

Optimal transport for machine learning

Learning with optimal transport

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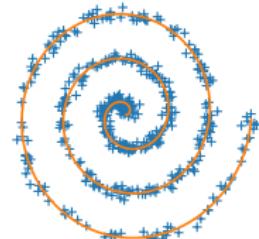
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Introduction

Three aspects of Machine Learning

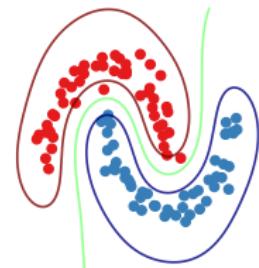
Unsupervised learning

- Extract information from unlabeled data
- Find labels (clustering) or subspaces/manifolds.
- Generate realistic data (GAN).



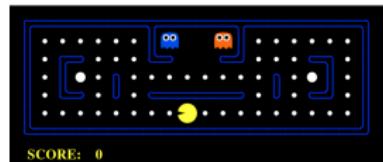
Supervised Learning

- Learning to predict from labeled dataset.
- Regression, Classification.
- Can use unsupervised information (DA, Semi-sup.)

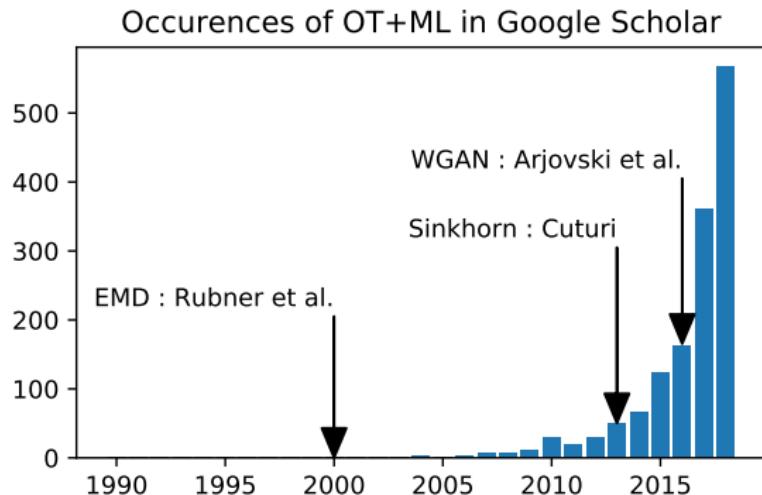


Reinforcement Learning

- Let the machine experiment.
- Learn from its mistakes.
- Framework for learning to play games.



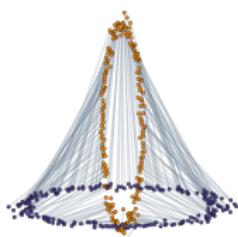
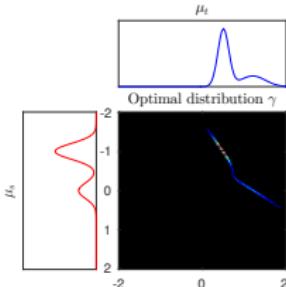
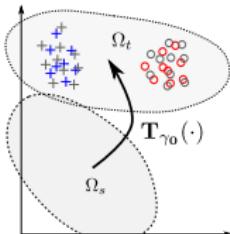
Optimal transport for machine learning



Short history of OT for ML

- Recently introduced to ML (well known in image processing since 2000s).
- Computationnal OT allow numerous applications (regularization).
- Deep learning boost (numerical optimization and GAN).

Three aspects of optimal transport



Transporting with optimal transport

- Color adaptation in image [Ferradans et al., 2014].
- Domain adaptation [Courty et al., 2016].
- OT mapping estimation [Perrot et al., 2016].

Divergence between histograms

- Use the ground metric to encode complex relations between the bins.
- Loss for multilabel classifier [Frogner et al., 2015]
- Loss for spectral unmixing [Flamary et al., 2016b].

Divergence between empirical distributions

- Non parametric divergence between non overlapping distributions.
- Objective function for GAN [Arjovsky et al., 2017].
- Estimate discriminant subspace [Flamary et al., 2016a].

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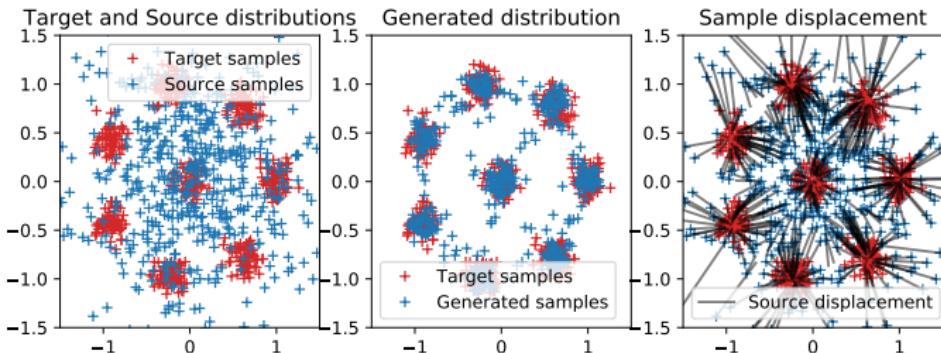
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Mapping with optimal transport

Mapping with optimal transport



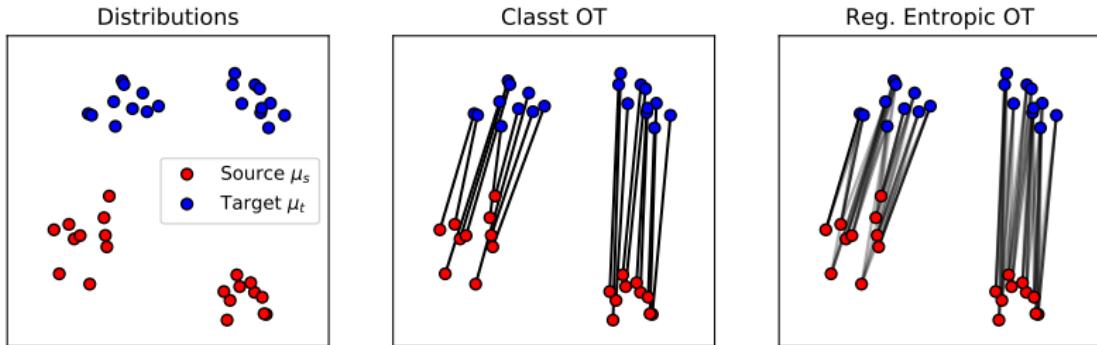
Mapping estimation

- Mapping do not exist in general between empirical distributions.
- Barycentric mapping [Ferradans et al., 2014].
- Smooth mapping estimation [Perrot et al., 2016, Seguy et al., 2017].

Why map ?

- Sensible displacement to align distributions.
- Color adaptation in image [Ferradans et al., 2014].
- Domain adaptation and transfer learning [Courty et al., 2016].

Transporting the discrete samples

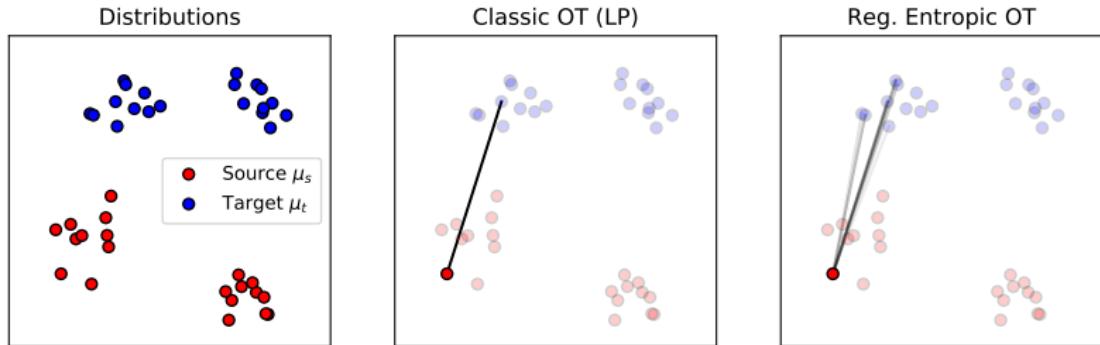


Barycentric mapping [Ferradans et al., 2014]

$$\hat{T}_{\gamma_0}(\mathbf{x}_i^s) = \arg \min_{\mathbf{x}} \sum_j \gamma_0(i, j) c(\mathbf{x}, \mathbf{x}_j^t). \quad (1)$$

- The mass of each source sample is spread onto the target samples (line of γ_0).
- The mapping is the barycenter of the target samples weighted by γ_0 .
- Closed form solution for the quadratic loss.
- Limited to the samples in the distribution (no out of sample).
- Trick: learn OT on few samples and apply displacement to the nearest point.

