Computational Optimal Transport for Machine and Deep Learning

Introduction to domain adaptation

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ENS DE LYON

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Acknowledgments

Slides adapted from those of Rémi Flamary

Euclidean to Fréchet barycenter

Let $\mathbf{x}_1, \cdots, \mathbf{x}_N \in \mathbb{R}^d$ and $(\lambda_1, \cdots, \lambda_N) \in \Sigma_N$ (histogram).

Standard barycenter

$$\hat{\mathbf{x}} = \sum_{i=1}^{N} \lambda_i \mathbf{x}_i = \underset{\bar{\mathbf{x}} \in \mathbb{R}^d}{\arg\min} \sum_{i=1}^{N} \lambda_i \|\bar{\mathbf{x}} - \mathbf{x}_i\|_2^2 \, . \tag{1}$$

Euclidean to Fréchet barycenter

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Fréchet barycenter

$\mathbf{x}_1, \cdots, \mathbf{x}_N \in X^N$ where (X, d) metric space.

$$\hat{\mathbf{x}} = \arg\min_{\overline{\mathbf{x}} \in X} \sum_{i=1}^{N} \lambda_i d^2(\overline{\mathbf{x}}, \mathbf{x}_i) \,. \tag{3}$$

Wasserstein barycenter

Let $\alpha_1, \cdots, \alpha_N \in \mathcal{P}(\mathbb{R}^d)$ probability measures and $(\lambda_1, \cdots, \lambda_N) \in \Sigma_N$.

Wasserstein barycenter

It is a probability measure $\hat{\mu}$ solving

$$\hat{\mu} = \underset{\overline{\mu} \in \mathcal{P}(\mathbb{R}^d)}{\arg\min} \sum_{i=1}^{N} \lambda_i W_2^2(\overline{\mu}, \alpha_i) \,. \tag{4}$$

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Discrete case when $N = 2$: Mccan's interpolant

When $\alpha_1 = \sum_{i=1}^n a_i \delta_{\mathbf{x}_i}$ (source), $\alpha_2 = \sum_{j=1}^m b_j \delta_{\mathbf{y}_j}$ (target) are discrete. If P is an optimal coupling $\hat{\mu} = \sum_{ij} P_{ij} \delta_{(1-t)\mathbf{x}_i + t\mathbf{y}_j}$: $n + m - 1$ points.

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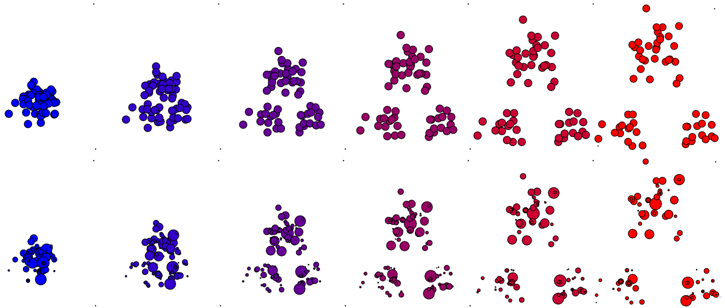

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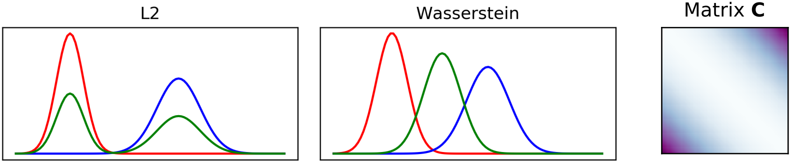

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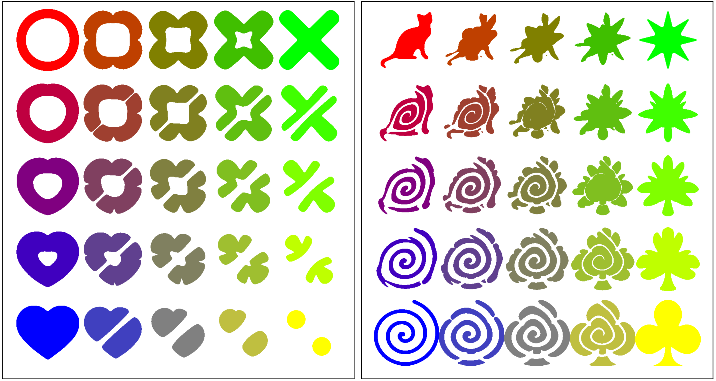


