Practical Optimal Transport for Machine Learning

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Divergences statistiques et géométriques pour l'apprentissage machine

Overview

Planning of the course:

- (Morning) 1h30 of introductory course to *computational optimal transport* (Nicolas)
- (Afternoon) 1h30 of introduction to Unbalanced OT and Transport between metric spaces (Laetitia)
- (Afternoon) 1h30 ofpractical sessions in Python (POT)
- (Tomorrow Morning) 1h30 of of applications of OT to Machine Learning (Rémi)

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What is optimal transport ?

The natural geometry of probability measures


Monge


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Koopmans

Nobel '75


Dantzig


Brenier


Otto


McCann


Villani

Fields '10

The origins of optimal transport

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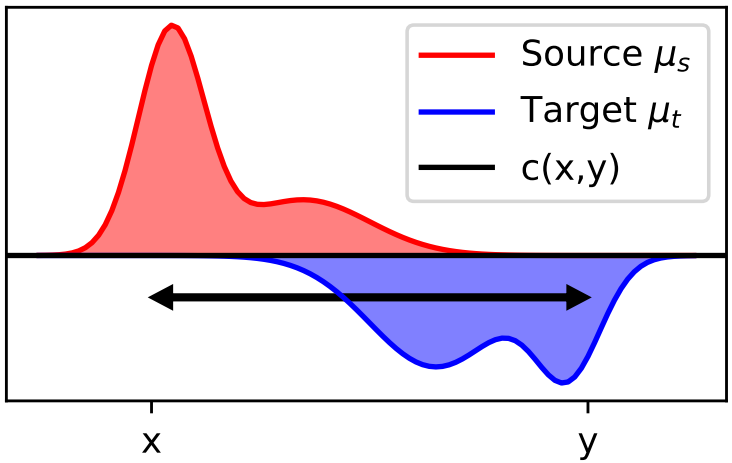
MÉMOIRE
SUR LA
THÉORIE DES DÉBLAIS
ET DES REMBLAIS.

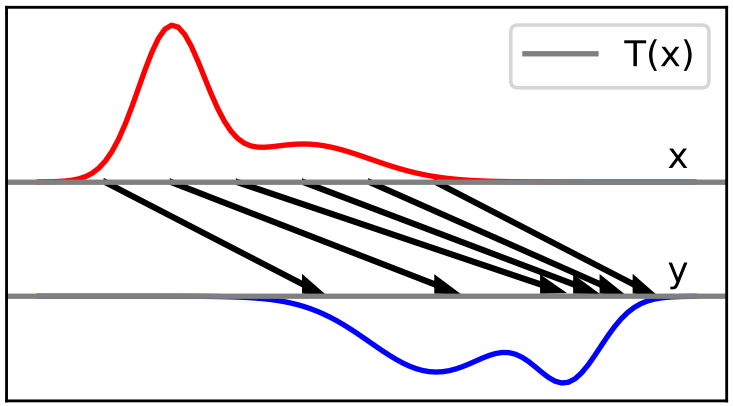
Par M. MONGE.

Problem [Monge, 1781]

- How to move dirt from one place (déblais) to another (remblais) while minimizing the effort ?
- Find a mapping T between the two distributions of mass (transport).
- Optimize with respect to a displacement cost $c(x, y)$ (optimal).

The origins of optimal transport





Problem [Monge, 1781]

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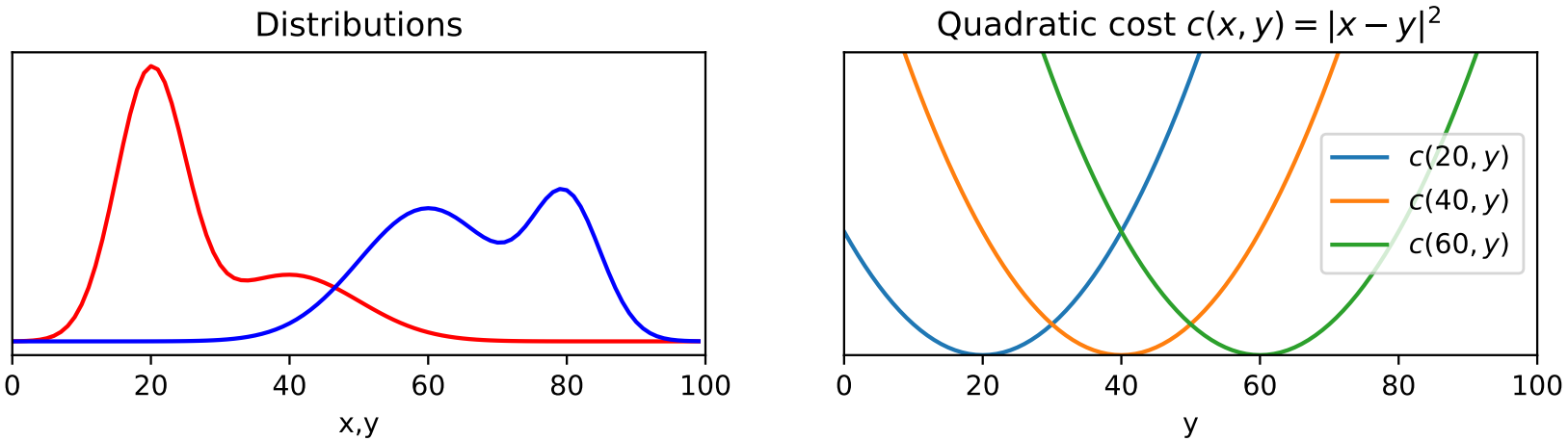
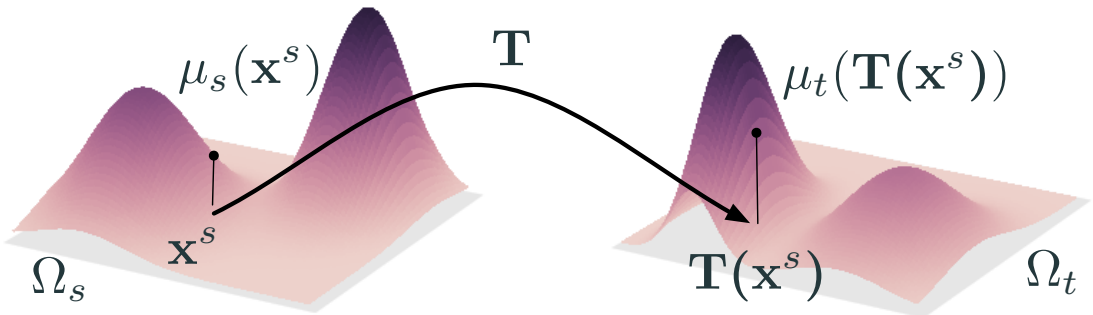
Optimal transport (Monge formulation)



- Probability measures μ_s and μ_t on and a cost function $c : \Omega_s \times \Omega_t \to \mathbb{R}^+$.
- The Monge formulation [Monge, 1781] aim at finding a mapping $T : \Omega_s \to \Omega_t$

$$\inf_{T\#\mu_s = \mu_t} \quad \int_{\Omega_s} c(\mathbf{x}, T(\mathbf{x}))\mu_s(\mathbf{x})d\mathbf{x} \tag{1}$$

What is $T\#\mu_s = \mu_t$?



- $T\#$ is the so called push forward operator
- it transfers measures from one space Ω_s to another space Ω_t
- it is equivalent to:

$$\mu_t(A) = \mu_s(T^{-1}(A))$$

$$\int_{\Omega_t} g(y) d\mu_t(y) = \int_{\Omega_s} g(T(x)) d\mu_s(x)$$

- for smooth measures $\mu_s = \rho(x)dx$ and $\mu_t = \eta(x)dx$

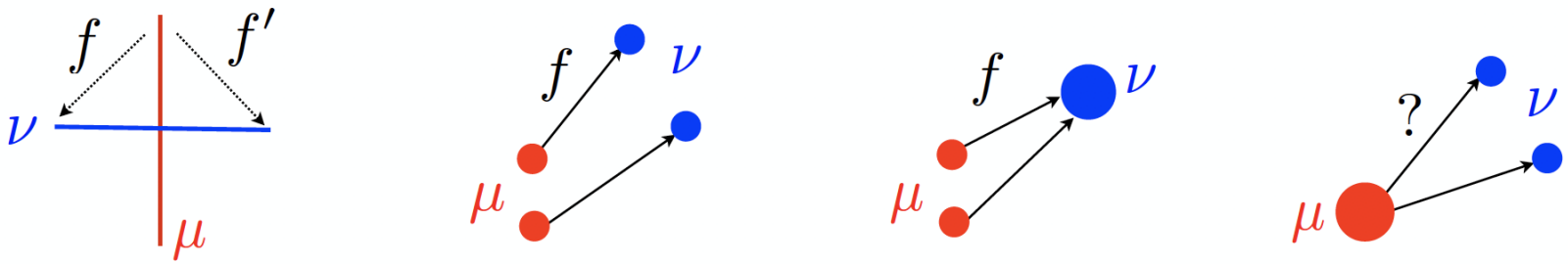
$$T\#\mu_s = \mu_t \equiv \rho(T(x))|\mathsf{det}(\partial T(x))| = \eta(x)$$

- a.k.a. change of variable formula

Non-existence / Non-uniqueness

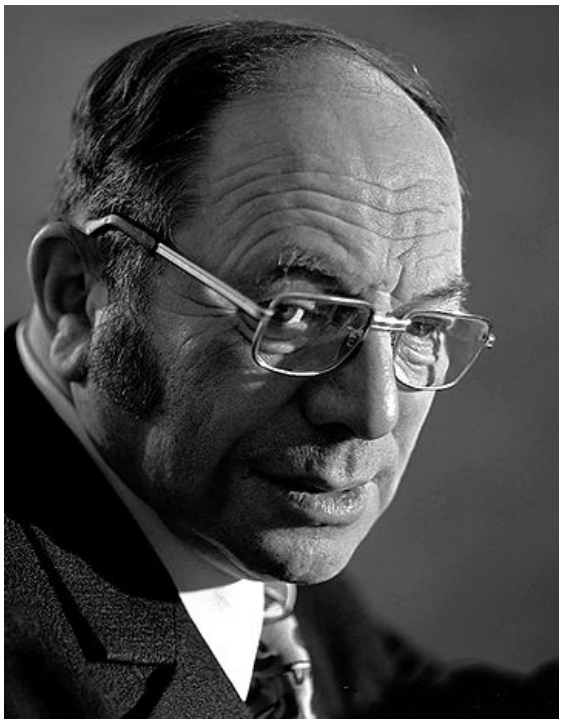
Solving for this push-forward operator is a non-convex optimization problem,

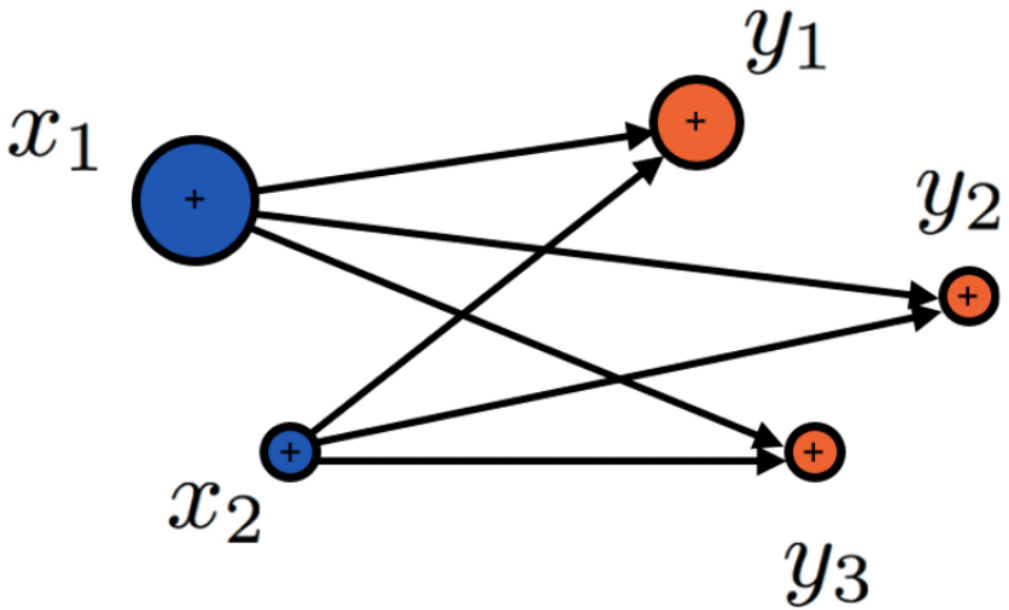
- for which existence is not guaranteed,
- nor unicity



Note: [Brenier, 1991] proved existence and unicity of the Monge map for $c(x, y) = \|x - y\|^2$ and distributions with densities (i.e. continuous).