Transporting the discrete samples

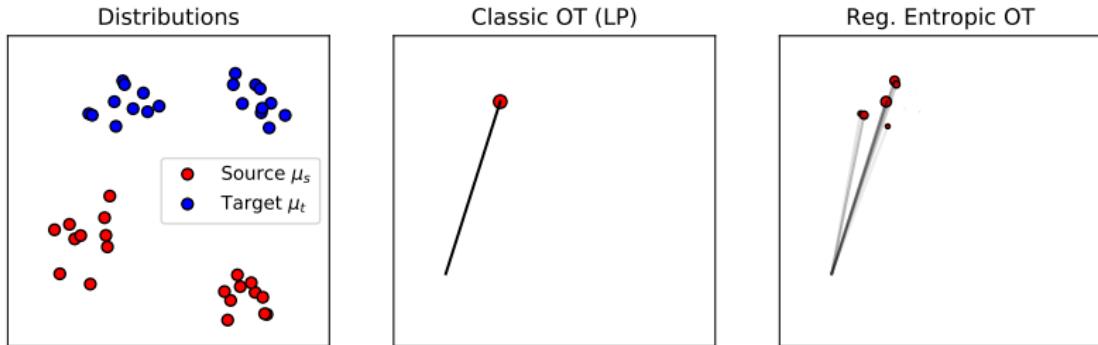


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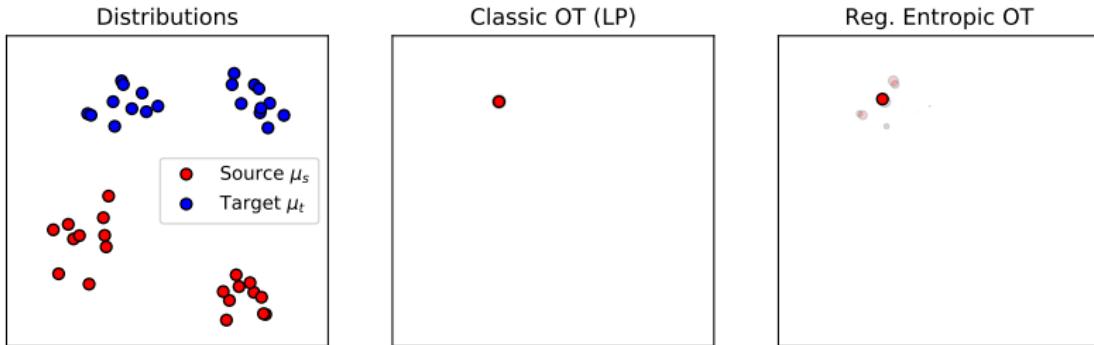


Barycentric mapping [Ferradans et al., 2014]

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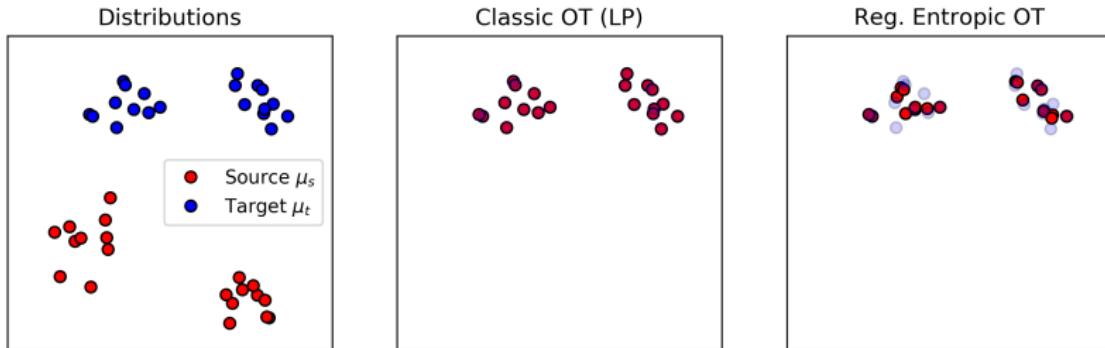


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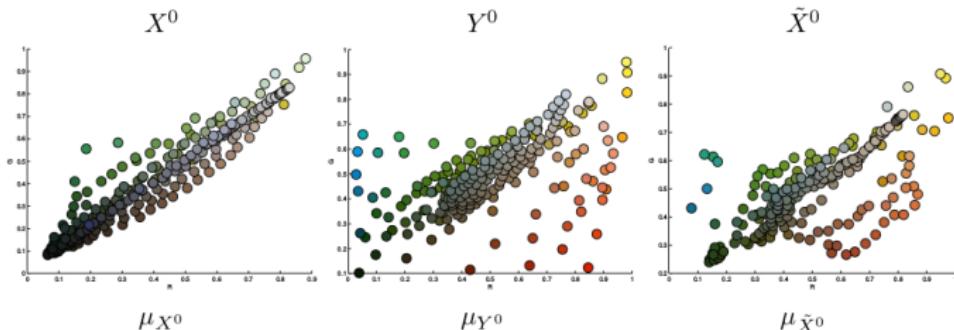
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Histogram matching in images

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

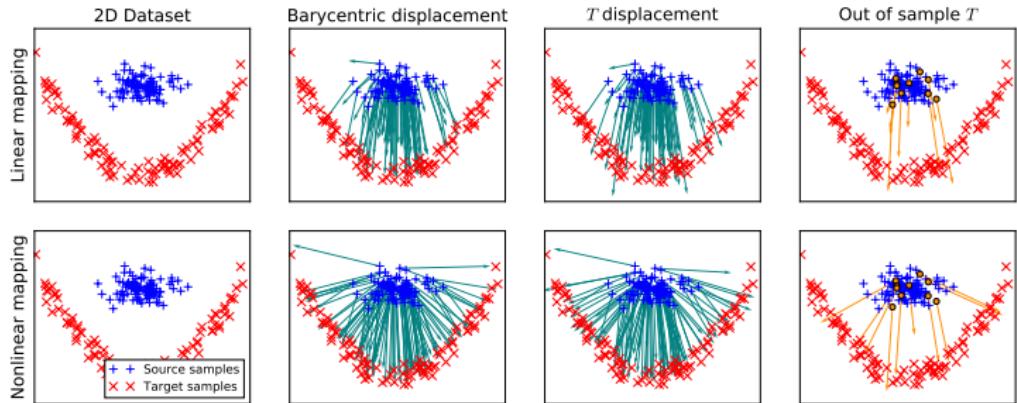


Histogram matching in images

Image colorization [Ferradans et al., 2014]



Joint OT and mapping estimation

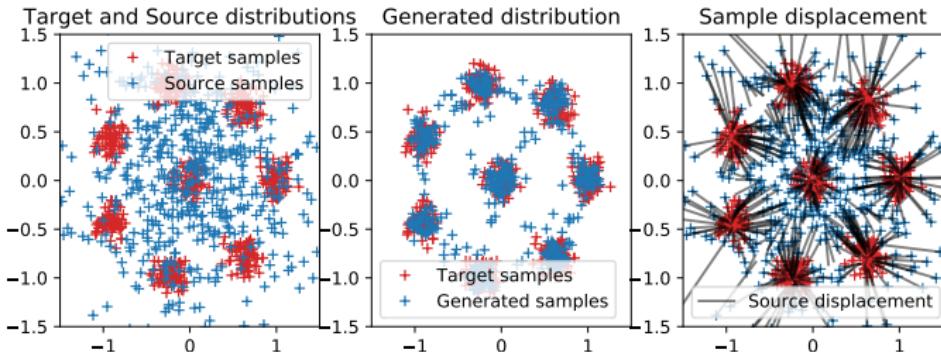


Simultaneous OT matrix and mapping [Perrot et al., 2016]

$$\min_{T, \gamma \in \mathcal{P}} \quad \langle \gamma, \mathbf{C} \rangle_F + \sum_i \|T(\mathbf{x}_i^s) - \hat{T}_\gamma(\mathbf{x}_i^s)\|^2 + \lambda \|T\|^2$$

- Estimate jointly the OT matrix and a smooth mapping approximating the barycentric mapping.
- The mapping is a regularization for OT.
- Controlled generalization error (statistical bound).
- Linear and kernel mappings T , limited to small scale datasets.

