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Contributions to Optimal Transport for Machine Learning: Ground Metric and Generalized Framework

Thesis defense of Tanguy KERDONCUFF

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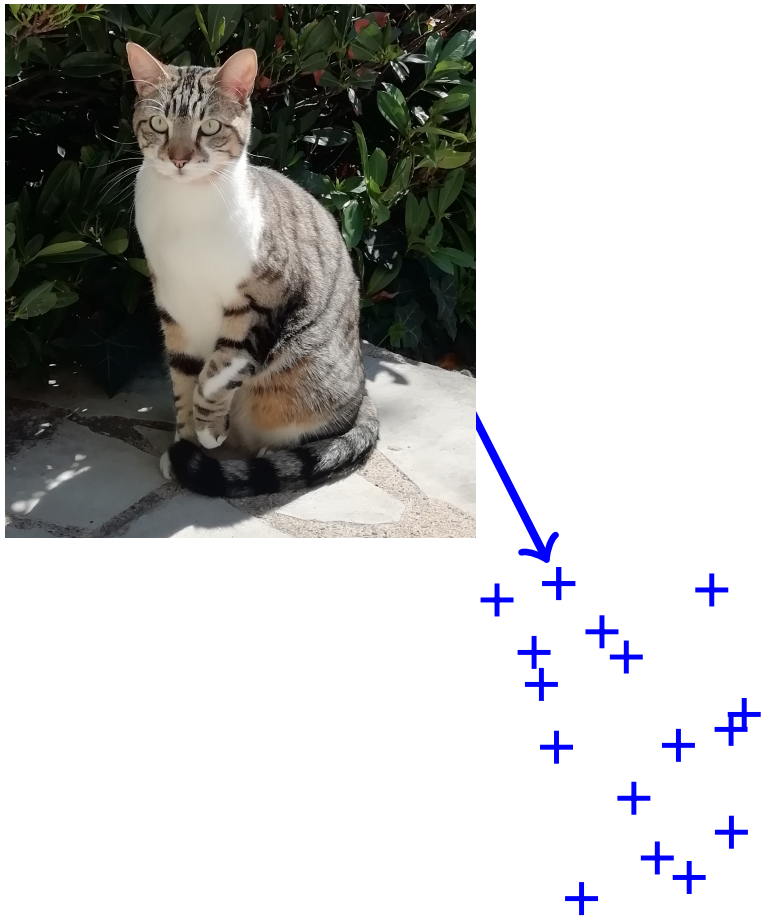
Rémi EMONET Maître de conférences, Université de Saint-Étienne Co-encadrant

November 16, 2021

Basic Machine Learning examples



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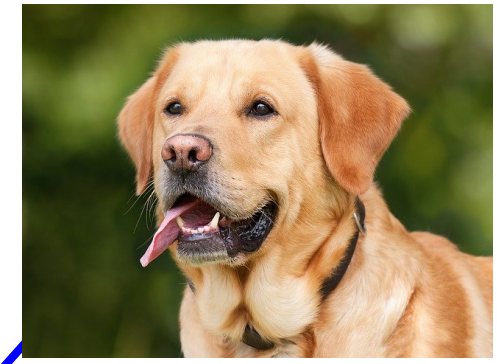

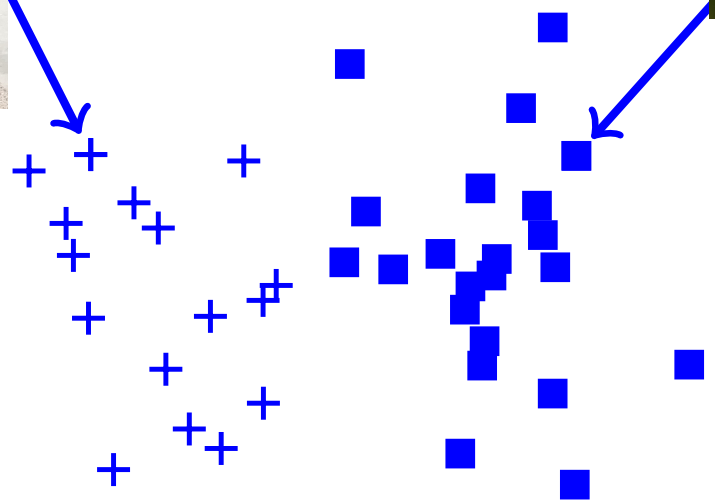

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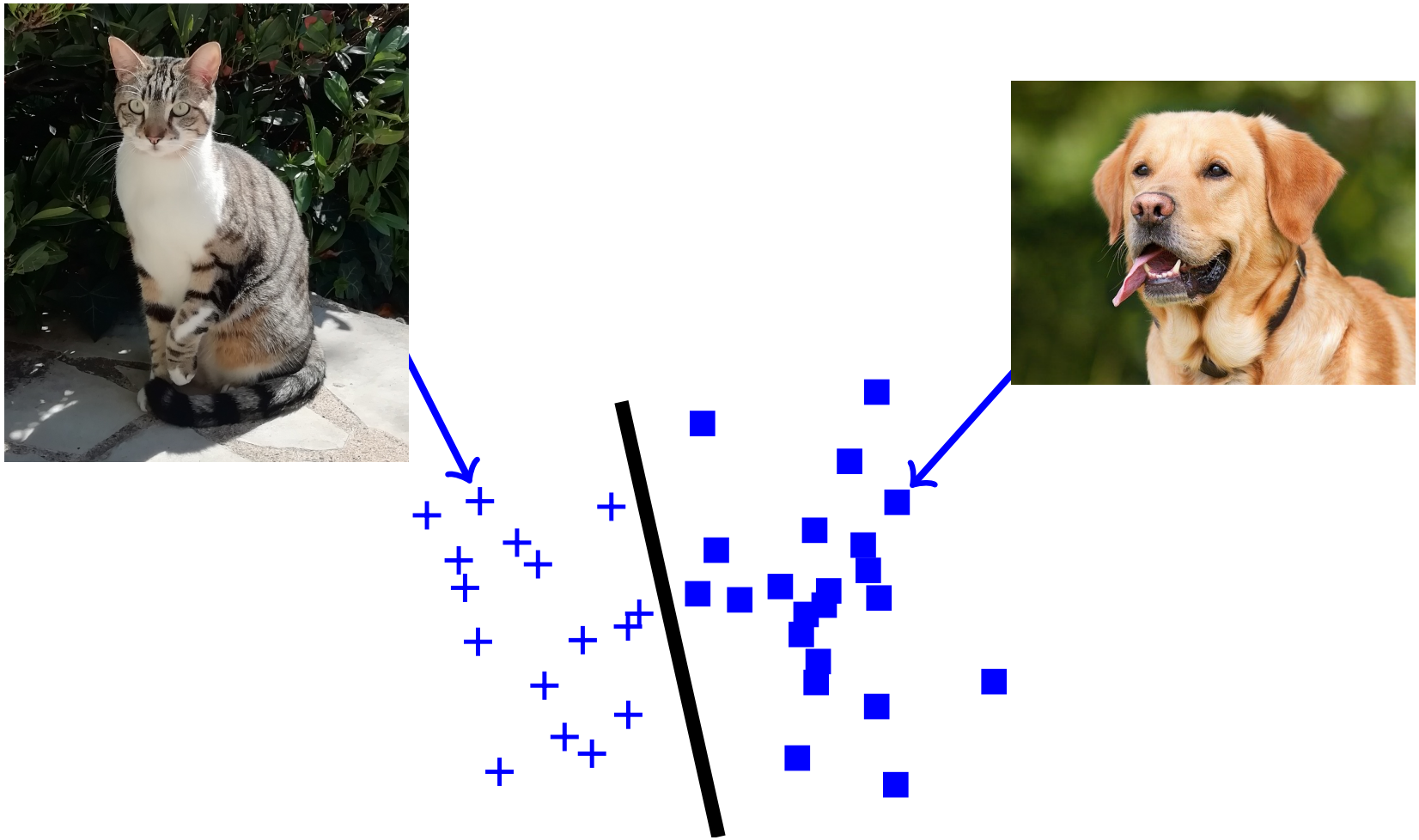