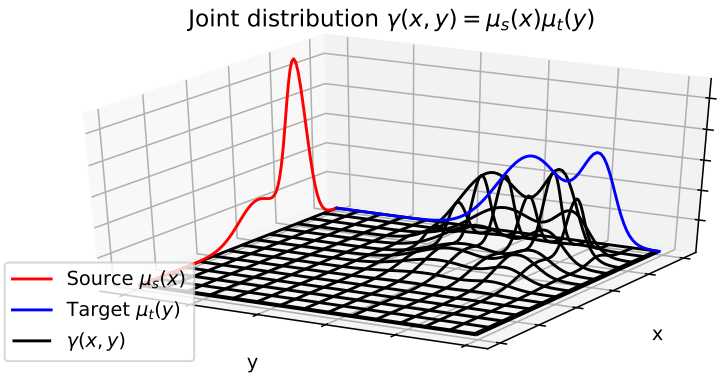
Kantorovich relaxation

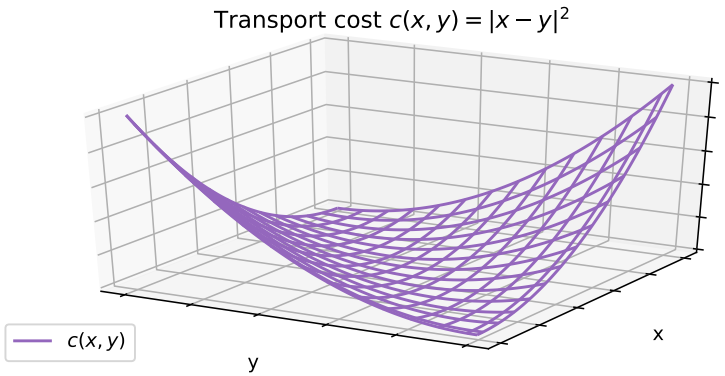




- Leonid Kantorovich (1912–1986), Economy nobelist in 1975, proposed a different formulation of the problem
- with applications mainly for ressource allocation problems

Optimal transport (Kantorovich formulation)





- The Kantorovich formulation [Kantorovich, 1942] seeks for a probabilistic coupling $\boldsymbol{\gamma} \in \mathcal{P}(\Omega_s \times \Omega_t)$ between Ω_s and Ω_t:

$$\boldsymbol{\gamma}_0 = \underset{\boldsymbol{\gamma}}{\operatorname{argmin}} \int_{\Omega_s \times \Omega_t} c(\mathbf{x}, \mathbf{y}) \boldsymbol{\gamma}(\mathbf{x}, \mathbf{y}) d\mathbf{x} d\mathbf{y}, \tag{2}$$

$$\text{s.t.} \quad \boldsymbol{\gamma} \in \mathcal{P} = \left\{ \boldsymbol{\gamma} \geq \mathbf{0}, \int_{\Omega_t} \boldsymbol{\gamma}(\mathbf{x}, \mathbf{y}) \mathbf{dy} = \mu_{\mathbf{s}}, \int_{\Omega_s} \boldsymbol{\gamma}(\mathbf{x}, \mathbf{y}) \mathbf{dx} = \mu_{\mathbf{t}} \right\}$$

- $\boldsymbol{\gamma}$ is a joint probability measure with marginals μ_s and μ_t.
- Linear Program that always have a solution.

The 3 ways of optimal transport

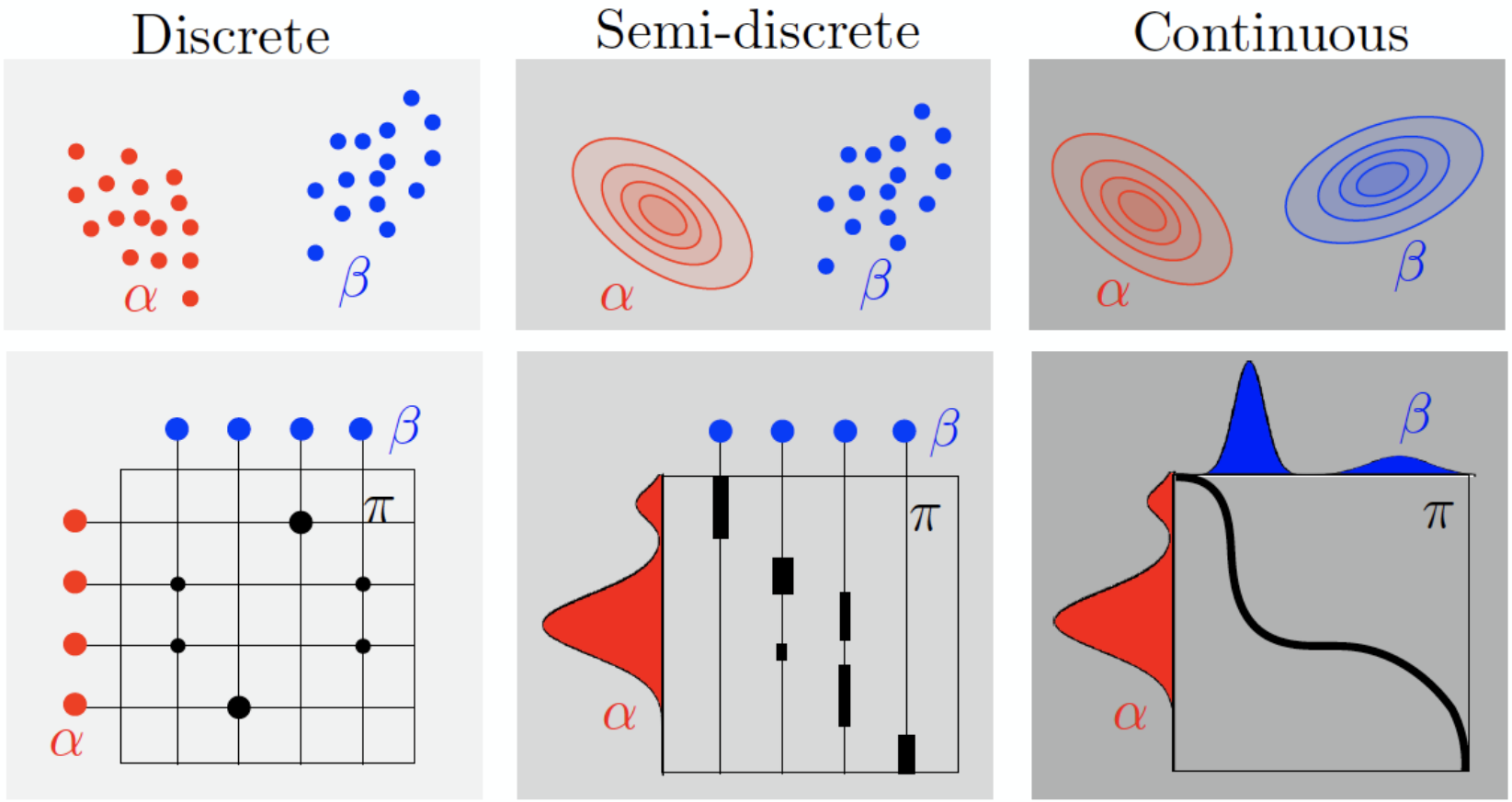


Image from Gabriel Peyré

Couplings

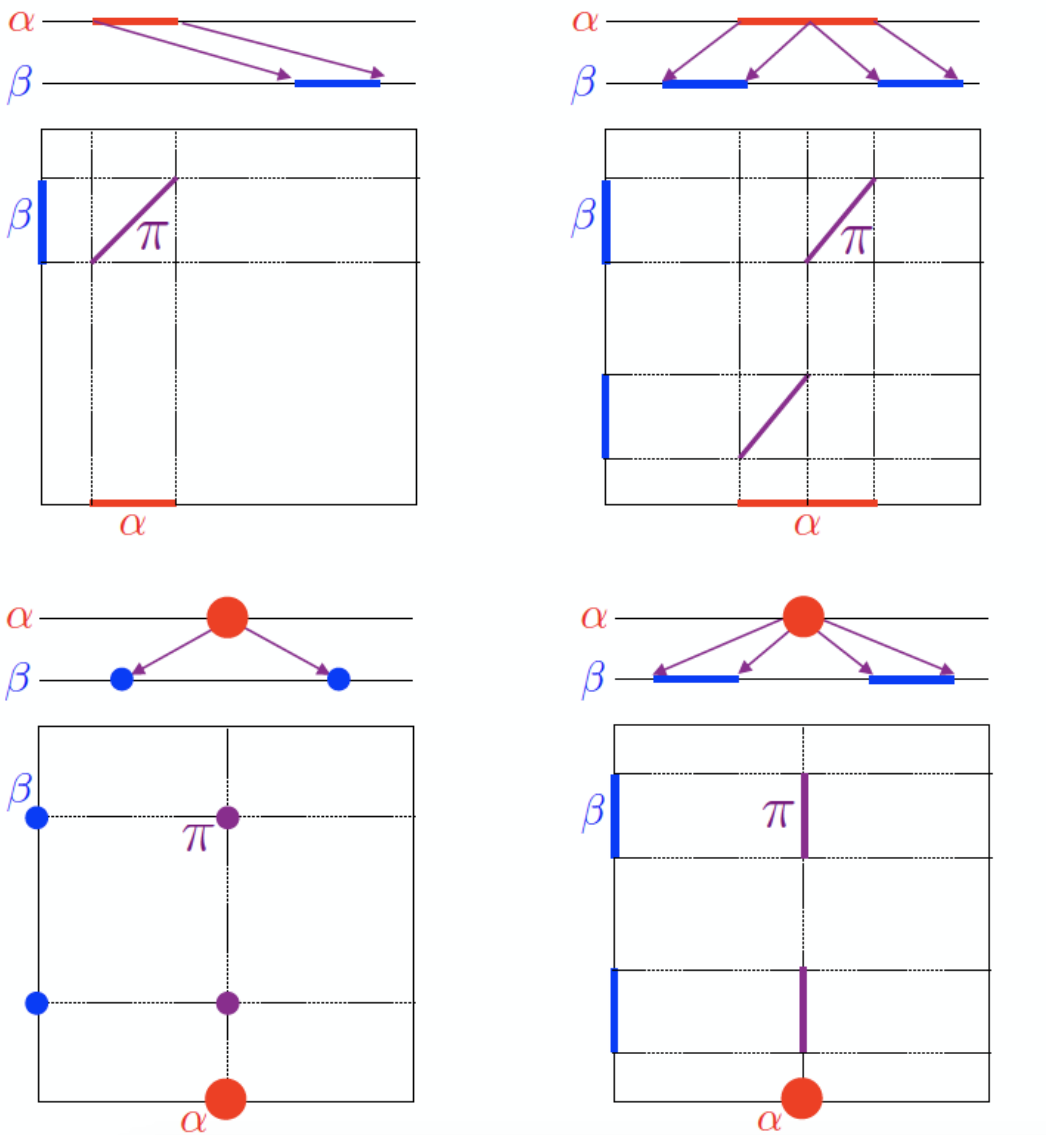


Image from Gabriel Peyré

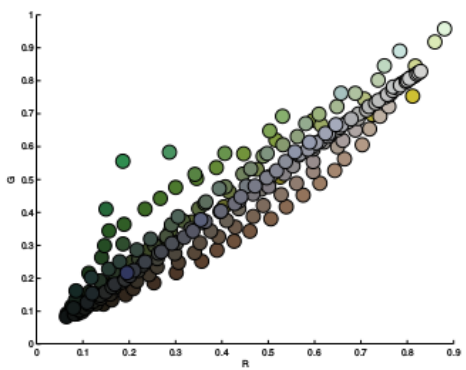
Histogram matching in images : color grading

Pixels as empirical distribution [Ferradans et al., 2014]

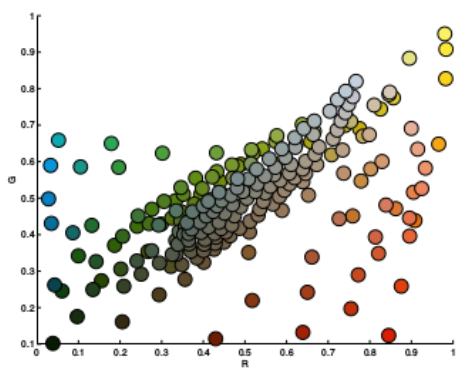
X^0

Y^0

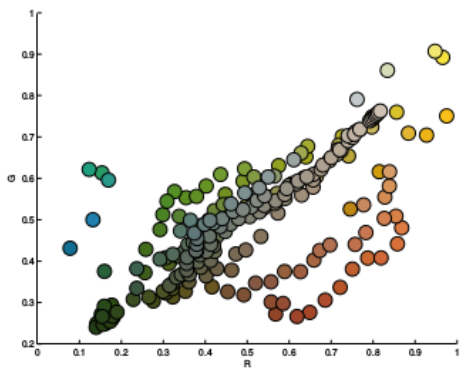
$\tilde{X}^0$



μ_{X^0}



μ_{Y^0}



$\mu_{\tilde{X}^0}$

Histogram matching in images : color grading

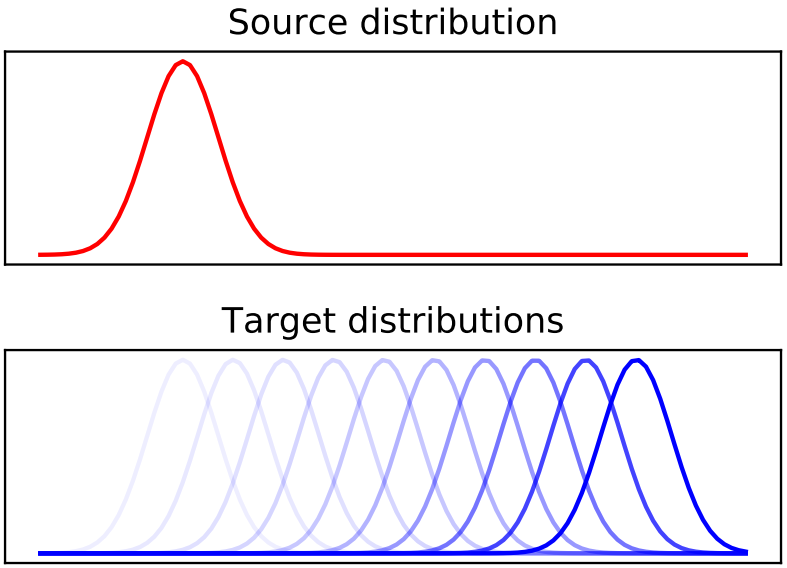
Image colorization [Ferradans et al., 2014]