Large scale optimal transport and mapping estimation

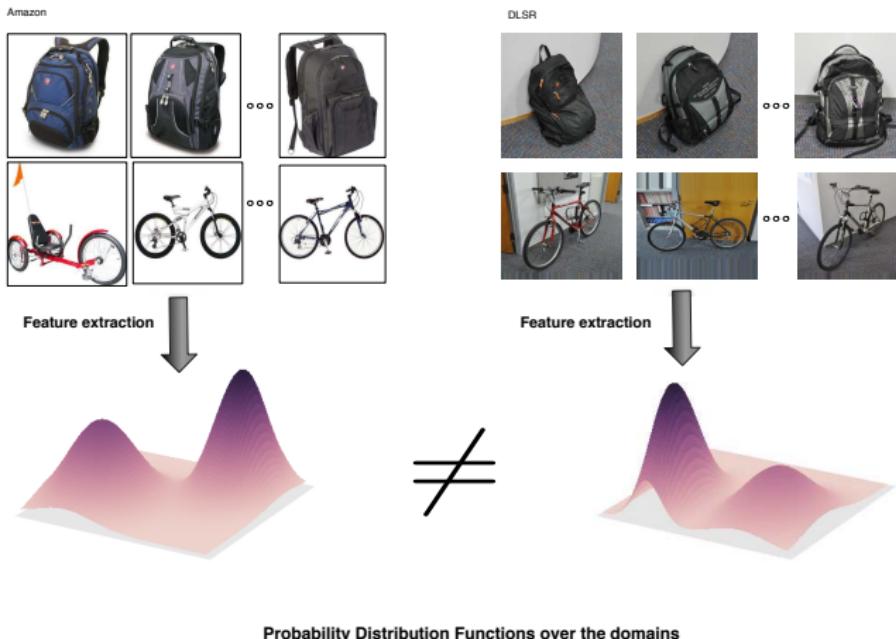


Large scale mapping estimation [Seguy et al., 2017]

- 2-step procedure:
 - 1 Stochastic estimation of regularized $\hat{\gamma}$.
 - 2 Stochastic estimation of T with a neural network.
- OT solved with Stochastic Gradient Ascent in the dual.
- Convergence to the true OT and mapping for small regularization.

0	0	3	9	2	9
1	7	7	6	8	6
0	3	8	1	4	4
9	4	1	5	6	1
7	2	4	5	1	7
5	3	6	6	9	1

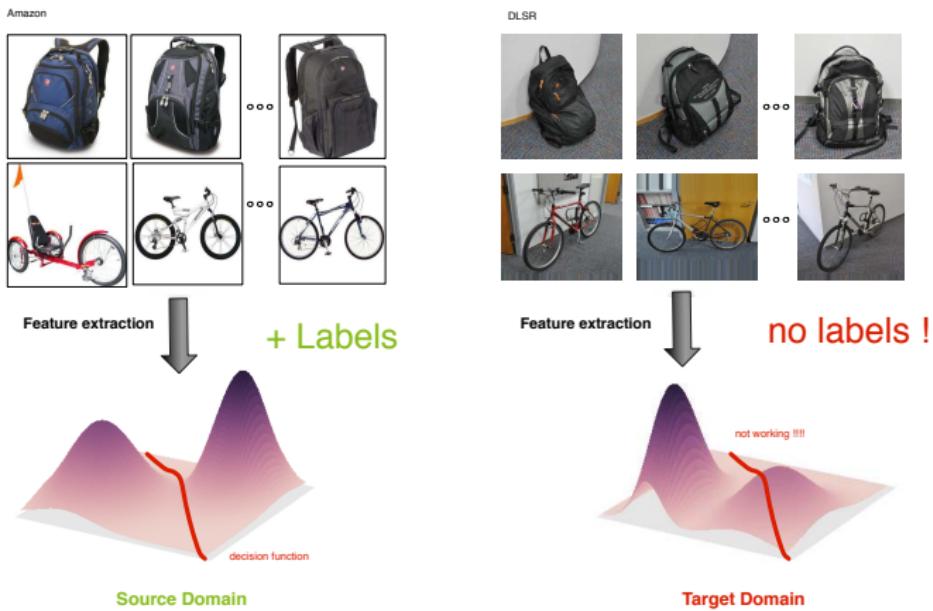
Domain Adaptation problem



Our context

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

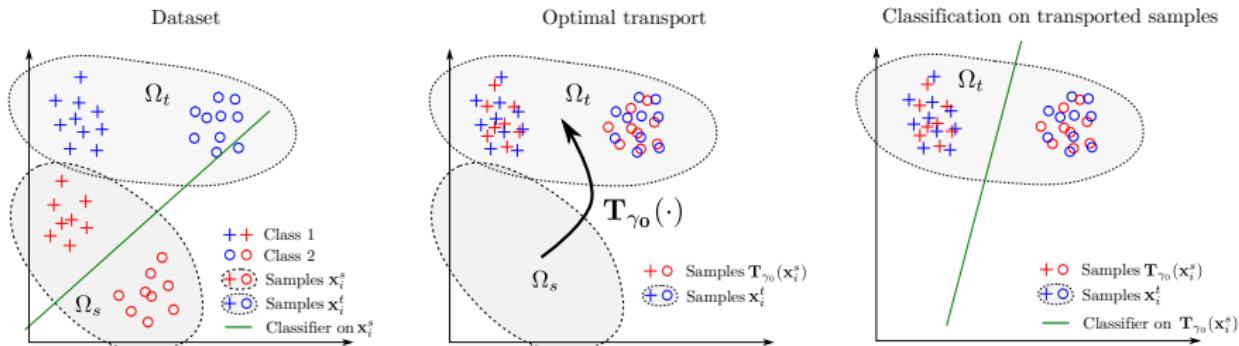
Unsupervised domain adaptation problem



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

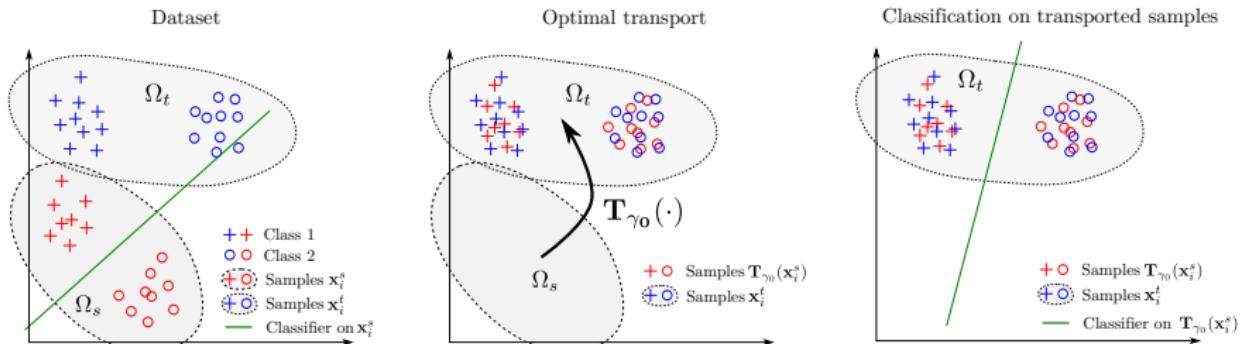
OT for domain adaptation : Step 1



Step 1 : Estimate optimal transport between distributions.

- Choose the ground metric (squared euclidean in our experiments).
- Using regularization allows
 - Large scale and regular OT with entropic regularization [Cuturi, 2013].
 - Class labels in the transport with group lasso [Courty et al., 2016].
- Efficient optimization based on Bregman projections [Benamou et al., 2015] and
 - Majoration minimization for non-convex group lasso.
 - Generalized Conditionnal gradient for general regularization (cvx. lasso, Laplacian).

OT for domain adaptation : Steps 2 & 3



Step 2 : Transport the training samples onto the target distribution.

- The mass of each source sample is spread onto the target samples (line of γ_0).
- Transport using barycentric mapping [Ferradans et al., 2014].
- The mapping can be estimated for out of sample prediction [Perrot et al., 2016, Seguy et al., 2017].

Step 3 : Learn a classifier on the transported training samples

- Transported sample keep their labels.
- Classic ML problem when samples are well transported.