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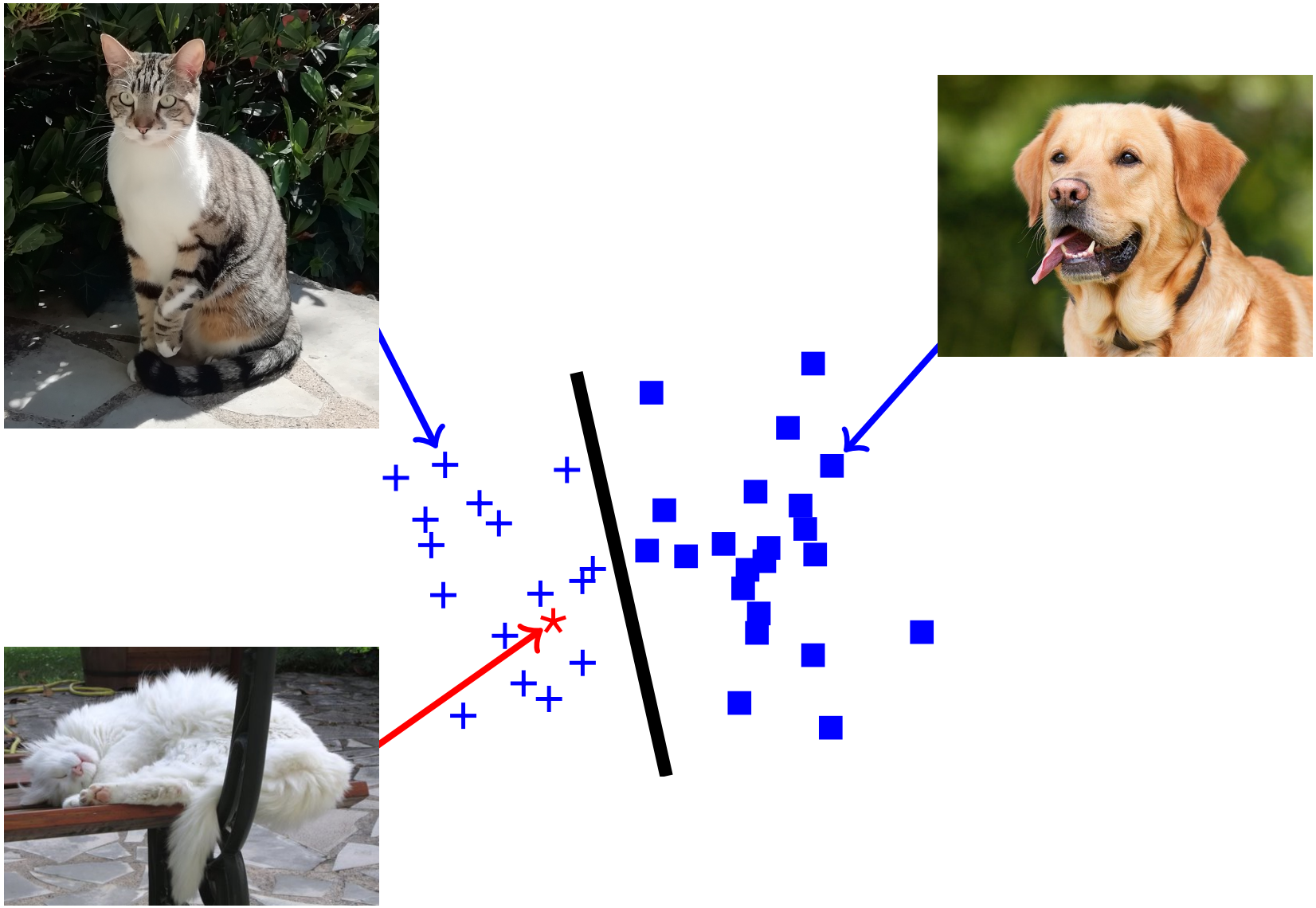
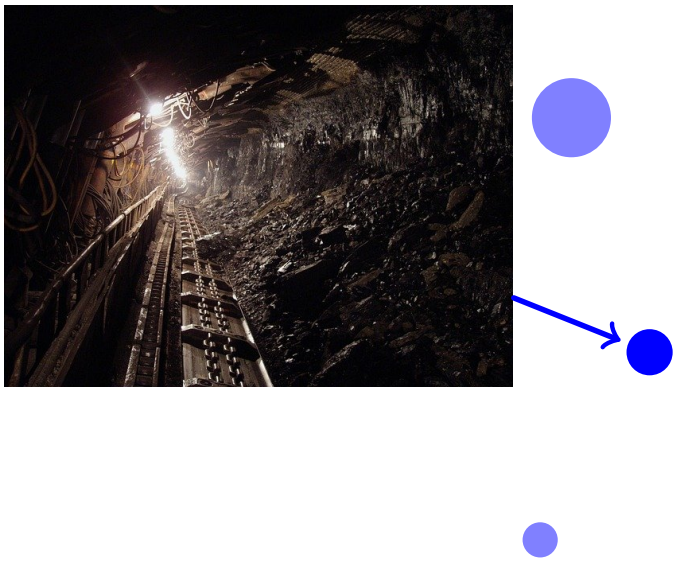


Intuition of the Optimal Transport



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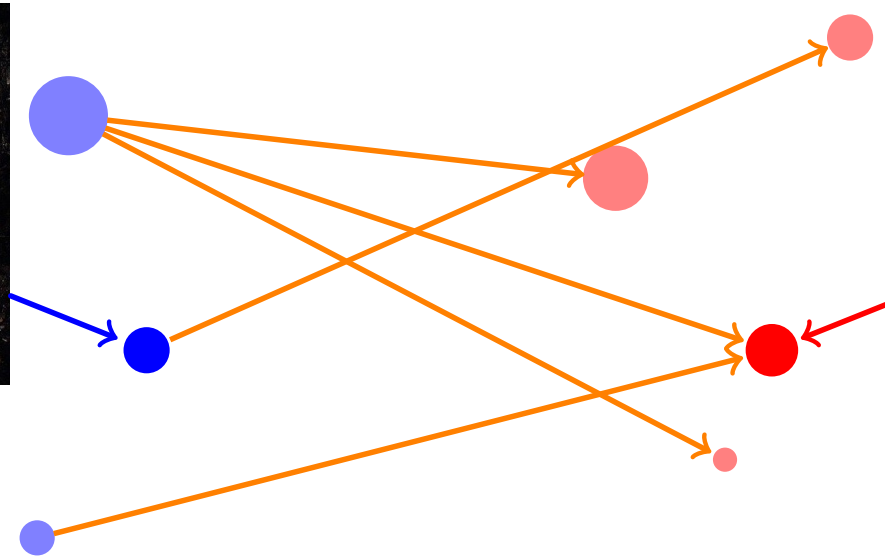