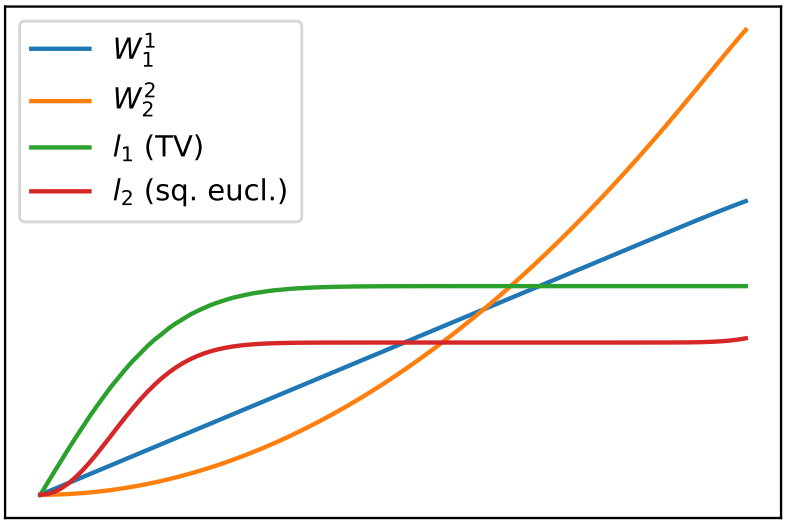
Matching words embedding

- Words are embedded in a high-dimensional space with neural networks
- Matching two documents is an OT problem, with the cost being the l_2 distance in the embedded space

Outline

Wasserstein distance





Wasserstein distance

$$W_p^p(\mu_s, \mu_t) = \min_{\gamma \in \mathcal{P}} \int_{\Omega_s \times \Omega_t} c(\mathbf{x}, \mathbf{y}) \gamma(\mathbf{x}, \mathbf{y}) d\mathbf{x} d\mathbf{y} = \mathop{\mathbb{E}}_{(\mathbf{x},\mathbf{y}) \sim \gamma} [c(\mathbf{x}, \mathbf{y})] \tag{3}$$

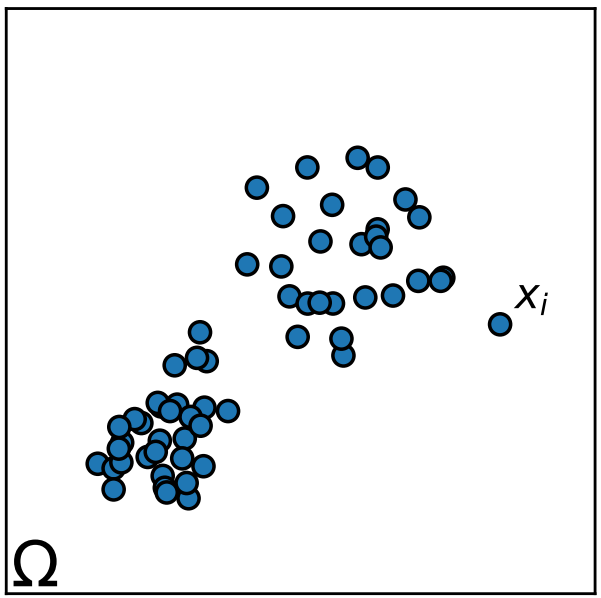
where $c(\mathbf{x}, \mathbf{y}) = \|\mathbf{x} - \mathbf{y}\|^p$

- A.K.A. Earth Mover's Distance (W_1^1) [Rubner et al., 2000].
- Do not need the distribution to have overlapping support.
- Works for continuous and discrete distributions (histograms, empirical).

Discrete distributions: Empirical vs Histogram

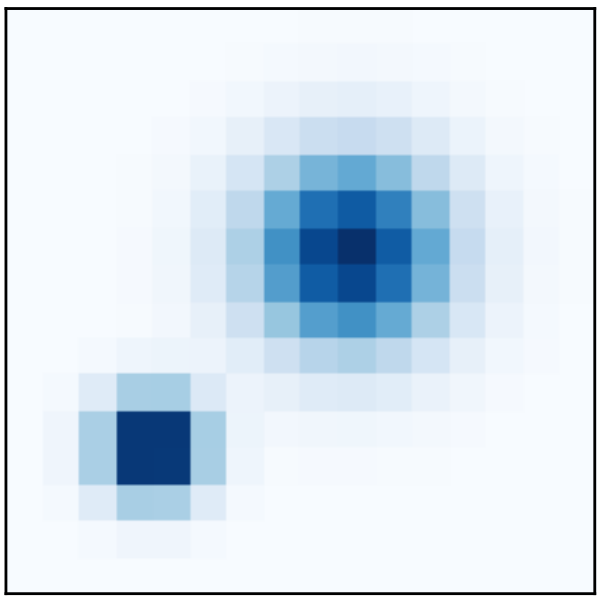
Discrete measure: $\mu = \sum_{i=1}^{n} \mu_i \delta_{\mathbf{x}_i}, \quad \mathbf{x}_i \in \Omega, \quad \sum_{i=1}^{n} \mu_i = 1$

Lagrangian (point clouds)



- Constant weight: $\mu_i = \frac{1}{n}$
- Quotient space: Ω^n, Σ_n

Eulerian (histograms)



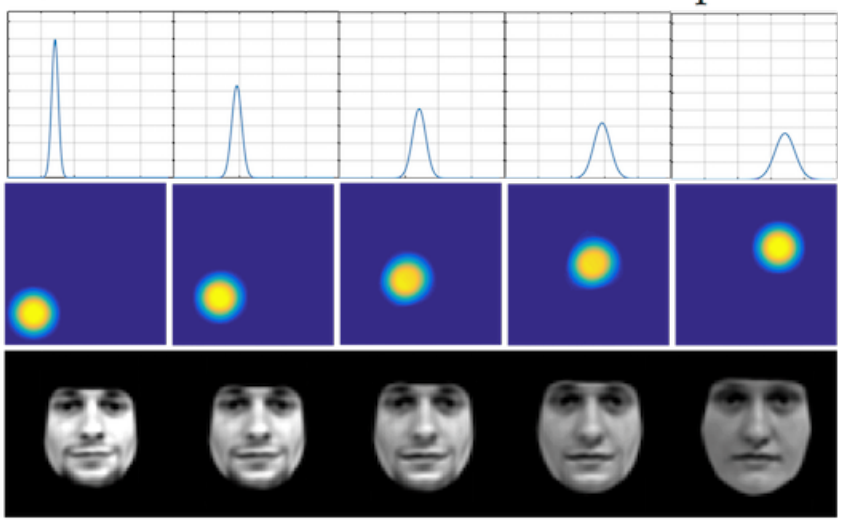
- Fixed positions $\mathbf{x}_i$ e.g. grid
- Convex polytope Σ_n (simplex): $\left\{(\mu_i)_i \geq 0; \sum_i \mu_i = 1\right\}$

Wasserstein space

The space of probability distribution equipped with the Wasserstein metric $(\mathcal{P}_p(X), W_2^2(X))$ defines a geodesic space with a Riemannian structure [Santambrogio, 2014].

- Geodesics are shortest curves on $\mathcal{P}_p(X)$ that link two distributions

Geodesic in the 2-Wasserstein space

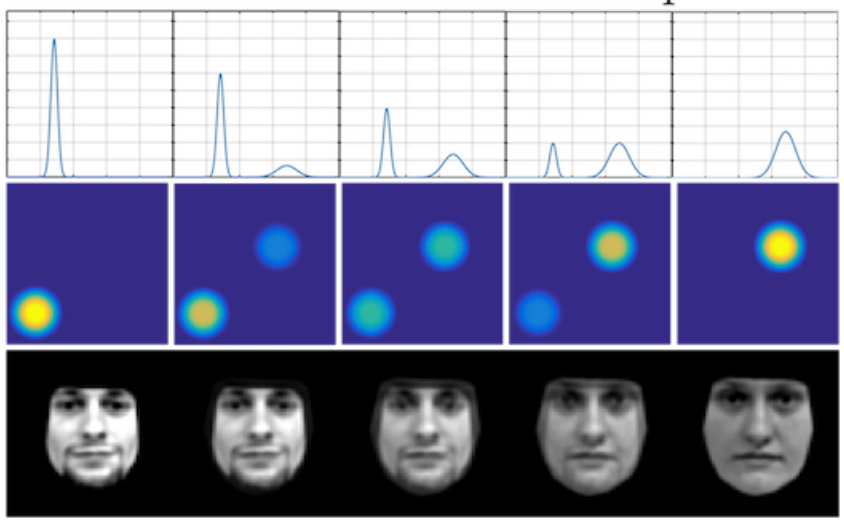


$t = 0 \quad t = 0.25 \quad t = 0.5 \quad t = 0.75 \quad t = 1$

$$\rho^*(.,t) = ((1-t)id + tf^*)_{\#}\mu$$

$$d\rho^*(x,t) = I^*(x,t)dx$$

Geodesic in the Euclidean space

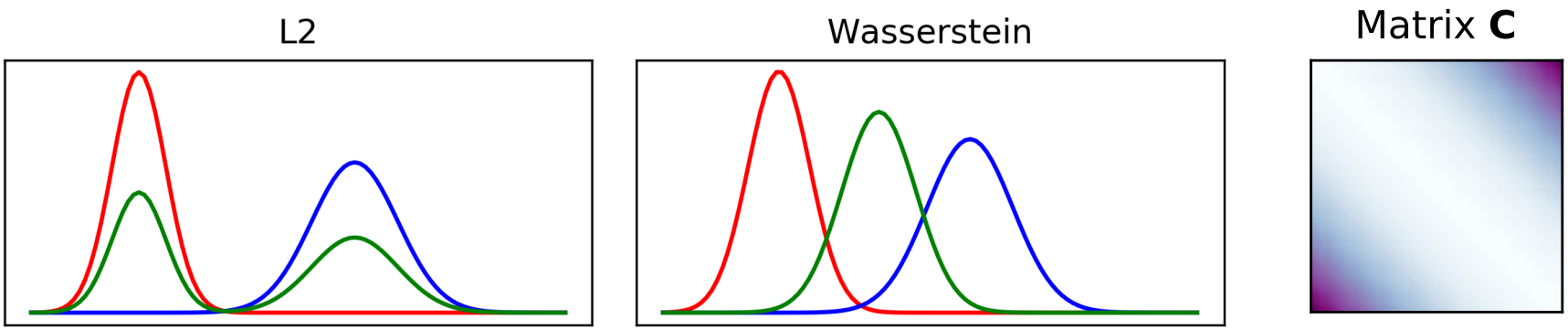


$t = 0 \quad t = 0.25 \quad t = 0.5 \quad t = 0.75 \quad t = 1$

$$I(x,t) = (1-t)I_0(x) + tI_1(x)$$

Illustration by S. Kolhouri

Wasserstein barycenter

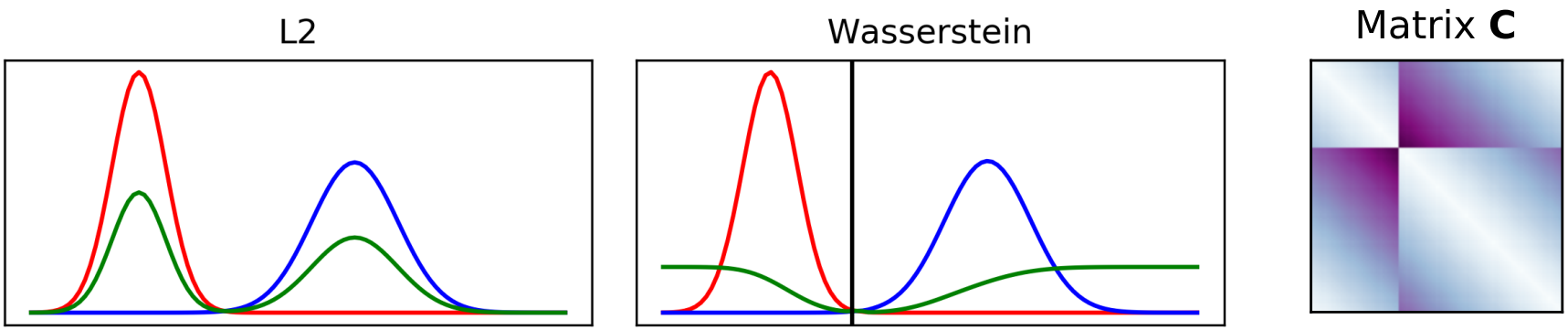


Barycenters [Agueh and Carlier, 2011]

$$\bar{\mu} = \arg\min_{\mu} \quad \sum_{i}^{n} \lambda_i W_p^p(\mu^i, \mu)$$

- $\lambda_i > 0$ and $\sum_i^n \lambda_i = 1$.
- Uniform barycenter has $\lambda_i = \frac{1}{n}, \forall i$.
- Interpolation with n=2 and $\boldsymbol{\lambda} = [1-t, t]$ with $0 \leq t \leq 1$ [McCann, 1997].
- Regularized barycenters using Bregman projections [Benamou et al., 2015].
- The cost and regularization impacts the interpolation trajectory.

