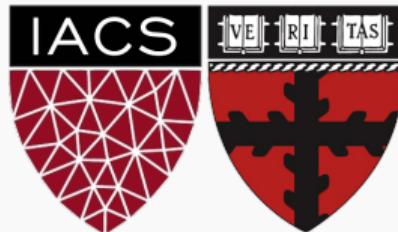


# Advanced Section #2: Optimal Transport

AC 209B: Data Science 2

Javier Zazo

Pavlos Protopapas



# Lecture Outline

---

Historical overview

Definitions and formulations

Metric properties about optimal transport

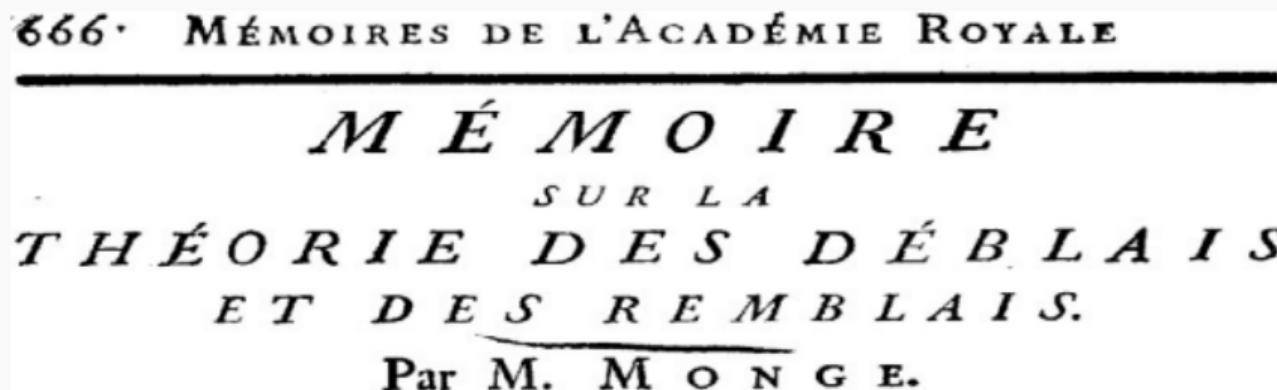
Application I: Supervised learning with Wasserstein Loss

Application II: Domain adaptation

## Historical overview

---

# The origins of optimal transport



- ▶ Gaspard Monge proposed the first idea in 1781.
- ▶ How to move dirt from one place (d'eblais) to another (remblais) with minimal effort?
- ▶ Enunciated the problem of finding a mapping  $F$  between two distributions of mass.
- ▶ Optimization with respect to a displacement cost  $c(x, y)$ .

# Transportation problem I

- Formulated by Frank Lauren Hitchcock in 1941.

## Factories & warehouses example

- Fixed number of factories, each of which produces good at a fixed output rate.
- Fixed number of warehouses, each of which has a fixed storage capacity.
- There is a cost to transport goods from a factory to a warehouse.
- **Goal:** Find the transportation of goods from factory → warehouse with lowest possible cost.

# Transportation problem II: Example

## Factories:

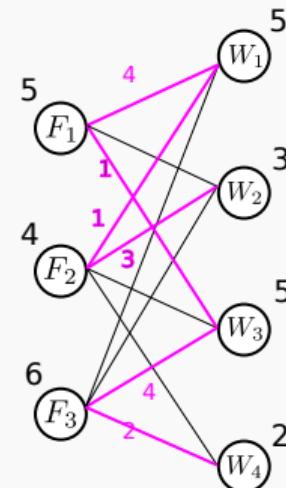
- $F_1$  makes 5 units.
- $F_2$  makes 4 units.
- $F_3$  makes 6 units.

## Warehouses:

- $W_1$  can store 5 units.
- $W_2$  can store 3 units.
- $W_3$  can store 5 units.
- $W_4$  can store 2 units.

## Transportation costs:

	$W_1$	$W_2$	$W_3$	$W_4$
$F_1$	5	4	7	6
$F_2$	2	5	3	5
$F_3$	6	3	4	4



## Transportation problem III:

---

- ▶ One factory can transport product to multiple warehouses.
- ▶ One warehouse can receive product from multiple factories.
- ▶ The Transportation problem can be formulated as an ordinary linear constrained optimization problem (LP):

$$\begin{aligned} \min_{x_{ij}} \quad & 5x_{11} + 4x_{12} + 7x_{13} + 6x_{14} + 2x_{21} + 5x_{22} \\ & + 3x_{23} + 2x_{24} + 6x_{31} + 3x_{32} + 4x_{33} + 4x_{34} \\ \text{s.t.} \quad & x_{11} + x_{12} + x_{13} + x_{14} = 5 \\ & x_{21} + x_{22} + x_{23} + x_{24} = 4 \\ & x_{31} + x_{32} + x_{33} + x_{34} = 6 \\ & x_{11} + x_{21} + x_{31} \leq 5 \\ & x_{12} + x_{22} + x_{32} \leq 3 \\ & x_{13} + x_{23} + x_{33} \leq 5 \\ & x_{14} + x_{24} + x_{34} \leq 2 \end{aligned}$$

## Definitions and formulations

---

# Definitions

---

- ▶ Probability simplex:

$$\Delta_n = \left\{ a_i \in \mathbb{R}_+^n \mid \sum_{i=1}^n a_i = 1 \right\}$$

- ▶ Discrete probability distribution:  $\mathbf{p} = (p_1, p_2, \dots, p_n) \in \Delta_n$ .
- ▶ Space  $\mathcal{X}$ : support for the distribution (coordinates vector/array, temperature, etc.).
- ▶ **Discrete measure:** given weights  $\mathbf{p} = (p_1, p_2, \dots, p_n)$  and  $\mathbf{x} = (x_1, x_2, \dots, x_n)$  locations,

