Optimal Transport Theory

for Machine Learning

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A Geometric Motivation

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

Goal

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

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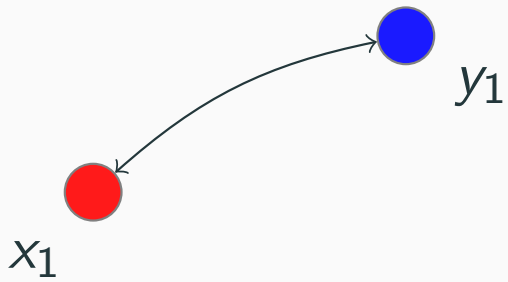

Distance between μ and ν...

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

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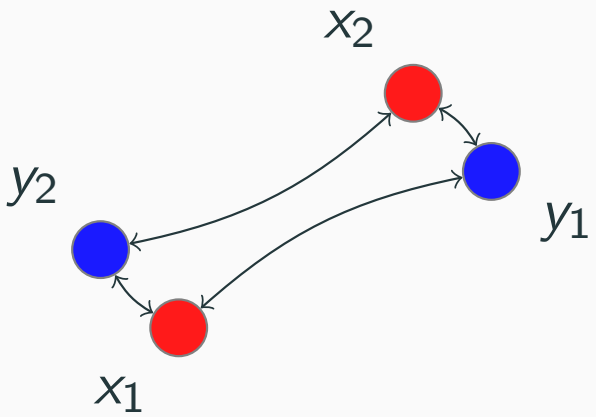

$$\mu = \frac{1}{n}\sum_{i=1}^{n} \delta_{x_i}, \quad \nu = \frac{1}{n}\sum_{j=1}^{n} \delta_{y_j}$$

Distance between μ and ν...

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

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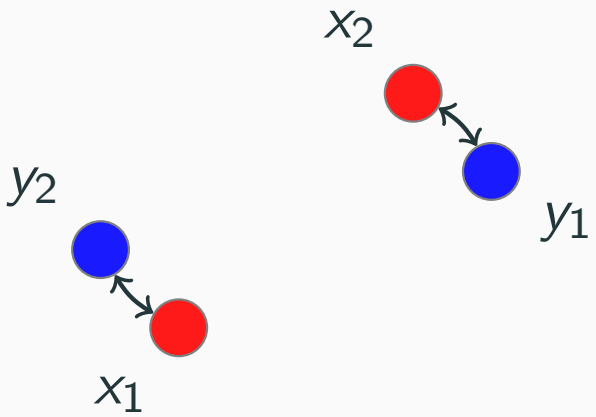

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Distance between μ and ν...

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

A Geometric Motivation

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

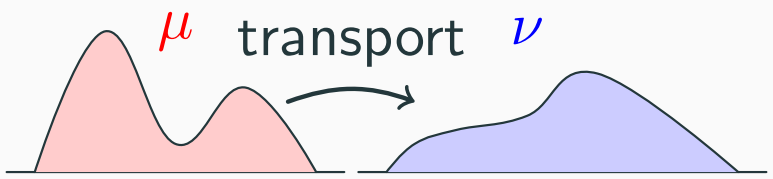
Distance between μ and ν...

?

Origin and Ramifications

Monge Problem (1781)

Move dirt from one configuration to another with least effort



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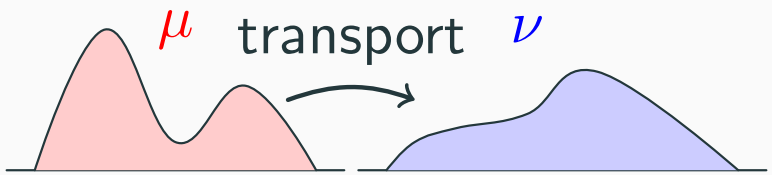
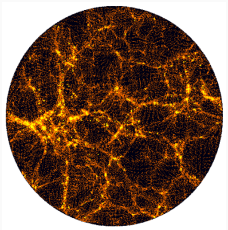
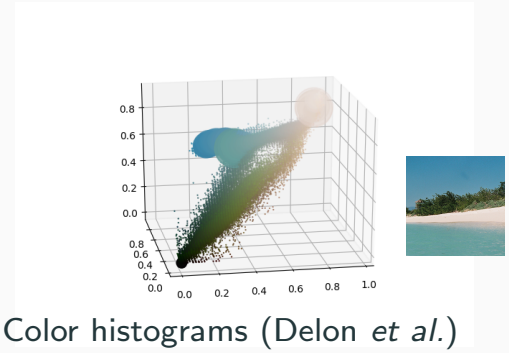


Strong modelization power:

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

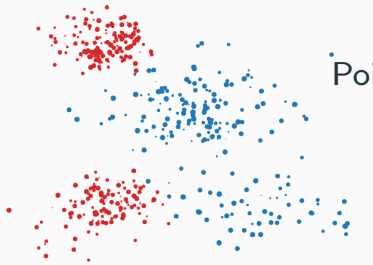
Early universe
(Brenier *et al.* '08)





Color histograms (Delon *et al.*)

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



Point clouds

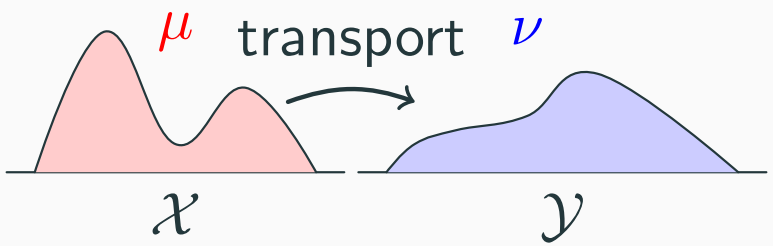
Outline

Outline

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 $\nu \in \mathcal{P}(\mathcal{Y})$