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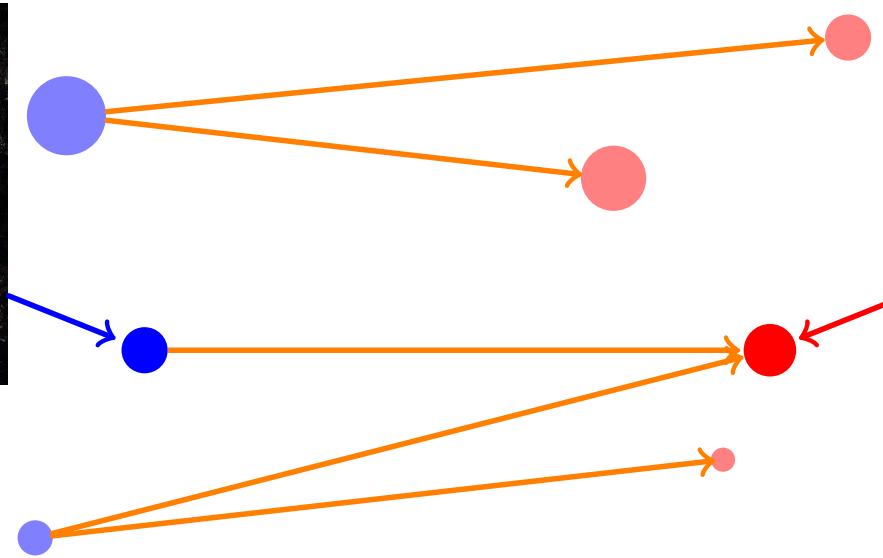
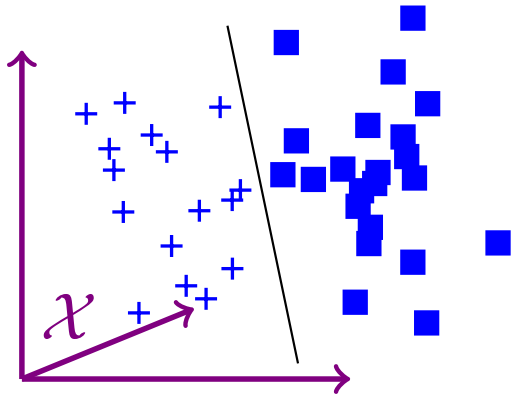
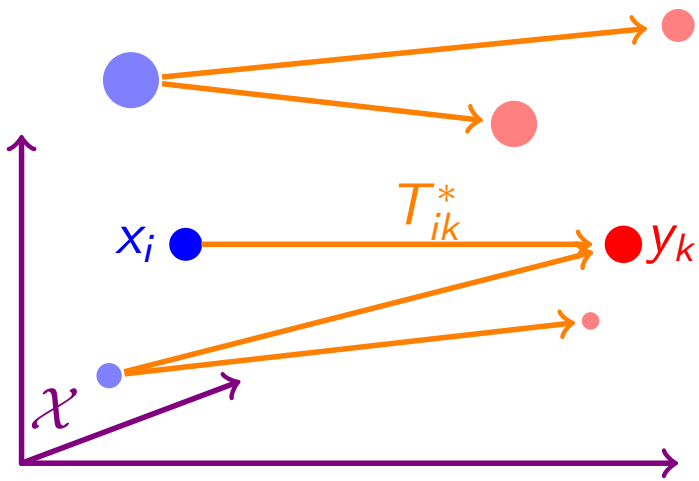


Overview

Machine Learning

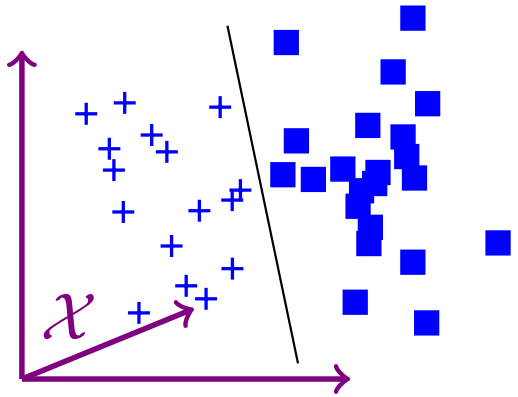


Optimal Transport



Overview

Machine Learning



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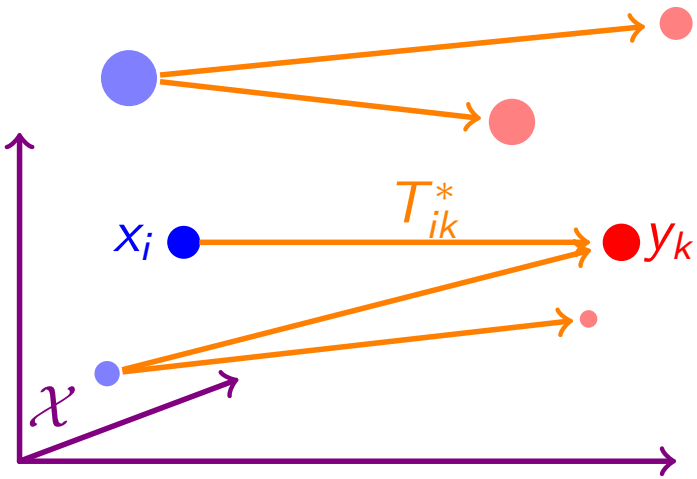
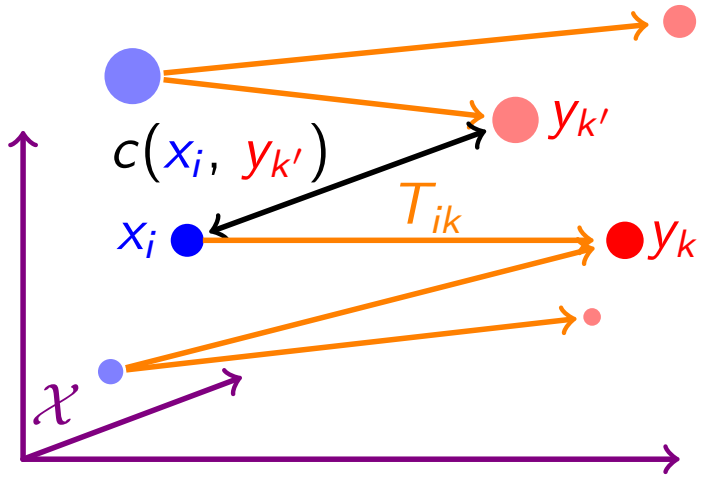
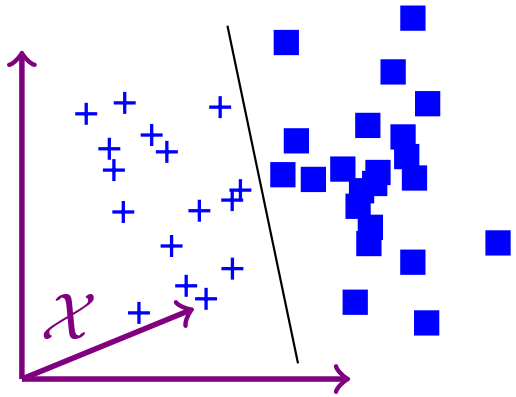


