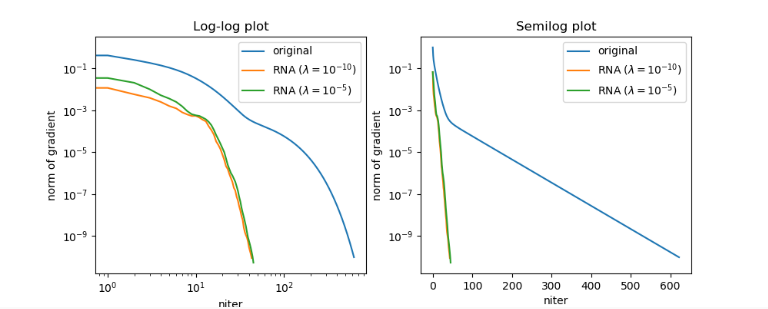
- Sinkhorn's algorithm allows to build an ϵ-accurate feasible transport plan in $\tilde{O}(n^2/\epsilon^2)$
- best bound in $\tilde{O}(n^2/\epsilon)$ (active research)

[Refs (see ref therein)]:
Lin, Ho, Jordan (2019). *On Efficient Optimal Transport [...]*
Dvurechensky, Gasnikov, Kroshnin (2018). *Computational Optimal Transport [...]*
Blanchet, Jambulapati, Kent, Sidford (2018). *Towards Optimal Running Times for Optimal Transport*

Fast In Practice

Overrelaxation and Nonlinear Acceleration

- average/extrapolate the iterates, possibly adaptively
- typical fixed-point algorithms accelerations
- preserves the iteration complexity and parallelizable

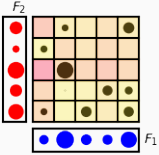


[Refs]:
Scieur, D'Aspremont, Bach (2016). *Regularized Nonlinear Acceleration*
Thibault, Chizat, Dossal, Papadakis (2017). *Overrelaxed Sinkhorn Algorithm for Regularized Optimal Transport*

Generalization

Solving barycenters, unbalanced OT, inverse problems...

$$\min \sum C_{i,j}\gamma_{i,j} + F_1(\gamma \cdot 1_n) + F_2(\gamma^T \cdot 1_n) + \beta^{-1}\,\mathrm{KL}(\gamma, \mu \otimes \nu)$$



Scaling iterates (alternate maximization on the dual)

1. initialize $b = 1_n$ and repeat until convergence
   1.1 $a \leftarrow \mathrm{prox}_{F_1}(Kb) \oslash (Kb)$ **[descent on rows]**
   1.2 $b \leftarrow \mathrm{prox}_{F_2}(K^T a) \oslash (K^T a)$ **[descent on columns]**
2. return $\gamma^*_{i,j} = a_i K_{i,j} b_j$.

$$\mathrm{prox}_F(\bar{s}) := \arg\min_s \{F(s) + \epsilon\,\mathrm{KL}(s|\bar{s})\}$$

[Refs]:
Chizat, Peyré, Schmitzer, Vialard (2016). *Scaling algorithms for unbalanced optimal transport problems*

Outline

Density Fitting

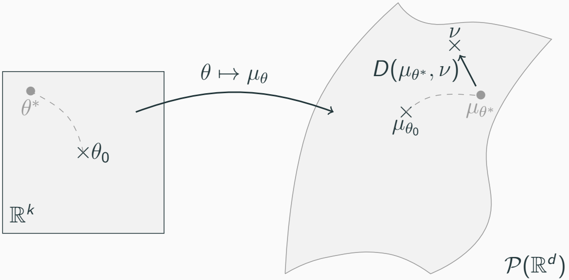
Ingredients

- a parametric family $\theta \in \mathbb{R}^k \to \mu_\theta \in \mathcal{P}(\mathbb{R}^d)$
- a target $\nu \in \mathcal{P}(\mathbb{R}^d)$

General problem

Chose a loss $D : \mathcal{P}(\mathbb{R}^d)^2 \to [0, \infty]$ and solve

$$\min_{\theta \in \mathbb{R}^k} D(\mu_\theta, \nu).$$



Examples (I)

Statistical inference

- μ_θ is an exponential family
- ν is known through samples $\hat{\nu} = \frac{1}{n}\sum_{i=1}^n \delta_{x_i}$