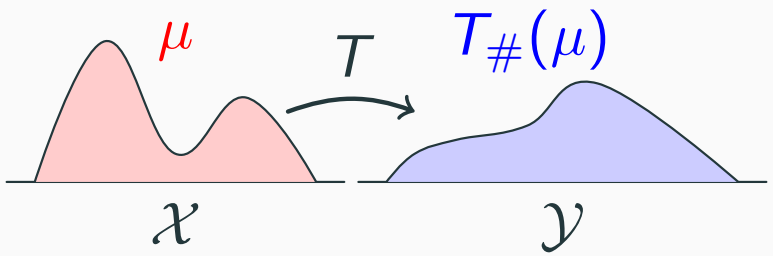


Transport map

Definition (pushforward)

Let $T : \mathcal{X} \to \mathcal{Y}$ be a map. The *pushforward measure* of μ by T, denoted $T_{\#}\mu$, 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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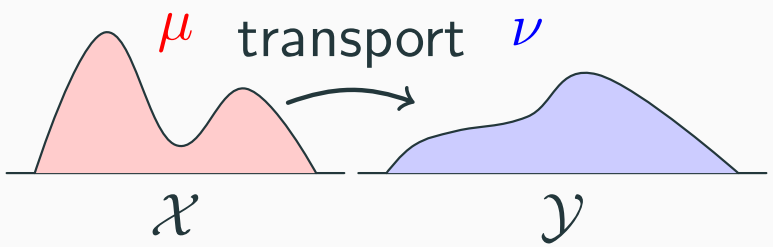


Definition (Monge problem)

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

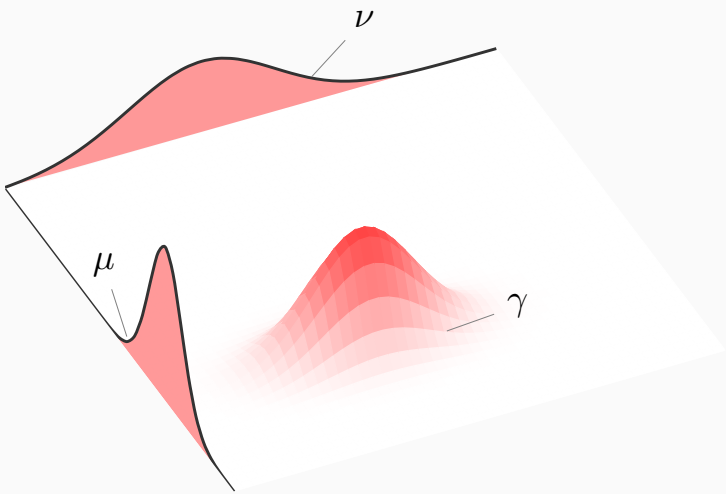
$\rightsquigarrow$ in some cases: no solution, no feasible point...

Transport Plans

Definition (Set of transport plans)

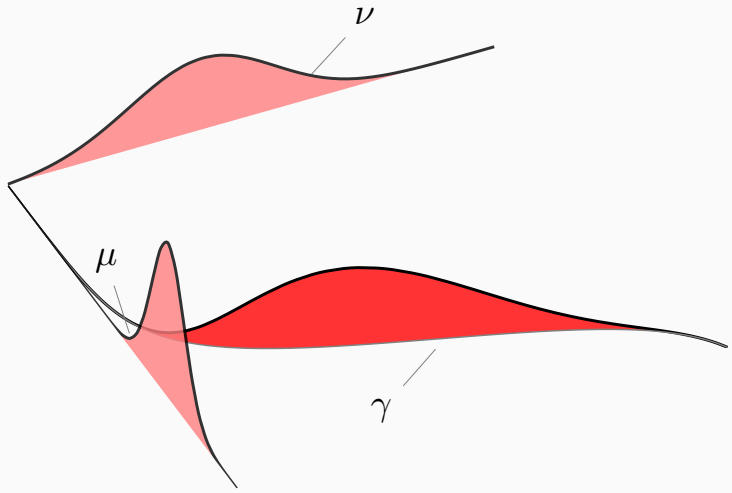
Positive measures on $\mathcal{X} \times \mathcal{Y}$ with specified marginals :

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



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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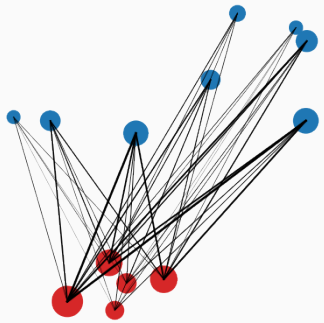

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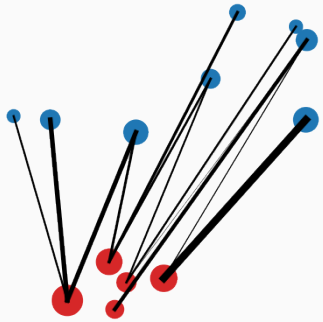

Cycle-free coupling

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

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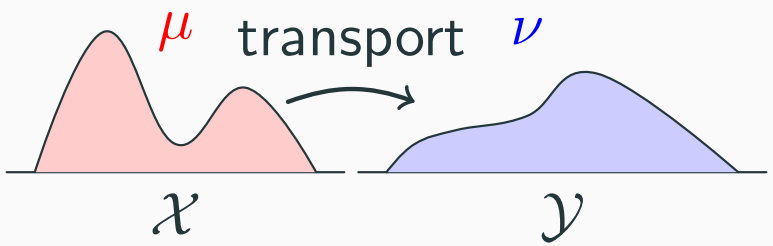
Definition (Optimal transport problem)