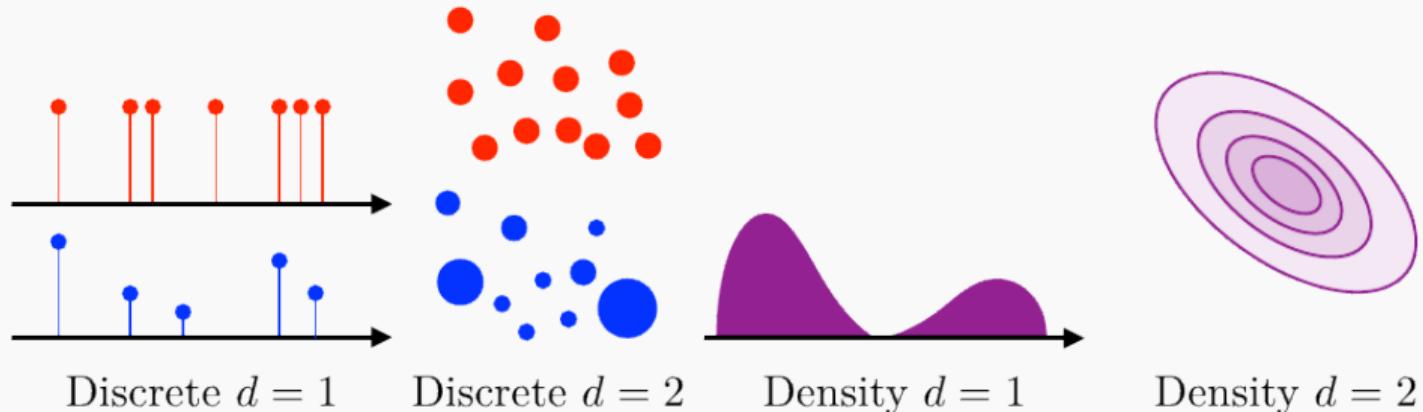
$$\alpha = \sum_i p_i \delta_{x_i}$$

- ▶ **Radon measure:**  $\alpha \in \mathcal{M}(\mathcal{X})$ ,
  - $\mathcal{X}$  is equipped with a distance, integrating it against a continuous function  $f$

$$\int_{\mathcal{X}} f(x) d\alpha(x) \stackrel{\mathbb{R}^d}{=} \int_{\mathcal{X}} f(x) \rho_{\alpha}(x) dx$$

## More definitions

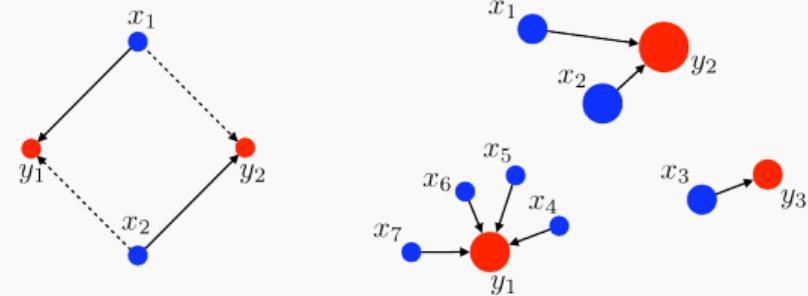
- Set of positive measures:  $\mathcal{M}_+$ , such that  $\int_{\mathcal{X}} f(x)d\alpha(x) \rightarrow \mathbb{R}_+$ .
- **Set of probability measures:**  $\mathcal{M}_+^1$ , such that  $\int_{\mathcal{X}} d\alpha(x) = 1$ .



# Assingment and Monge problems

- ▶  $n$  origin elements (**factories**),
- ▶  $m = n$  destination elements (**warehouses**),
- ▶ we look for a permutation (an assignment in the general case) of elements

$$\min_{\sigma \in \text{Perm}(n)} \quad \frac{1}{n} \sum_{i=1}^n C_{i,\sigma(i)}$$



- ▶ The set of  $n$  discrete elements has  $n!$  possible permutations.
- ▶ Works after Monge, aimed to simplify the problem, such as Hitchcock in 1941, or Kantorovich in 1942.

# Kantorovich relaxation

---

- **Goal:** find a minimal transport plan  $\mathbf{F}$  such that

$$\mathbf{F} \in U(\mathbf{p}, \mathbf{q}) = \{ \mathbf{F} \in \mathbb{R}_+^{n \times n} \mid \mathbf{F}\mathbf{1} = \mathbf{p} \text{ and } \mathbf{F}^T\mathbf{1} = \mathbf{q} \}$$

- $\mathbf{F}\mathbf{1} = \mathbf{p}$  sum the rows of  $\mathbf{F} \rightarrow$  all goods are transported from  $\mathbf{p}$ .
- $\mathbf{F}^T\mathbf{1} = \mathbf{q}$  sum the columns of  $\mathbf{F} \rightarrow$  all goods are received in  $\mathbf{q}$ .
- $\mathbf{p}$  and  $\mathbf{q}$  are probability distributions  $\rightarrow$  mass is conserved and equals 1.

# Relation to linear programming

- The Kantorovich problem is an LP:

$$\boxed{\begin{aligned} L_{\mathbf{C}}(\mathbf{p}, \mathbf{q}) &= \min_{\mathbf{F} \geq 0} \text{tr}(\mathbf{FC}) \\ \mathbf{F}\mathbf{1} &= \mathbf{p}, \quad \mathbf{F}^T\mathbf{1} = \mathbf{q} \end{aligned}} \tag{1}$$

- LP programs can be solved with *simplex method, interior point methods, dual descent methods*, etc. The problem is **convex**.
- One option is to use LP solvers: Clp, Gurobi, Mosek, SeDuMi, CPLEX, ECOS, etc.
- **Spezialized methods exist** (and Python, C, Julia, etc. libraries)
  - Network simplex
  - Approximate methods: Sinkhorn, smoothed versions, etc.

# Kantorovich formulation for arbitrary measures

- Now  $\mathbf{C}$  needs to be a function:

$$c(x, y) : \mathcal{X} \times \mathcal{Y} \rightarrow \mathbb{R}_+$$

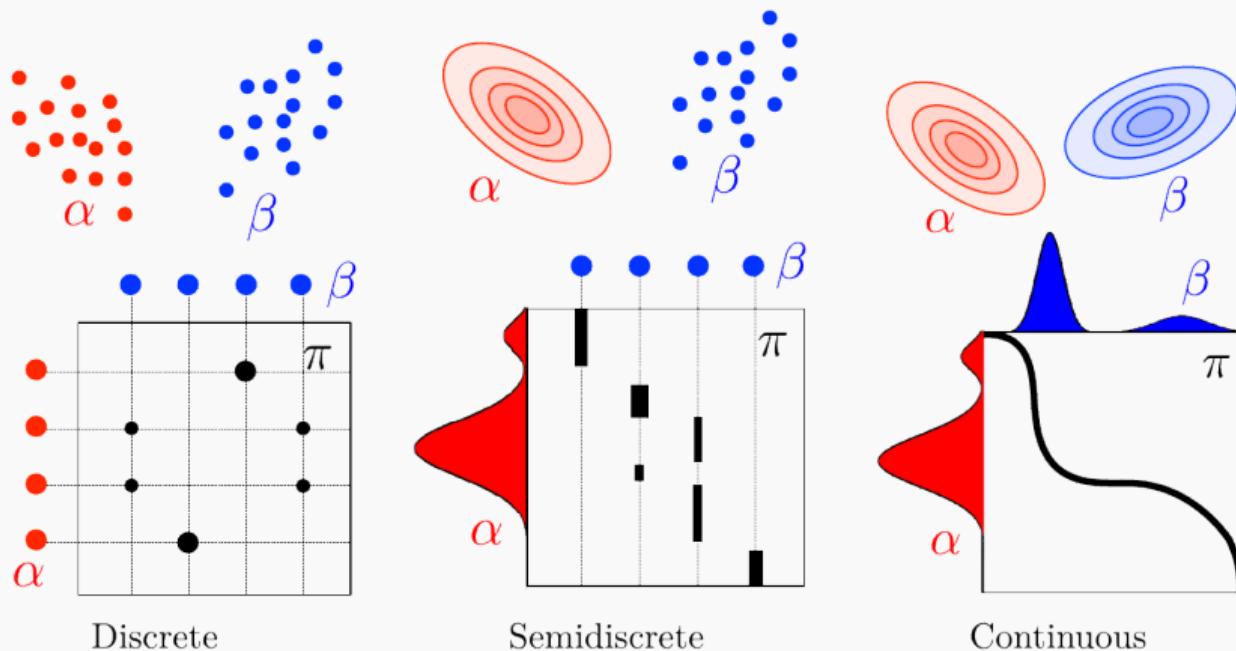
- Discrete measures  $\alpha = \sum_i p_i \delta_{x_i}$  and  $\beta = \sum_i q_i \delta_{y_i}$ :
  - $c(x, y)$  is still a matrix where costs depends on locations of measures.
- For arbitrary probabilistic measures:
  - Define a coupling  $\pi \in \mathcal{M}_+^1(\mathcal{X}, \mathcal{Y}) \rightarrow$  joint probability distribution of  $\mathcal{X}$  and  $\mathcal{Y}$ .