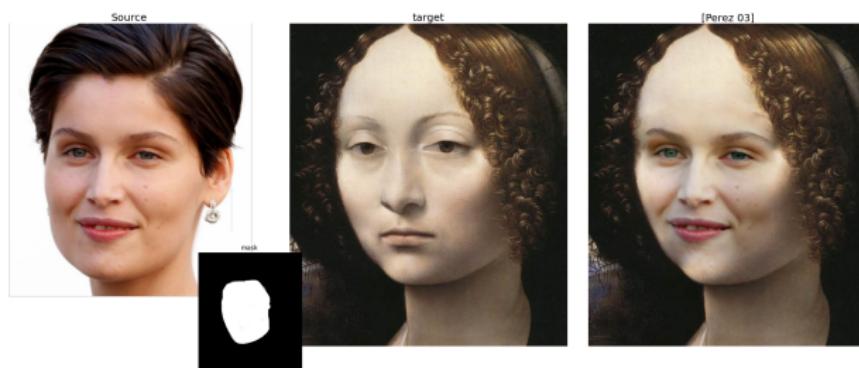
Seamless copy in images



Poisson image editing [Pérez et al., 2003]

- Use the color gradient from the source image.
- Use color border conditions on the target image.
- Solve Poisson equation to reconstruct the new image.

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Seamless copy with gradient adaptation [Perrot et al., 2016]

- Transport the gradient from the source to target color gradient distribution.
- Solve the Poisson equation with the mapped source gradients.
- Better respect of the color dynamic and limits false colors.

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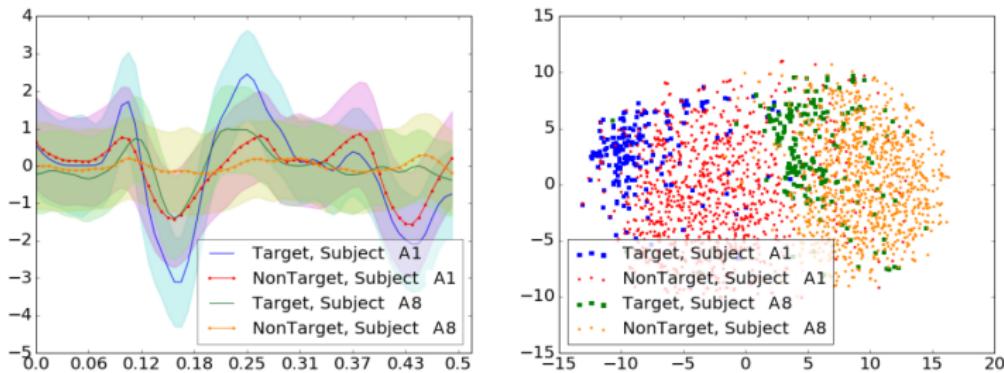
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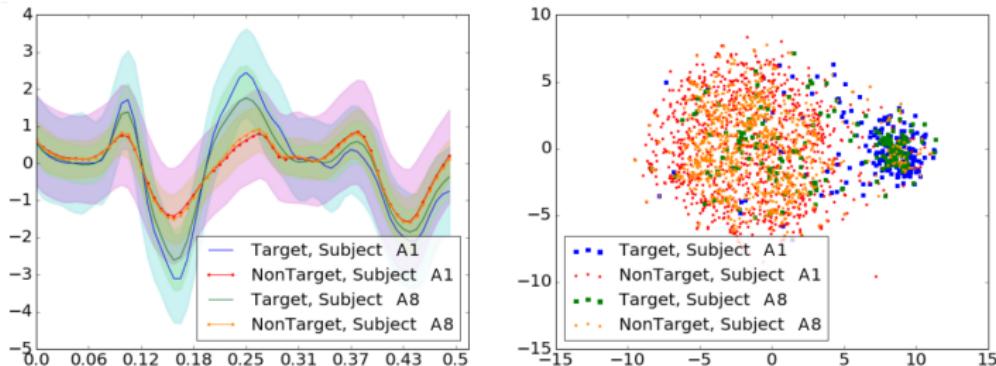
OTDA for biomedical data (1)



Multi-subject P300 classification [Gayraud et al., 2017]

- Objective : reduce calibration for BCI users.
- P300 signal is different accross subjects so adapting models is hard.
- Perform XDAWN [Rivet et al., 2009] as pre-processing.
- Use OTDA to adapt each subject in the dataset to a new subject.
- Train independent classifier on transported data and perform aggregation.

OTDA for biomedical data (1)



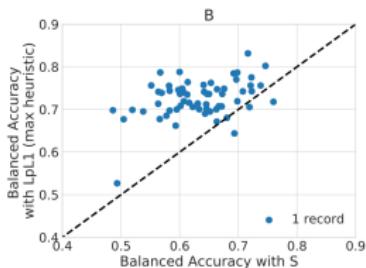
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OTDA for biomedical data (2)

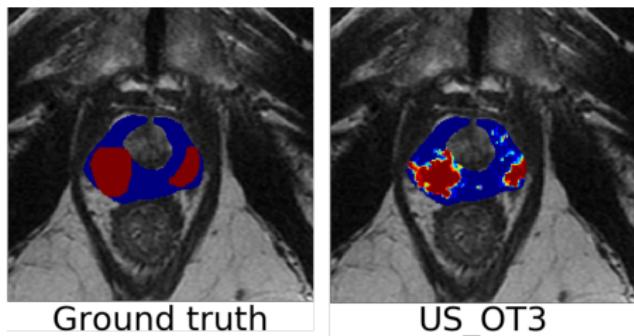
EEG sleep stage classification [Chambon et al., 2018]

- Use pre-trained neural network.
- Adapt with OTDA on the penultimate layer.
- OTDA best DA approach to adapt between EEG recordings.



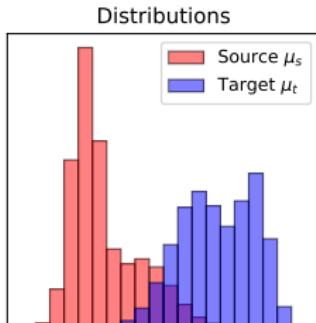
Prostate cancer classification [Gautheron et al., 2017]

- Adaptation of MRI voxel features from 1.5T to 3T.
- Achieve good performance across subjects and modality with no target labels.



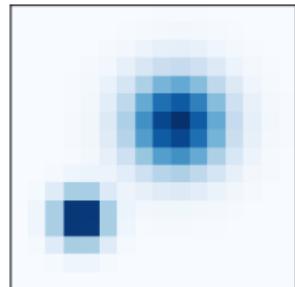
Learning from histograms with Optimal Transport

Learning from histograms



classification
image
learning
problem
optimal

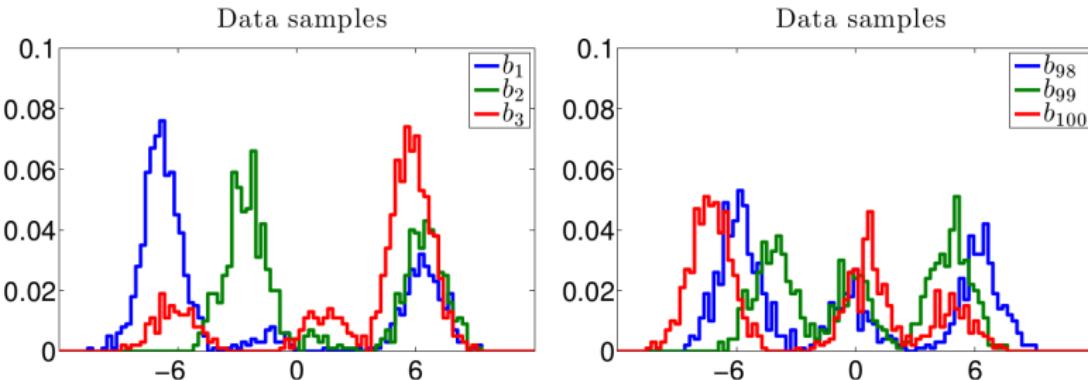
images
sensor
feature
signal
large
spatial
used
data
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target
linear
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sparse
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features



Data as histograms

- Fixed bin positions x_i e.g. grid, simplex $\Delta = \{(\mu_i)_i \geq 0; \sum_i \mu_i = 1\}$
- A lot of datasets comes under the form of histograms.
- Images are photo counts (black and white), text as word counts.
- Natural divergence is Kullback–Leibler.
- Not all data can be seen as histograms (positivity+constant mass)!