Ground Metric



Overview

Machine Learning



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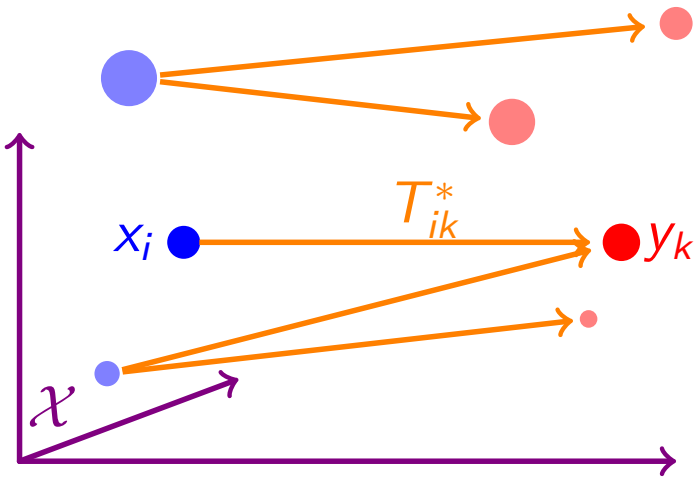

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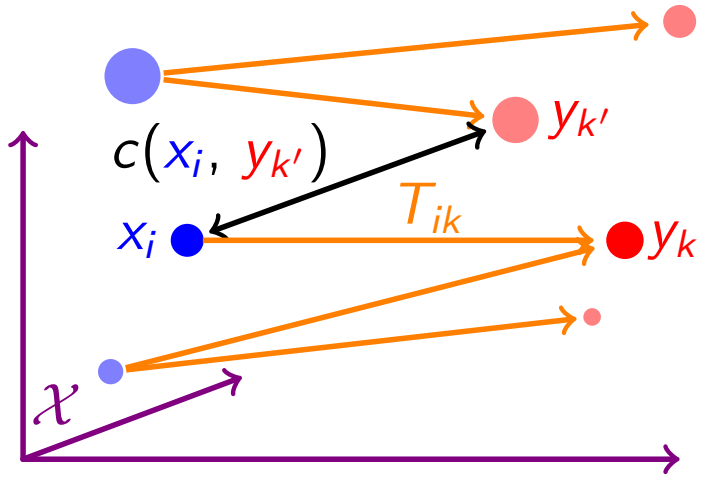
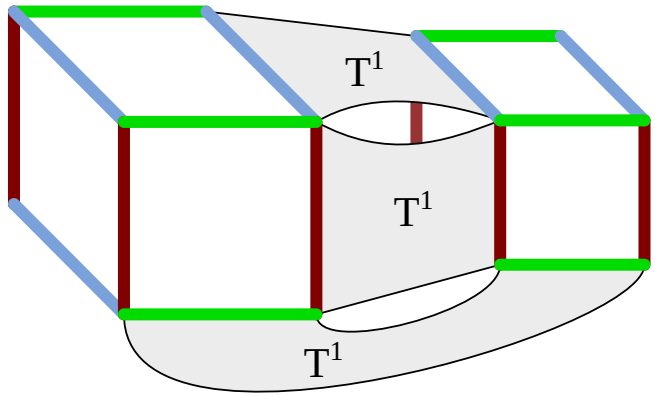


Generalized Framework



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Discrete Optimal Transport

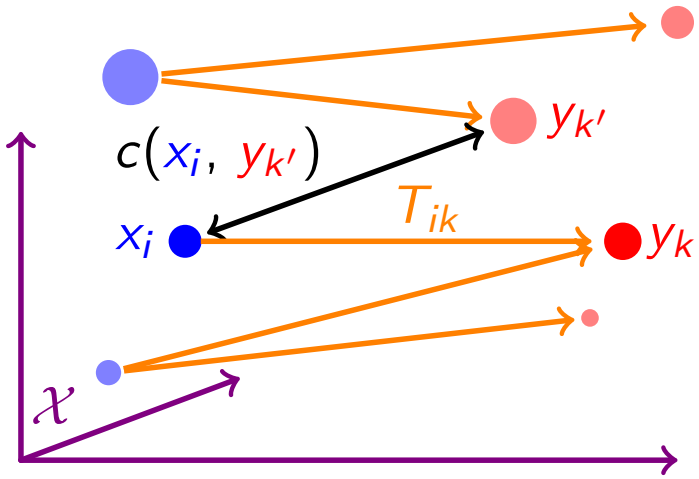


Figure 1: Optimal Transport between two distributions using the ground cost c to compare points.

Discrete Optimal Transport

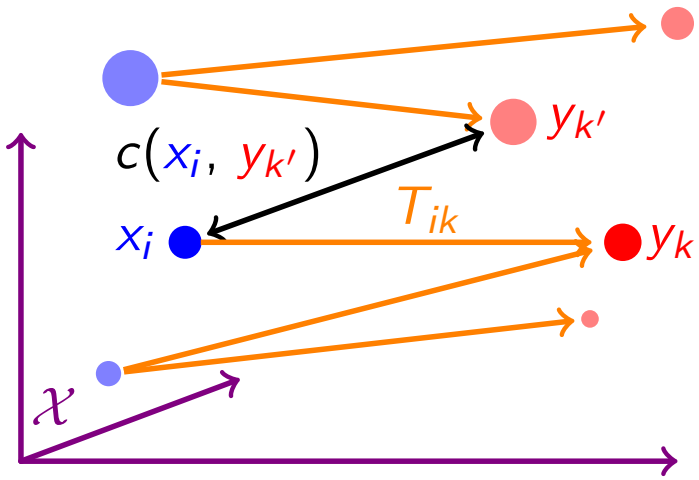


Figure 1: Optimal Transport between two distributions using the ground cost c to compare points.