Wasserstein barycenter



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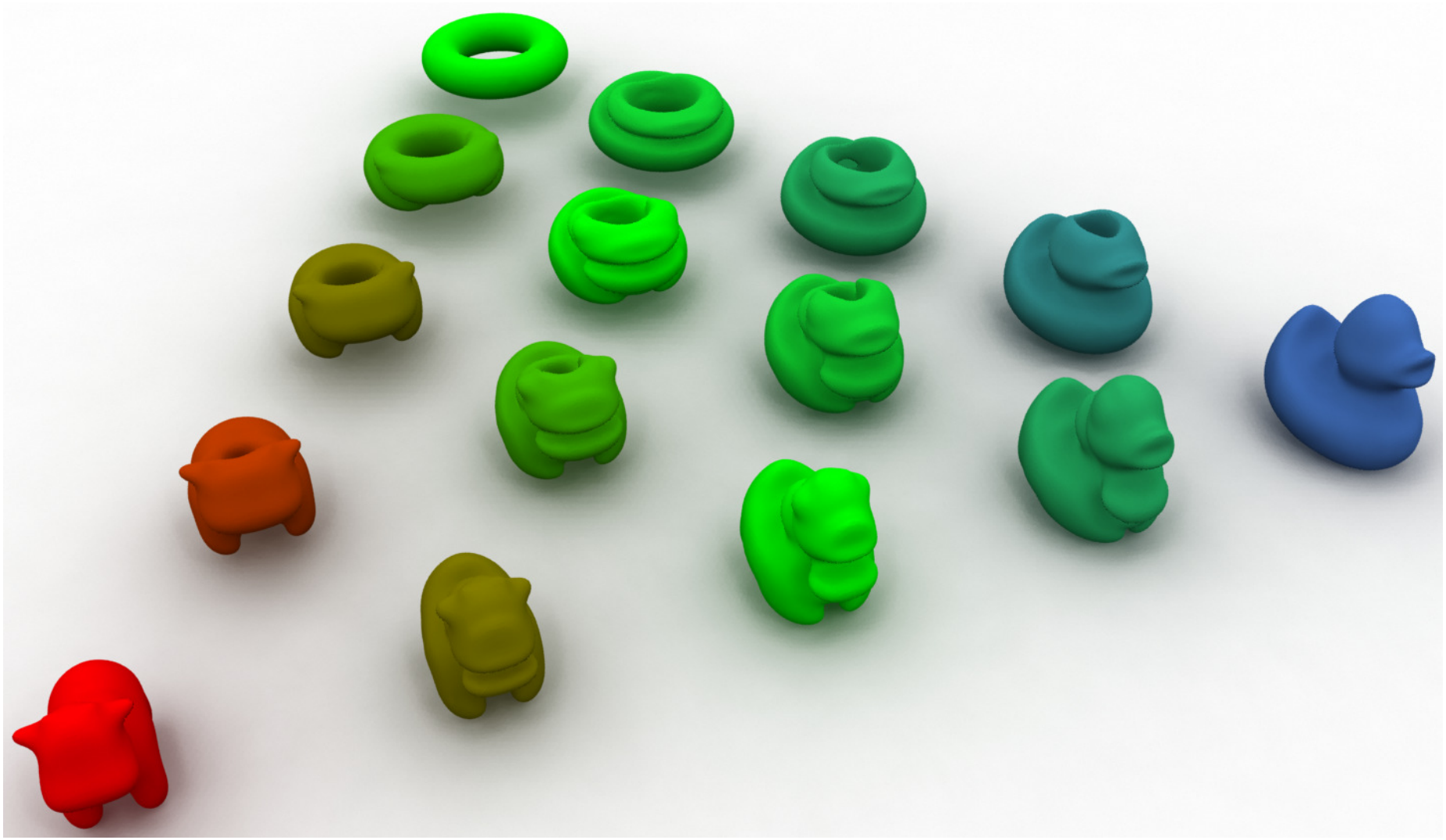
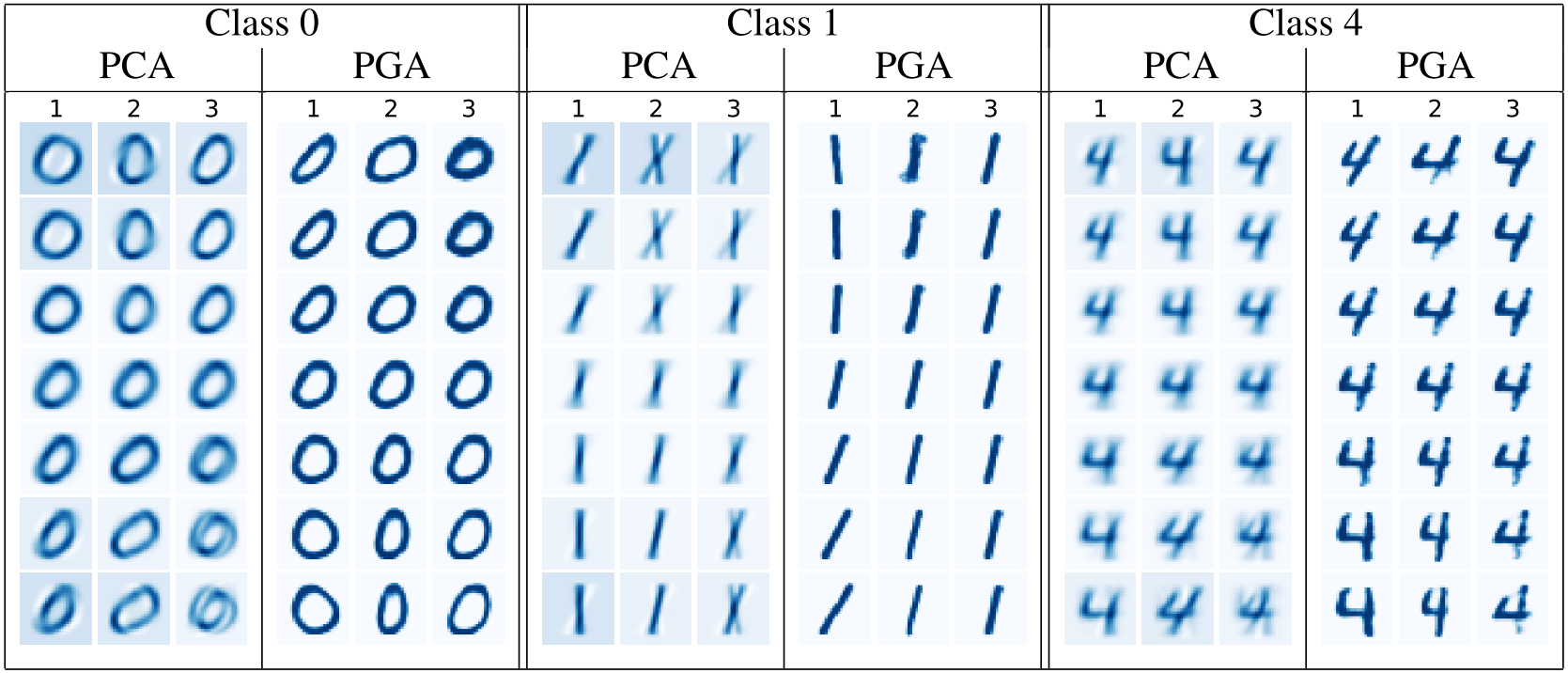
3D Wasserstein barycenter

Shape interpolation [Solomon et al., 2015]



Principal Geodesics Analysis



Geodesic PCA in the Wasserstein space [Bigot et al., 2017]

- Generalization of Principal Component Analysis to the Wassertsein manifold.
- Regularized OT [Seguy and Cuturi, 2015].
- Approximation using Wasserstein embedding [Courty et al., 2017].
- Also note recent Wasserstein Dictionary Learning approaches [Schmitz et al., 2017].

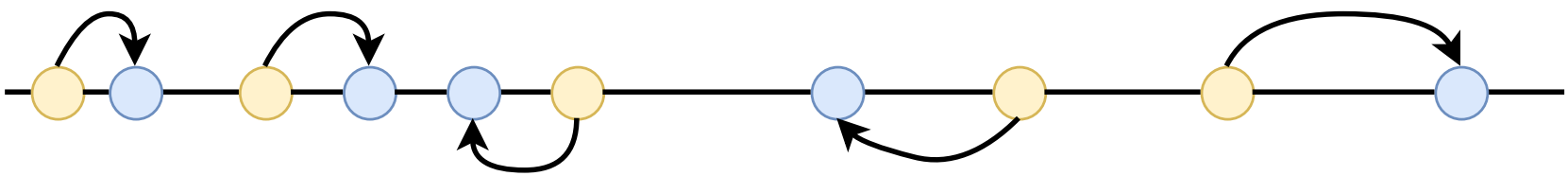
Outline

Special case: 1D distribution

We consider the case where $c(x, y)$ is a strictly convex and increasing function of $|x - y|$.

- if $x_1 < x_2$ and $y_1 < y_2$, it is easy to check that $c(x_1, y_1) + c(x_2, y_2) < c(x_1, y_2) + c(x_2, y_1)$
- As such, any optimal transport plan respects the ordering of the elements, and the solution is given by the monotone rearrangement of μ_1 onto μ_2

This gives very simple algorithm to compute the transport in $O(N \log N)$, by sorting both x_i and y_i and summing the absolute values of differences.



Special case: 1D distribution

Consider the cumulative distribution functions F_μ associated to the μ distribution.

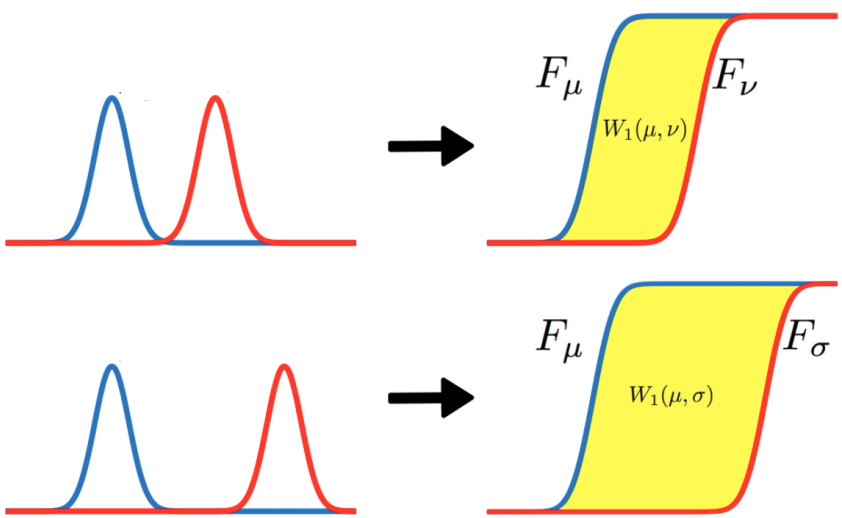
- It is defined such that $F_\mu(t) = \mu(-\infty, t]$.

We will note $F_\mu^{-1}(q),\ q \in [0, 1]$ the corresponding generalized inverse distribution (or quantile function)

- defined as $F_\mu^{-1}(q) = \inf\{x \in \mathbb{R} : F_\mu(x) \geq q\}$.

Then,

$$W_1(\mu_s, \mu_t) = \int_0^1 c(F_{\mu_s}^{-1}(q), F_{\mu_t}^{-1}(q))dq$$



Sliced-Wassertein on $\mathbb{R}^d$

Wasserstein on $\mathbb{R}$:

$$\forall p \geq 1, \forall \mu, \nu \in \mathcal{P}_p(\mathbb{R}),\ W_p^p(\mu, \nu) = \int_0^1 |F_\mu^{-1}(u) - F_\nu^{-1}(u)|^p \ \mathrm{d}u \tag{4}$$

This property gives a method for computing Wasserstein in higher dimensions ($n > 1$).

The principle is simple. Slice the distribution along lines, project the measures onto it and compute $1D$ Wasserstein along those projections.

Sliced-Wasserstein [Rabin et al., 2011b]

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

$$SW_p^p(\mu, \nu) = \int_{S^{d-1}} W_p^p(P_\#^\theta \mu, P_\#^\theta \nu) \ \mathrm{d}\lambda(\theta), \tag{5}$$

where $P^\theta(x) = \langle x, \theta \rangle$, λ uniform measure on S^{d-1}.

Properties:

- Distance
- Topogically equivalent to the Wasserstein distance
- Monte-Carlo approximation in $O(Ln \log n)$

This has been extended to a more genral setting. Consider the Radon transform $\mathcal{R}$:

$$\mathcal{R}(\mu, \theta) = \int_{\mathbb{S}^{d-1}} \mu(\mathbf{x})\delta(t - \theta.\mathbf{x})dx$$

where $t \in \mathbb{R}$ parametrizes the support and $\forall \theta \in \mathbb{S}^{d-1}$ (unit sphere in $\mathbb{R}^d$). Then, the p-sliced Wasserstein distance is given by:

p-sliced Wasserstein distance pSW [Bonneel et al., 2015]

$$pSW_p^p(\mu_s, \mu_t) = \int_{\mathbb{S}^{d-1}} W_p^p(\mathcal{R}(\mu_s, \theta), \mathcal{R}(\mu_t, \theta))d\theta$$

Special cases: Wasserstein on the Circle

Let $\mu, \nu \in \mathcal{P}(S^1)$ where $S^1 = \mathbb{R}/\mathbb{Z}$.