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



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

Duality

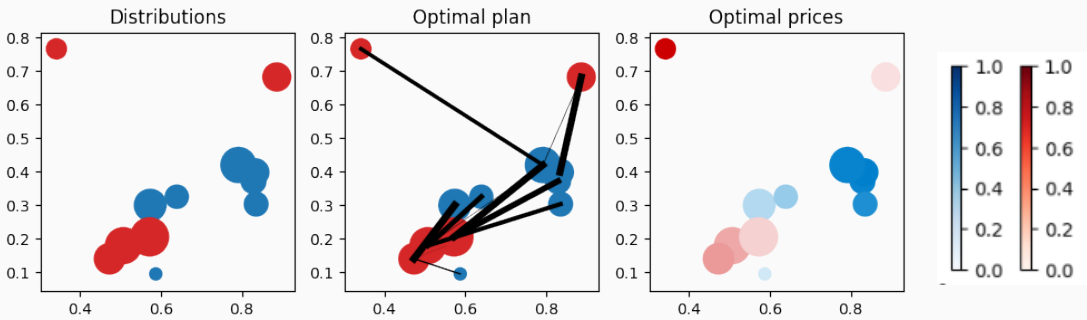
Theorem (Kantorovich duality)

$$\min_{\gamma \in \Pi(\mu,\nu)} \int_{\mathcal{X}\times\mathcal{Y}} c(x,y)d\gamma(x,y) \qquad \text{(Primal)}$$

$$=$$

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

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



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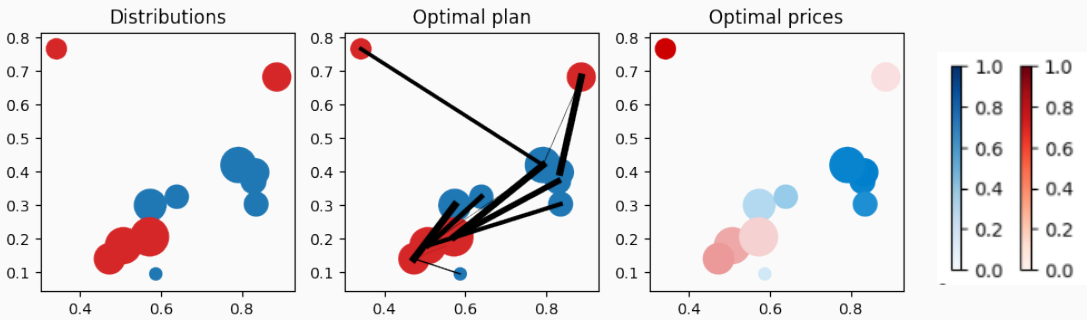


At optimality

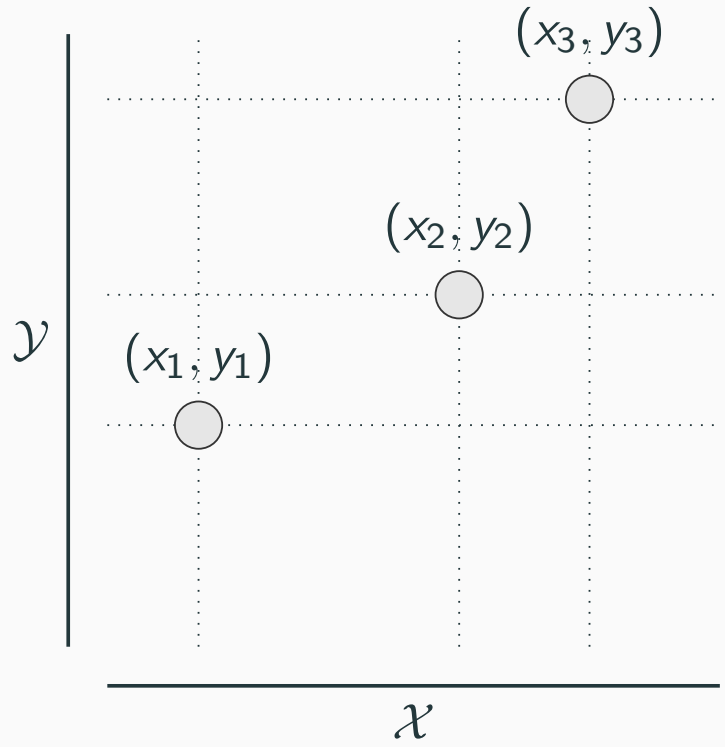
- $\phi(x)+\psi(y) = c(x,y)$ for γ almost every (x,y)
- γ is concentrated on a "c-cyclically monotone" set

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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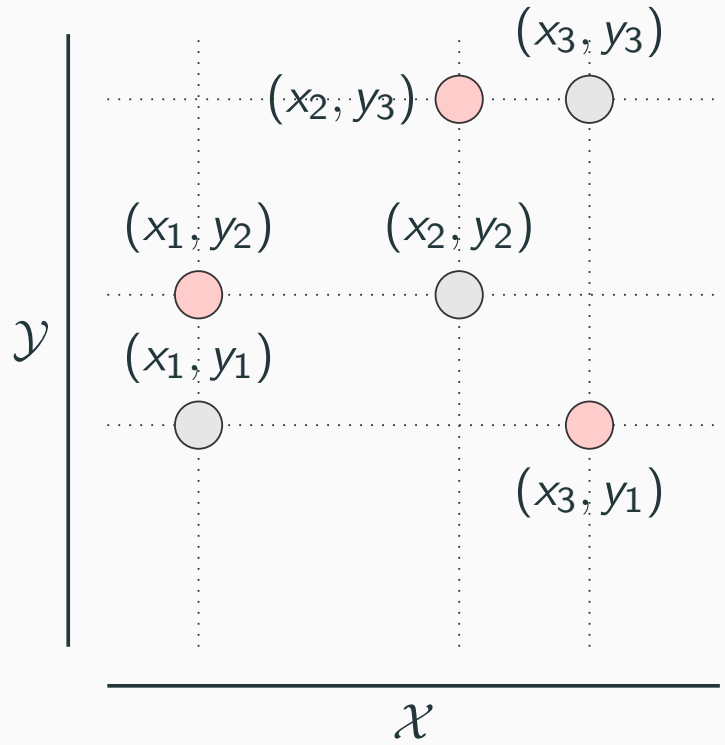