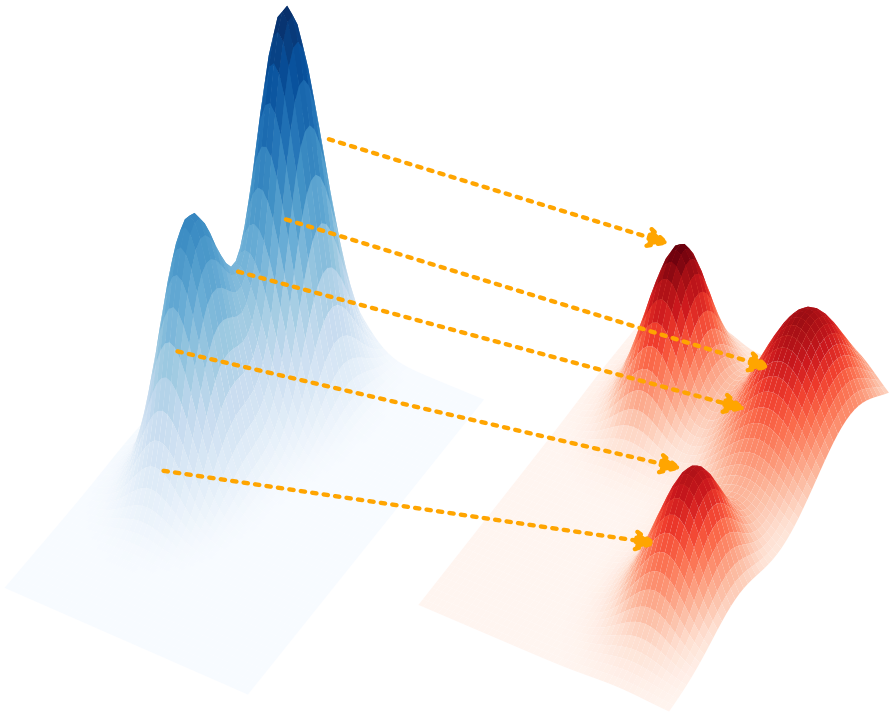
Optimal Transport [Monge, 1781; Kantorovich, 1942; Villani, 2008]

- Two empirical distributions: $\mu = \sum_{i=1}^{I} a_i \delta_{x_i}$ and $\nu = \sum_{k=1}^{K} b_k \delta_{y_k}$.
- Set of transport plans: $\Pi(\mu, \nu) = \{T \in \mathbb{R}_+^{I \times K} \,|\, T^\top \mathbb{1}_I = b, T\mathbb{1}_K = a\}$

$$\min_{T \in \Pi(\mu,\nu)} \sum_{i,k=1}^{I,K} c(x_i, y_k) T_{ik} = \min_{T \in \Pi(\mu,\nu)} \langle C, T \rangle \tag{1}$$

Continuous Optimal Transport (OT)

Figure 2: Optimal Transport between two continuous distributions $\mu \in \mathcal{P}(\mathcal{X})$ and $\nu \in \mathcal{P}(\mathcal{Y})$.



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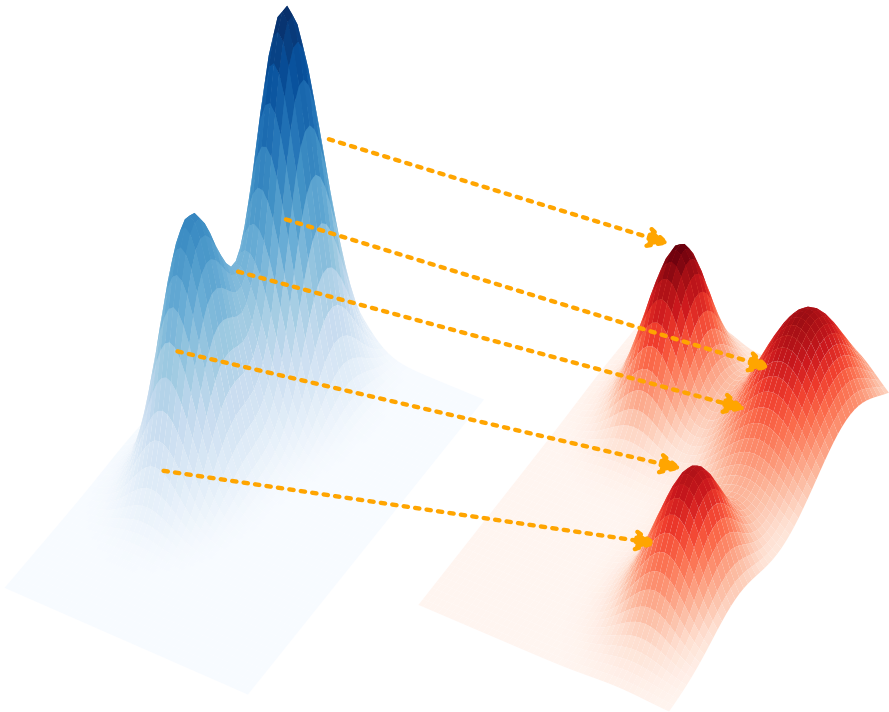


Optimal Transport [Kantorovich, 1942; Villani, 2008]

- Set of transport plans: $\Pi(\mu, \nu)$ containing all $\pi \in \mathcal{P}(\mathcal{X} \times \mathcal{Y})$ with marginal μ and ν.

$$\min_{\pi \in \Pi(\mu,\nu)} \int_{\mathcal{X}\times\mathcal{Y}} c(x,y) d\pi(x,y) \tag{2}$$

Possible solvers

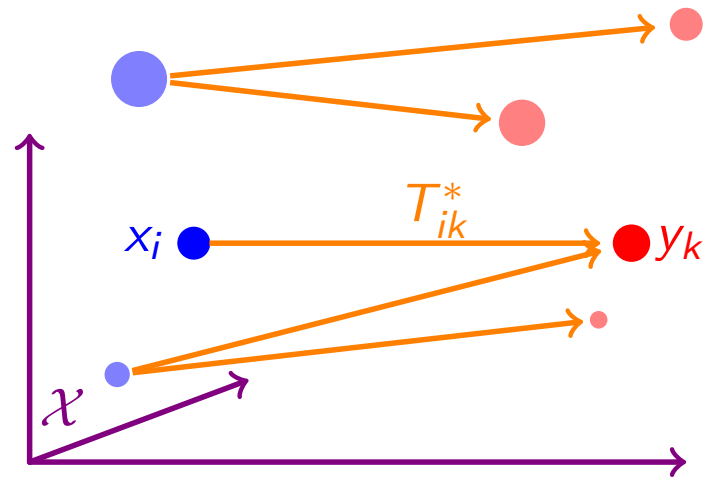
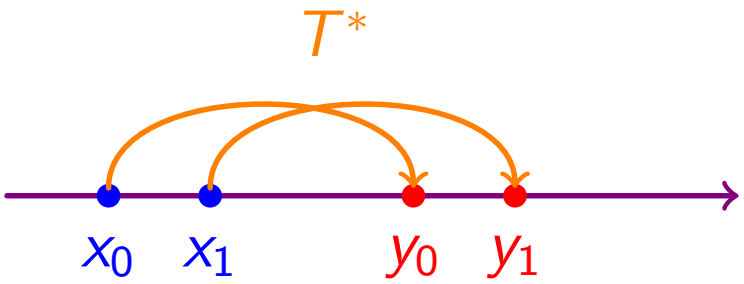


Figure 3: EMD: Based on the min cost flow problem [Ahuja et al., 1988] and $N^3 log(N)$ in the worst case.



$$c(x, y) = (x - y)^2$$

Figure 4: 1D Optimal Transport: Can be computed in $Nlog(N)$ by sorting the two lists.