Dictionary learning on histograms

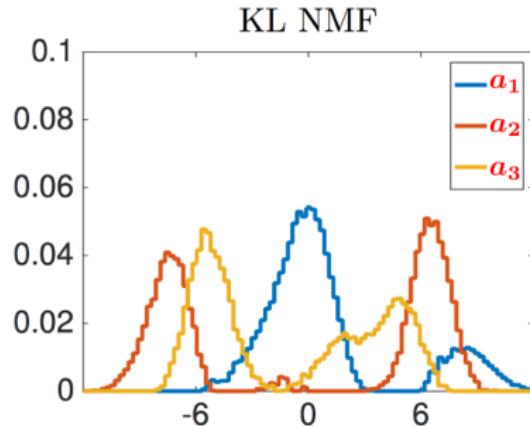
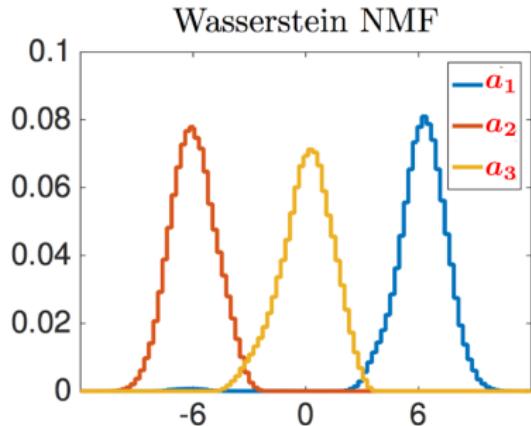


DL with Wasserstein distance [Sandler and Lindenbaum, 2011]

$$\min_{\mathbf{D}, \mathbf{H}} \sum_i W_{\mathbf{C}}(\mathbf{v}_i, \mathbf{D}\mathbf{h}_i)$$

- NMF: columns of \mathbf{D} and \mathbf{H} are on the simplex.
- Metric \mathbf{C} can encode spatial relations between the bins of the histograms.
- Ground metric learning [Zen et al., 2014].
- Fast DL with regularized OT [Rolet et al., 2016].

Dictionary learning on histograms

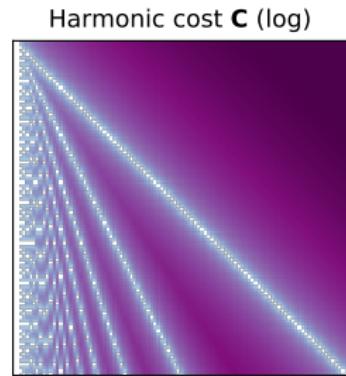
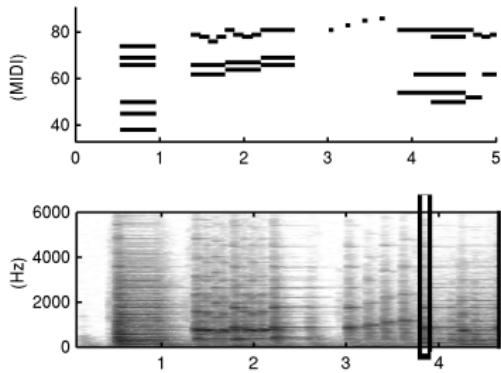


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Optimal Spectral Transportation (OST)

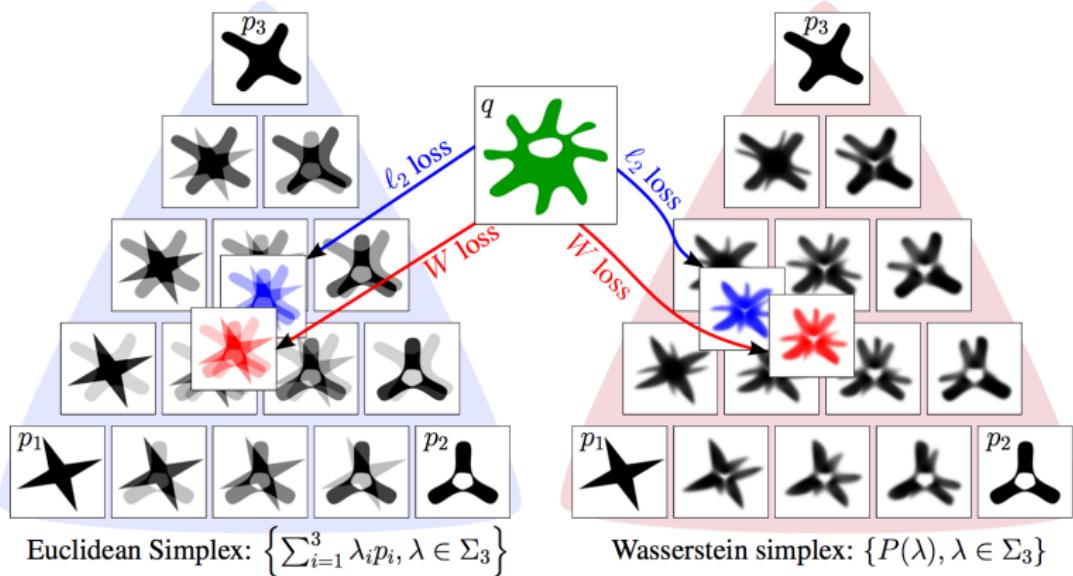


OT linear spectral unmixing of musical data [Flamary et al., 2016b]

$$\min_{\mathbf{h} \in \Delta} W_C(\mathbf{v}, \mathbf{D}\mathbf{h}) \quad (2)$$

- Objective : robustness to harmonic magnitude and small frequency shift
- Encode harmonic structure in the cost matrix (harmonic robustness).
- Can use simple dictionary (diracs on fundamental frequency).
- Very fast solver for sparse and entropic regularization.

Wasserstein dictionary learning

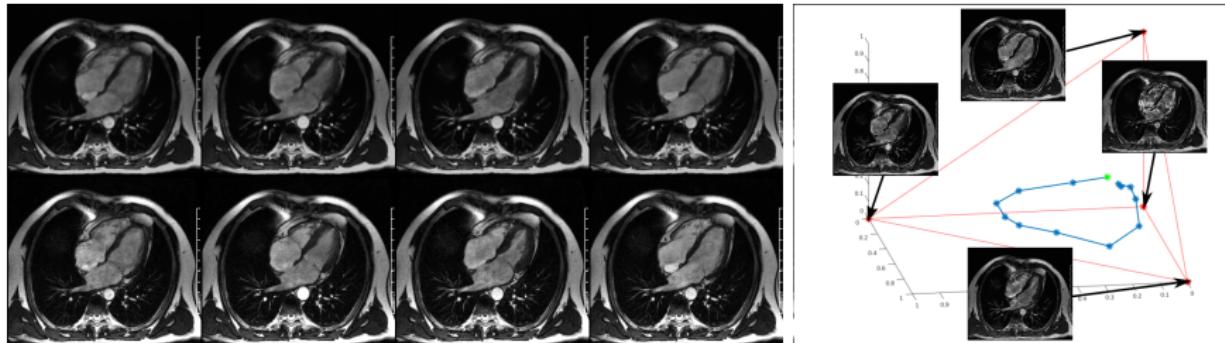


Nonlinear unmixing with Wasserstein simplex [Schmitz et al., 2017]

$$\min_{\mathbf{D}, \mathbf{H}} \quad \sum_i L(\mathbf{v}_i, WB(\mathbf{D}, \mathbf{h}_i))$$

with $WB(\mathbf{D}, \mathbf{h}) = \arg \min_{\mathbf{a}} \sum_i h_i W_C(\mathbf{d}_i, \mathbf{a})$

Wasserstein dictionary learning (2)



Nonlinear unmixing with Wasserstein simplex [Schmitz et al., 2017]

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with $WB(\mathbf{D}, \mathbf{h}) = \arg \min_{\mathbf{a}} \sum_i h_i W_C(\mathbf{d}_i, \mathbf{a})$

- Linear model is a barycenter for the squared ℓ_2 distance.
- Use Wasserstein barycenter for non-linear modeling.
- Application to cardiac sequence in MRI.
- One cardiac cycle is a trajectory in the simplex of the dictionary.

Principal Geodesics Analysis

Class 0			Class 1			Class 4		
PCA			PGA			PCA		
1	2	3	1	2	3	1	2	3
0	0	0	0	0	0	1	X	X
0	0	0	0	0	0	1	1	1
0	0	0	0	0	0	1	1	1
0	0	0	0	0	0	1	1	1
0	0	0	0	0	0	1	1	1
0	0	0	0	0	0	1	1	1
0	0	0	0	0	0	1	X	X
0	0	0	0	0	0	1	1	1

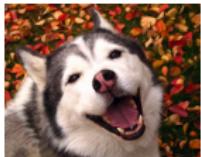
Geodesic PCA in the Wasserstein space [Bigot et al., 2017]

- Generalization of Principal Component Analysis to the Wasserstein manifold.
 - Regularized OT [Seguy and Cuturi, 2015].
 - Approximation using Wasserstein embedding [Courty et al., 2017a].