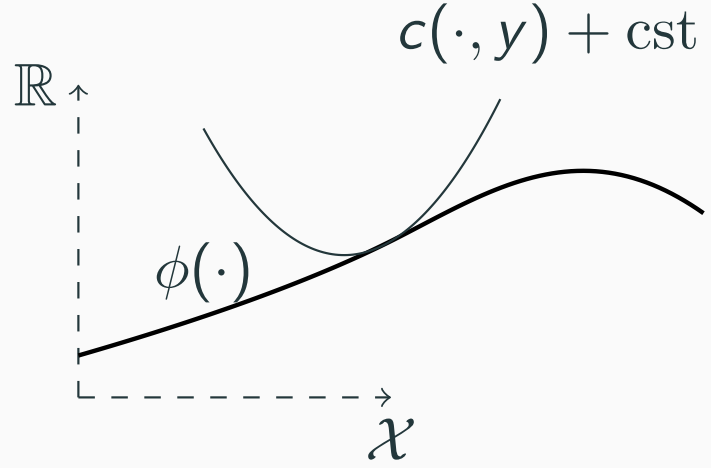
Generalizing Convex Analysis Tools (II)

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 :

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

Special Cases

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

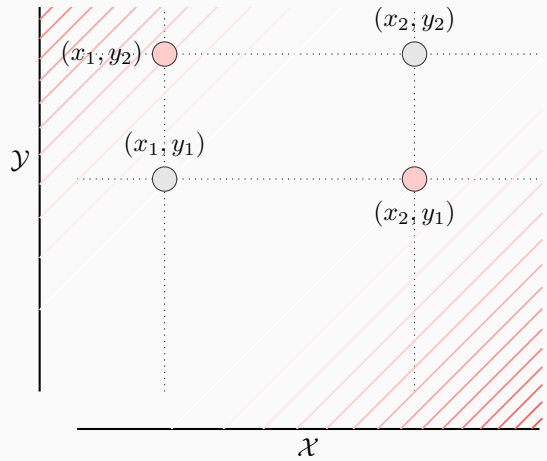
Theorem (Monotone Rearrangement)

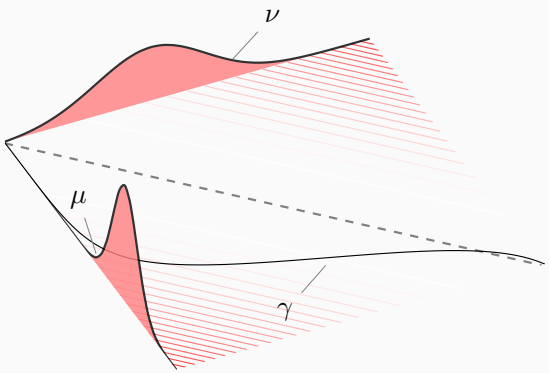
If $\mu, \nu \in \mathcal{P}(\mathbb{R})$ and $c(x, y) = h(y - x)$ with h strictly convex:

- 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. $\square$



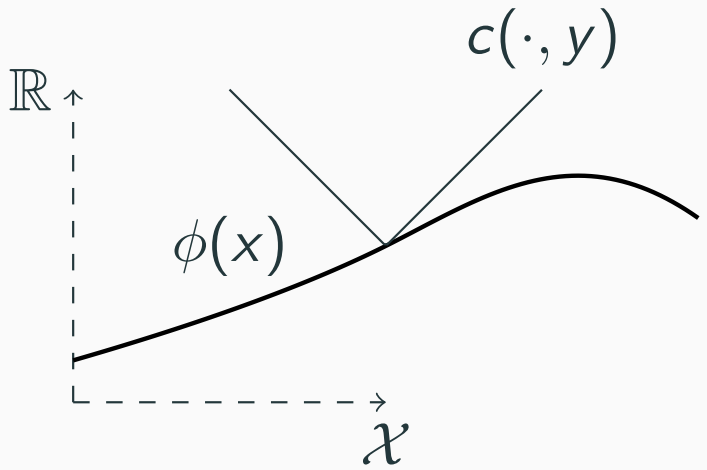


Distance Cost

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

- ϕ c-concave $\Leftrightarrow$ ϕ 1-Lipschitz $\Leftrightarrow$
  $|\phi(x) - \phi(y)| \leq \text{dist}(x, y),\ \forall x, y$
- $\phi^c(y) = \inf_x d(x, y) - \phi(x) = -\phi(y)$
- consequence :

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



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.