- Parametrize S^1 by $[0, 1[$
- $\forall x, y \in [0, 1[,\ d_{S^1}(x, y) = \min(|x - y|, 1 - |x - y|)$
- For a cost function $c(x, y) = h(d_{S^1}(x, y))$ with $h : \mathbb{R} \to \mathbb{R}^+$ increasing and convex
- $\forall \mu, \nu \in \mathcal{P}(S^1)$, [Rabin et al., 2011a]

$$W_c(\mu, \nu) = \inf_{\alpha \in \mathbb{R}} \int_0^1 h(|F_\mu^{-1}(t) - (F_\nu - \alpha)^{-1}(t)|)\ \mathrm{d}t. \tag{6}$$

- To find α: binary search [Delon et al., 2010]

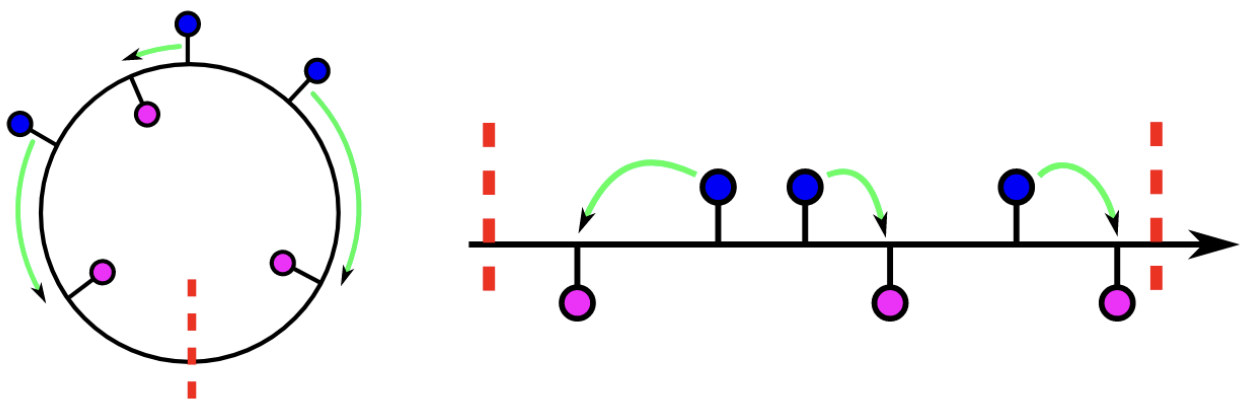


Image from [Rabin et al., 2011a]

Particular Cases

- For $h = \mathrm{Id}$, [Hundrieser et al., 2021]

$$W_1(\mu, \nu) = \int_0^1 |F_\mu(t) - F_\nu(t) - \mathrm{LevMed}(F_\mu - F_\nu)| \, \mathrm{d}t, \tag{7}$$

where

$$\mathrm{LevMed}(f) = \inf \left\{ t \in \mathbb{R}, \ \beta(\{x \in [0,1[, \ f(x) \leq t\}) \geq \frac{1}{2} \right\}. \tag{8}$$

- For $h(x) = x^2$ and $\nu = \mathrm{Unif}(S^1)$,[Bonet et al., 2022]

$$W_2^2(\mu, \nu) = \int_0^1 |F_\mu^{-1}(t) - t - \hat{\alpha}|^2 \, \mathrm{d}t \quad \text{with} \quad \hat{\alpha} = \int x \, \mathrm{d}\mu(x) - \frac{1}{2}. \tag{9}$$

In particular, if $x_1 < \cdots < x_n$ and $\mu_n = \frac{1}{n} \sum_{i=1}^n \delta_{x_i}$, then

$$W_2^2(\mu_n, \nu) = \frac{1}{n} \sum_{i=1}^n x_i^2 - \left(\frac{1}{n} \sum_{i=1}^n x_i \right)^2 + \frac{1}{n^2} \sum_{i=1}^n (n + 1 - 2i) x_i + \frac{1}{12}. \tag{10}$$

Sliced-Wasserstein on the Sphere

The slicing strategy can be extended to manifolds ! In this case slices are geodesics of the considered manifold. Example on the Sphere [Bonet et al., 2022]:

- Great circle: Intersection between 2-plane and S^{d-1}
- Parametrize 2-plane by the Stiefel manifold

$$\mathbb{V}_{d,2} = \{U \in \mathbb{R}^{d\times 2},\ U^T U = I_2\}$$

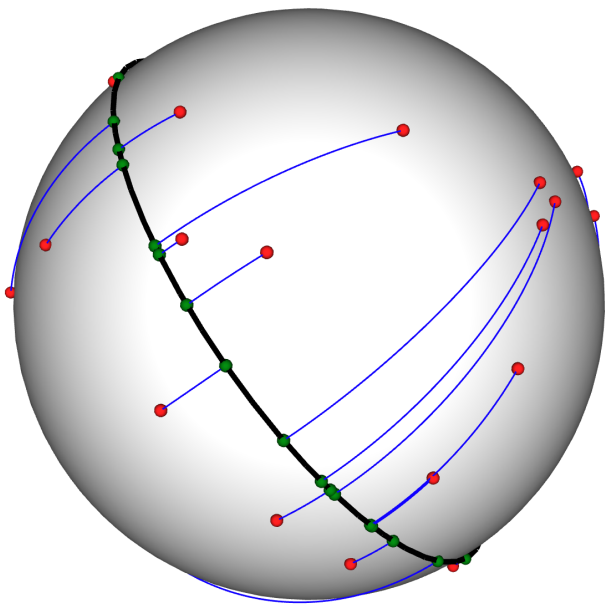
- Projection on great circle C: For a.e. $x \in S^{d-1}$,

$$P^C(x) = \operatorname*{argmin}_{y\in C}\ d_{S^{d-1}}(x, y),$$

where $d_{S^{d-1}}(x, y) = \arccos(\langle x, y\rangle)$.

- For $U \in \mathbb{V}_{d,2}$, $C = \operatorname{span}(UU^T) \cap S^{d-1}$,

$$P^U(x) = U^T \operatorname*{argmin}_{y\in C} d_{S^{d-1}}(x, y)$$
$$= \frac{U^T x}{\|U^T x\|_2}.$$



Special case: transport between Gaussians

In the case where $\mu_s \sim \mathcal{N}(\mathbf{m}_1, \Sigma_1)$ and $\mu_t \sim \mathcal{N}(\mathbf{m}_2, \Sigma_2)$ the Wasserstein distance with $c(\mathbf{x}, \mathbf{y}) = \|\mathbf{x} - \mathbf{y}\|_2^2$ reduces to:

W_2^2 between Gaussians

$$W_2^2(\mu_s, \mu_t) = ||\mathbf{m}_1 - \mathbf{m}_2||_2^2 + \mathcal{B}(\Sigma_1, \Sigma_2)^2$$

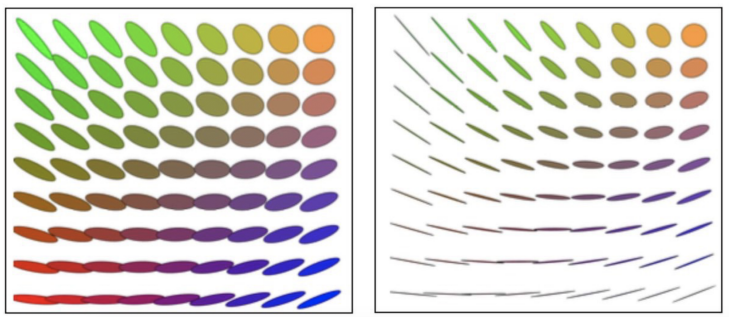
where $\mathbb{B}(,)$ is the so-called Bures metric:

$$\mathcal{B}(\Sigma_1, \Sigma_2)^2 = \text{trace}(\Sigma_1 + \Sigma_2 - 2(\Sigma_1^{1/2}\Sigma_2\Sigma_1^{1/2})^{1/2}).$$

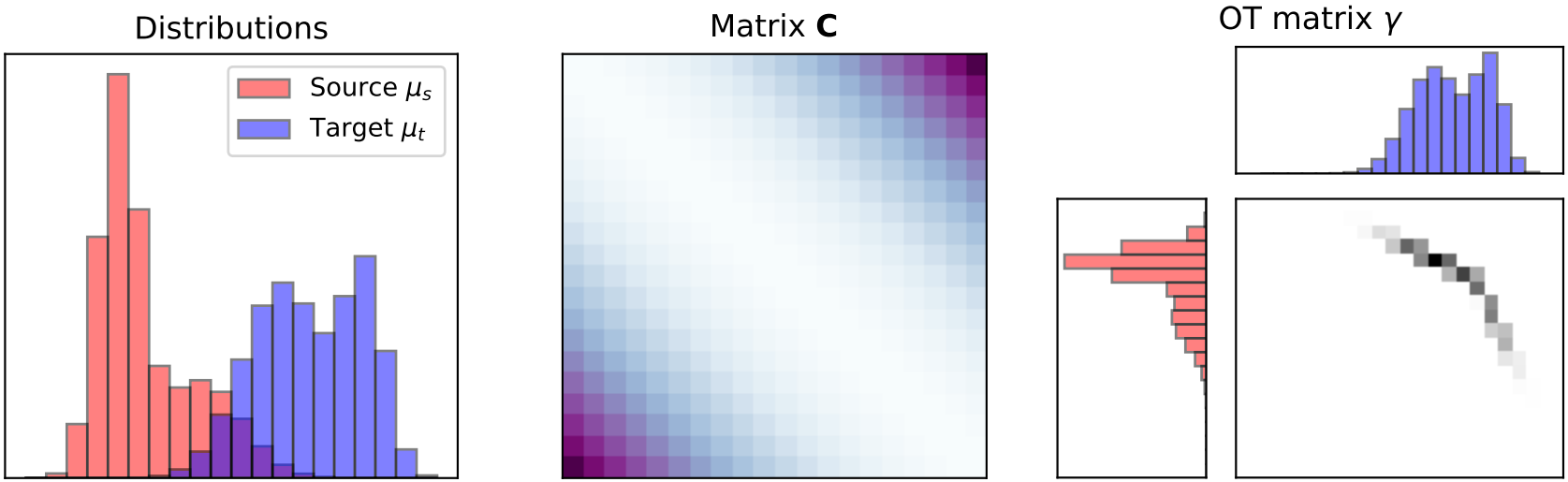
The optimal map T is given by

$$T(\mathbf{x}) = \mathbf{m}_2 + A(\mathbf{x} - \mathbf{m}_1)$$

with $A = \Sigma_1^{-1/2}(\Sigma_1^{1/2}\Sigma_2\Sigma_1^{1/2})^{1/2}\Sigma_1^{-1/2}$



Optimal transport with discrete distributions



OT Linear Program

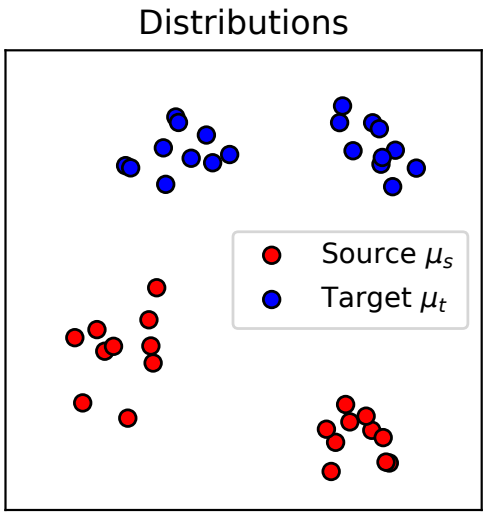
$$\gamma_0 = \underset{\gamma \in \mathcal{P}}{\operatorname{argmin}} \quad \left\{ \langle \gamma, \mathbf{C} \rangle_F = \sum_{i,j} \gamma_{i,j} c_{i,j} \right\}$$

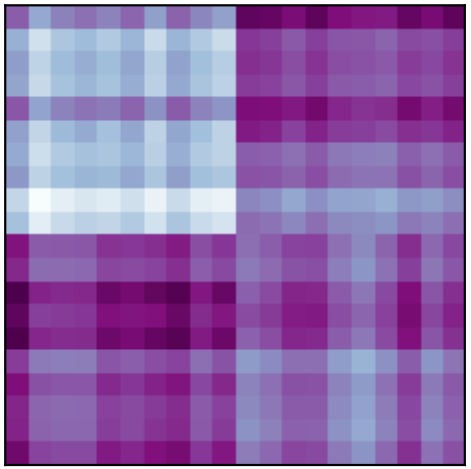
where $\mathbf{C}$ is a cost matrix with $c_{i,j} = c(\mathbf{x}_i^s, \mathbf{x}_j^t)$ and the marginals constraints are

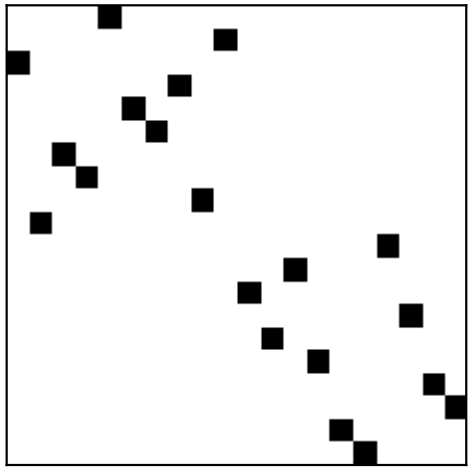
$$\mathcal{P} = \left\{ \gamma \in (\mathbb{R}^+)^{\mathbf{n_s} \times \mathbf{n_t}} \,|\, \gamma \mathbf{1}_{\mathbf{n_t}} = \mu_{\mathbf{s}}, \gamma^{\mathbf{T}} \mathbf{1}_{\mathbf{n_s}} = \mu_{\mathbf{t}} \right\}$$

Solved with Network Flow solver of complexity $O(n^3 \log(n))$.

Optimal transport with discrete distributions







OT Linear Program

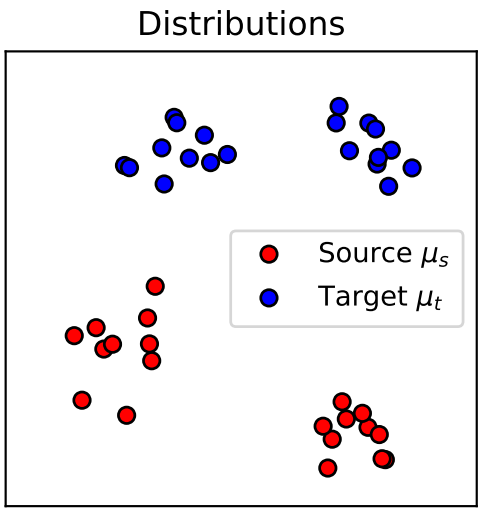
$$\gamma_0 = \underset{\gamma \in \mathcal{P}}{\operatorname{argmin}} \quad \left\{ \langle \gamma, \mathbf{C} \rangle_F = \sum_{i,j} \gamma_{i,j} c_{i,j} \right\}$$

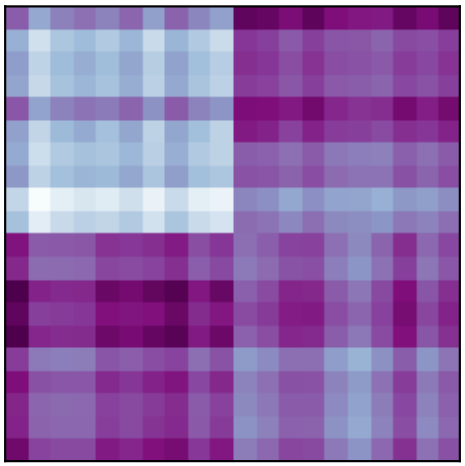
where $\mathbf{C}$ is a cost matrix with $c_{i,j} = c(\mathbf{x}_i^s, \mathbf{x}_j^t)$ and the marginals constraints are

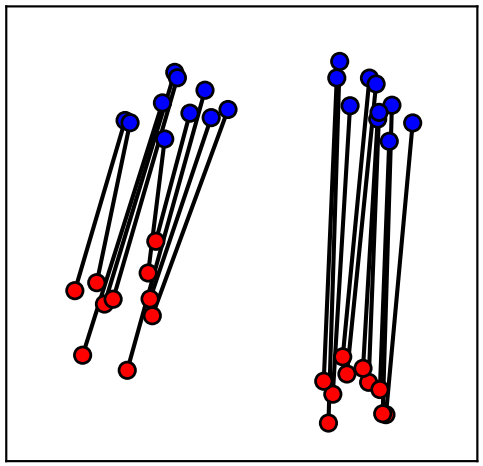
$$\mathcal{P} = \left\{ \boldsymbol{\gamma} \in (\mathbb{R}^+)^{\mathbf{n_s} \times \mathbf{n_t}} \,|\, \boldsymbol{\gamma} \mathbf{1}_{\mathbf{n_t}} = \boldsymbol{\mu_s}, \boldsymbol{\gamma}^{\mathbf{T}} \mathbf{1}_{\mathbf{n_s}} = \boldsymbol{\mu_t} \right\}$$

Solved with Network Flow solver of complexity $O(n^3 \log(n))$.