Entropy regularization

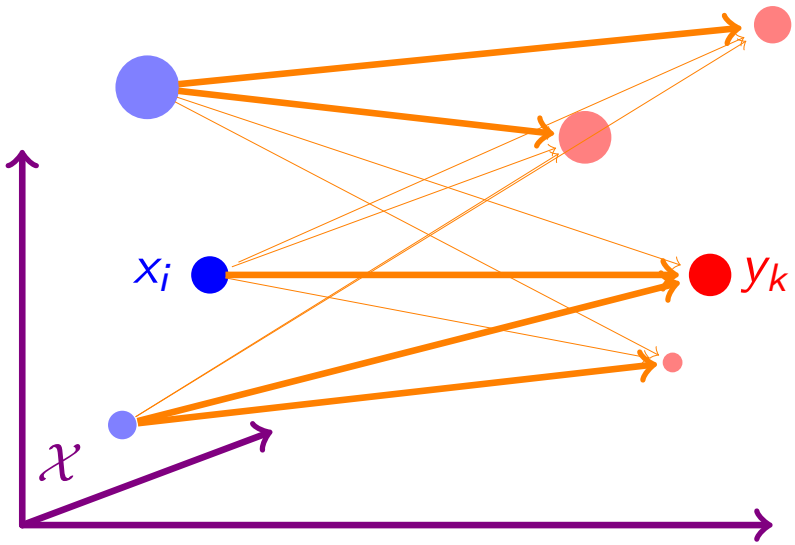


Figure 5: Solution of the entropy regularized Optimal Transport problem. The transport plan T is not sparse anymore.

Entropy regularization

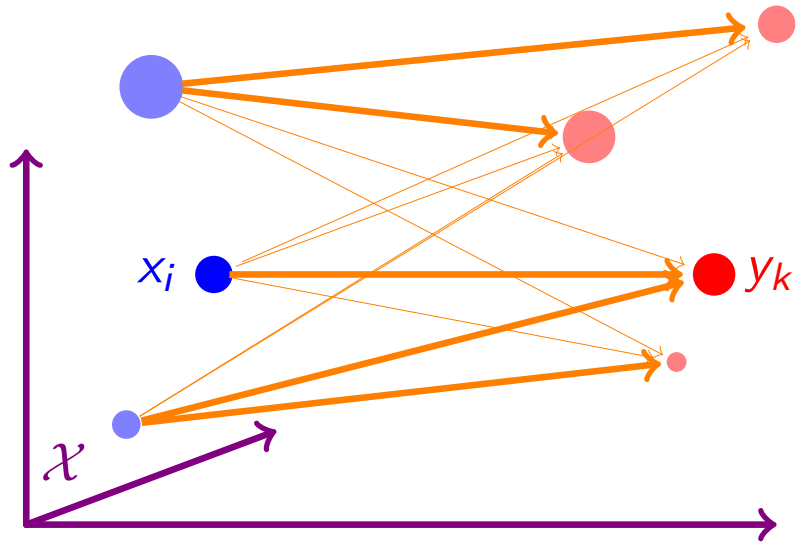


Figure 5: Solution of the entropy regularized Optimal Transport problem. The transport plan T is not sparse anymore.

Regularized OT Cuturi [2013]; Sinkhorn and Knopp [1967]

- Kullback-Leibler regularization $KL(T||T') = \sum_{i,k=1}^{I,K} T_{ik} log(\frac{T_{ik}}{T'_{ik}})$:

$$\min_{T \in \Pi(\mu,\nu)} \sum_{i,k=1}^{I,K} c(x_i, y_k) T_{ik} + \epsilon KL(T||ab^\top) \tag{3}$$

Entropy regularization

- Unique solution
- The optimal transport plan changes continuously
- Can take into account a prior on the transport plan
- Fast and simple solver available ($P \times N^2$)

Regularized OT Cuturi [2013]; Sinkhorn and Knopp [1967]

- Kullback-Leibler regularization $KL(T||T') = \sum_{i,k=1}^{I,K} T_{ik} log(\frac{T_{ik}}{T'_{ik}})$:

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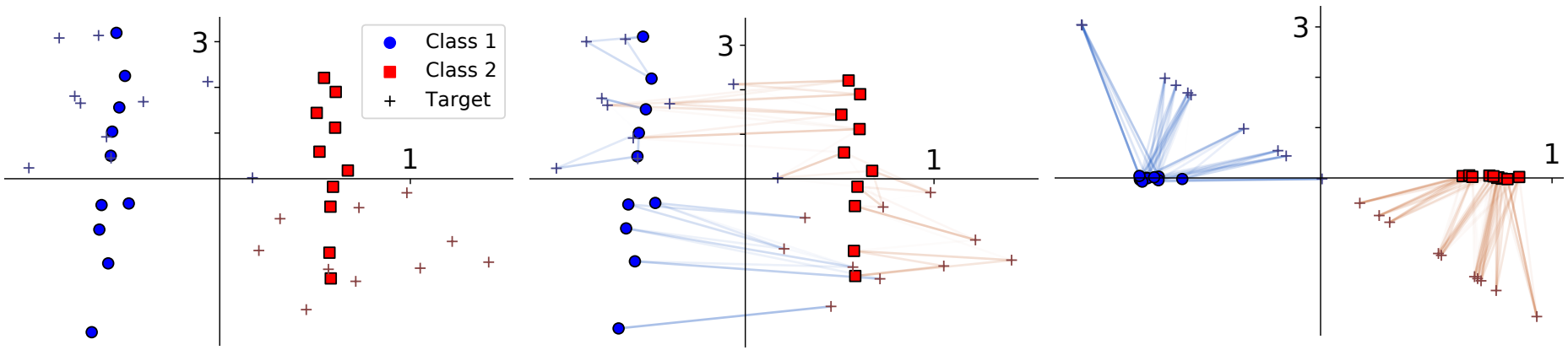
Metric Learning for Optimal Transport

Based on a published paper at the International Joint Conference on Artificial Intelligence (IJCAI) [Kerdoncuff et al., 2020]



Domain Adaptation (DA): Intuition

- Internship supervision of Thibaud Leteno, in collaboration with DGFiP, on companies **fraud detection**.