Multi-label learning with Wasserstein Loss



Siberian husky



Eskimo dog



Flickr : street, parade, dragon
Prediction : people, protest, parade



Flickr : water, boat, reflection, sun-shine
Prediction : water, river, lake, summer;

Learning with a Wasserstein Loss [Frogner et al., 2015]

$$\min_f \quad \sum_{k=1}^N W_1^1(f(\mathbf{x}_i), \mathbf{l}_i)$$

- Empirical loss minimization with Wasserstein loss.
- Multi-label prediction (labels \mathbf{l} seen as histograms, f output softmax).
- Cost between labels can encode semantic similarity between classes.
- Good performances in image tagging.

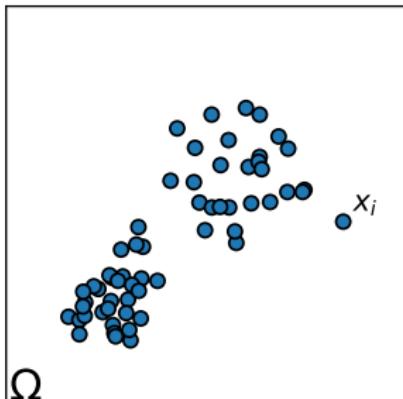
Learning from empirical distributions with Optimal Transport

Empirical distributions A.K.A datasets

$$\mu = \sum_{i=1}^n a_i \delta_{\mathbf{x}_i}, \quad \mathbf{x}_i \in \Omega, \quad \sum_{i=1}^n a_i = 1$$

Empirical distribution

- Two realizations never overlap.
- Training base of all machine learning approaches.
- How to measure discrepancy?
- Maximum Mean Discrepancy (ℓ_2 after convolution).
- Wasserstein distance.



Generative Adversarial Networks (GAN)

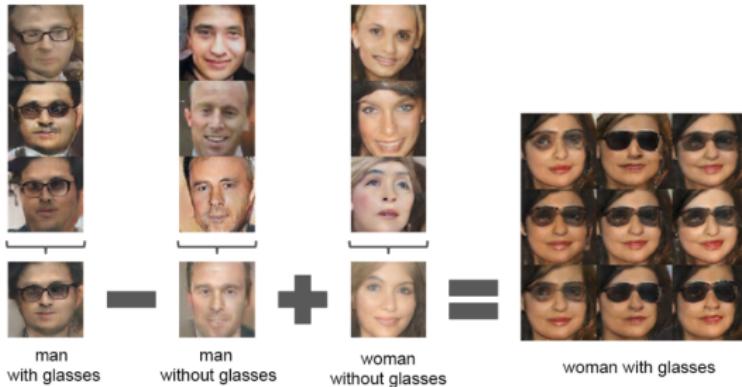


Generative Adversarial Networks (GAN) [Goodfellow et al., 2014]

$$\min_G \max_D E_{\mathbf{x} \sim \mu_d} [\log D(\mathbf{x})] + E_{\mathbf{z} \sim \mathcal{N}(0, \mathbf{I})} [\log(1 - D(G(\mathbf{z})))]$$

- Learn a generative model G that outputs realistic samples from data μ_d .
- Learn a classifier D to discriminate between the generated and true samples.
- Make those models compete (Nash equilibrium [Zhao et al., 2016]).

Generative Adversarial Networks (GAN)

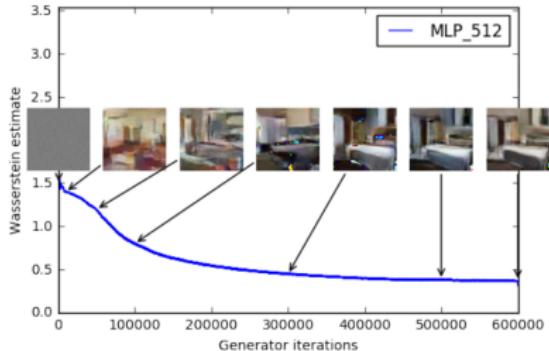
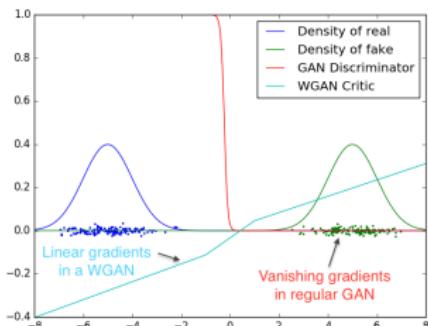


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- Learn a generative model G that outputs realistic samples from data μ_d .
- Learn a classifier D to discriminate between the generated and true samples.
- Make those models compete (Nash equilibrium [Zhao et al., 2016]).
- Generator space has semantic meaning [Radford et al., 2015].
- **But extremely hard to train (vanishing gradients).**

Wasserstein Generative Adversarial Networks (WGAN)



Wasserstein GAN [Arjovsky et al., 2017]

$$\min_G \quad W_1^1(G\#\mu_z, \mu_d), \quad (3)$$

- Minimizes the Wasserstein distance between the data μ_d and the generated data $G\#\mu_z$ whe $\mu_z = \mathcal{N}(0, \mathbf{I})$.
- No vanishing gradients ! Better convergence in practice.
- Wasserstein in the dual (separable w.r.t. the samples).

$$\min_G \sup_{\phi \in \text{Lip}^1} \quad \mathbb{E}_{\mathbf{x} \sim \mu_d} [\phi(\mathbf{x})] - \mathbb{E}_{\mathbf{z} \sim \mu_z} [\phi(G(\mathbf{z}))]$$

- ϕ is a neural network that acts as an *actor critic*

WGAN: the devil in the approximation

Neural network belonging to Lip^1 ?

- Not really! [Arjovsky et al., 2017] proposes to do weight clipping that force an upper bound on the Lipschitz constant.
- It is actually the supremum over K-Lipschitz functions that is approximated by a neural network

$$\max_{f \in \text{NN class}} L_{\text{WGAN}}(f, G) \leq \sup_{\|\phi\|_L \leq K} L_{\text{WGAN}}(\phi, G) = K \cdot W_1^1(G(\mathbf{z}), \mu_d)$$

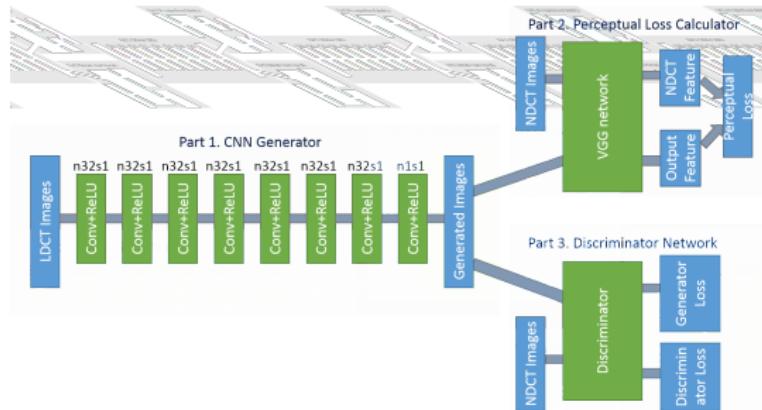
- Actually **not** equivalent to solve the optimal transport, but gradients are aligned.

Improved WGAN [Gulrajani et al., 2017]

$$\min_G \sup_{f \in \text{NN class}} \mathbb{E}_{\mathbf{x} \sim \mu_d}[f(\mathbf{x})] - \mathbb{E}_{\mathbf{z} \sim \mu_z}[f(G(\mathbf{z}))] + \lambda \mathbb{E}_{\mathbf{x} \sim \mu_d}[(\|\nabla f(\mathbf{x})\|_2 - 1)^2]$$

Relaxation of the constraint (for W_1 the gradient of the potential is 1 almost everywhere).