Optimal transport with discrete distributions







OT Linear Program

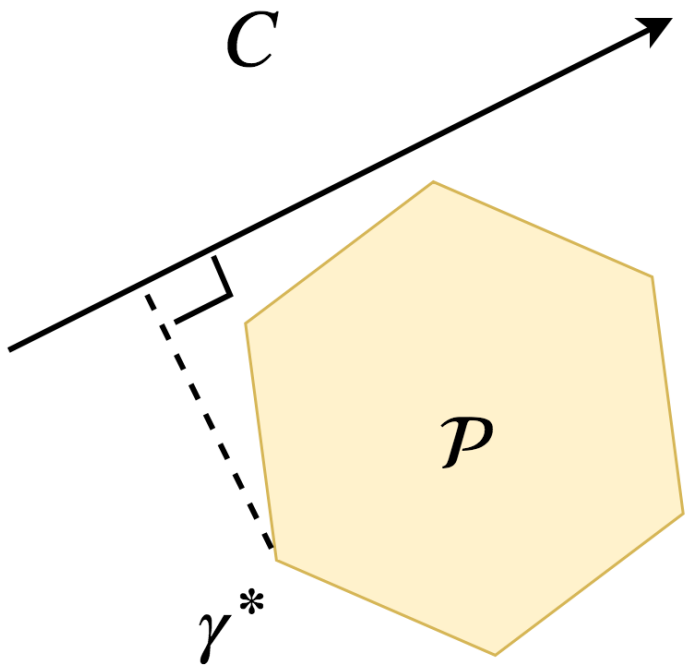
$$\boldsymbol{\gamma}_0 = \underset{\boldsymbol{\gamma} \in \mathcal{P}}{\operatorname{argmin}} \quad \left\{ \langle \boldsymbol{\gamma}, \mathbf{C} \rangle_F = \sum_{i,j} \gamma_{i,j} c_{i,j} \right\}$$

where $\mathbf{C}$ is a cost matrix with $c_{i,j} = c(\mathbf{x}_i^s, \mathbf{x}_j^t)$ and the marginals constraints are

$$\mathcal{P} = \left\{ \boldsymbol{\gamma} \in (\mathbb{R}^+)^{\mathbf{n_s} \times \mathbf{n_t}} \,|\, \boldsymbol{\gamma} \mathbf{1}_{\mathbf{n_t}} = \boldsymbol{\mu_s}, \boldsymbol{\gamma}^{\mathbf{T}} \mathbf{1}_{\mathbf{n_s}} = \boldsymbol{\mu_t} \right\}$$

Solved with Network Flow solver of complexity $O(n^3 \log(n))$.

Optimal transport with discrete distributions



- $\mathcal{P}$ is the Birkhoff polytope
- No unique solution in some cases, numerical instabilities
- Not differentiable !

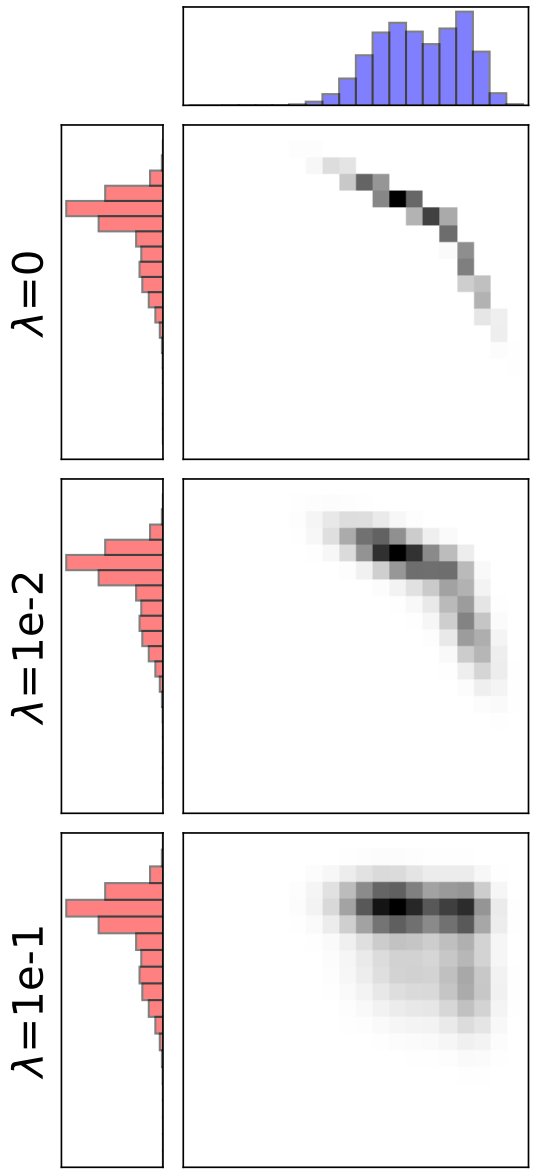
$$\gamma_0^\lambda = \underset{\gamma \in \mathcal{P}}{\operatorname{argmin}} \quad \langle \gamma, \mathbf{C} \rangle_F + \lambda \Omega(\gamma), \qquad (11)$$

Regularization term $\Omega(\gamma)$

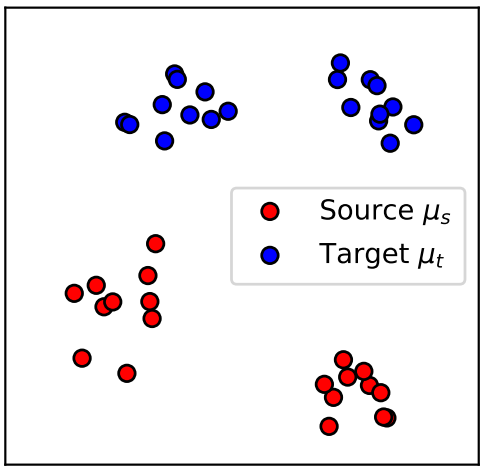
- Entropic regularization [Cuturi, 2013].
- Group Lasso [Courty et al., 2016].
- KL, Itakura Saito, β-divergences, [Dessein et al., 2016].

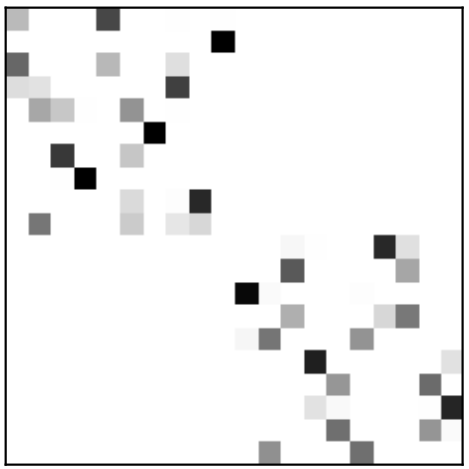
Why regularize?

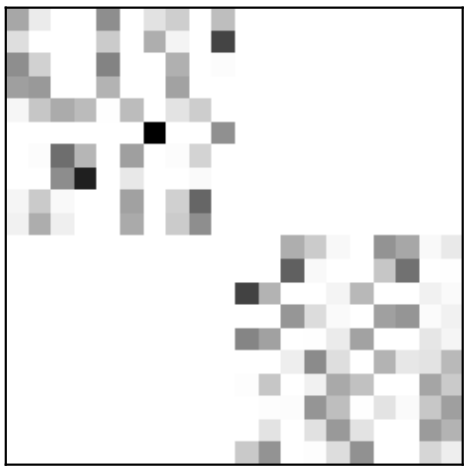
- Smooth the "distance" estimation:
$$W_\lambda(\mu_s, \mu_t) = \langle \gamma_0^\lambda, \mathbf{C} \rangle_F$$
- Encode prior knowledge on the data.
- Better posed problem (convex, stability).
- Fast algorithms to solve the OT problem.



Entropic regularized optimal transport





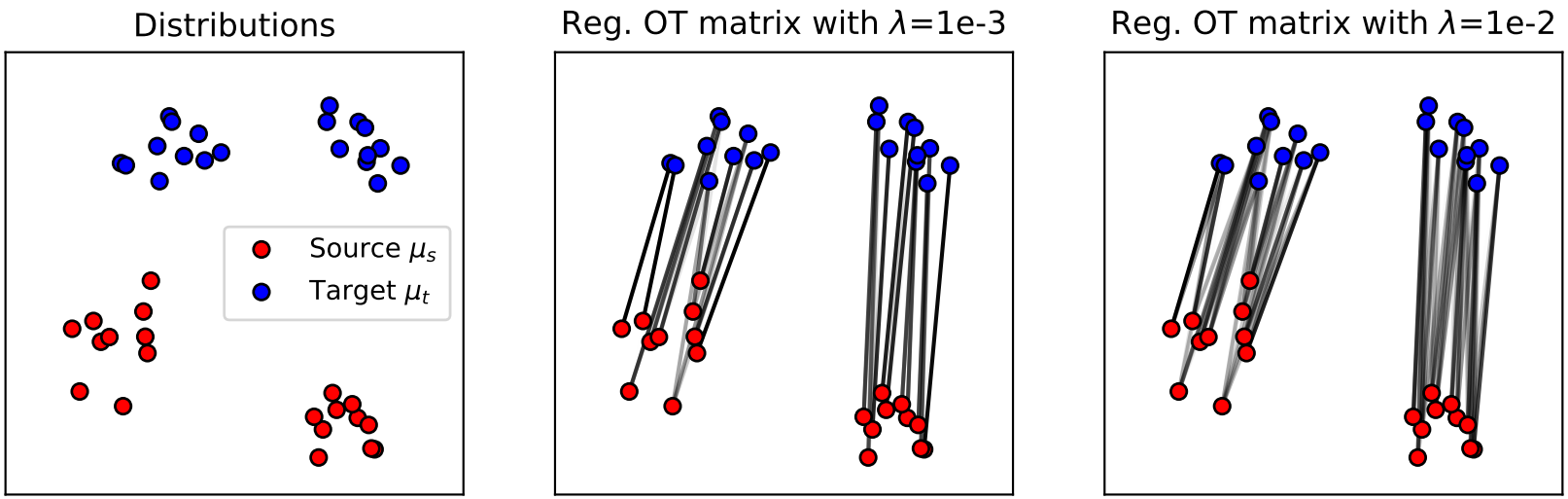


Entropic regularization [Cuturi, 2013]

$$\Omega(\boldsymbol{\gamma}) = \sum_{i,j} \boldsymbol{\gamma}(i,j)(\log \boldsymbol{\gamma}(i,j) - 1)$$

- Regularization with the negative entropy of $\boldsymbol{\gamma}$.

Entropic regularized optimal transport



Entropic regularization [Cuturi, 2013]

$$\Omega(\gamma) = \sum_{i,j} \gamma(i,j)(\log \gamma(i,j) - 1)$$

- Regularization with the negative entropy of γ.

Resolving the entropy regularized problem

Entropy-regularized transport

The solution of entropy regularized optimal transport problem is of the form

$$\boldsymbol{\gamma}_0^\lambda = \text{diag}(\mathbf{u}) \exp(-\mathbf{C}/\lambda) \text{diag}(\mathbf{v})$$

Why ? Consider the Lagrangian of the optimization problem:

$$\mathcal{L}(\boldsymbol{\gamma}, \alpha, \beta) = \sum_{ij} \boldsymbol{\gamma}_{ij} \mathbf{C}_{ij} + \lambda \boldsymbol{\gamma}_{ij} (\log \boldsymbol{\gamma}_{ij} - 1) + \alpha^{\mathbf{T}} (\boldsymbol{\gamma} \mathbf{1}_{n_t} - \mu_s) + \beta^{\mathbf{T}} (\boldsymbol{\gamma}^T \mathbf{1}_{n_s} - \mu_t)$$

$$\begin{aligned} \partial \mathcal{L}(\boldsymbol{\gamma}, \alpha, \beta)/\partial \boldsymbol{\gamma}_{ij} &= \mathbf{C}_{ij} + \lambda \log \boldsymbol{\gamma}_{ij} + \alpha_i + \beta_j \\ \partial \mathcal{L}(\boldsymbol{\gamma}, \alpha, \beta)/\partial \boldsymbol{\gamma}_{ij} = 0 &\implies \boldsymbol{\gamma}_{ij} = \exp(\frac{\alpha_i}{\lambda}) \exp(-\frac{\mathbf{C}_{ij}}{\lambda}) \exp(\frac{\beta_j}{\lambda}) \end{aligned}$$

- Through the **Sinkhorn theorem** $\text{diag}(\mathbf{u})$ and $\text{diag}(\mathbf{v})$ exist and are unique.
- Can be solved by the **Sinkhorn-Knopp** algorithm (implementation in parallel, GPU).