Figure: Peyré, Cuturi, et al. 2019

The barycentric mapping

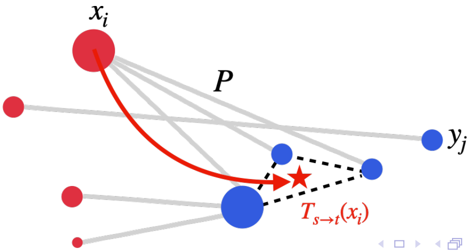
Let $\mu_s = \sum_{i=1}^{n} a_i \delta_{\mathbf{x}_i}$ (source), $\mu_t = \sum_{j=1}^{m} b_j \delta_{\mathbf{y}_j}$ (target). Let P be optimal coupling between μ_s, μ_t with cost c.

Weighted barycenter with OT plan

- Source to target

$$T_{s\to t} : \mathbf{x}_i \to \arg\min_{\bar{\mathbf{y}}} \sum_{j=1}^{m} P_{ij} c(\bar{\mathbf{y}}, \mathbf{y}_j) \tag{5}$$

- When $c = \ell_2^2$, mapping the entire data $T_{s\to t}(\mathbf{X}) = \mathrm{diag}(P1_m)^{-1} P\mathbf{Y}$.
- If $P = ab^\top$, $T_{s\to t}(\mathbf{x}_i) = \sum_{j=1}^{m} b_j \mathbf{y}_j$.



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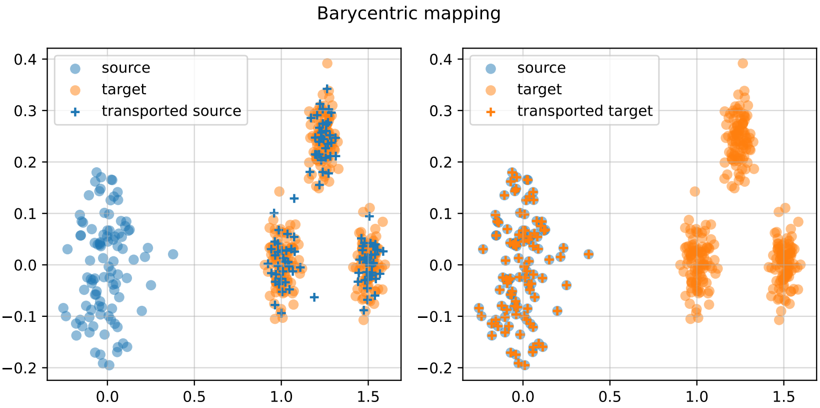

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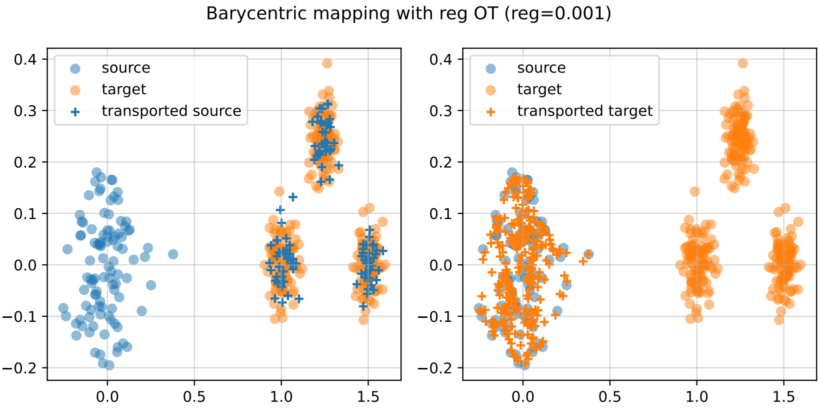

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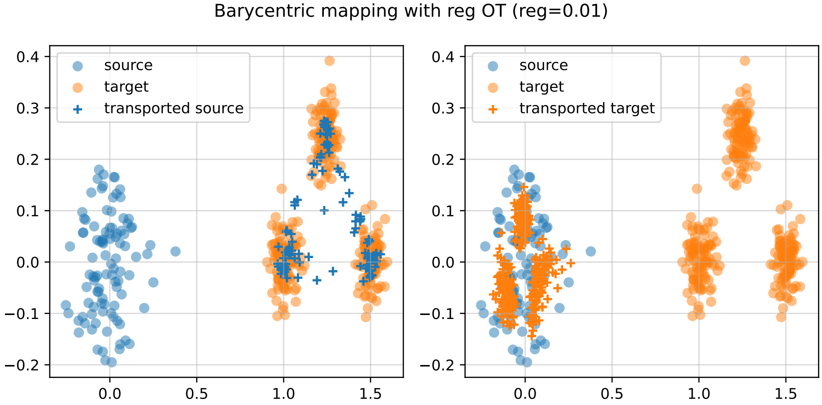

