Optimal Transport for Machine Learning

Part 2: Machine learning applications

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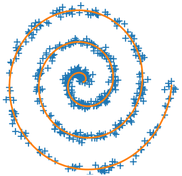
Introduction

Three aspects of Machine Learning

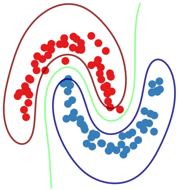
Unsupervised learning

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



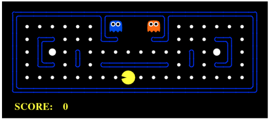
Supervised Learning

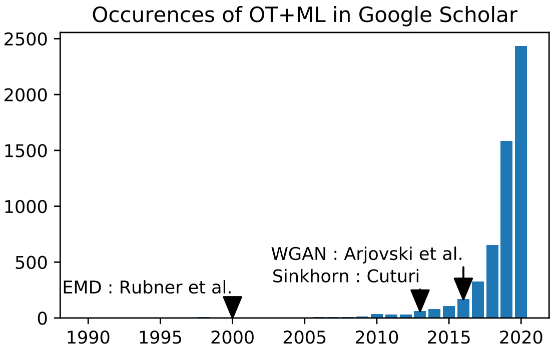
- Learning to predict from labeld dataset.
- Regression, Classification.
- Can use unsupervised information (DA, Semi-sup.)



Reinforcement Learning

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

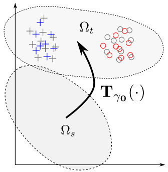


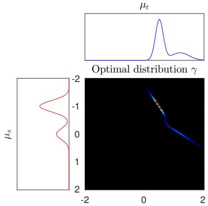


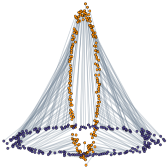
Short history of OT for ML

- 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 for ML







Transporting with optimal transport

- Color adaptation in image [Ferradans et al., 2014].
- Style transfer [Mroueh, 2019].
- Domain adaptation [Courty 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]
- Adversarial regularization [Fatras et al., 2021].

Divergence between empirical distributions

- Non parametric divergence between non overlapping distributions.
- Generative modeling [Arjovsky et al., 2017].
- Data imputation [Muzellec et al., 2020].

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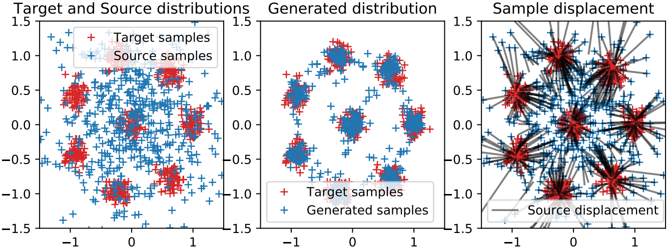
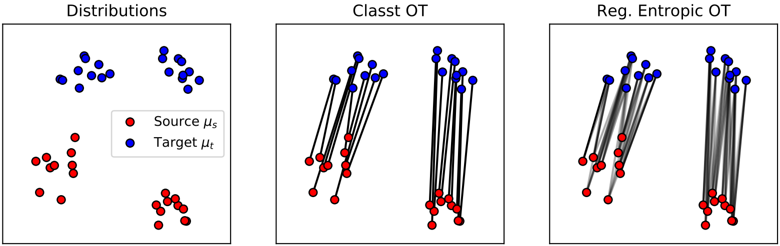
Mapping with optimal transport



Mapping estimation

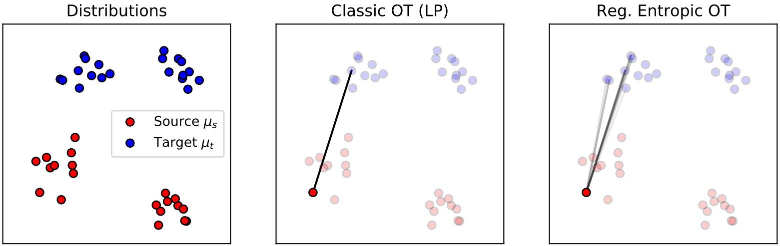
- Barycentric mapping using the OT matrix [Ferradans et al., 2014].
- Linear Monge mapping when data supposed Gaussian [Flamary et al., 2019].
- Smooth mapping estimation
  [Perrot et al., 2016, Seguy et al., 2017, Paty et al., 2020].
- Estimation for W_2 using input convex neural networks [Makkuva et al., 2020].
- Can be used to linearize the Wasserstein space [Mérigot et al., 2020]



Barycentric mapping [Ferradans et al., 2014]

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

- 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.