Wasserstein GAN loss on Biomedical images

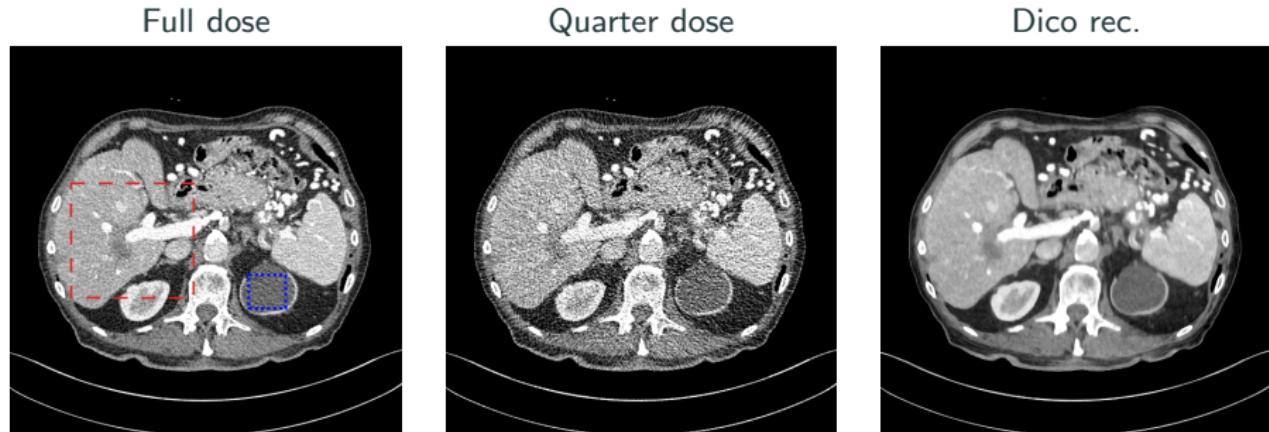


Reconstructing low dose CT images [Yang et al., 2018]

$$\min_G W_1^1(G\#\mu_l, \mu_f) + \lambda_1 E_{\mathbf{x} \sim \mu_l} [\|VGG(\mathbf{x}_l) - VGG(G(\mathbf{x}_l))\|^2], \quad (4)$$

- Use Wasserstein to make reconstruction of quarter dose CT images (μ_l) similar to high dose (resolution) CT images (μ_f).
- Perceptual loss based on VGG [Simonyan and Zisserman, 2014] embedding to keep image information.

Wasserstein GAN loss on Biomedical images



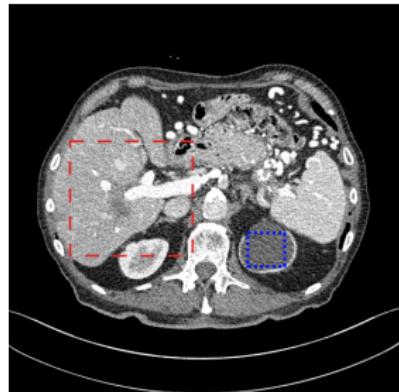
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Wasserstein GAN loss on Biomedical images

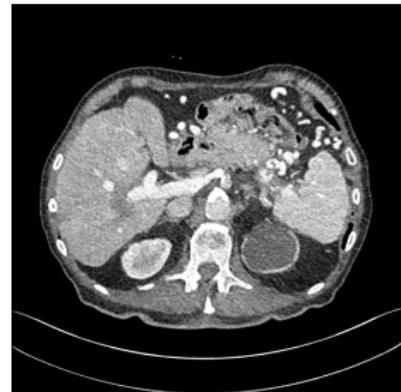
Full dose



Quarter dose



WGAN-VGG rec.

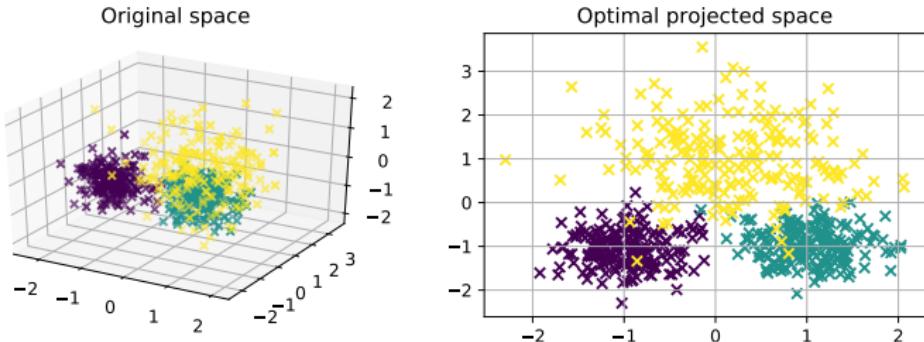


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Wasserstein Discriminant Analysis (WDA)

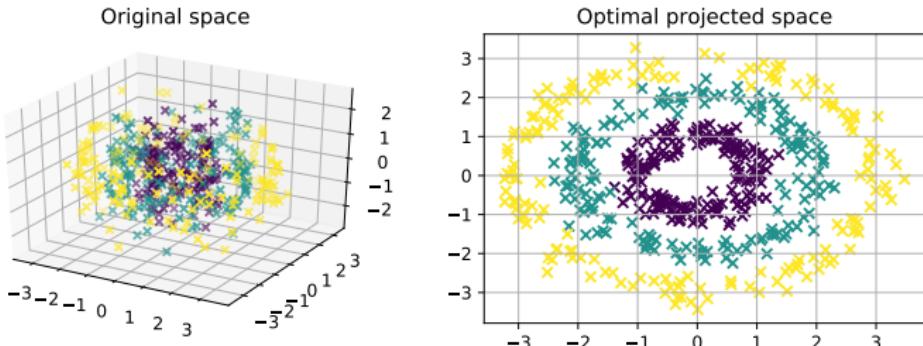


$$\max_{\mathbf{P} \in \mathcal{S}} \frac{\sum_{c,c' > c} W_\lambda(\mathbf{P}\mathbf{X}^c, \mathbf{P}\mathbf{X}^{c'})}{\sum_c W_\lambda(\mathbf{P}\mathbf{X}^c, \mathbf{P}\mathbf{X}^c)} \quad (5)$$

- \mathbf{X}^c are samples from class c .
- \mathbf{P} is an orthogonal projection;

- Converges to Fisher Discriminant when $\lambda \rightarrow \infty$.
- Non parametric method that allows nonlinear discrimination.
- Problem solved with gradient ascent in the Stiefel manifold \mathcal{S} .
- Gradient computed using automatic differentiation of Sinkhorn algorithm.

Wasserstein Discriminant Analysis (WDA)

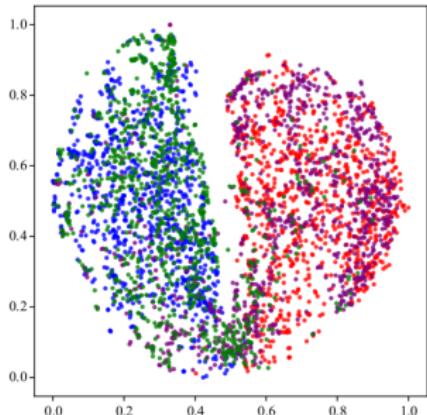
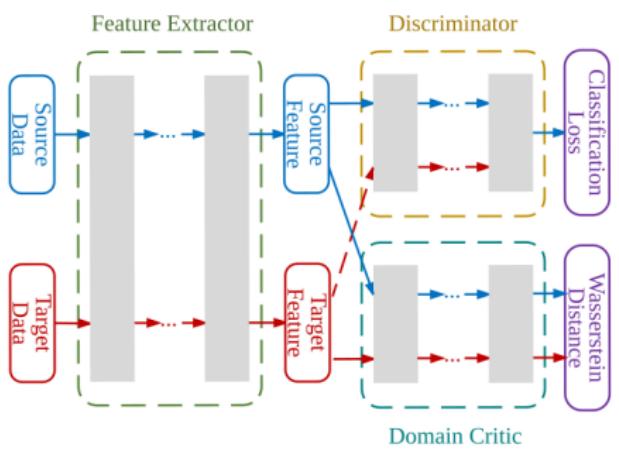


$$\max_{\mathbf{P} \in \mathcal{S}} \frac{\sum_{c,c' > c} W_\lambda(\mathbf{P}\mathbf{X}^c, \mathbf{P}\mathbf{X}^{c'})}{\sum_c W_\lambda(\mathbf{P}\mathbf{X}^c, \mathbf{P}\mathbf{X}^c)} \quad (5)$$

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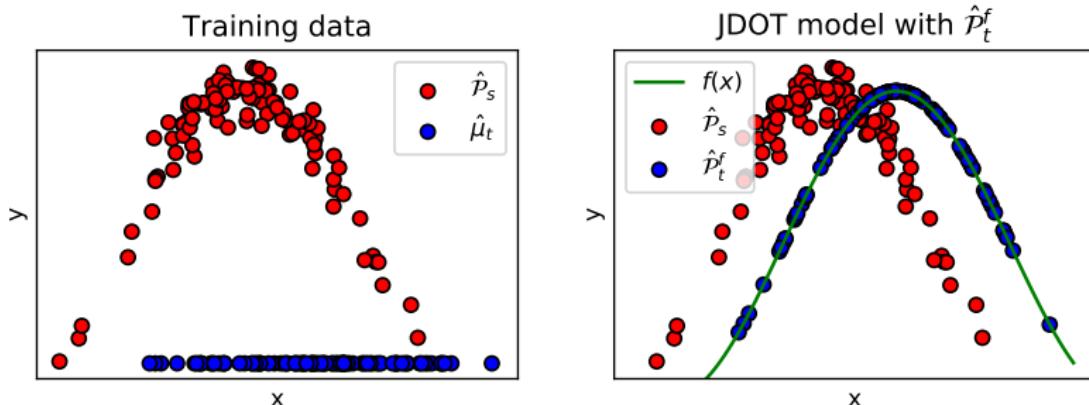
Domain adaptation with Wasserstein distance



Domain adaptation for deep learning [Shen et al., 2018]

- Modern DA aim at aligning source and target in the deep representation : DANN [Ganin et al., 2016], MMD [Tzeng et al., 2014], CORAL [Sun and Saenko, 2016].
- Wasserstein distance (WGAN loss [Arjovsky et al., 2017]) used as objective for the adaptation [Shen et al., 2018].