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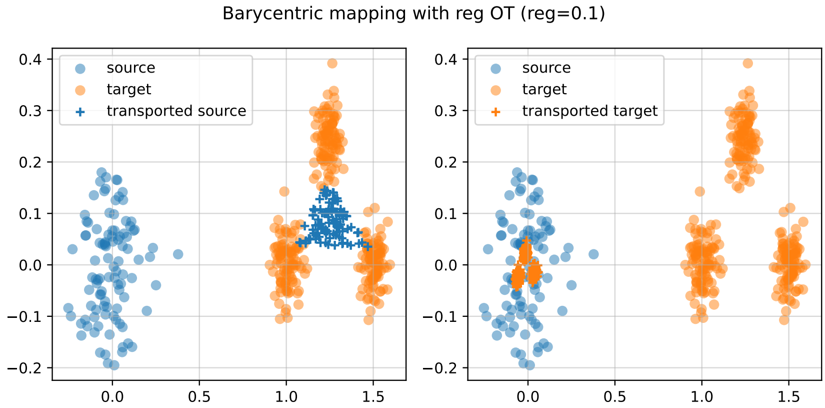

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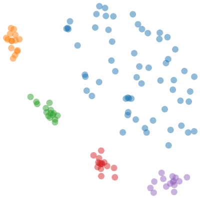
Supervised ML

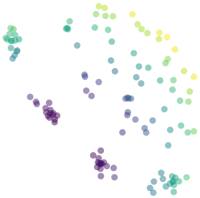
Samples + labels:

$$\mathbf{X} = \begin{bmatrix} \mathbf{x}_1^\top \\ \mathbf{x}_2^\top \\ \vdots \\ \mathbf{x}_n^\top \end{bmatrix} \quad \mathbf{c} = \begin{bmatrix} c_1 \\ c_2 \\ \vdots \\ c_n \end{bmatrix}$$

Classification



Regression



Supervised learning

- The dataset contains the samples $(\mathbf{x}_i, c_i)_{i=1}^n$ where $\mathbf{x}_i$ is the feature sample and c_i its label/class.
- The values to predict (label) can be concatenated in a vector $\mathbf{c}$

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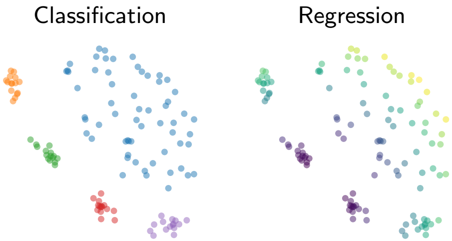

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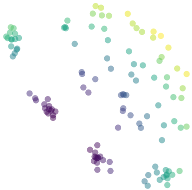
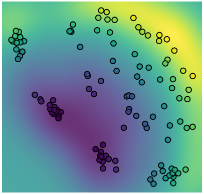
- The values to predict (label) can be concatenated in a vector $\mathbf{c}$
- Semi-supervised learning: few labeled points are available, but a large number of unlabeled points are given.

Regression



$\Longrightarrow$

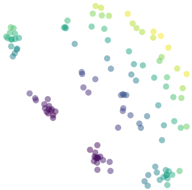


Objective

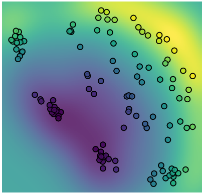
$$(\mathbf{x}_i, c_i)_{i=1}^n \quad \Rightarrow \quad f : \mathbb{R}^d \rightarrow \mathbb{R}$$

- Train a function $f(\mathbf{x}) = c \in \mathbb{R}$ predicting a continuous value.
- Can be extended to multi-value prediction ($\mathbb{R}^p$).

Regression



$$\Rightarrow$$



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Hyperparameters

- Type of function (linear, kernel, neural network).
- Performance measure.
- Regularization.