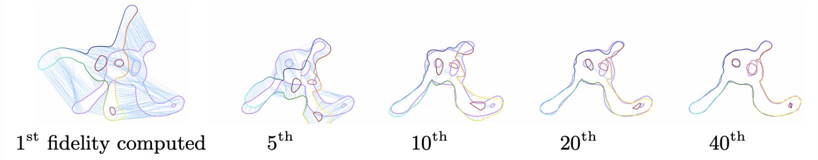
Choosing $D = \mathrm{KL}$ gives the maximum likelihood estimator:

$$\min_{\theta\in\mathbb{R}^k} \mathrm{KL}(\nu|\mu_\theta) \rightsquigarrow \min_{\theta\in\mathbb{R}^k} \mathbb{E}_{x\sim\nu}\left[-\log\left(\frac{\mathrm{d}\mu_\theta}{\mathrm{d}\mathcal{L}}(x)\right)\right]$$
$$\rightsquigarrow \max_{\theta\in\mathbb{R}^k} \frac{1}{n}\sum_{i=1}^n \log\left(\frac{\mathrm{d}\mu_\theta}{\mathrm{d}\mathcal{L}}(x_i)\right)$$

Examples (II)

Shapes matching

- μ_θ is $(f_\theta)_\# \mu$ where f_θ is a smooth deformation of $\mathbb{R}^d$ and μ a reference shape
- ν is a target shape
- goal : find a smooth deformation f_{θ^*} from μ to ν



(Feydy et al. '17)

[Refs]:

Feydy, Charlier, Vialard, Peyré (2017). *Optimal Transport for Diffeomorphic Registration*

Examples (III)

Generative modeling

- μ_θ is $(f_\theta)_\# \mu$ where f_θ is a neural network and μ is a simple distribution (Gaussian) on a low dimensional space
- ν is a target distribution observed through samples
- goal : generate new samples from ν using $f_\theta(X)$, $X \sim \mu$

Random bedrooms (Arjovsky et al. '14)

[Refs]:
Arjovsky, Chintala, Bottou (2014). *Wasserstein GAN*
Genevay, Peyré, Cuturi (2017). *Learning Generative Models with Sinkhorn Divergences*

Properties Needed

Gradient-based minimization

Choose step-size η, start from $\theta^{(0)}$ and (ideally) define

$$\theta^{(k+1)} = \theta^{(k)} - \eta \nabla_\theta [D(\mu_{\theta^{(k)}}, \nu)].$$

Requires

- differentiability
- low computational complexity
- low sample complexity
- to incorporate geometry

Outline

Classes of losses

- φ-divergence (includes KL, Hellinger, TV,...)
- integral probability metrics (includes MMD, W_1)
- Sinkhorn divergences
- Wasserstein loss

φ-divergences

Definition

Let $\varphi : \mathbb{R}_+ \to \mathbb{R}_+$ be a convex function with $\varphi(1) = 0$ and superlinear (to simplify):

$$D_\varphi(\mu, \nu) = \begin{cases} \int_{\mathbb{R}^d} \varphi\left(\frac{\mathrm{d}\mu}{\mathrm{d}\nu}(x)\right) \mathrm{d}\nu(x) & \text{if } \mu \ll \nu \\ +\infty & \text{otherwise} \end{cases}$$

- pointwise comparison of the density (no geometry)
- recovers KL when $\varphi(s) = s \log(s)$
- computational cost $O(n)$ (on a discrete space)
- estimation: depends on the class of density considered

Integral Probability Metrics

Definition

Let $\mathcal{F}$ a subset of functions $\mathbb{R}^d \to \mathbb{R}$ that contains 0 and define

$$D_{\mathcal{F}}(\mu,\nu) = \sup_{f\in\mathcal{F}} \int_{\mathbb{R}^d} f(x)\mathrm{d}(\mu-\nu)(x)$$

It $\mathcal{F}$ is the set of 1-Lipschitz functions then $D_{\mathcal{F}} = W_1$.