$$U(\alpha, \beta) = \left\{ \pi \in \mathcal{M}_+^1(\mathcal{X}, \mathcal{Y}) \mid P_{\mathcal{X}\sharp}\pi = \alpha \text{ and } P_{\mathcal{Y}\sharp}\pi = \beta \right\}$$

- The continuous problem:

$$\mathcal{L}_c(\alpha, \beta) = \min_{\pi \in U(\alpha, \beta)} \int_{\mathcal{X} \times \mathcal{Y}} c(x, y) d\pi(x, y) = \min_{(X, Y)} \left\{ \mathbb{E}_{(X, Y)}(c(X, Y)) \mid X \sim \alpha, Y \sim \beta \right\}$$

# Example of transport maps for arbitrary measures



## Metric properties about optimal transport

---

# Metric properties of the discrete optimal transport

- Wasserstein distance is also referred as OT, or Earth mover's distance (EMD).

## Discrete Wasserstein distance

Consider  $\mathbf{p}, \mathbf{q} \in \Delta_n$  and

$$\mathbf{C} \in \mathcal{C}_n = \left\{ \mathbf{C} \in \mathbb{R}_+^{n \times n} \mid \mathbf{C} = \mathbf{C}^T, \text{diag}(\mathbf{C}) = 0 \text{ and } \forall(i, j, k) \quad C_{i,j} \leq C_{i,k} + C_{k,j} \right\}.$$

Then,

$$W_p(\mathbf{p}, \mathbf{q}) = L_{\mathbf{C}^p}(\mathbf{p}, \mathbf{q})^{1/p}$$

defines a  **$p$ -Wasserstein** distance on  $\Delta_n$ .

- Recall that  $L_{\mathbf{C}}(\mathbf{p}, \mathbf{q})$  refers to the discrete Kantorovich problem:

$$L_{\mathbf{C}}(\mathbf{p}, \mathbf{q}) = \left\{ \min \text{tr}(\mathbf{F}\mathbf{C}) \mid \mathbf{F} \geq 0, \quad \mathbf{F}\mathbf{1} = \mathbf{p}, \quad \mathbf{F}^T\mathbf{1} = \mathbf{q} \right\}$$

# Proof that p-Wasserstein constitutes a distance

- We need to show **positivity**, **symmetry** and **triangular inequality**.
- Since  $\text{diag}(\mathbf{C}) = 0$ ,  $W_p(\mathbf{p}, \mathbf{p}) = 0$ , and  $\mathbf{F}^* = \text{diag}(\mathbf{p})$ .
- Because of strict positivity of off-diagonal elements,  $W_p(\mathbf{p}, \mathbf{q}) = \text{tr}(\mathbf{CF}) > 0$  for  $\mathbf{p} \neq \mathbf{q}$ .
- Since  $W_p(\mathbf{p}, \mathbf{q}) = \text{tr}(\mathbf{CF})$ , and  $\mathbf{C}$  is symmetric,  $W_p(\mathbf{p}, \mathbf{q}) = W_p(\mathbf{q}, \mathbf{p})$ .
- For triangularity, define  $\mathbf{p}$ ,  $\mathbf{q}$  and  $\mathbf{t}$  and

$$\mathbf{F} = \text{sol}(W_p(\mathbf{p}, \mathbf{q})) \quad \mathbf{G} = \text{sol}(W_p(\mathbf{q}, \mathbf{t})).$$

- For simplicity, assume  $\mathbf{q} > 0$  (detailed proof in the lecture notes). Define

$$\mathbf{S} = \mathbf{F} \text{diag}(1/\mathbf{q}) \mathbf{G} \in \mathbb{R}_+^{n \times n}.$$

- Note that  $\mathbf{F} \in U(\mathbf{p}, \mathbf{t})$ , i.e., is a feasible transport plan:

$$\mathbf{S}\mathbf{1} = \mathbf{F} \text{diag}(1/\mathbf{q}) \underbrace{\mathbf{G}\mathbf{1}}_{\mathbf{q}} = \mathbf{F} \underbrace{\text{diag}(\mathbf{q}/\mathbf{q})}_{\mathbf{1}} = \mathbf{F}\mathbf{1} = \mathbf{p}$$

$$\mathbf{S}^T \mathbf{1} = \mathbf{G}^T \text{diag}(1/\mathbf{q}) \underbrace{\mathbf{F}^T \mathbf{1}}_{\mathbf{q}} = \mathbf{G}^T \underbrace{\text{diag}(\mathbf{q}/\mathbf{q})}_{\mathbf{1}} = \mathbf{G}^T \mathbf{1} = \mathbf{t}$$

# Wasserstein distance for arbitrary measures

## Wasserstein distance for arbitrary measures

Consider  $\alpha(x) \in \mathcal{M}_+^1(\mathcal{X})$ ,  $\beta(y) \in \mathcal{M}_+^1(\mathcal{Y})$ ,  $\mathcal{X} = \mathcal{Y}$ , and for some  $p \geq 1$ ,

- ▶  $c(x, y) = c(y, x) \geq 0$ ;
- ▶  $c(x, y) = 0$  if and only if  $x = y$ ;
- ▶  $\forall (x, y, z) \in \mathcal{X}^3, c(x, y) \leq c(x, z) + c(z, y)$

Then,

$$W_p(\alpha, \beta) = \mathcal{L}_{c^p}(\alpha, \beta)^{1/p}$$

defines a  **$p$ -Wasserstein** distance on  $\mathcal{X}$ .