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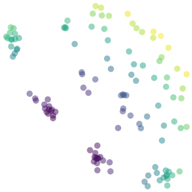

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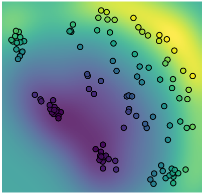

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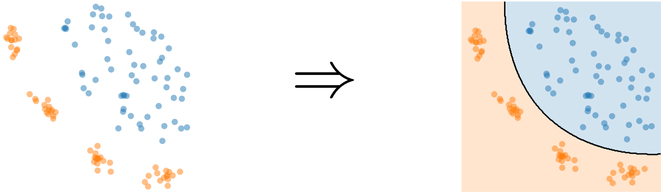
Methods

- Least Square (LS).
- Ridge regression, Lasso.
- Kernel regression.
- Deep learning.

Binary classification

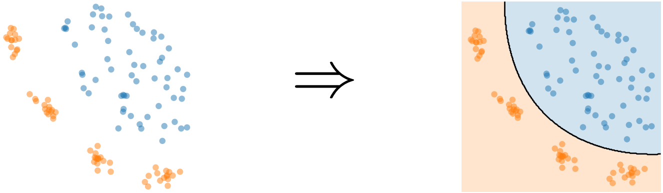


Objective

$$(\mathbf{x}_i, c_i)_{i=1}^n \quad \Rightarrow \quad f : \mathbb{R}^d \to \{-1, 1\}$$

- Train a function $f(\mathbf{x}) = c \in \mathcal{C}$ predicting a binary value ($e.g.\{-1, 1\}$).
- $f(\mathbf{x}) = 0$ defines the boundary on the partition of the feature space.

Binary classification



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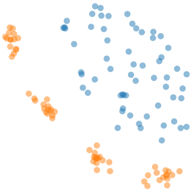

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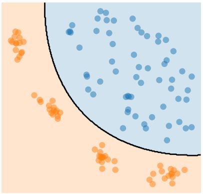

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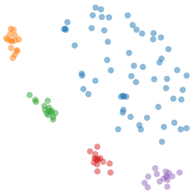
Hyperparameters

- Type of function (linear, kernel, neural network).
- Performance measure.
- Regularization.

Methods

- Bayesian classifier (LDA, QDA)
- Linear and kernel discrimination
- Decision trees, random forests.
- Deep learning.

Multiclass classification



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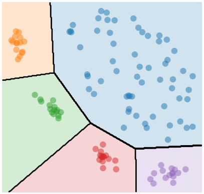

Objective

$$(\mathbf{x}_i, c_i)_{i=1}^n \quad \Rightarrow \quad f : \mathbb{R}^d \to \{1, \ldots, K\}$$

- Train a function $f(\mathbf{x}) = c \in \{1, \ldots, K\}$ predicting an integer value.

Empirical risk minimization

Minimizing the train error

To find f the idea is to **minimize the averaged error** on the training samples:

$$\min_f \frac{1}{n} \sum_{i=1}^{n} \ell(c_i, f(\mathbf{x}_i)) \tag{ERM}$$

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- ℓ is a loss function

$$\ell(\text{true value, predicted value}) = \text{how good is my prediction}$$

- It is called **empirical risk minimization (ERM)**
- Given the loss, finds the "best" f on the training data
- E.g. linear regression

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Domain adaptation

Traditional supervised learning

- We want to learn predictor such that $c \approx f(\mathbf{x})$.
- Actual $p(x, c)$ unknown.
- We have access to training dataset $(\mathbf{x}_i, c_i)_{i=1,\ldots,n}$ $(\hat{p}(x, c))$.
- We choose a loss function $\ell(c, f(\mathbf{x}))$ that measure the discrepancy.

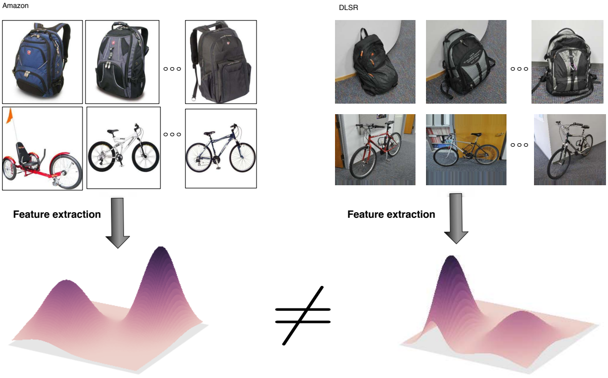
Empirical risk minimization

We week for a predictor f minimizing

$$\min_f \left\{ \mathbb{E}_{(\mathbf{x},c)\sim\hat{p}(x,c)} \; \ell(c, f(\mathbf{x})) = \sum_j \ell(c_j, f(\mathbf{x}_j)) \right\} \tag{6}$$

- Well known generalization results for predicting on new data.