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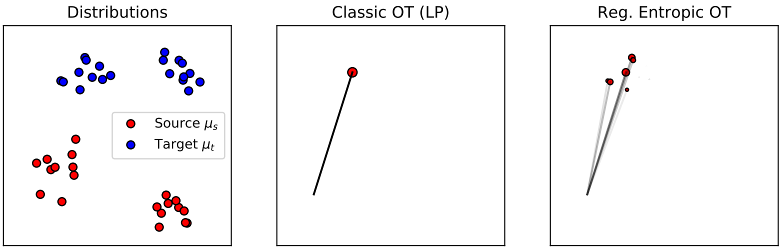
Transporting the discrete samples



Barycentric mapping [Ferradans et al., 2014]

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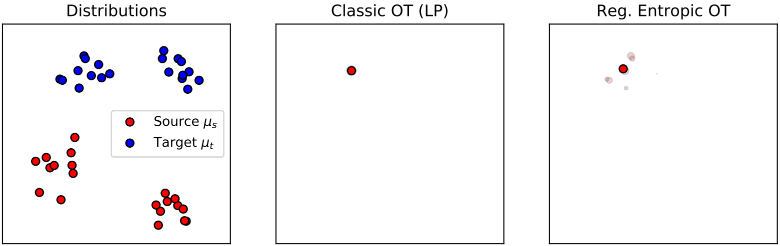

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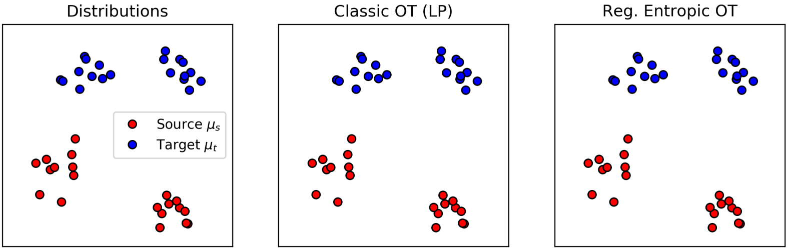

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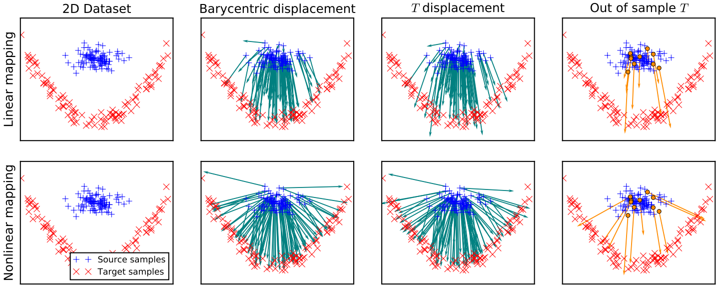
Joint OT and mapping estimation

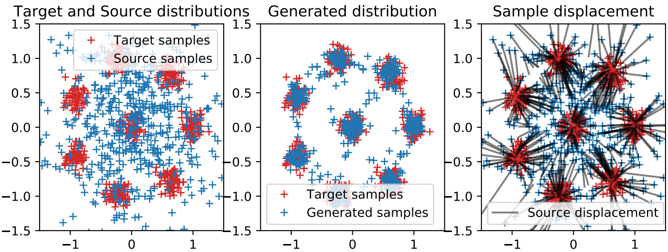


Simultaneous OT matrix and mapping [Perrot et al., 2016]

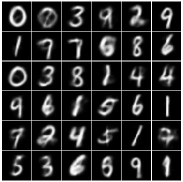
$$\min_{T,\boldsymbol{\gamma}\in\mathcal{P}} \quad \langle\boldsymbol{\gamma},\mathbf{C}\rangle_F + \sum_i \|T(\mathbf{x}_i^s) - \hat{T}_{\boldsymbol{\gamma}}(\mathbf{x}_i^s)\|^2 + \lambda\|T\|^2$$

- 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

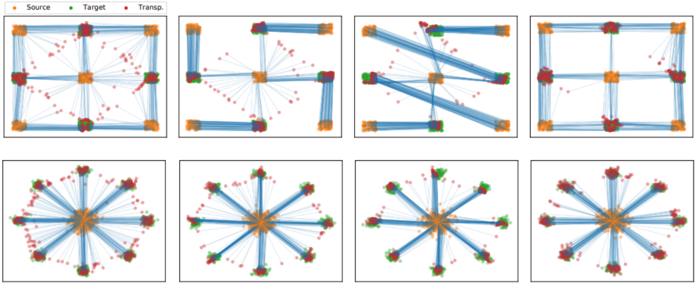


Large scale mapping estimation [Seguy et al., 2017]



- 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 mapping for small regularization.
- Convergence to the smooth mapping for large n [Pooladian and Niles-Weed, 2021].