- ▶ Recall, that the Kantorovich problem for arbitrary measures is given by:

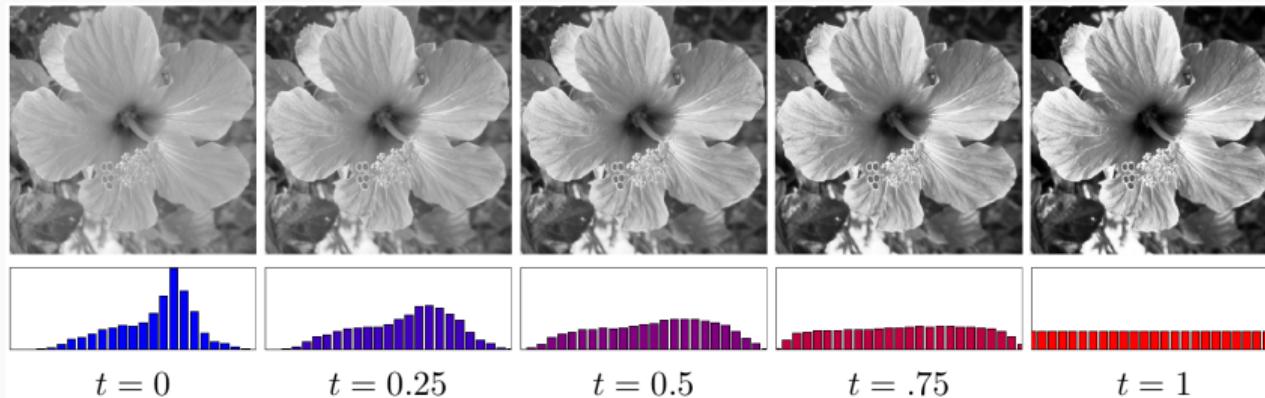
$$\mathcal{L}_c(\alpha, \beta) = \min_{\pi \in U(\alpha, \beta)} \int_{\mathcal{X} \times \mathcal{Y}} c(x, y) d\pi(x, y)$$

# Special cases I

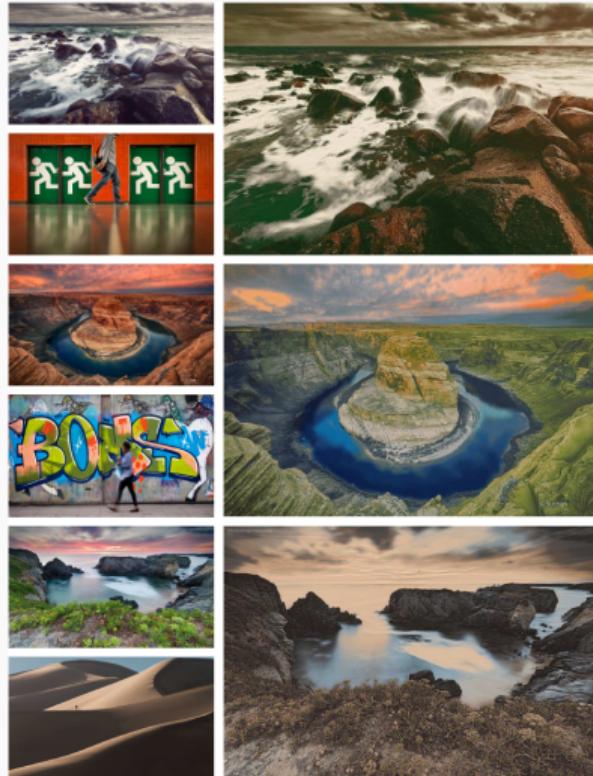
- ▶ Binary cost matrix: If  $\mathbf{C} = \mathbf{1}\mathbf{1}^T - \mathbf{I}$ , then  $L_{\mathbf{C}}(\mathbf{p}, \mathbf{q}) = \|\mathbf{p} - \mathbf{q}\|_1$ .
- ▶ 1D case of empirical measures:
  - $\mathcal{X} = \mathbb{R}; \alpha = \frac{1}{n} \sum_i \delta_{x_i}, \beta = \frac{1}{n} \sum_i \delta_{y_i}$ ;
  - $x_1 \leq x_2, \dots \leq x_n$  and  $y_1 \leq y_2, \dots \leq y_n$  ordered observations.

$$W_p(\mathbf{p}, \mathbf{q})^p = \sum_{i=1}^n |x_i - y_i|^p$$

- ▶ Histogram equalization:



# Color transfer



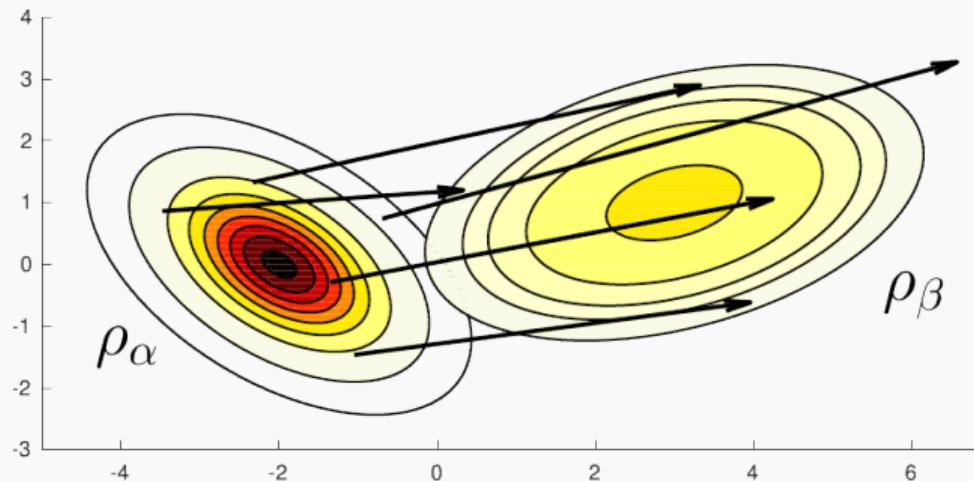
## Special cases II: Distance between Gaussians

- If  $\alpha = \mathcal{N}(\mathbf{m}_\alpha, \Sigma_\alpha)$  and  $\beta = \mathcal{N}(\mathbf{m}_\beta, \Sigma_\beta)$  are two gaussians in  $\mathbb{R}^d$ ,
- The following map:

$$T : x \rightarrow \mathbf{m}_\beta + A(x - \mathbf{m}_\alpha)$$

where  $A = \Sigma_\alpha^{-1/2} (\Sigma_\alpha^{1/2} \Sigma_\beta \Sigma_\alpha^{1/2})^{1/2} \Sigma_\alpha^{-1/2}$  constitutes an optimal transport plan.