1. Usual Goal: Predict the companies that might defraud
2. Goal in **DA** context: Predict the companies that might defraud in a **Covid crisis** context

Intuition of Optimal Transport for Domain Adaptation

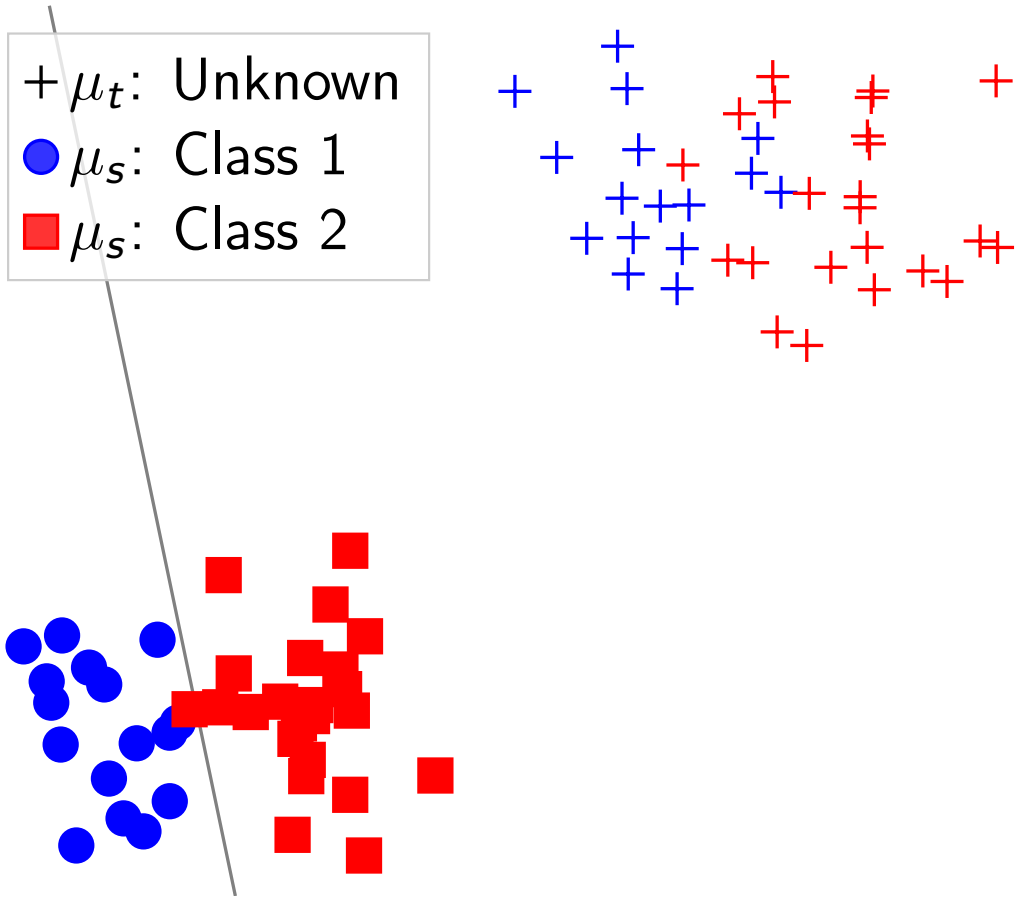


Figure 5: Optimal Transport for Domain Adaptation

Intuition of Optimal Transport for Domain Adaptation

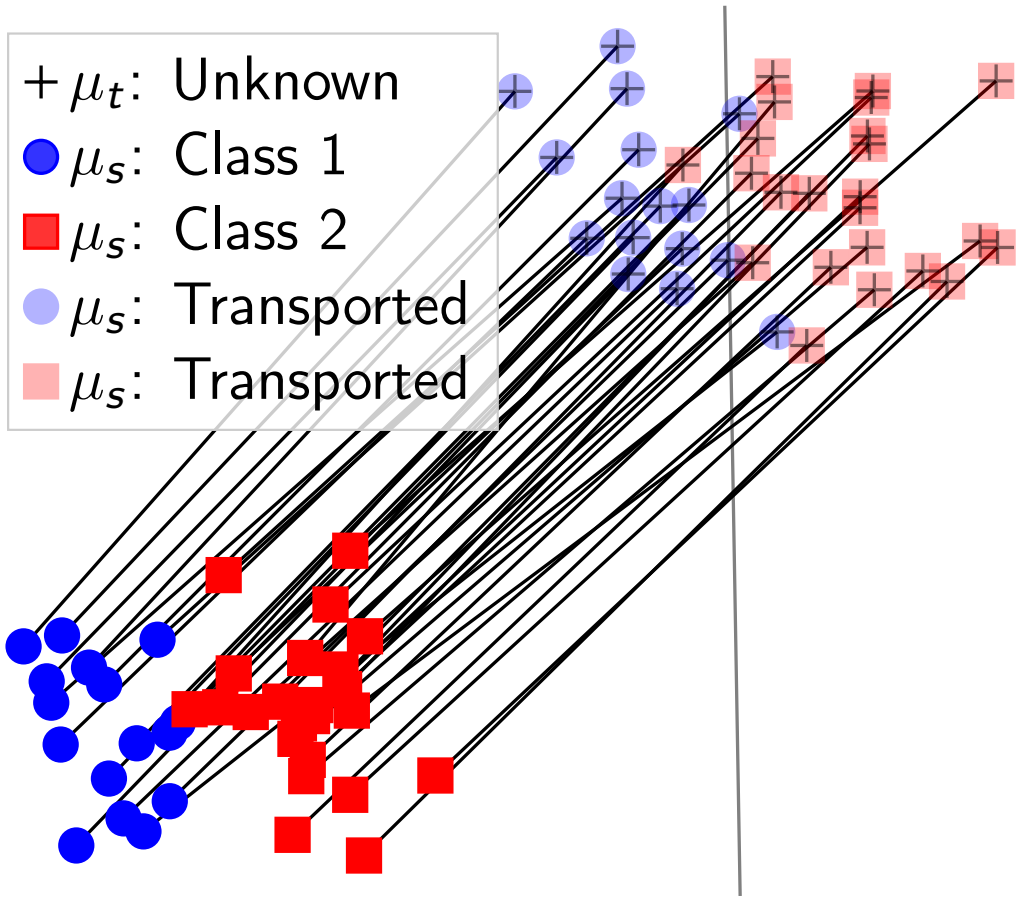


Figure 6: Optimal Transport for Domain Adaptation

Intuition of Optimal Transport for Domain Adaptation

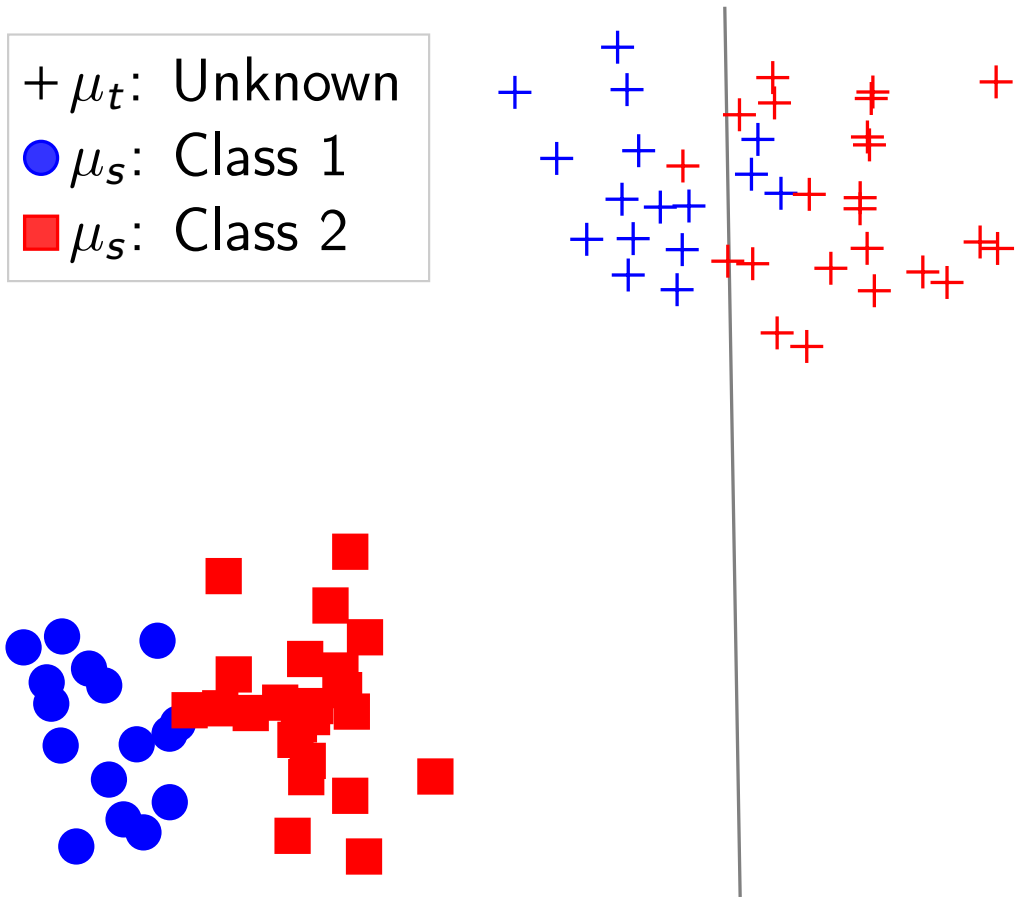


Figure 7: Optimal Transport for Domain Adaptation

Optimal Transport for Domain Adaptation

Optimal Transport for Domain Adaptation [Courty et al., 2017]

$$\min_{T \in \Pi(\hat{\mu}_s, \hat{\mu}_t)} \langle T, C \rangle + \epsilon KL(T || ab^\top) + \lambda_c \left(\sum_{k=1}^{K} \sum_{cl=1}^{\#classes} \| T(\mathcal{I}_{cl}, k) \|_2 \right) \quad (4)$$

✓ Points of different classes should **not** be sent to same location

Metric learning

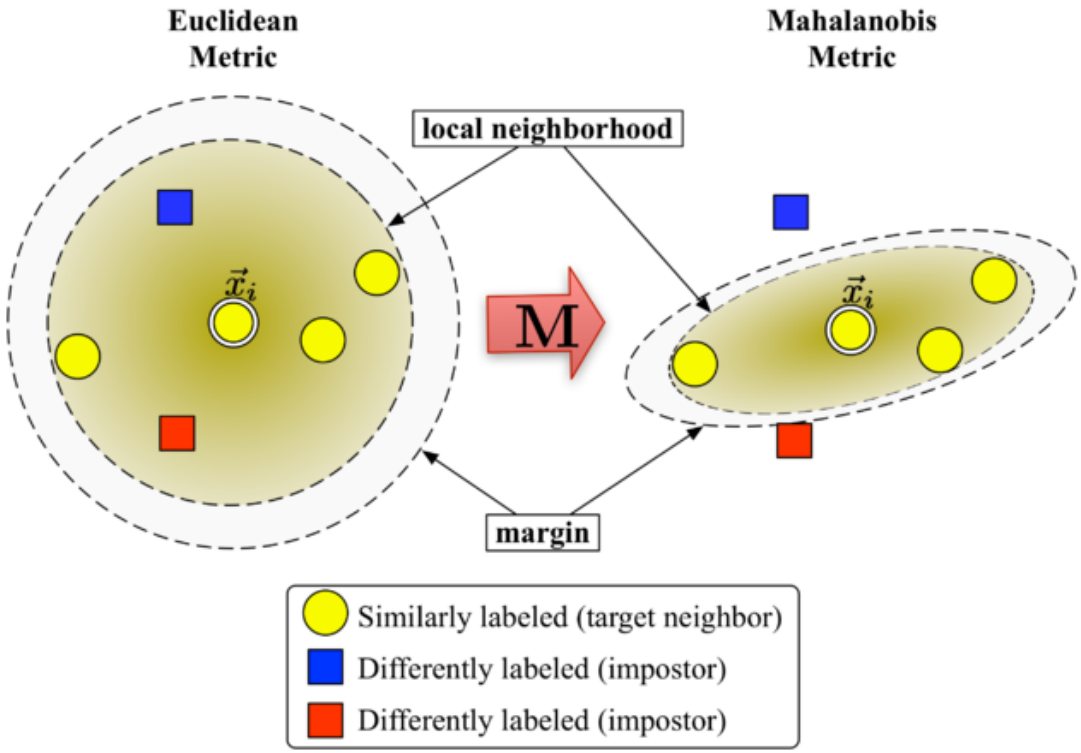


Figure 8: LMNN [Weinberger and Saul, 2009] CC-BY Mlguy (wikipedia)

Mahalanobis metric