Monge Mapping with input convex neural networks

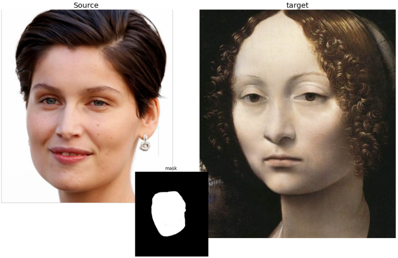


(a) Barycentric-OT (b) W1-LP (c) W2GAN (d) Our approach

Principle [Makkuva et al., 2020]

- For the quadratic cost OT between two smooth distribution Brenier theorem states that the Monge mapping is the gradient of a convex function.
- Neural network can be designed to be convex wrt their input (ICNN) [Amos et al., 2017].
- [Makkuva et al., 2020] proposed to estimate directly the Monge as a gradient of an ICNN from the empirical distributions. mapping usin

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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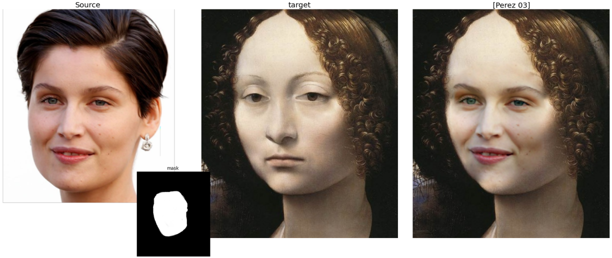

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Seamless copy with gradient adaptation [Perrot et al., 2016]

- 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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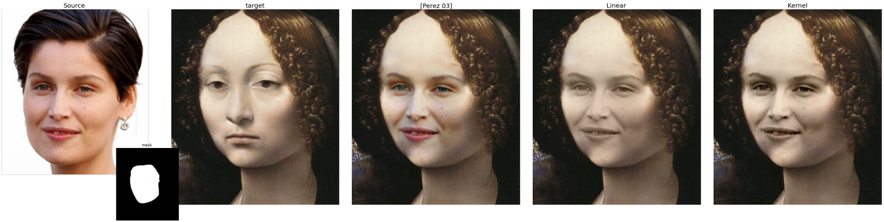

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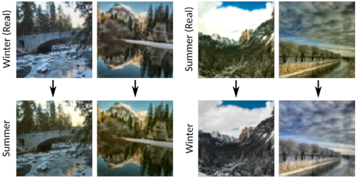
Example and webcam demo: `https://github.com/ncourty/PoissonGradient`

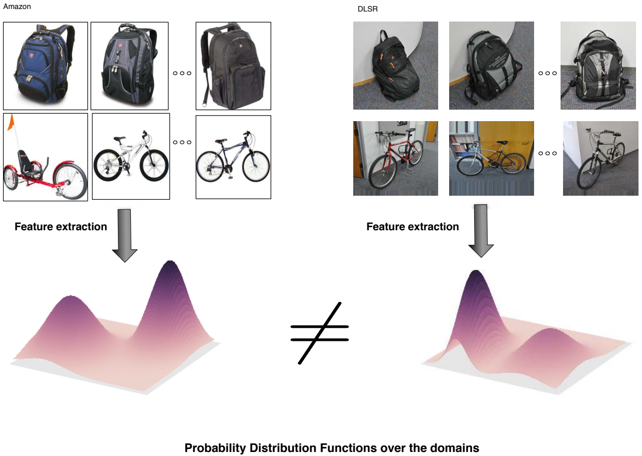
Monge mapping for Image-to-Image translation



Principle

- Encode image as a distribution in a DNN embedding.
- Transform between images using estimated Monge mapping.
- Linear Monge Mapping (Wasserstein Style Transfer [Mroueh, 2019]).
- Nonlinear Monge Mapping using input Convex Neural Networks [Korotin et al., 2019].
- Allows for transformation between two images but also style interpolation with Wasserstein barycenters.