Wasserstein distance

Definition

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

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

- W_2 metrizes weak convergence + 2-nd order moments
- if $(\mathcal{X}, \mathrm{dist})$ 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

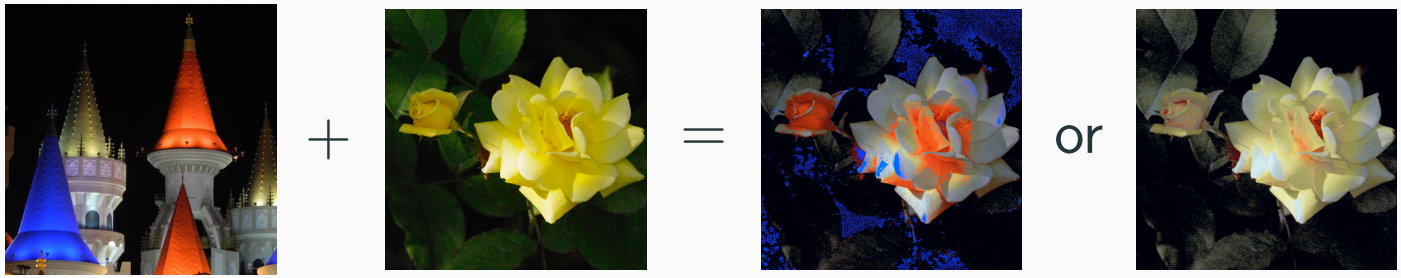
Properties of the distance W_2 on $\mathbb{R}^d$

- 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 geodesic space
- some explicit cases (real line)

Outline

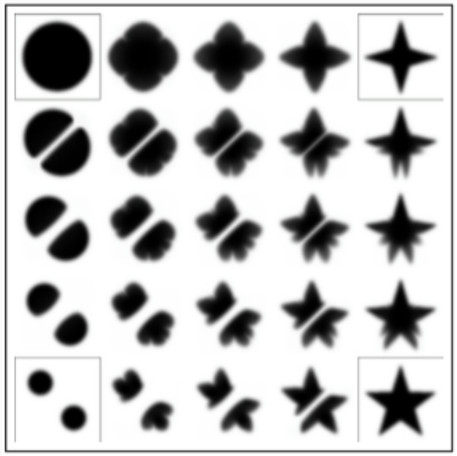
Histogram and shapes processing

Color transfer

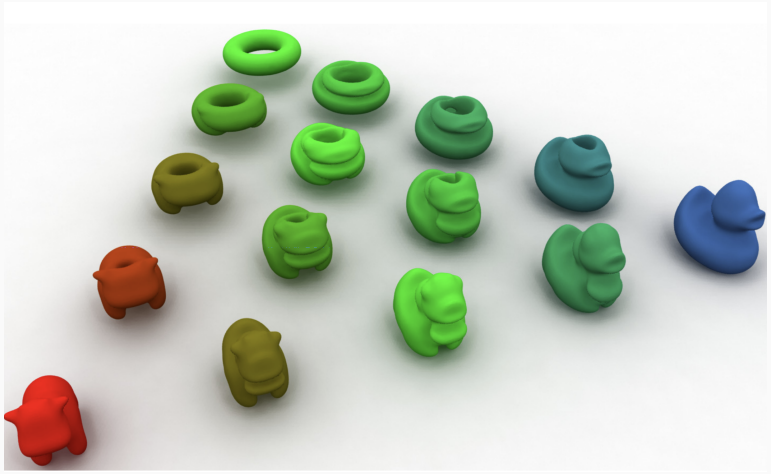


color target OT or unbalanced OT

Barycenters



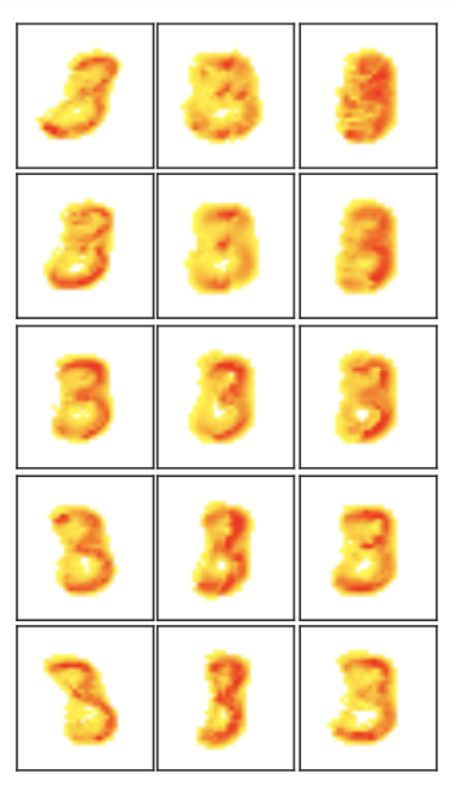
(Benamou et al. '15)



(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!



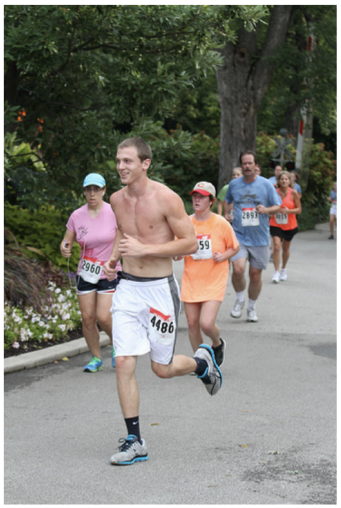
Three PCs from the MNIST dataset (Seguy and Cuturi, 2015)

[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.