- Furthermore,  $W_2^2(\alpha, \beta) = \|\mathbf{m}_\alpha - \mathbf{m}_\beta\|^2 + \text{tr}(\Sigma_\alpha + \Sigma_\beta - 2(\Sigma_\alpha^{1/2} \Sigma_\beta \Sigma_\alpha^{1/2})^{1/2})^2$ .



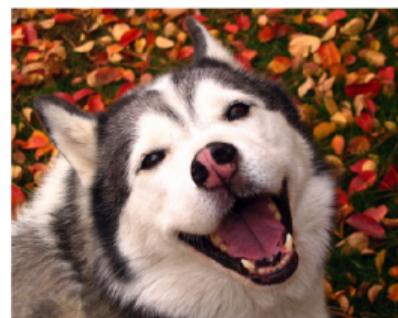
## Application I: Supervised learning with Wasserstein Loss

# Learning with Wasserstein Loss

- ▶ Natural metric on the outputs that can be used to improve predictions.
- ▶ Wasserstein distance provides a natural notion of dissimilarity for probability measures → Can encourage smoothness on the predictions.
  - In ImageNet, 1000 categories may have inherent semantic relationships.
  - Speech recognition systems, output correspond to keywords that also have semantic relations → this correlation can be exploited.



Siberian husky



Eskimo dog

# Semantic relationships: Flickr dataset



(a) **Flickr user tags:** street, parade, dragon; **our proposals:** people, protest, parade; **baseline proposals:** music, car, band.



(b) **Flickr user tags:** water, boat, reflection, sunshine; **our proposals:** water, river, lake, summer; **baseline proposals:** river, water, club, nature.



(a) **Flickr user tags:** zoo, run, 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:** running, country, lake.



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

# Problem setup

---

- ▶ **Goal:** Learn a mapping  $\mathcal{X} \subset \mathbb{R}^d \rightarrow \mathcal{K} \subset \mathcal{Y} = \mathbb{R}_+^K$ , where  $|\mathcal{K}| = K$ .
- ▶ Assume  $\mathcal{K}$  possesses a metric  $d_{\mathcal{K}}(\cdot, \cdot)$ , or ground metric.
- ▶ Learning over a hypothesis space  $\mathcal{H}$  of predictors:  $h_{\theta} : \mathcal{X} \rightarrow \mathcal{Y}$ , param. by  $\theta \in \Theta$ .
  - These can be a logistic regression, output of a NN, etc.
- ▶ Empirical risk minimization:

$$\min_{h_{\theta} \in \mathcal{H}} \mathbb{E} \{l(h_{\theta}(x), y)\} \approx \frac{1}{N} \sum_{i=1}^N l(h_{\theta}(x_i), y_i)$$

## Discrete Wasserstein loss

---

- ▶ Assuming  $h_\theta$  outputs a probability measure (or a discrete probability distribution), and  $\mathbf{y}_i$  corresponds to the one-hot encoding of the label classes,

$$W_c(\alpha, \beta) = \sum_{i=1}^N L_{\mathbf{C}}(h_{\theta(x_i)}, \mathbf{y}_i)$$

where  $\mathbf{C}$  encodes the ground metric given by  $c(x, y)$ .

- ▶ In order to optimize the loss function, how do we compute gradients?
  - Gradients are easy to compute in the dual domain.

# Dual problem formulation

1. Construct the Lagrangian:

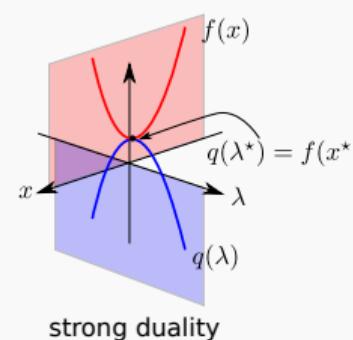
$$L(x, \lambda, \nu) = f(x) + \sum_i \lambda_i g_i(x) + \sum_j \nu_j h_j(x).$$

2. **Dual function:** the minimum of the Lagrangian over  $x$ :

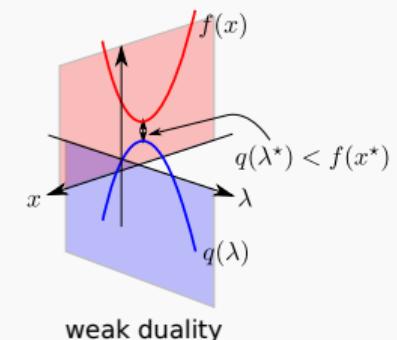
$$q(\lambda, \nu) = \min_x L(x, \lambda, \nu).$$

3. **Dual problem:** maximization of the dual function over  $\lambda_i \geq 0$ :

$$\begin{aligned} & \max_{\lambda \in \mathbb{R}^m, \nu \in \mathbb{R}^p} q(\lambda, \nu) \\ & \text{s.t. } \lambda_i \geq 0 \quad \forall i. \end{aligned} \tag{2}$$



strong duality



weak duality

# Dual problem of the discrete Kantorovich problem

## Dual of the discrete Kantorovich problem

Given  $\mathbf{p} \in \mathbb{R}^n$ ,  $\mathbf{q} \in \mathbb{R}^n$  and  $\mathbf{C} \in \mathbb{R}^{n \times n}$ , the dual of  $L_{\mathbf{C}}(\mathbf{p}, \mathbf{q})$  has the following form:

$$\begin{aligned} & \max_{\mathbf{r}, \mathbf{s}} \quad \mathbf{p}^T \mathbf{r} + \mathbf{q}^T \mathbf{s} \\ \text{s.t.} \quad & \mathbf{r} \mathbf{1}^T + \mathbf{1}^T \mathbf{s} \leq \mathbf{C} \end{aligned} \tag{3}$$

where  $\mathbf{r} \in \mathbb{R}^n$ ,  $\mathbf{s} \in \mathbb{R}^n$ .

- ▶ Because the primal OT Kantorovich problem is a feasible LP for  $\mathbf{p}$  and  $\mathbf{q}$  probability distributions, the dual problem is also feasible and strong duality holds.
- ▶ The dual problem can play an important part in devising algorithms to solve the Kantorovich problem.
- ▶ Interpretation of prices of dual variables.