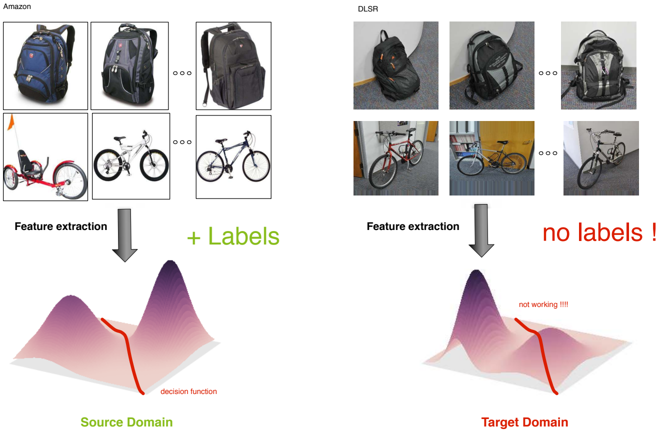
Domain Adaptation problem



Our context

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

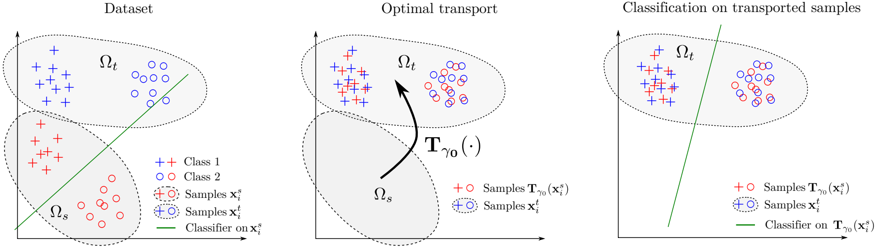
Unsupervised domain adaptation problem



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

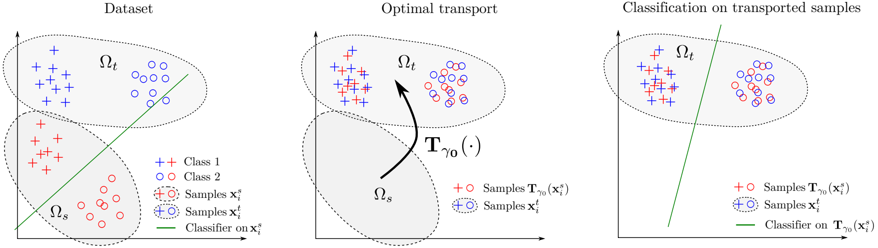
OT for domain adaptation : Step 1



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



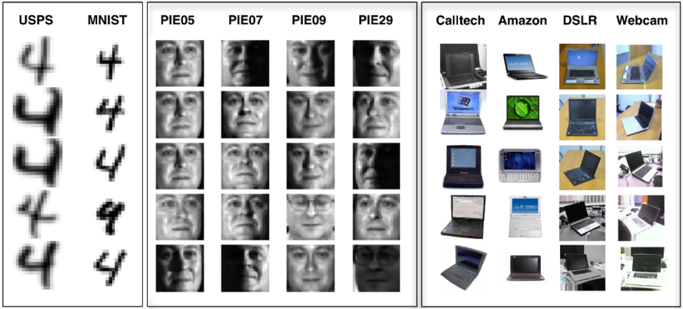
Step 2 : Transport the training samples onto the target distribution.

- 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.

Visual adaptation datasets



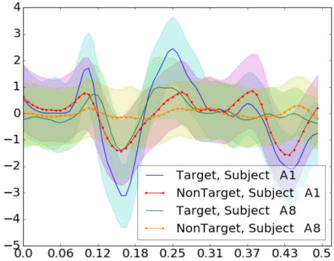
Datasets

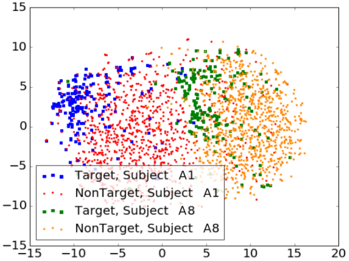
- **Digit recognition**, MNIST VS USPS (10 classes, d=256, 2 dom.).
- **Face recognition**, PIE Dataset (68 classes, d=1024, 4 dom.).
- **Object recognition**, Caltech-Office dataset (10 classes, d=800/4096, 4 dom.).

Numerical experiments

- State of the art performances on the 3 datasets.
- Works well on deep features adaptation and extension to semi-supervised DA.

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.

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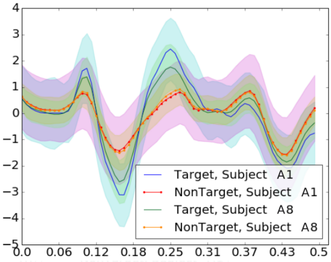

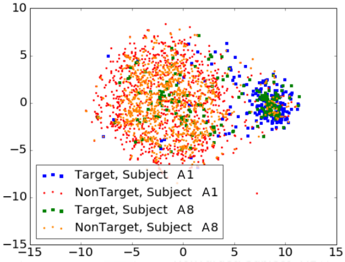

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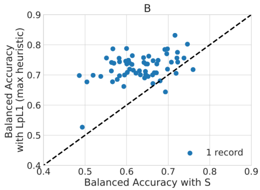
OTDA for biomedical data (2)

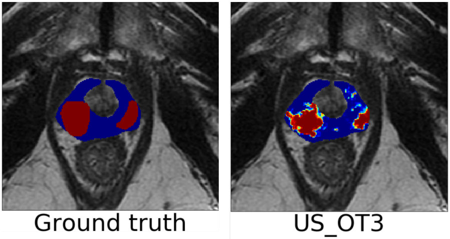
EEG sleep stage classification [Chambon et al., 2018]

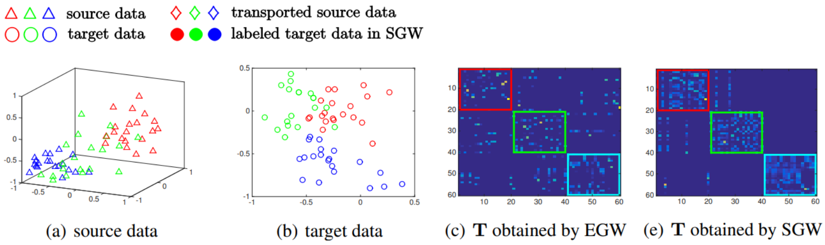
- Use pre-trained neural network.
- Adapt with OTDA on the penultimate layer.
- OTDA best DA approach to adapt between EEG recordings.