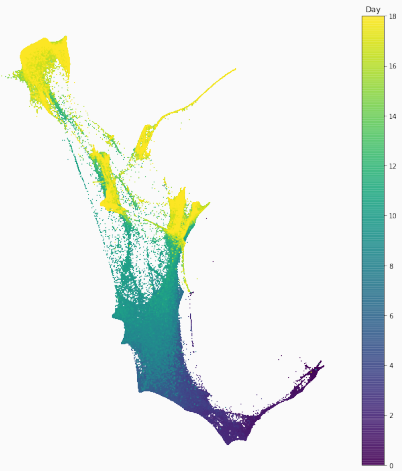
(c) **Flickr user tags**: spring, race, training; **our proposals**: road, bike, trail; **baseline proposals**: dog, surf, bike.

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

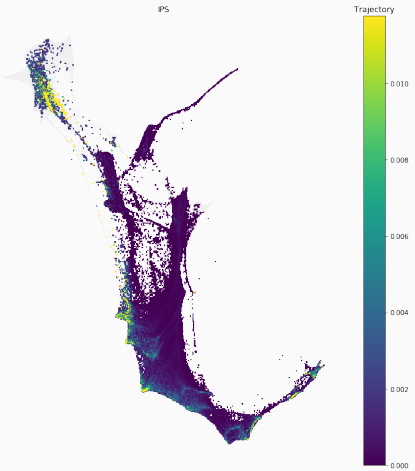
[Refs]:
Frogner, Zhang, Mobahi, Araya, Poggio (2015). *Learning with a Wasserstein loss.*

Learning from population dynamics

- Goal: given a population of undistinguishable particles μ_t at times $t = 1, 2, \ldots,$ recover the motion of individual particles
- Solution: compute optimal transport maps from μ_t to μ_{t+1}



Dynamic of cells in "gene space"



Dynamic of a single cell type

[Refs]:
Shiebinger et al. (2017). *Optimal-transport analysis of single-cell gene expression identifies developmental trajectories in reprogramming.*

Generative models

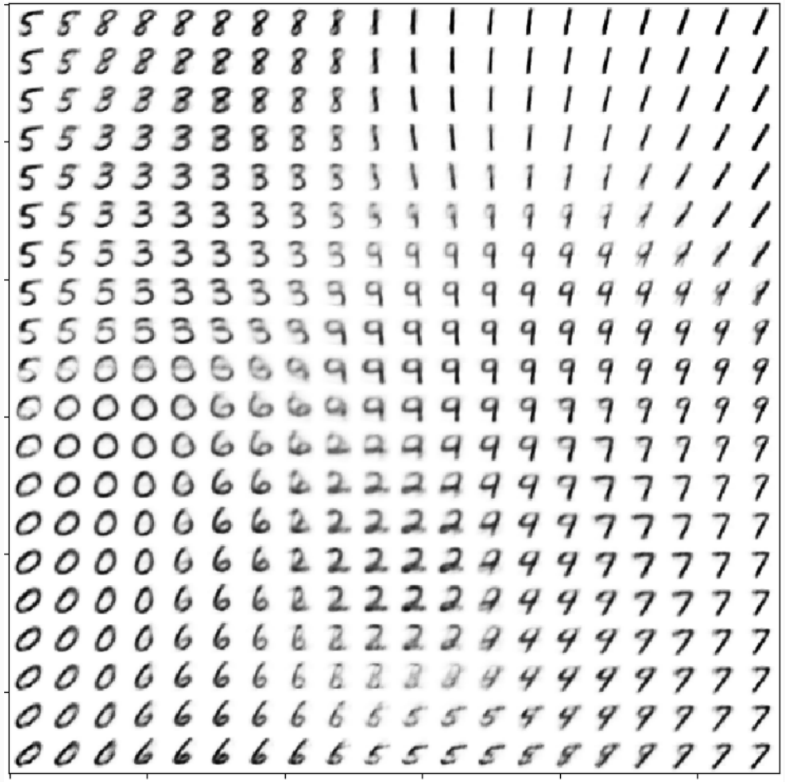
Loss for density fitting:

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 later in this talk



Generating figure from MNIST
(Genevay et al. 2018)

[Refs]:

Genevay, Peyré, Cuturi (2017). *Learning Generative Models with Sinkhorn Divergences*.

Outline

Discrete Optimal Transport

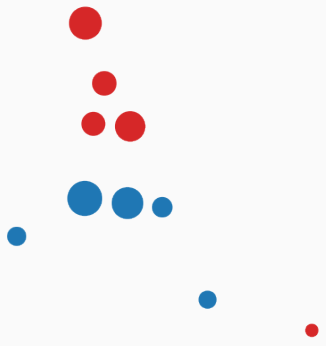
Discrete Setting

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

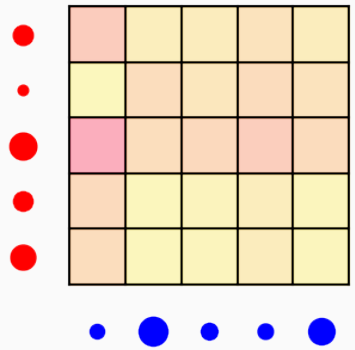
Linear Program

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

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



μ and ν on $\mathbb{R}^2$



Matrix representation

Discrete Optimal Transport

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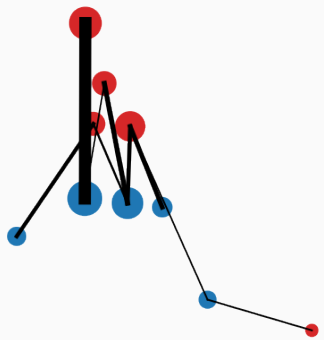

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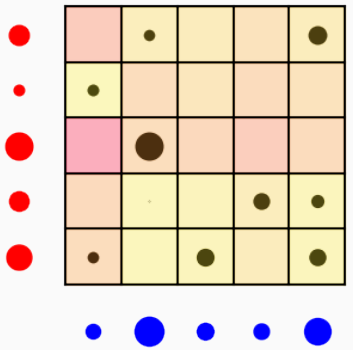