Domain Adaptation problem

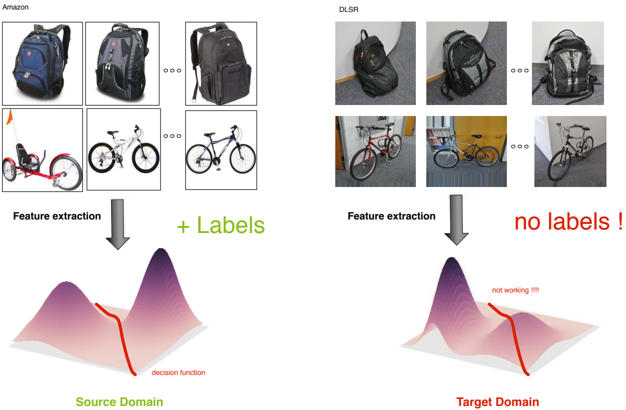


Probability Distribution Functions over the domains

Our context

- Classification problem with data coming from different sources (domains).
- Distributions are different but related.

Unsupervised domain adaptation problem

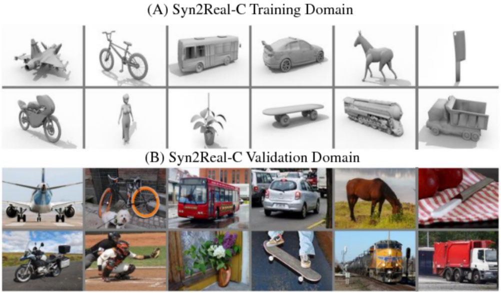


Problems

- Labels only available in the **source domain**, and classification is conducted in the **target domain**.
- Classifier trained on the source domain data performs badly in the target domain

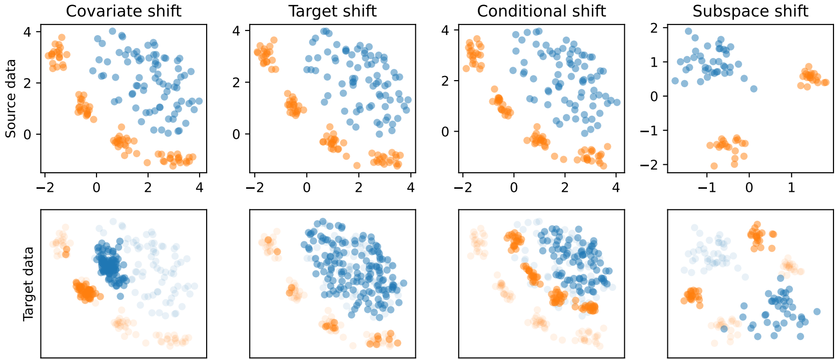
Is Domain Adaptation a real problem ?

- Ubiquitous problem in Deep Learning ! People can not afford to label billions of data for every single problems
- Novel interesting challenges if one considers learning from synthetic data



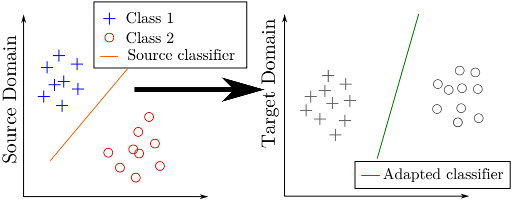
The pig picture

Many shifts are possible.



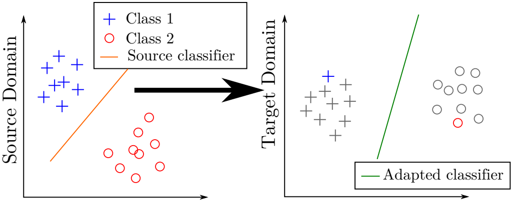
Unsupervised and semi-supervised DA

Unsupervised DA



- Source : $\{\mathbf{x}_i^s, c_i^s\}_{i=1}^{n_s}$
- Target : $\{\mathbf{x}_j^t\}_{j=1}^{n_t}$
- Requires assumptions on the shift (CS, TS, CD, SSB).

Semi-Supervised DA



- Source : $\{\mathbf{x}_i^s, c_i^s\}_{i=1}^{n_s}$
- Target : $\{\mathbf{x}_j^t\}_{j=1}^{n_t}$, $\{c_j^t\}_{j=1}^{n_l}$
- The few $n_l \ll n_t$ labeled target samples can help guide the learning on target.

Domain adaptation

Problem: how to learn a classifier that can be good on several domains with only labels in one of the domain ?