# Dual problem of the discrete Kantorovich problem: Proof

- Semilagrangian of the primal problem:

$$J(\mathbf{F}; \mathbf{r}, \mathbf{s}) = \text{tr}(\mathbf{C}\mathbf{F}^T) + \mathbf{r}^T(\mathbf{p} - \mathbf{F}\mathbf{1}) + \mathbf{s}^T(\mathbf{q} - \mathbf{F}^T\mathbf{1})$$

- Dual problem:

$$\max_{\mathbf{r}, \mathbf{s}} \mathbf{r}^T \mathbf{p} + \mathbf{s}^T \mathbf{q} + \min_{\mathbf{F} \geq 0} \text{tr}(\mathbf{C}\mathbf{F}^T) - \underbrace{\mathbf{r}^T \mathbf{F} \mathbf{1}}_{\text{tr}(\mathbf{F}^T \mathbf{r} \mathbf{1}^T)} - \underbrace{\mathbf{s}^T \mathbf{F}^T \mathbf{1}}_{\mathbf{F}^T \mathbf{1} \mathbf{s}^T}$$

where  $\mathbf{Q} = \mathbf{C} - \mathbf{r}\mathbf{1}^T - \mathbf{1}\mathbf{s}^T$

$$\min_{\mathbf{F} \geq 0} \text{tr}(\mathbf{C}\mathbf{F}^T) - \underbrace{\mathbf{r}^T \mathbf{F} \mathbf{1}}_{\text{tr}(\mathbf{F}^T \mathbf{r} \mathbf{1}^T)} - \underbrace{\mathbf{s}^T \mathbf{F}^T \mathbf{1}}_{\mathbf{F}^T \mathbf{1} \mathbf{s}^T} = \begin{cases} 0 & \text{if } \mathbf{Q} \geq 0 \\ -\infty & \text{otherwise} \end{cases}$$

- Giving

$$\begin{aligned} \max_{\mathbf{r}, \mathbf{s}} \quad & \mathbf{r}^T \mathbf{p} + \mathbf{s}^T \mathbf{q} \\ \text{s.t.} \quad & \mathbf{r}\mathbf{1}^T + \mathbf{1}^T \mathbf{s} \leq \mathbf{C} \end{aligned}$$

# Gradient of the Wasserstein Loss

- Back to the Wasserstein loss function:  $L_{\mathbf{C}}(h_{\theta(x_i)}, \mathbf{y}_i)$ .

- If we write it in dual form:

$$\begin{aligned} \max_{\mathbf{r}, \mathbf{s}} \quad & \mathbf{r}^T h_{\theta(x_i)} + \mathbf{s}^T \mathbf{y}_i \\ \text{s.t.} \quad & \mathbf{r} \mathbf{1}^T + \mathbf{1}^T \mathbf{s} \leq \mathbf{C}. \end{aligned}$$

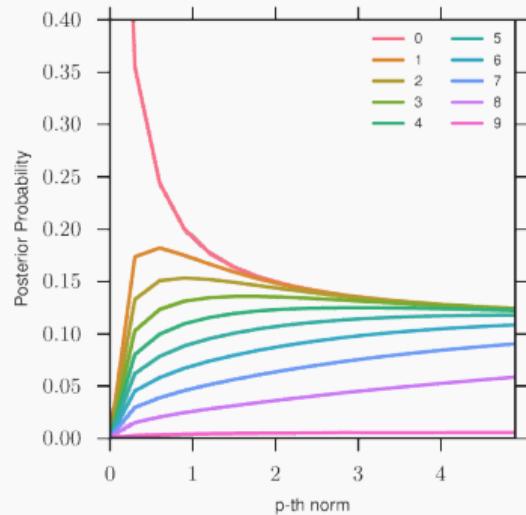
- We can take conditional subgradient w.r.t.  $h_{\theta}(x)$ :

$$\frac{d}{dh_{\theta}(x)} W_p(h_{\theta}(x), y) = \mathbf{r}$$

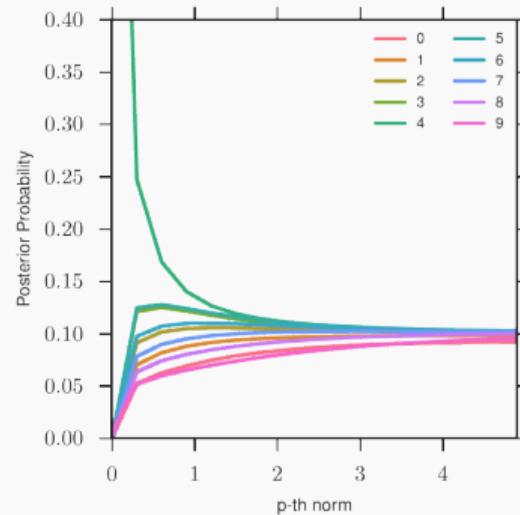
- Note that the Wasserstein loss is subdifferentiable.
- Computing the Wasserstein loss for  $N$  examples can be costly in high dimensions...
- Once we have the subgradient, we can backpropagate to update  $\theta$  with SGD.

# Effects of the ground metric I

- Authors compare discriminative power of  $W_p$  for different  $p$  norm values.



(a) Posterior prediction for images of digit 0.

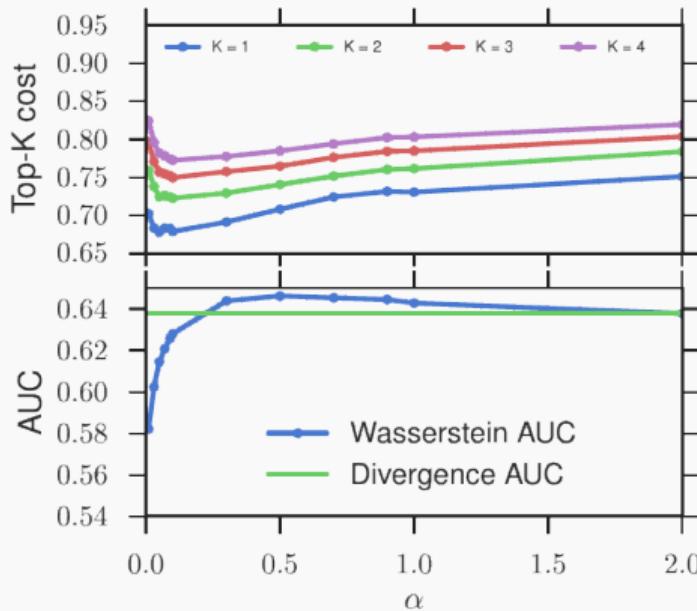


(b) Posterior prediction for images of digit 4.