Maximum Mean Discrepancy

Let $\mathcal{F}$ be the 1-ball of a RKHS $\mathcal{H}$ with kernel k, then

$$D_{\mathcal{F}}(\mu,\nu) = \|\mu-\nu\|_k^2 \quad \text{where} \quad \|\mu\|_k^2 := \iint k(x,y)\mathrm{d}\mu(x)\otimes\mathrm{d}\mu(y)$$

- computational cost $O(n^2)$
- sample complexity : accuracy in $O(1/n)$

[Refs]:
Sriperumbudur et al.(2012). *On the Empirical Estimation of Integral Probability Metrics.*

Optimal Transport

We know the definition...

$$C(\mu, \nu) = \min_{\gamma \in \Pi(\mu,\nu)} \int c \mathrm{d}\gamma$$

- "a lot" of geometry
- computational cost: $O(n^3)$ or $O(n^2/\epsilon^2)$

Sample Complexity

- $|\mathbb{E}[W_2^2(\hat{\mu}_n, \hat{\nu}_n) - W_2^2(\mu, \nu)|] = O(n^{-2/d})$ for $d > 4$
- there exists better estimators if the density is assumed smooth

[Refs]:
Weed, Bach (2017). *Sharp asymptotic and finite-sample rates of convergence of empirical measures in Wasserstein distance*
Weed, Berthet (2019). *Estimation of smooth densities in Wasserstein distance.*

Sinkhorn divergence

$$C_\beta(\mu,\nu) = \min_{\gamma\in\Pi(\mu,\nu)} \int c\mathrm{d}\gamma + \beta^{-1}\,\mathrm{KL}(\gamma|\mu\otimes\nu)$$

Definition

$$D_\beta(\mu,\nu)^2 := 2C_\beta(\mu,\nu) - C_\beta(\mu,\mu) - C_\beta(\nu,\nu)$$

Properties

- converges to $C(\mu,\nu)$ as $\beta\to\infty$
- converges to $\|\mu-\nu\|^2_{-c}$ as $\beta\to 0$
- it is positive definite if $e^{-\beta c}$ is a positive definite kernel

[Refs]:
Feydy, Séjourné, Vialard, Amari, Trouvé, Peyré (2018). *Interpolating between Optimal Transport and MMD using Sinkhorn Divergences*
Ramdas, Trillos, Cuturi, (2017). *On Wasserstein two-sample testing and related families of nonparametric tests.*

Sinkhorn divergence (II)

Proposition (sample complexity)

$$\mathbb{E}[|D_\beta(\mu,\nu) - D_\beta(\hat{\mu}_n, \hat{\nu}_n)|] = O(1/\sqrt{n})$$

Computational Properties

- computation through Sinkhorn algorithm in $O(n^2 \log(1/\epsilon))$
- or, with stochastic algorithms
  $\rightsquigarrow$ SGD achieves the $O(1/\sqrt{n})$ rate

$\rightsquigarrow$ the "constants" deteriorate as $\beta \to \infty$.

[Refs]:
Mena, Weed (2019). *Statistical bounds for entropic optimal transport: sample complexity and the central limit theorem.*
Genevay, Chizat, Bach, Cuturi, Peyré (2018). *Sample Complexity of Sinkhorn divergences.*
Genevay, Cuturi, Peyré, Bach (2016). *Stochastic Optimization for Large-scale Optimal Transport*

Comparison

Loss D	computational compl.	sample compl.	geometry
φ-divergence	$-$	$-$	- -
MMD	$O(n^2)$	$O(n^{-1})$	-
Sinkhorn div.	$\tilde{O}(n^2 \log 1/\epsilon)$	$O(n^{-1/2})$	$+$
Wasserstein	$\tilde{O}(n^3)$ or $\tilde{O}(n^2/\epsilon^2)$	$O(n^{-2/d})$	$++$

- (disclaimer) these quantities are not exactly comparable
- ideally, deal with computational and statistical aspects jointly
- for density fitting, study ideally the complexity of the whole scheme

Part 1: qualitative overview

- **classical theory**
- **selection of properties and variants**

Part 2: Algorithms and Approximations

- **computational aspects**
- **entropic regularization**
- **statistical aspects**

[Some reference textbooks:]
- Peyré, Cuturi (2018). Computational Optimal Transport
- Santambrogio (2015). Optimal Transport for Applied Mathematicians
- Villani (2008). Optimal Transport, Old and New