Prostace cancer classification [Gautheron et al., 2017]

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

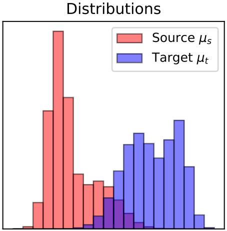


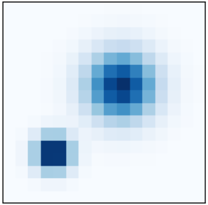


Semi-supervised Heterogeneous Domain Adaptation [Yan et al., 2018]

- OT for DA initially proposed by [Courty et al., 2016].
- Use the OT matrix to transfer labels or samples between datasets.
- GW find correspondences across spaces but very noisy.
- Semi-supervised strategy allows very good performances.
- Alternative : Co-optimal transport that find correspondances between the variables and samples simultaneously [Redko et al., 2020].

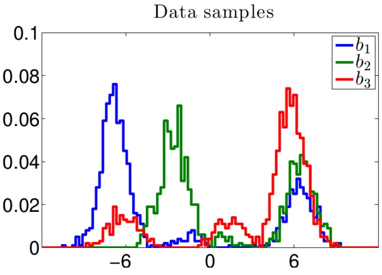
Outline





Data as histograms

- Fixed bin positions $\mathbf{x}_i$ e.g. grid, simplex $\Delta = \left\{(\mu_i)_i \geq 0; \sum_i \mu_i = 1\right\}$
- 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)!

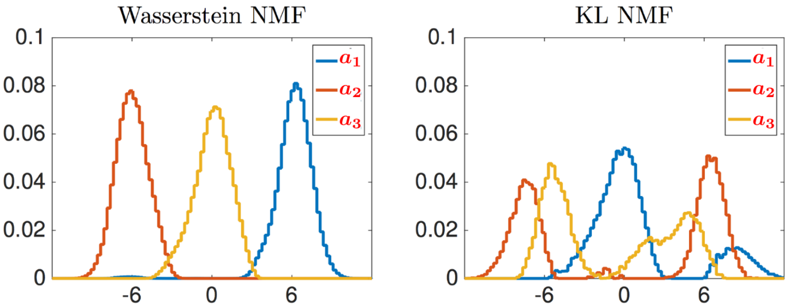


DL with Wasserstein distance [Sandler and Lindenbaum, 2011]

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

- 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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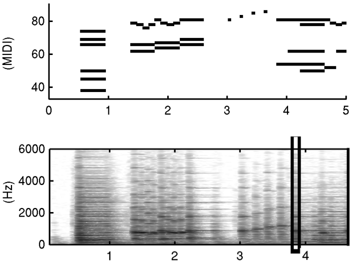
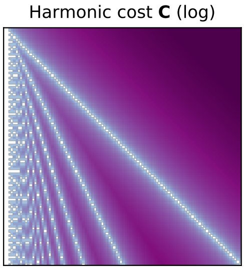
Optimal Spectral Transportation (OST)





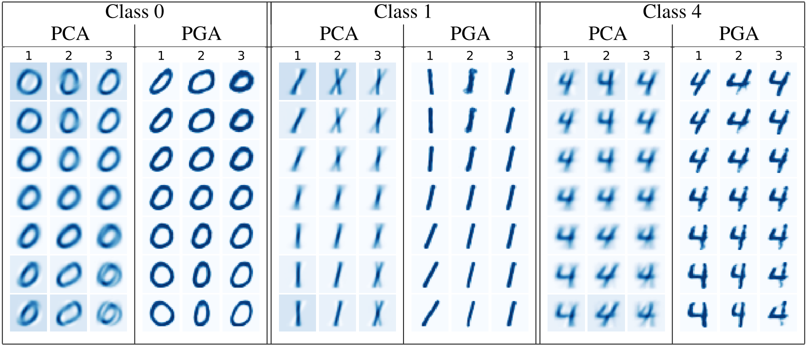
OT linear spectral unmixing of musical data [Flamary et al., 2016]

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

- 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.

Demo : `https://github.com/rflamary/OST`

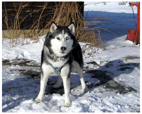
Principal Geodesics Analysis



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., 2017a].

Multi-label learning with Wasserstein Loss



Siberian husky

Eskimo dog

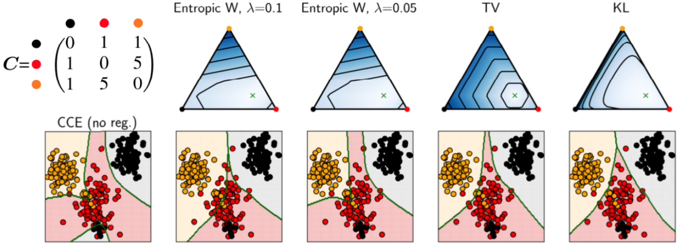
Flickr : street, parade, dragon
Prediction : people, protest, parade

Flickr : water, boat, ref ection, 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.



Principle [Fatras et al., 2021]

$$R_{\mathbf{C}}(f,\mathbf{x}) = \max_{\|\mathbf{v}\|\leq\epsilon} W_{\mathbf{C}}(f(\mathbf{x}+\mathbf{v}), f(\mathbf{x}))$$

- Use (virtual) adversarial examples to promote a better generalization of DNN (close samples should have close predictions) [Miyato et al., 2018].
- The ground metric $\mathbf{C}$ in regularization $R_{\mathbf{C}}(f,\mathbf{x})$ encodes pairwise class relations and will promote smooth/complex between them.
- State of the art performance for learning with label noise when using semantic relations between the classes for $\mathbf{C}$ (word2vec).