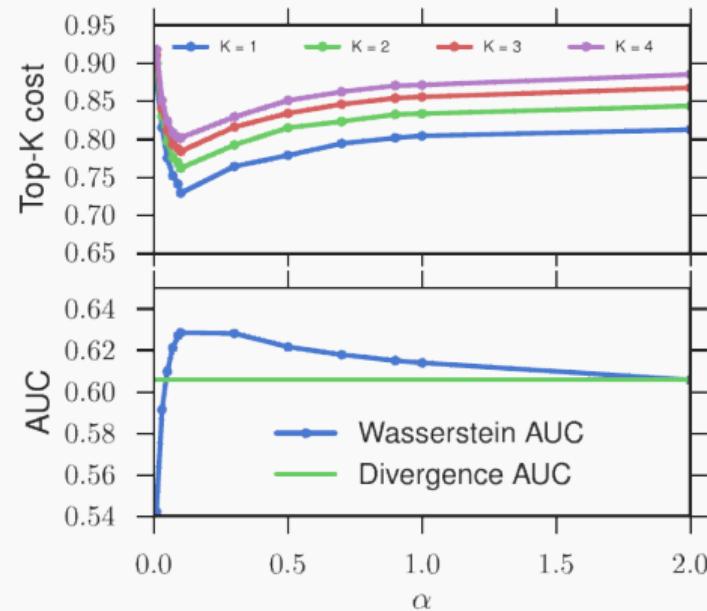
## Effects of the ground metric II

- KL loss vs. Wasserstein loss on the Flickr database:

$$l(x_i, y_i) = W_p(h_\theta(x_i), y_i) + \alpha KL$$



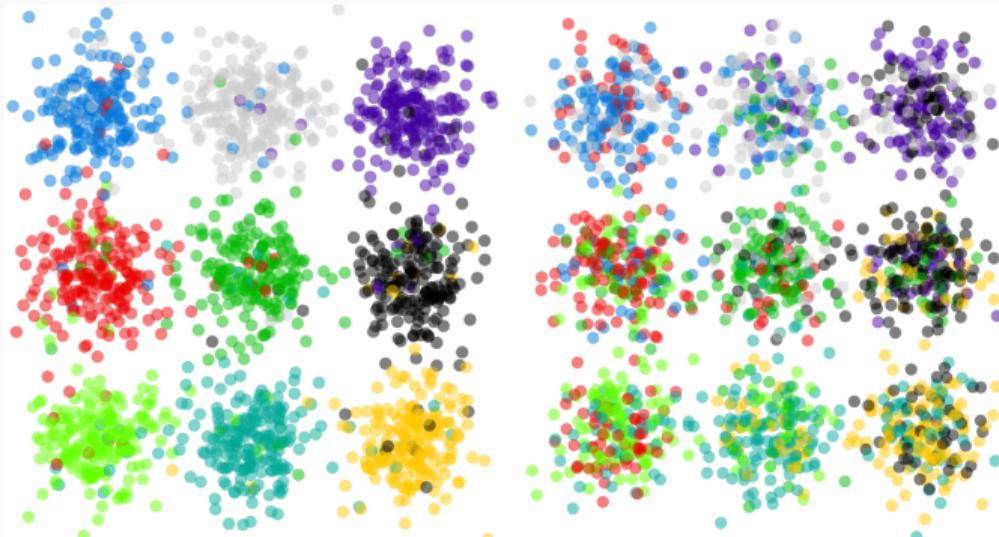
(a) Original Flickr tags dataset.



(b) Reduced-redundancy Flickr tags dataset.

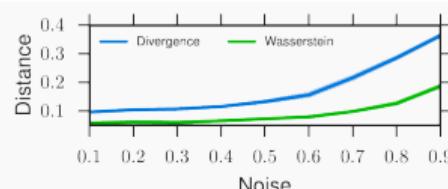
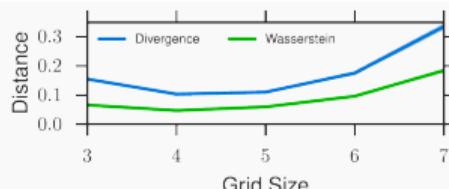
# Homework proposal

- ▶ Train a Wasserstein loss classifier on the plane with semantic classes.



(a) Noise level 0.1

(b) Noise level 0.5



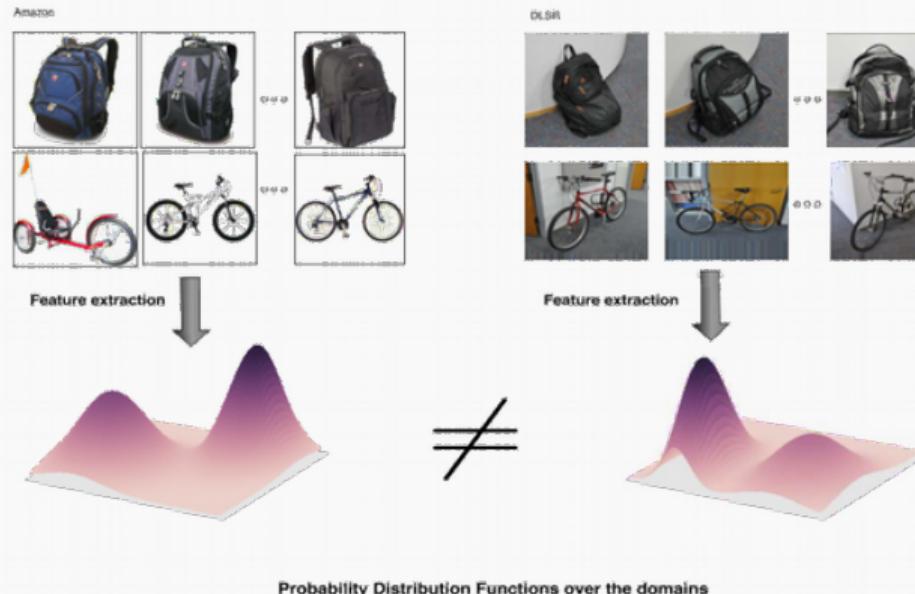
# Thank you for listening!

---

- ▶ There are more things I wanted to talk about.
  1. **Approximate methods** such as Sinkhorn, or smooth OT, to scale problem dimensions.
  2. **Domain adaptation** transport a database of unlabelled data, to a domain where such labels exist, according to a Wasserstein transport plan.
  3. **Ground metric learning** allows to learn the cost matrix from data, potentially improving performance compared to a p-Wasserstein loss as we have seen in examples.
  4. Barycenter estimation: for clustering, or interpolation between histograms.
  5. Transfer learning.
  6. Unbalanced optimal transport.
  7. Wasserstein discriminant analysis.
  8. Etc.