Sinkhorn-Knopp algorithm

The Sinkhorn-Knopp algorithm performs alternatively a scaling along the rows and columns of $\mathbf{K} = \exp(-\frac{\mathbf{C}}{\lambda})$ to match the desired marginals.

Algorithm 1 Sinkhorn-Knopp Algorithm (SK).

Require: $\mathbf{a}, \mathbf{b}, \mathbf{C}, \lambda$

$\mathbf{u}^{(0)} = \mathbf{1}, \mathbf{K} = \exp(-\mathbf{C}/\lambda)$

for i in $1, \dots, n_{it}$ **do**

$\mathbf{v}^{(i)} = \mathbf{b} \oslash \mathbf{K}^\top \mathbf{u}^{(i-1)}$ // Update right scaling

$\mathbf{u}^{(i)} = \mathbf{a} \oslash \mathbf{K}\mathbf{v}^{(i)}$ // Update left scaling

end for

return $\mathbf{T} = \text{diag}(\mathbf{u}^{(n_{it})})\mathbf{K}\text{diag}(\mathbf{v}^{(n_{it})})$

- Complexity $O(kn^2)$, where k iterations are required to reach convergence
- Fast implementation in parallel, GPU friendly
- Convolutive/Heat structure for K [Solomon et al., 2015]

Sinkhorn as Bregman projections

Recalling that the Kullback Leibler (KL) divergence between two distribution is

$$\mathrm{KL}(\boldsymbol{\gamma}, \rho) = \sum_{ij} \boldsymbol{\gamma}_{ij} \log \frac{\boldsymbol{\gamma}_{ij}}{\rho_{ij}} = < \boldsymbol{\gamma}, \log \frac{\boldsymbol{\gamma}}{\rho} >_F,$$

Benamou *et al.* [Benamou et al., 2015] showed that solving for the OT problem is actually a Bregman projection

OT as a Bregman projection

$\boldsymbol{\gamma}^\star$ is the solution of the following Bregman projection

$$\boldsymbol{\gamma}^\star = \underset{\boldsymbol{\gamma} \in \mathcal{P}}{\operatorname{argmin}} \, \mathrm{KL}(\boldsymbol{\gamma}, \zeta), \tag{12}$$

where $\zeta = \exp(-\frac{C}{\lambda})$.

- Sinkhorn in this case is an iterative projection scheme, with alternative projections on marginal constraints.
- Generalizes well for barycenters computation

Dual formulation of optimal transport

- Yet, solving for γ is impractical to intractable when dealing with high-dimensional distributions
- especially if one is interested in computing the gradients of the Wasserstein distance
- Other solving strategies should be taken into consideration
- Recalling that any LP problem can be turnt into its dual form:

$$\begin{array}{rrcl} \textbf{primal form}: & & & \\ \text{minimize} & z & = & \mathbf{c}^T\mathbf{x}, \\ \text{so that} & \mathbf{A}\mathbf{x} & = & \mathbf{b} \\ \text{and} & \mathbf{x} & \geq & \mathbf{0} \end{array} \quad \Bigg| \quad \begin{array}{rrcl} \textbf{dual form}: & & & \\ \text{maximize} & \tilde{z} & = & \mathbf{b}^T\mathbf{y}, \\ \text{so that} & \mathbf{A}^T\mathbf{y} & \leq & \mathbf{c} \end{array}$$

- Weak duality: $\tilde{z}$ is a lower bound of z, Strong duality $\tilde{z} = z$
- Strong duality is usually achieved via Farkas Theorem

Duality: general case with continuous distributions

We now introduce two functions scalar functions ϕ and ψ (also known as Kantorovich potentials) that will act as our dual variables. Then, we consider the optimal problem is equivalent (by the Rockafellar-Fenchel theorem) to:

$$\max_{\phi,\psi} \left\{ \int \phi d\mu_s + \int \psi d\mu_t \;\; | \;\; \phi(x) + \psi(y) \leq c(x,y) \right\} \tag{13}$$

Note that the marginal constraint has been turned into an equality constraint on ϕ and ψ

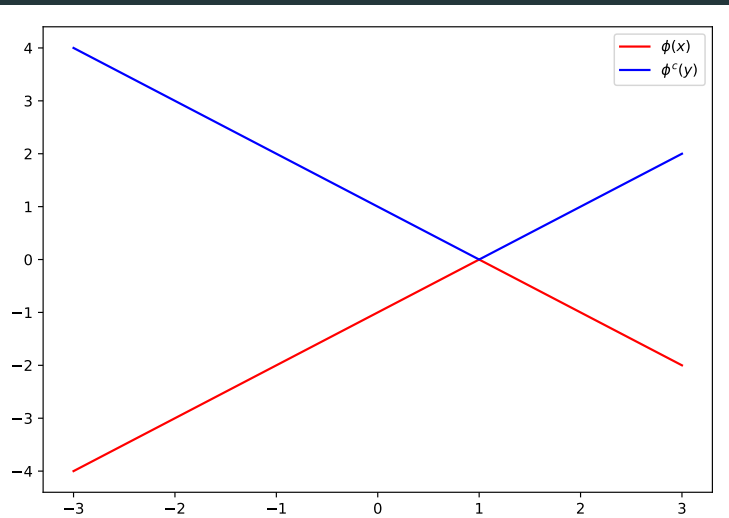
Introducing the *c-transform* (or *c-conjugate*) H^c which is in spirit close to a Legendre transform:

$$\phi^c \stackrel{\text{def}}{=} H^c(\phi) = \inf_x c(x,y) - \phi(x) \tag{14}$$

then the following problem is equivalent:

$$\max_{\phi} \left\{ \int \phi d\mu_s + \int \phi^c d\mu_t \;\; | \;\; \phi(x) + \phi^c(y) \leq c(x,y) \right\} \tag{15}$$

Case $c(x, y) = |x - y|$ (a.k.a W_1^1)



Whenever $c(x, y) = |x - y|$, then:

- existence of a solution but not unique
- For any $\phi \in \text{Lip}^1$ (set of 1-Lipschitz functions), we have $\phi^c(x) = -\phi(x)$

The optimal transport problem then amounts to find $\phi \in \text{Lip}^1$ as

$$\sup_{\phi \in \text{Lip}^1} \int \phi d(\mu_s - \mu_t) = \sup_{\phi \in \text{Lip}^1} \mathop{\mathbb{E}}_{\mathbf{x} \sim \mu_s} [\phi(x)] - \mathop{\mathbb{E}}_{\mathbf{y} \sim \mu_t} [\phi(y)] \tag{16}$$

- also known as **Kantorovich-Rubinstein duality**
- ϕ can be learnt as a neural network constrained to the set Lip^1, see next section on GAN

Case $c(x, y) = |x - y|^2/2$ (a.k.a W_2^2)

Whenever the cost is quadratic, $c(x, y) = |x - y|^2/2$, then:

- $T(x)$ the transport mapping exists and is unique
- More remarkably, it is a gradient of a convex functions $\Phi(x)$

$$T(x) = x - \nabla\phi(x) = \nabla(\frac{x^2}{2} - \phi(x)) = \nabla(\Phi(x)) \tag{17}$$

Brenier's Theorem

Let $\mu, \nu \in \mathcal{P}_2(\mathbb{R}^d)$, μ absolutely continuous with respect to the Lebesgue measure. Then, the optimal coupling γ^* is unique and of the form $\gamma^* = (Id, \nabla\Phi)_{\#}\mu$ with Φ a convex function.

- can be optimized for instance with Input Convex Neural Networks (ICNN) [Amos et al., 2017] to model the convex functions

Dual: empirical version

In the case when we have access to discrete distributions, μ_s (resp. μ_t) is characterized by a set of locations $\mathbf{X^s}$ and masses $\mathbf{a} \in \mathbb{R}^{n^s}$ (resp. $\mathbf{X^t}$ and $\mathbf{b} \in \mathbb{R}^{n^t}$)

Discrete dual version of OT

$$W(\mu_s, \mu_t) = \max_{\alpha \in \mathbb{R}^{n^s}, \beta \in \mathbb{R}^{n^t}, \alpha_i + \beta_j \leq c(\mathbf{X^s_i}, \mathbf{X^t_j})} \alpha^T \mathbf{a} + \beta^T \mathbf{b} \tag{18}$$

i.e. find a scalar values per sample

Regularized case

Adding regularization to the original problem turns the dual computation to an unconstrained problem !

In the case of entropy regularization, *i.e.*

$$W_\lambda(\mu_s, \mu_t) = \min_{\gamma \in \mathcal{P}} \quad \langle \gamma, \mathbf{C} \rangle_F + \lambda \Omega(\gamma) \text{ with } \Omega(\gamma) = \sum_{i,j} \gamma(i,j) \log \gamma(i,j),$$

the dual now reads (in a discrete settings, measures are collections of Diracs):

$$\max_{\alpha, \beta} \alpha^T \mu_s + \beta^T \mu_t - \frac{1}{\lambda} \exp(\frac{\alpha}{\lambda})^T \mathbf{K} \exp(\frac{\beta}{\lambda}) \tag{19}$$

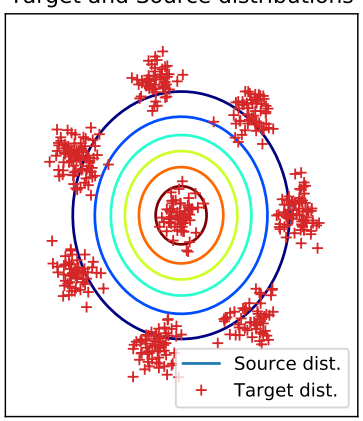
with $\mathbf{K} = \exp(-\frac{\mathbf{C}}{\lambda})$.

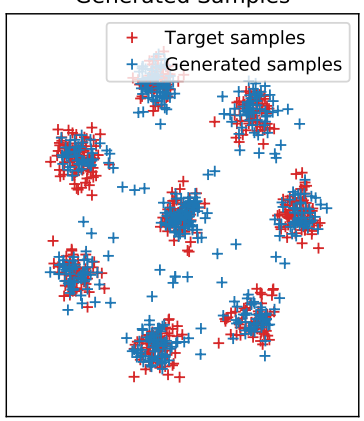
Remark: The Sinkhorn algorithm is a gradient ascent on the dual variables !

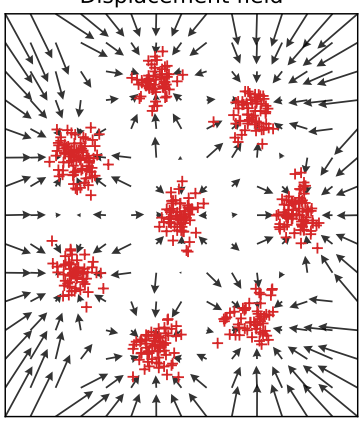
Regularized case

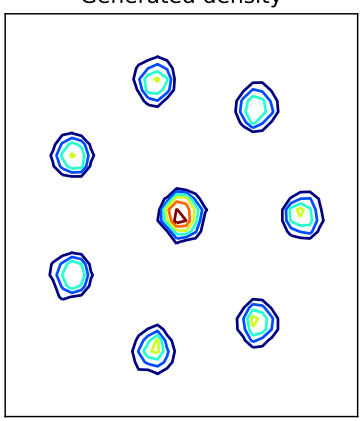
With this unconstrained problem, incremental gradients techniques (SGD, SAG) can be used to solve the problem !

- [Genevay et al., 2016] used the semi-dual formulation (one variable is removed by replacing it with its c-transform) int the first stochastic version of Optimal Transport problem
- [Seguy et al., 2017] used the full dual version with entropic and L2 regularizations, together with neural networks to parameterize the problem.









2 ways of minimizing the Wasserstein distance

In machine learning applications, one can be interested in finding distributions that minimize the Wasserstein distance wrt. a reference measure. There are two ways of understanding this:

- case 1: **for a fixed support** $\mathbf{X}$, find the corresponding probability masses $\mathbf{m}$
- case 2: **for a fixed vector of probability masses** $\mathbf{m}$, e.g. uniform distribution, find the corresponding support $\mathbf{X}$

Case 1: fixed support

Recalling the form of the dual

$$W(\mu, \mu_t) = \max_{\alpha \in \mathbb{R}^{n^s}, \beta \in \mathbb{R}^{n^t}, \alpha_i + \beta_j \leq c(\mathbf{x}, \mathbf{x_j^t})} \alpha^T \mathbf{m} + \beta^T \mathbf{b} \tag{20}$$

- $W(\mu, \mu_t)$ is convex wrt. $\mathbf{m}$
- $\partial_{\mathbf{m}} W(\mu, \mu_t) = \alpha^*$
- **Entropy regularized case**: $W_\lambda(\mu, \mu_t)$ is convex and $\nabla_{\mathbf{m}} W_\lambda(\mu, \mu_t) = \lambda \log \mathbf{u}$

Case 2: fixed probability masses $\mathbf{m}$

Recalling the form of the primal problem

$$W_2^2(\mu, \mu_t) = \min_{\boldsymbol{\gamma} \in \mathcal{P}} \quad < \boldsymbol{\gamma}, \mathbf{1_{n^s}} \mathbf{1_{n^t}^T} \mathbf{X}^2 + \mathbf{X^t}^{2T} \mathbf{1_{n^t}} \mathbf{1_{n^s}} - 2\mathbf{X}\mathbf{X^t} > \tag{21}$$

- $W_2^2(\mu, \mu_t)$ decreases if $\mathbf{X} \leftarrow \mathbf{X^t} \boldsymbol{\gamma}^{*T} \text{diag}(\mathbf{m}^{-1})$
- explicit gradient for the regularized case.
- Barycentric interpolation !
- see Rémi next slides

General case: autodifferentiation

Automatic differentiation to the rescue !