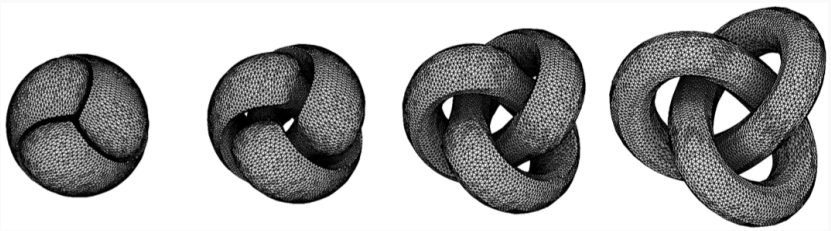
Matrix representation

Exact solvers

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

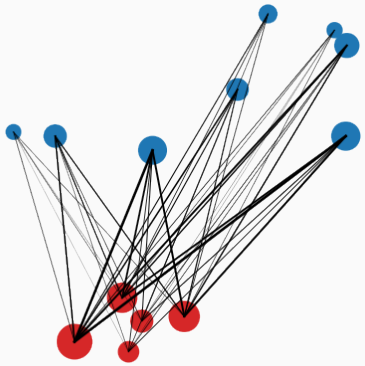
Efficient methods in $\mathbb{R}^2$ or $\mathbb{R}^3$

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

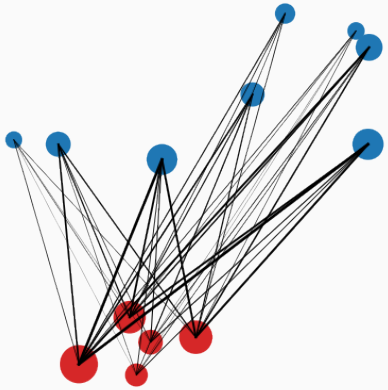


(Levy, 15')

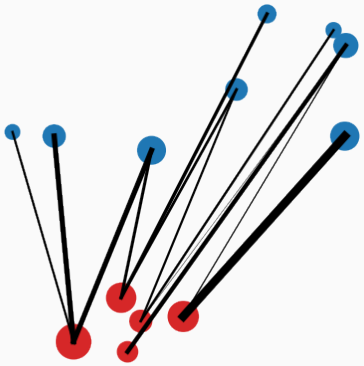
Approximate Solver



Product coupling

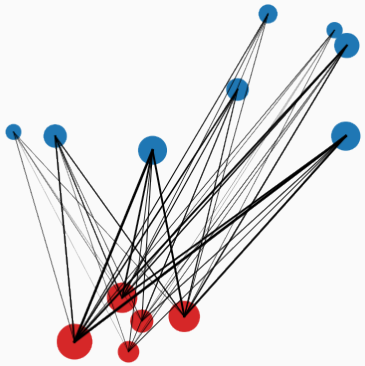


$0 < \eta < \infty$

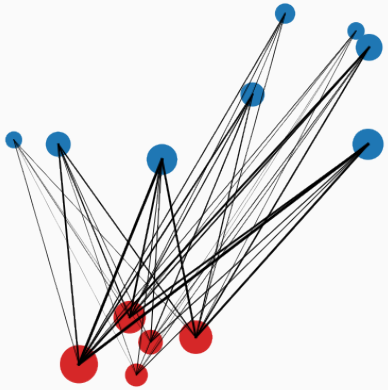


Optimal coupling

Approximate Solver



Product coupling



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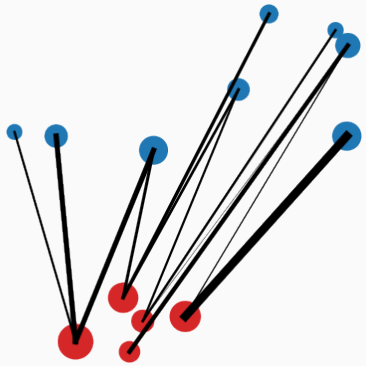
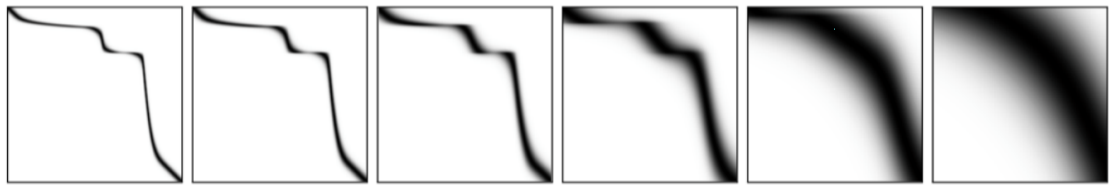


Optimal coupling

Entropic regularization

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

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



Optimal transport plan as η increases (Nenna et al. '15)

Sinkhorn's algorithm

Proposition (Optimality Condition)

Define the matrix $K_{i,j} = \exp(-\eta^{-1} \cdot C_{i,j})$. There exists $a, b \in \mathbb{R}_+^n$ such that at optimality:

$$\gamma^* = \mathrm{diag}(a) K \mathrm{diag}(b) \quad \Leftrightarrow \quad \gamma^*_{i,j} = a_i K_{i,j} b_j$$