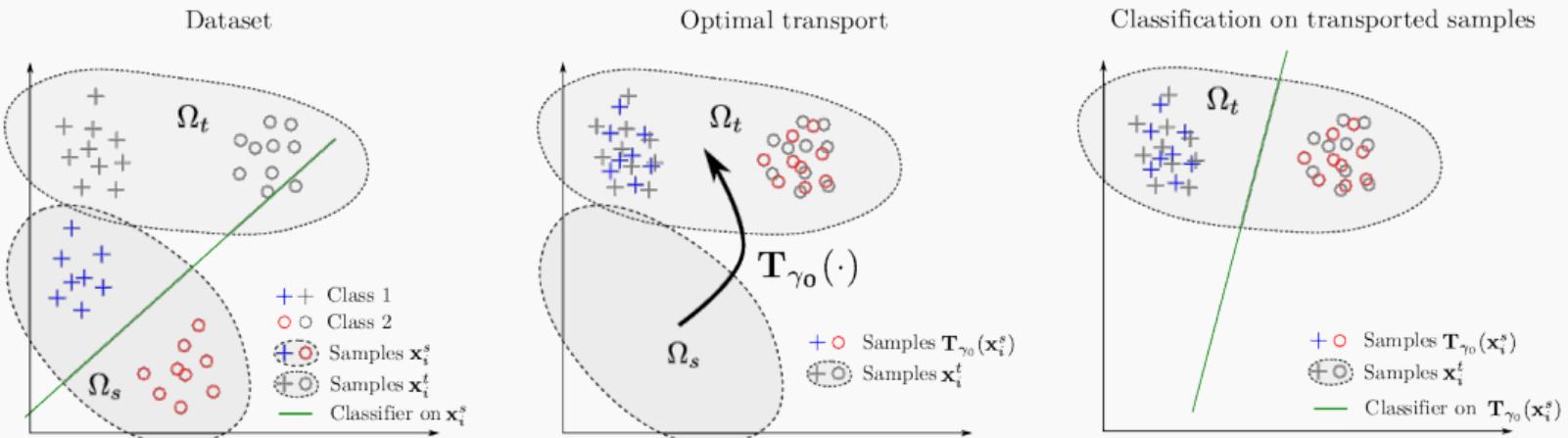
## Application II: Domain adaptation

# Problem intuition



- We consider unsupervised domain adaptation → labels only in source domain.
- **Assumption:** data is processed to make the domains similar.
- Transformation follows a **least effort principle**.

# Procedure



1. Estimate the marginals  $\mu_s$  and  $\mu_t$  from source and target sample distributions.
2. Find a transport map  $T$  from  $\mu_s$  to  $\mu_t$ .
3. Use  $T$  to transport labeled samples  $\mathbf{x}_s$  and train a classifier from them.

## Related work

---

- ▶ The approach defines a local transformation for each sample in the domain.
- ▶ It can be seen as a graph matching problem → marginal distribution conservation.
- ▶ **Related work:**
  1. Projection methods: inner products, region transformation, extraction of common features.
  2. Unsupervised: common latent space representations; feature extraction is key.
  3. Gradual alignment of feature representation: kernel methods.

## Problem description

---

- ▶  $\mathcal{K}$  set of possible labels; only available for  $\mathcal{X}$ .
- ▶ Source sample data:  $((\mathbf{x}_i^s)_i^N, (y_i)_i^N)$ .
- ▶ Target sample data:  $((\mathbf{x}_i^t)_i^N)$ .
- ▶ Joint probability distribution in source:  $P_s(\mathbf{x}^s, y)$
- ▶ Marginal over  $x$ :  $\mu_s$ .
- ▶ Joint probability distribution in target:  $P_t(\mathbf{x}^t, y)$ .
- ▶ Marginal over  $x$ :  $\mu_t$ .

## Assumptions of the transportation

---

- The domain drift is to an unknown, possibly nonlinear transformation of the linear space

$$T : \mathcal{X} \rightarrow \mathcal{Y}$$

- From probabilistic perspective,  $T$  transforms  $\mu_s$  into  $\mu_t$ , i.e.,

$$T\sharp\mu_s : \mathcal{M}_+^1 \rightarrow \mathcal{M}_+^1 = \mu_t$$

$X_t$  are drawn from same pdf as  $T\sharp\mu_s$ .

- Transformation preserves conditional distribution, i.e.,

$$P_s(y|\mathbf{x}^s) = P_t(y|\mathbf{x}^t) \iff f_t(T(\mathbf{x}^s)) = f_s(\mathbf{x}^s)$$

# Problem formulation

---

- Empirical distributions:

$$\mu_s = \sum_{i=1}^{N_s} p_i^s \delta_{x_i^s}, \quad \mu_t = \sum_{i=1}^{N_t} p_i^t \delta_{x_i^t}$$

- Transport problem:

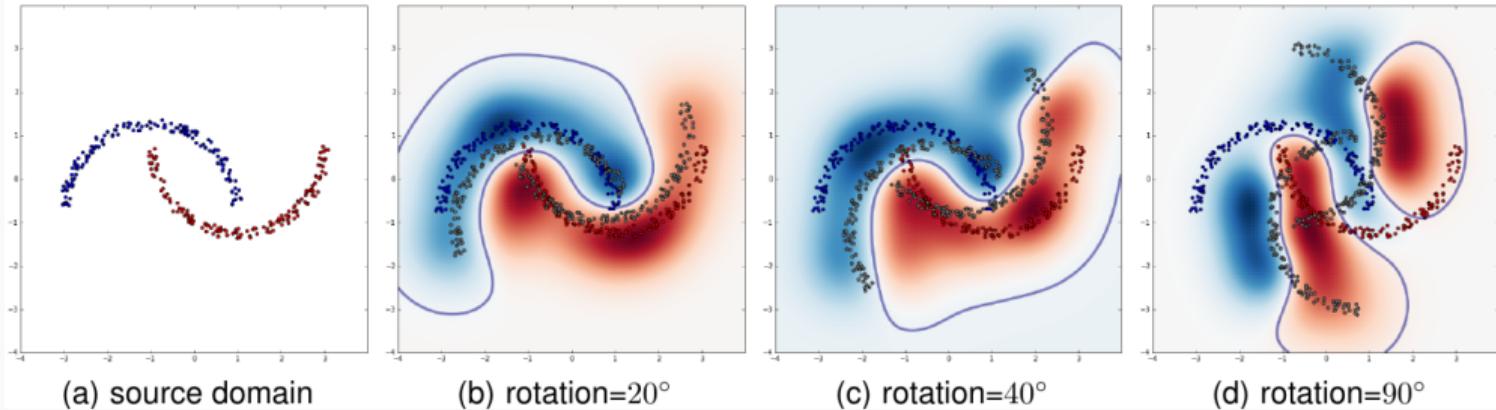
$$\mathbf{F} = \arg \min_{\mathbf{F} \in U(\mu_s, \mu_t)} \text{tr}(\mathbf{FC})$$

where  $C_{ij} = \|\mathbf{x}_s - \mathbf{x}_t\|^2$ .

- When  $N_s = N_t = N$  and for all  $i$ ,  $p_i^s = p_i^t = 1/N$ ,  $\mathbf{F}$  is simply a permutation matrix, which makes a correspondence of one to one from source to target domain.

# Results

- Once we have the transport plan, we can bring features with labels to the target domain and train a classifier.
- Regularization can be induced to improve results using labels
- Results:



Thanks again

---

Questions?