- Theory Mansour, Mohri, and Rostamizadeh 2009 measures the difficulty of this task in terms of discrepancy of the representations of the data.
- Possible solutions include:
  - Find domain invariant representation of the data.
  - Transform data from one domain into "similar" versions in the other domain (adversarial methods).
  - At any point a notion of divergence between the distributions is involved.

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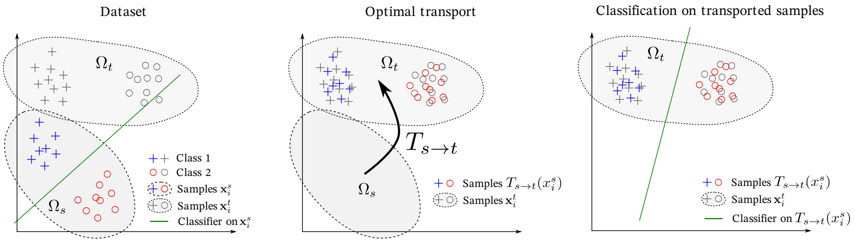
Optimal transport for domain adaptation



Assumptions

1. There exist an OT mapping T in the feature space between the two domains.
2. The transport preserves the joint distributions:

$$P^s(\mathbf{x}, c) = P^t(T(\mathbf{x}), c).$$

3-step strategy Courty et al. 2016

1. Estimate optimal transport between distributions (use regularization).
2. Transport the training samples on target domain.
3. Learn a classifier on the transported training samples.

Label propagation

4-step strategy Redko et al. 2019

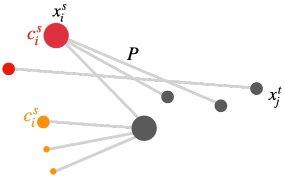
1. One-hot encoding of the classes in the source domain. E.g. if K classes $\{1, 2, \cdots, K\}$

$$c_i^s = 2 \rightarrow \mathbf{c}_i^s = \overbrace{(0, 1, \cdots, 0)}^{K}$$

2. Find a good OT plan P between source and target.
3. Propagate the labels of the source into the target.

$$\forall j \in [n_t],\ \widehat{\mathbf{c}}_j^t = \frac{1}{b_j} \sum_{i=1}^{n_s} P_{ij} \mathbf{c}_i^s = T_{t \rightarrow s}(\mathbf{c}_i^s)\,.$$

4. (optional) Find the class with maximal coordinate for prediction. E.g. $\widehat{\mathbf{c}}_j^t = (0.1, 0.8, 0.1) \rightarrow \widehat{c}_j^t = 2$.



Why it is a good idea ? (few intuitions)

Using duality theory

$$W_1(\alpha, \beta) = \sup_{f \in \mathrm{Lip}_1} \mathbb{E}_{\mathbf{x}\sim\alpha}[f(\mathbf{x})] - \mathbb{E}_{\mathbf{y}\sim\beta}[f(\mathbf{y})]\,.$$

Let $\mathrm{error}_s(f) = \mathbb{E}_{(\mathbf{x},c)\sim P^s}[\ell(c, f(\mathbf{x}))], \mathrm{error}_t(f) = \mathbb{E}_{(\mathbf{x},c)\sim P^t}[\ell(c, f(\mathbf{x}))]$ and

$$\mathcal{F}_{L,\ell} = \{f : X \to C, \ell(\cdot, f(\cdot)) \in \mathrm{Lip}_L\}\,.$$

Take

- Best error on target $f^\star \in \arg\min_{f\in\mathcal{F}_{L,\ell}} \ \mathrm{error}_t(f)$.
- Best error on source $f_s \in \arg\min_{f\in\mathcal{F}_{L,\ell}} \ \mathrm{error}_s(f)$.

Then

$$0 \le \mathrm{error}_t(f_s) - \mathrm{error}_t(f^\star) \le 2L \cdot W_1(P^s, P^t)\,.$$

Conclusion if P^s, P^t are closed in OT then perf should be good.

Deep domain adaptation Damodaran et al. 2018

Let $P^f = \frac{1}{n_t}\sum_{j=1}^{n_t} \delta_{(\mathbf{x}_j^t, f(\mathbf{x}_j^t))}$ and $\hat{P}^s = \frac{1}{n_s}\sum_{i=1}^{n_s} \delta_{(\mathbf{x}_i^s, c_i^s)}$. Solve

$$\min_f \ W_1(\hat{P}^s, P^f)\,.$$

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