Joint Distribution Optimal Transport for DA

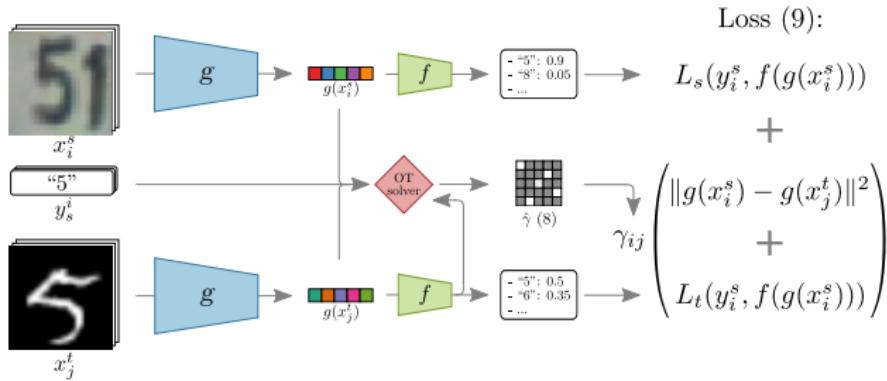


Learning with JDOT [Courty et al., 2017b]

$$\min_f \quad \left\{ W_1(\hat{\mathcal{P}}_s, \hat{\mathcal{P}}_t^f) = \inf_{\gamma \in \Pi} \sum_{ij} \mathcal{D}(\mathbf{x}_i^s, y_i^s; \mathbf{x}_j^t, f(\mathbf{x}_j^t)) \gamma_{ij} \right\} \quad (6)$$

- $\hat{\mathcal{P}}_t^f = \frac{1}{N_t} \sum_{i=1}^{N_t} \delta_{\mathbf{x}_i^t, f(\mathbf{x}_i^t)}$ is the proxy joint feature/label distribution.
- $\mathcal{D}(\mathbf{x}_i^s, y_i^s; \mathbf{x}_j^t, f(\mathbf{x}_j^t)) = \alpha \|\mathbf{x}_i^s - \mathbf{x}_j^t\|^2 + \mathcal{L}(y_i^s, f(\mathbf{x}_j^t))$ with $\alpha > 0$.
- We search for the predictor f that better align the joint distributions.
- OT matrix does the label propagation (no mapping).
- JDOT can be seen as minimizing a generalization bound.

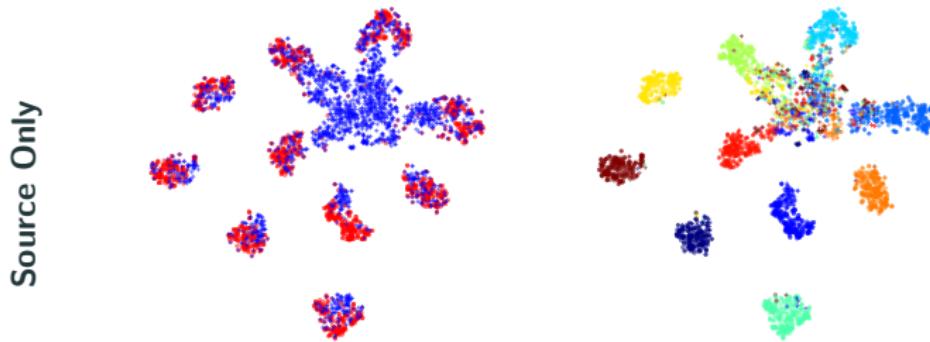
JDOT for large scale deep learning



DeepJDOT [Damodaran et al., 2018]

- Learn simultaneously the embedding g and the classifier f .
- JDOT performed in the joint embedding/label space.
- Use minibatch to estimate OT and update g, f at each iterations.
- Scales to large datasets and estimate a representation for both domains.
- TSNE projections of embeddings (MNIST→MNIST-M).

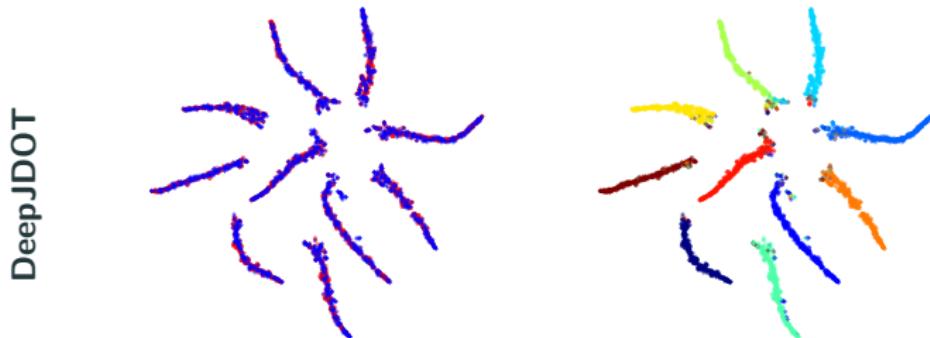
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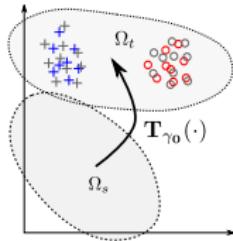
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Conclusion

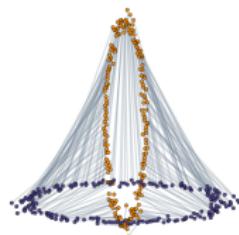
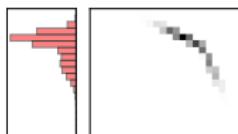
Optimal transport for machine learning

Mapping with optimal transport



- Optimal displacement from one distribution to another.
- Can estimate smooth mapping for out of sample displacement.
- Domain, color and gradient adaptation, transfer learning.

OT matrix γ



Learning with optimal transport

- Natural divergence for machine learning and estimation.
- Cost encode complex relations in an histogram.
- Regularization is the key (performance, smoothness).
- Recent optimization procedures opened it to medium/large scale datasets.
- Sensible loss between non overlapping distributions.
- Works with both histograms and empirical distributions.

Thank you

Python code available on GitHub:

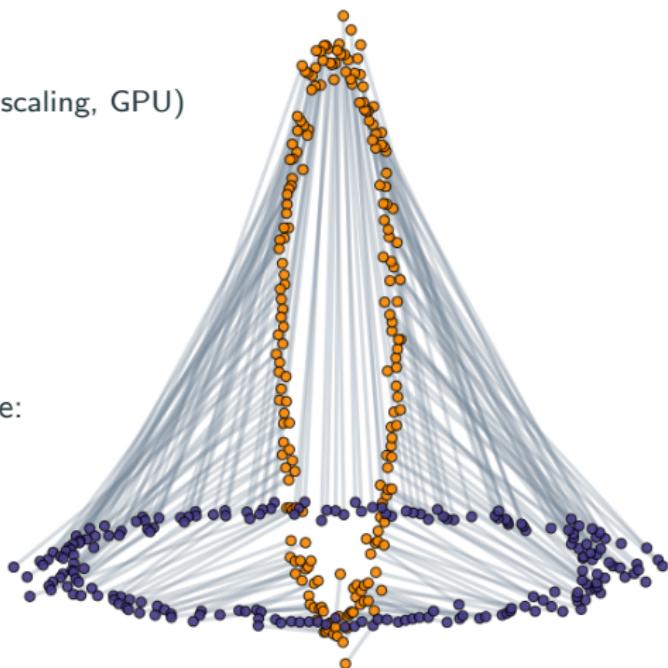
<https://github.com/rflamary/POT>

- OT LP solver, Sinkhorn (stabilized, ϵ -scaling, GPU)
- Domain adaptation with OT.
- Barycenters, Wasserstein unmixing.
- Wasserstein Discriminant Analysis.

Slides and papers available on my website:

<https://remi.flamary.com/>

Post doc available in Nice (France)



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