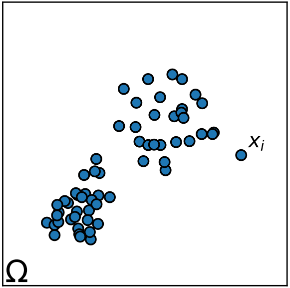
Outline

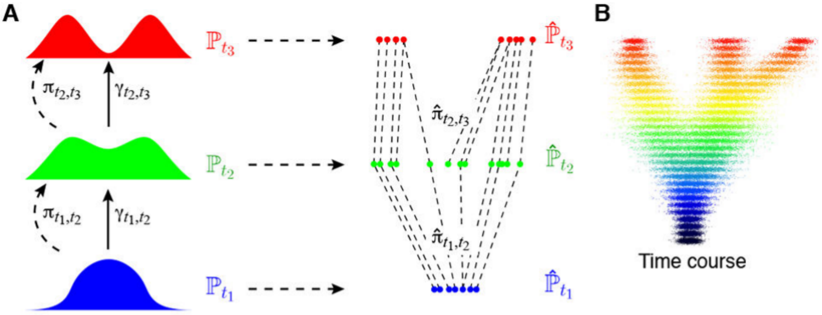
Empirical distributions A.K.A datasets

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

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.

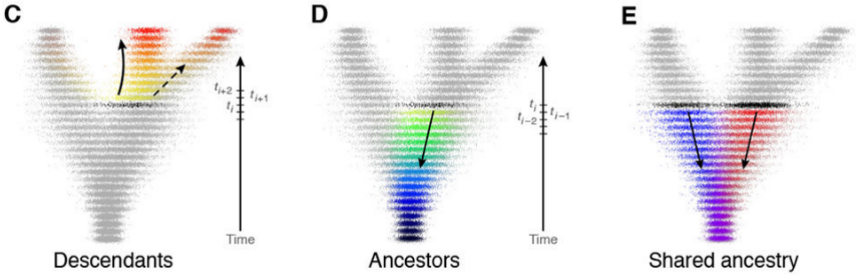




Principle [Schiebinger et al., 2019]

- Developmental trajectories of cells from stem cells to more specialized.
- Cell populations are samples at different times with scRNA-seq.
- Optimal transport can be used to find mapping/correspondances between across population measurements.
- Unbalanced OT is used to model cellular growth and death rates.

OT for modeling cell deelopment



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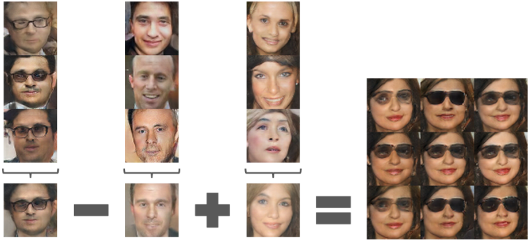
Generative Adversarial Networks (GAN)

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

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

- 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]).



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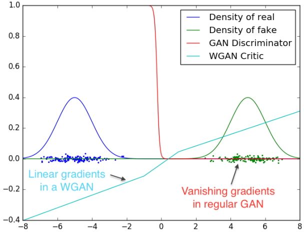
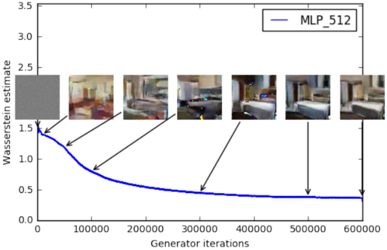
- Learn a classifier D to discriminate between the generated and true samples.
- Make those models compete (Nash equilibrium [Zhao et al., 2016]).
- Generator space has semantic meaning [Radford et al., 2015].
- But extremely hard to train (vanishing gradients).

Wasserstein Generative Adversarial Networks (WGAN)





Wasserstein GAN [Arjovsky et al., 2017]

$$\min_{G} \quad W_1^1(G\#\mu_z, \mu_d), \tag{3}$$

- 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

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

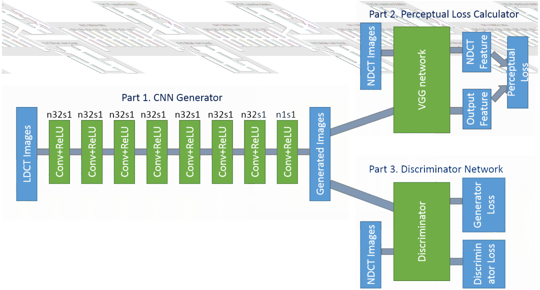
- Actually **not** equivalent to solve the optimal transport, but gradients are aligned.