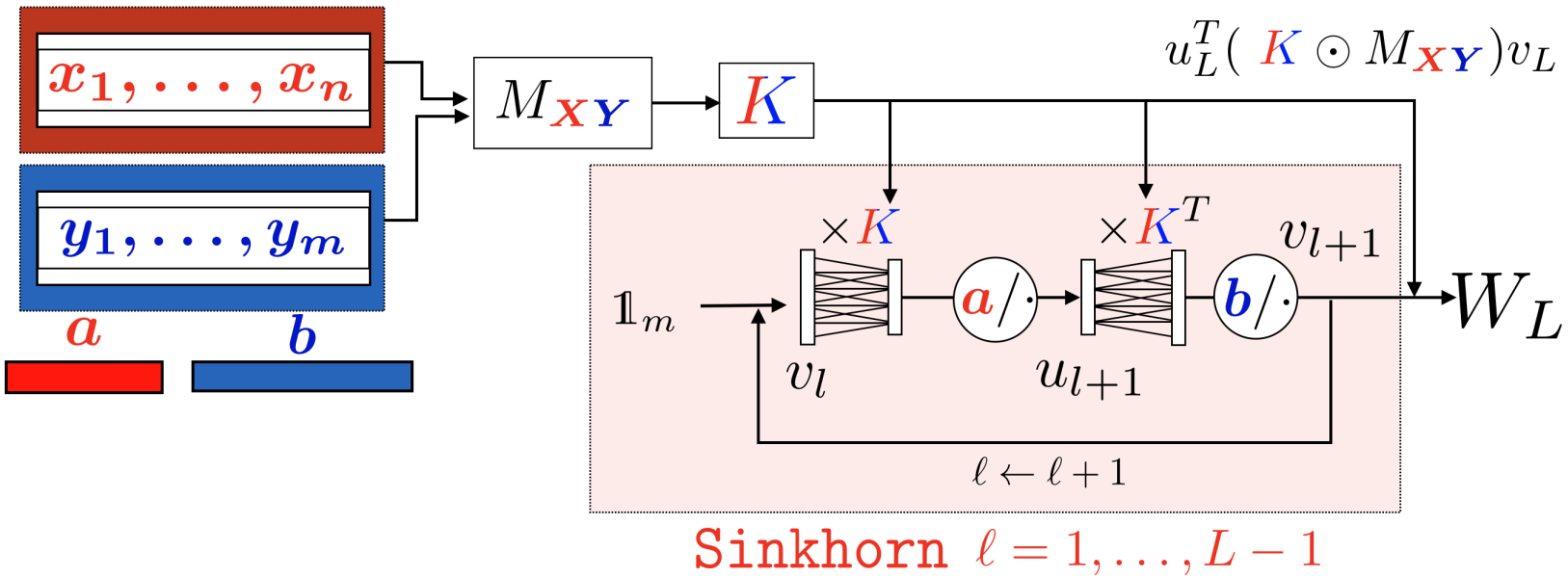


Image from Marco Cuturi

But also consider using the Enveloppe theorem, *i.e.* take the gradient in the optimal solution of the primal problem.

Contents

Outline

Gradient flows

Point of View:

- Define Wasserstein gradient flows
- Analogies with gradient flows in Euclidean space
- For more abstract views, see [Santambrogio, 2017, Ambrosio et al., 2008]
- Talk from Anna Korba https://mathtube.org/lecture/video/wasserstein-gradient-flows-machine-learning

Gradient Flows on $\mathbb{R}^p$

Let $X = \mathbb{R}^p$, d a distance (*e.g.* $d(x, y) = \|x - y\|_2$), $F : X \to \mathbb{R}$.

Goal:

$$\min_x \; F(x)$$

Gradient Flows on $\mathbb{R}^p$

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Goal:

$$\min_x \ F(x)$$

Definition (Gradient Flow on $\mathbb{R}^p$)
A gradient flow is a curve $x : [0, T] \to X$ which decreases as much as possible along the functional F.

i.e. If F is differentiable, x follows the Cauchy problem

$$\begin{cases} \frac{\mathrm{d}x}{\mathrm{d}t}(t) = -\nabla F(x(t)) \\ x(0) = x_0 \end{cases}$$

Gradient Flows on $\mathbb{R}^p$

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Solving the ODE in practice:

- Explicit Euler scheme ($x_k = x(k\tau)$):

$$x_{k+1} = x_k - \tau \nabla F(x_k)$$

- Implicit Euler scheme:

$$\begin{aligned} x_{k+1} = x_k - \tau \nabla F(x_{k+1}) &\iff 0 = \frac{x_{k+1} - x_k}{\tau} + \nabla F(x_{k+1}) \\ &\iff x_{k+1} \in \operatorname*{argmin}_{x \in X} \frac{\|x - x_k\|_2^2}{2\tau} + F(x) \\ &\iff x_{k+1} = \operatorname{prox}_{\tau F}(x_k) \end{aligned}$$

- Any ODE solver (Runge-Kutta...)

Other characterization

See [Santambrogio, 2017, Ambrosio et al., 2008]

- Energy Dissipation Equality (EDE):

$$\begin{aligned} &\frac{\mathrm{d}x}{\mathrm{d}t}(t) = -\nabla F(x(t)) \iff \forall 0 \leq s < t \leq 1, \\ &F(x(s)) - F(x(t)) = \int_s^t \left(\frac{1}{2}|x'(u)|^2 + \frac{1}{2}|\nabla F(x(u))|^2 \right) \mathrm{d}u, \end{aligned} \tag{22}$$

  where (speed)

$$|x'(t)| = \lim_{h \to 0} \frac{d\big(x(t+h), x(t)\big)}{h}$$

  and (descending slope)

$$|\nabla F|(x) = \limsup_{y \to x} \frac{|F(y) - F(x)|}{d(x,y)}.$$

- Evolution Variational Inequality (EVI): For F λ-geodesically convex,

$$x'(t) \in \partial F(x(t)) \iff \forall y \in X, \ \frac{\mathrm{d}}{\mathrm{d}t}\frac{1}{2}|x(t) - y|^2 \leq F(y) - F(x(t)) - \frac{\lambda}{2}|x(t) - y|^2 \tag{23}$$

JKO Scheme

Let $\mathcal{P}_2(\mathbb{R}^p) = \{\mu \in \mathcal{P}(\mathbb{R}^p),\ \int \|x\|^2 \,\mathrm{d}\mu(x) < +\infty\}$.

Define Gradient Flows in $(\mathcal{P}_2(\mathbb{R}^p), W_2)$ via the JKO Scheme [Jordan et al., 1998]: Let $F : \mathcal{P}_2(\mathbb{R}^p) \to \mathbb{R}$, $\mu_0 \in \mathcal{P}_2(\mathbb{R}^p)$,

$$\forall k \geq 0,\ \mu_{k+1}^\tau \in \underset{\mu \in \mathcal{P}_2(\mathbb{R}^p)}{\operatorname{argmin}} \ \frac{W_2^2(\mu, \mu_k^\tau)}{2\tau} + F(\mu) = \mathrm{JKO}_{\tau F}(\mu_k^\tau) \tag{24}$$

Define a piecewise constant interpolation μ^τ, *i.e.*

$$\forall t \in [k\tau, (k+1)\tau[,\ \mu_t^\tau = \mu_k^\tau$$

Wasserstein gradient flows: $t \mapsto \mu_t$ such that, for $\mu^\tau \xrightarrow[\tau \to 0]{} \mu$.

(also called (generalized) minimizing movement [Bonnotte, 2013, Liutkus et al., 2019])

Gradient Flow in $(\mathcal{P}_2(\mathbb{R}^d), W_2)$:

Iterated Minimization scheme (JKO Scheme) [Jordan et al., 1998]:

$$\mu_{k+1}^{\tau} \in \underset{\mu \in \mathcal{P}_2(\mathbb{R}^d)}{\operatorname{argmin}} \frac{1}{2\tau} W_2^2(\mu, \mu_k^{\tau}) + F(\mu)$$

Examples

- $F(\mu) = \int \rho(x) \log \rho(x) \, \mathrm{d}x + \int V(x)\rho(x)\mathrm{d}x$ if $\mathrm{d}\mu = \rho \mathrm{dLeb}$
  Solution in the limit $\tau \to 0$ to the PDE: (Fokker-Planck)

$$\partial_t \rho_t = \operatorname{div}(\rho_t \nabla V) + \Delta \rho_t$$

- $F(\mu) = \frac{1}{2} SW_2^2(\mu, \nu) + \lambda \mathcal{H}(\mu)$ [Bonnotte, 2013, Liutkus et al., 2019]
- $F(\mu) = \frac{1}{2} MMD^2(\mu, \nu)$ [Arbel et al., 2019]
- $F(\mu) = \frac{1}{2} \mathrm{KSD}^2(\mu, \nu)$ [Korba et al., 2021]

- If an associated SDE is known, simulate from it
  [Liu et al., 2021, Liutkus et al., 2019, Arbel et al., 2019, Korba et al., 2021]

Examples

Let $F(\mu) = \int V(x)\rho(x)\mathrm{d}x + \int \log(\rho(x))\rho(x)\mathrm{d}x$,

Gradient Flow solution of:

$$\partial_t \rho_t = \mathrm{div}(\rho_t \nabla V) + \Delta \rho_t$$

Associated SDE (Langevin Equation):

$$\mathrm{d}X_t = -\nabla V(X_t)\mathrm{d}t + \sqrt{2}\ \mathrm{d}W_t$$

First Algorithms of Resolution of WGFs

If SDE is unknow, need specific numerical methods to solve for Wasserstein Gradient Flows by the JKO Scheme:

- By approximating W_2:
  - By the entropic regularized OT problem + Dykstra's algorithm + $\mu = \sum_{i=1}^n \rho_i \delta_{x_i}$, $(x_i)_i$ grid [Peyré, 2015, Carlier et al., 2017]

$$\forall k,\ \mu_{k+1}^\tau \in \underset{\mu \in \mathcal{P}_2(\mathbb{R}^p)}{\operatorname{argmin}} \ \frac{W_\epsilon^2(\mu, \mu_k^\tau)}{2\tau} + F(\mu) \tag{25}$$

  - By the dual formulation of the entropic OT problem [Caluya and Halder, 2019, Frogner and Poggio, 2020]
  - By using SW_2 [Bonet et al., 2021] + Neural networks g^θ and implicit modeling, *i.e.* $\mu = g_{\#}^\theta p_Z$

$$\forall k,\ \mu_{k+1}^\tau \in \underset{\mu \in \mathcal{P}_2(\mathbb{R}^p)}{\operatorname{argmin}} \ \frac{SW_2^2(\mu, \mu_k^\tau)}{2\tau} + F(\mu) \tag{26}$$

- By using the dynamic formulation of the transport + grid discretization [Laborde, 2016, Carrillo et al., 2021]
- JKO-ICNN [Alvarez-Melis et al., 2021, Mokrov et al., 2021, Bunne et al., 2021]

Theorem (Brenier's Theorem)
Let $\mu, \nu \in \mathcal{P}_2(\mathbb{R}^d)$, μ absolutely continuous with respect to the Lebesgue measure. Then, the optimal coupling γ^* is unique and of the form $\gamma^* = (Id, \nabla\varphi)_{\#}\mu$ with φ is a convex function.

- Reformulate the problem as:

$$u_{k+1}^{\tau} \in \underset{u \in \text{cvx}}{\operatorname{argmin}} \ \frac{1}{2\tau} \int \|\nabla u(x) - x\|_2^2 \ \rho_k^{\tau}(x) \mathrm{d}x + F\big((\nabla u)_{\#}\rho_k^{\tau}\big)$$

- Implicitly define $\rho_{k+1}^{\tau} = (\nabla u_{k+1}^{\tau})_{\#}\rho_k^{\tau}$
- Use Input Convex Neural Networks (ICNN) [Amos et al., 2017] to model the convex functions:

$$\theta_{k+1}^{\tau} \in \underset{\theta \in \{\theta, u_\theta \in \text{ICNN}\}}{\operatorname{argmin}} \ \frac{1}{2\tau} \int \|\nabla_x u_\theta(x) - x\|_2^2 \ \rho_k^{\tau}(x) \mathrm{d}x + F\big((\nabla_x u_\theta)_{\#}\rho_k^{\tau}\big)$$

- Backpropagate through gradient

Resolution of Wasserstein Gradient Flows by the JKO Scheme:

- By approximating W_2
- By using the dynamic formulation of the transport + grid discretization [Laborde, 2016, Carrillo et al., 2021]
- JKOICNN: Modeling the Monge map with ICNNs [Alvarez-Melis et al., 2021, Mokrov et al., 2021, Bunne et al., 2021]

$$\theta_{k+1}^{\tau} \in \underset{\tau \in \{\theta, u_\theta \in \mathrm{ICNN}\}}{\operatorname{argmin}} \frac{1}{2\tau} \int \|\nabla u_\theta(x) - x\|_2^2 \, \mathrm{d}\mu_k^{\tau}(x) + F\big((\nabla_x u_\theta)_{\#}\mu_k^{\tau}\big) \tag{27}$$

- Modeling directly the Monge map

$$T_{k+1}^{\tau} \in \underset{T}{\operatorname{argmin}} \frac{1}{2\tau} \int \|T(x) - x\|_2^2 \, \mathrm{d}\mu_k^{\tau}(x) + F(T_{\#}\mu_k^{\tau}) \tag{28}$$

Summary

Optimal transport is a well theoretically grounded ways of comparing probability distributions

- that allows to compare empirical distributions in a non-parametric ways
- that leverages on a ground metric in the embedding space
- for which exist several algorithmic solutions

It comes in several flavours:

- Monge problem: find a mapping (transport map)
- Kantorovich problem: find a coupling (transport plan)

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