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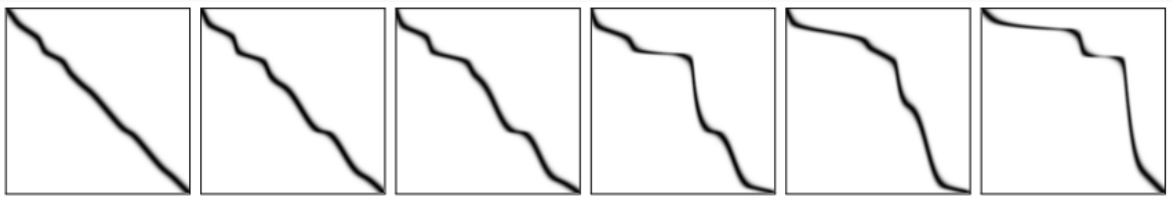
Sinkhorn's Algorithm

1. initialize $b = (1, \ldots, 1)$ 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, accelerations

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One iteration

- 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, accelerations

Solving OT

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

Outline

Density Fitting

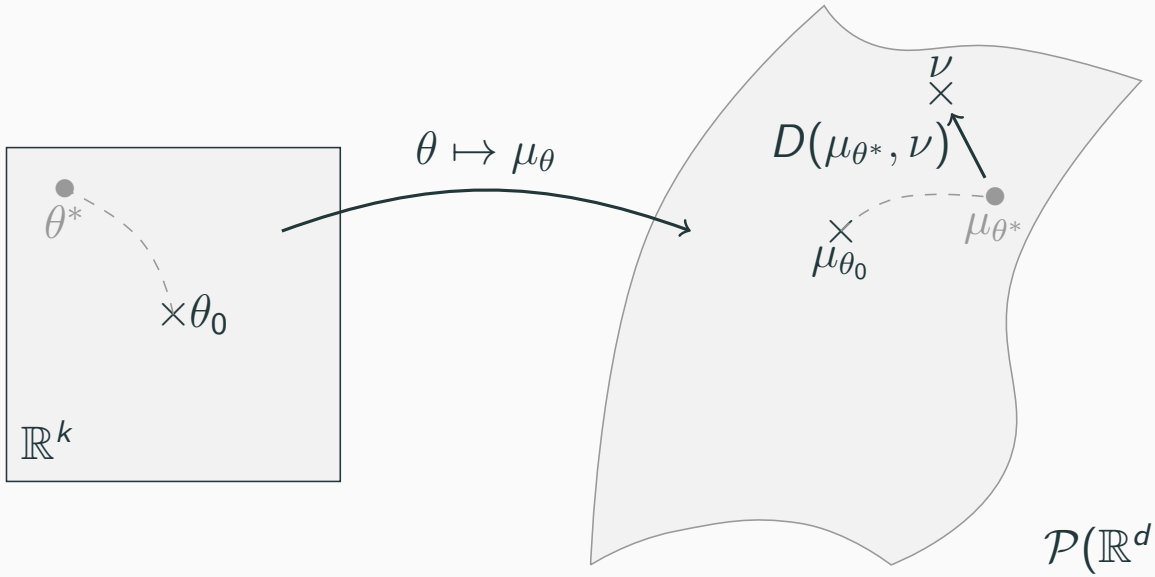
Ingredients

- 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 $\hat{\nu} = \frac{1}{n}\sum_{i=1}^{n} \delta_{x_i}$

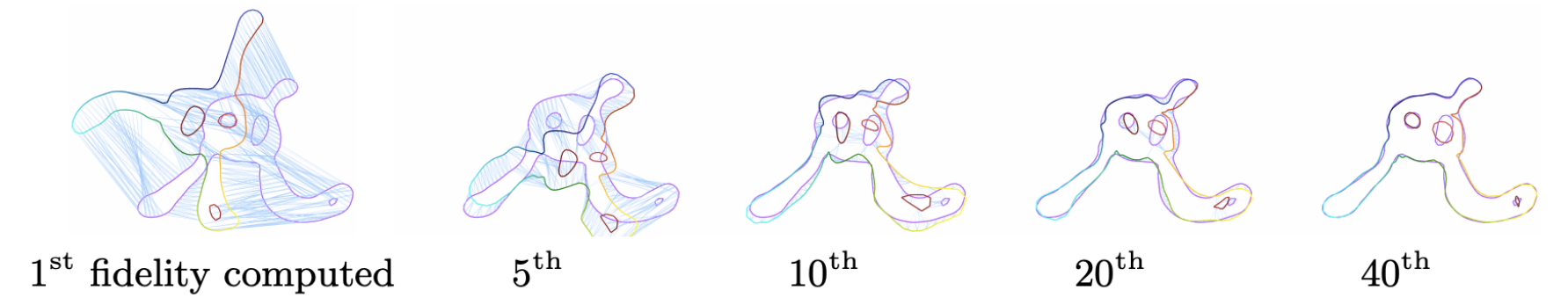
Choosing $D = \mathrm{KL}$ gives the maximum likelihood estimator:

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

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 (e.g. 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 α, start from $\theta^{(0)}$ and (ideally) define

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

Requires

- low computational complexity
- "informative" gradients
- low sample complexity

NB: Sample complexity

Let $x_1, \ldots, x_n$ be i.i.d. samples from μ and $y_1, \ldots, y_n$ be i.i.d. samples from ν. Let $\mu_n = \frac{1}{n} \sum \delta_{x_n}$ and $\nu_n = \frac{1}{n} \sum \delta_{y_n}$. How much the estimation $D(\hat{\mu}_n, \hat{\nu}_n)$ differs from $D(\mu, \nu)$ in terms of n?

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 $D_{\mathcal{F}} = W_1$.

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Maximum Mean Discrepancy

With $\mathcal{F}$ be the 1-ball of a RKHS $\mathcal{H}$ with positive definite kernel k,

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

- 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:

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

- "good" 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 under stronger assumptions

[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

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

Definition

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

Properties

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

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

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 $\eta \to 0$.

[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**