Improved WGAN [Gulrajani et al., 2017]

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

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

Wasserstein GAN loss on Biomedical images



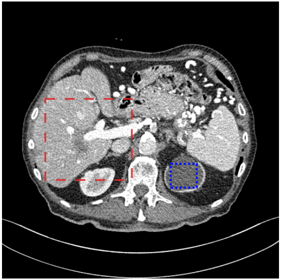
Reconstructing low dose CT images [Yang et al., 2018]

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

- 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

Full dose



Quarter dose

Dico rec.

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

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

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Wasserstein GAN loss on Biomedical images

Full dose | Quarter dose | WGAN-VGG rec.

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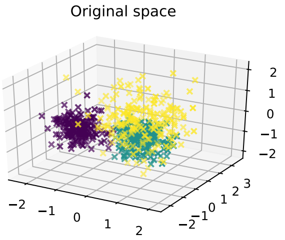
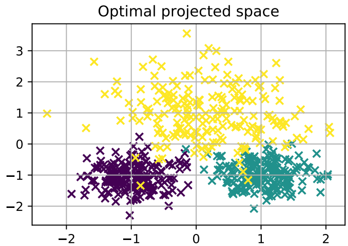
Wasserstein Discriminant Analysis (WDA)



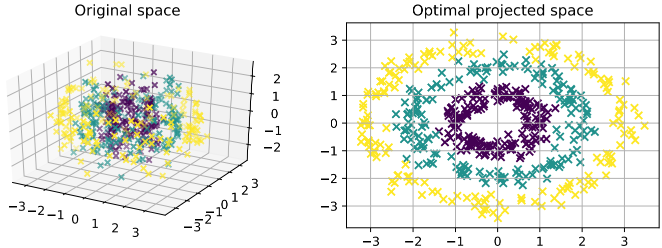


$$\max_{\mathbf{P}\in\mathcal{S}} \quad \frac{\sum_{c,c'>c} W_\lambda(\mathbf{P}\mathbf{X}^c, \mathbf{P}\mathbf{X}^{c'})}{\sum_c W_\lambda(\mathbf{P}\mathbf{X}^c, \mathbf{P}\mathbf{X}^c)} \quad (5)$$

- $\mathbf{X}^c$ 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)



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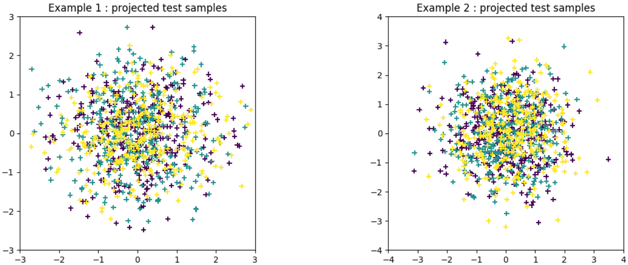

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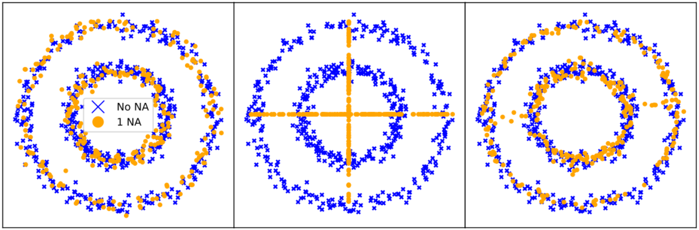
Data imputation with Optimal Transport

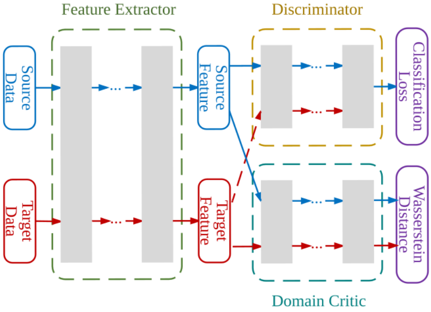


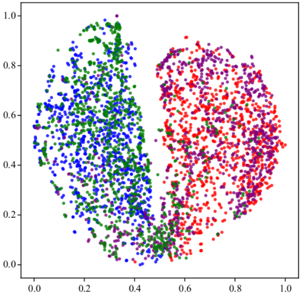
Missing Data imputation [Muzellec et al., 2020]

$$\min_{\mathbf{X}^{imp}} \quad \mathbb{E}[SD(\mu_m(\hat{\mathbf{X}}), \mu_m(\hat{\mathbf{X}}))]$$

- $\mathbf{X} \odot \mathbf{M}$ is the partially observed data with binary mask $\mathbf{M}$.
- $\hat{\mathbf{X}} = \mathbf{X} \odot \mathbf{M} + (1 - \mathbf{M}) \odot \mathbf{X}^{imp}$ is the data imputed by $\mathbf{X}^{imp}$
- $\mu_m(\mathbf{X})$ is a minibatch of $\mathbf{X}$, expectation is taken *w.r.t.* the minibatches.
- Out of sample imputation with model [Muzellec et al., 2020, Algo 2 & 3]
- Optimizing minibatch Wasserstein is a classical approach [Fatras et al., 2020].

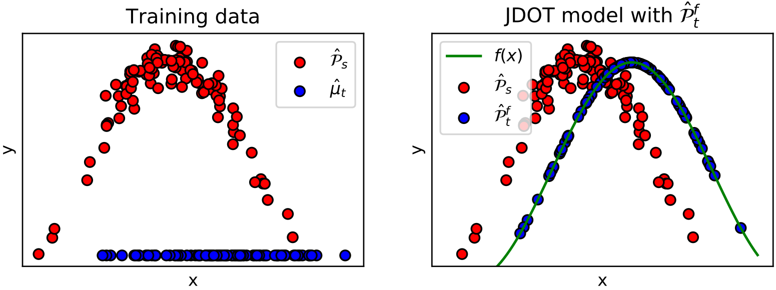
Domain adaptation with Wasserstein distance




(d) t-SNE of WDGRL features

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

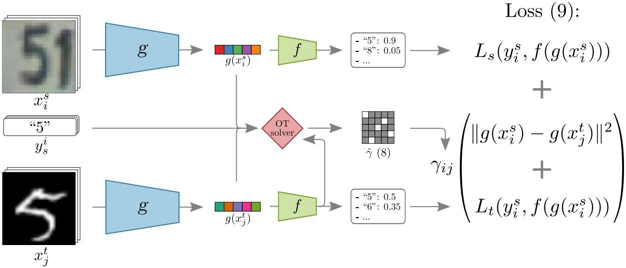
- Modern DA aim at aligning source and target in the deep representation : DANN [Ganin et al., 2016], MMD [Tzeng et al., 2014], CORAL [Sun and Saenko, 2016].
- Wasserstein distance (WGAN loss [Arjovsky et al., 2017]) used as objective for the adaptation [Shen et al., 2018].



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

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

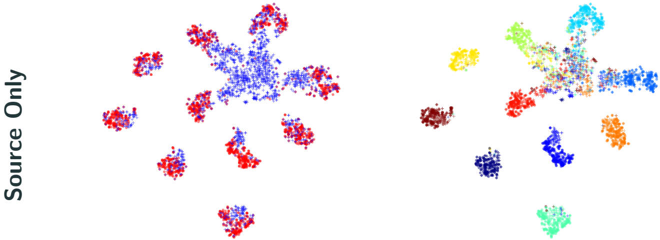
- $\hat{\mathcal{P}}_t{}^f = \frac{1}{N_t} \sum_{i=1}^{N_t} \delta_{\mathbf{x}_i^t, f\mathbf{x}_i^t}$ is the proxy joint feature/label distribution.
- $\mathcal{D}(\mathbf{x}_i^s, y_i^s; \mathbf{x}_j^t, f(\mathbf{x}_j^t)) = \alpha \|\mathbf{x}_i^s - \mathbf{x}_j^t\|^2 + \mathcal{L}(y_i^s, f(\mathbf{x}_j^t))$ 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.



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 [Fatras et al., 2020].
- Scales to large datasets and estimate a representation for both domains.
- TSNE projections of embeddings (MNIST→MNIST-M).

JDOT for large scale deep learning



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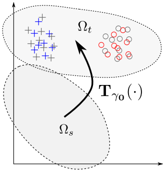
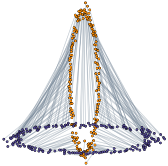
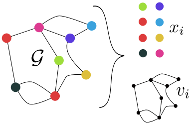
Outline

Three aspects of optimal transport







Transporting with optimal transport

- Learn to map between distributions.
- Estimate a smooth mapping from discrete distributions.
- Applications in domain adaptation.

Divergence between histograms/empirical distributions

- Use the ground metric to encode complex relations between the bins of histograms for data fitting.
- OT losses are non-parametric divergences between non overlapping distributions.
- Used to train minimal Wasserstein estimators.

Divergence between structured objects and spaces

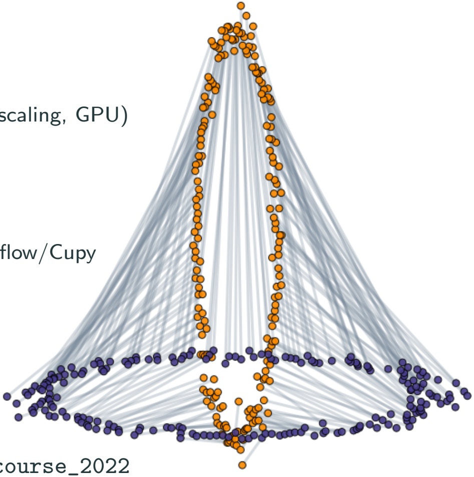
- Modeling of structured data and graphs as distribution.
- OT losses (Wass. or (F)GW) measure similarity between distributions/objects.
- OT find correspondance across spaces for adaptation.

Thank you

Python code available on GitHub:

https://github.com/PythonOT/POT

- OT LP solver, Sinkhorn (stabilized, $\epsilon-$scaling, GPU)
- Domain adaptation with OT.
- Barycenters, Wasserstein unmixing.
- Gromov Wasserstein.
- Solvers for Numpy/Pytorch/Jax/tensorflow/Cupy



Link for the practical session:

https://github.com/PythonOT/OTML_course_2022

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