- $C_M^2(x, x') = (x - x')M(x - x')^T = \|Lx - Lx'\|_2^2$ with $L^T L = M$

Metric Learning for Optimal Transport (MLOT)

Algorithm 1 MLOT

Require: η (gradient step) $\boldsymbol{X}^s$ $\boldsymbol{X}^t$ $\boldsymbol{Y}^s$

1: $\boldsymbol{V}_s = PCA(\boldsymbol{X}^s)$, $\boldsymbol{V}_t = PCA(\boldsymbol{X}^t)$

2: $\boldsymbol{L}_s = \boldsymbol{V}_s^\top \boldsymbol{V}_s$, $\boldsymbol{L}_t = \boldsymbol{V}_t^\top \boldsymbol{V}_t$

3: **for** $i = 1$ **to** P **do**

4: $\quad T = \underset{T \in \Pi(\hat{\mu}_s, \hat{\mu}_t)}{\operatorname{argmin}} \langle T, C^2(\boldsymbol{L}_s, \boldsymbol{L}_t) \rangle - \epsilon \mathcal{H}(T) + \lambda_c \Omega_{cl}(T)$

5: $\quad \boldsymbol{L}_s = \boldsymbol{L}_s - \eta \nabla_{\boldsymbol{L}_s} (\langle T, C^2(\boldsymbol{L}_s, \boldsymbol{L}_t) \rangle + \lambda_l \Omega_l(\boldsymbol{L}_s))$

6: **end for**

7: $\tilde{\boldsymbol{X}}_s = T \boldsymbol{L}_t \boldsymbol{X}^t$

8: classifier = classifier method$(\tilde{\boldsymbol{X}}_s, \boldsymbol{Y}^s)$

9: $\hat{\boldsymbol{Y}}^t$ = classifier$(\boldsymbol{X}^t)$

10: **return** $\hat{\boldsymbol{Y}}^t$

Illustration of the usefulness of Metric Learning

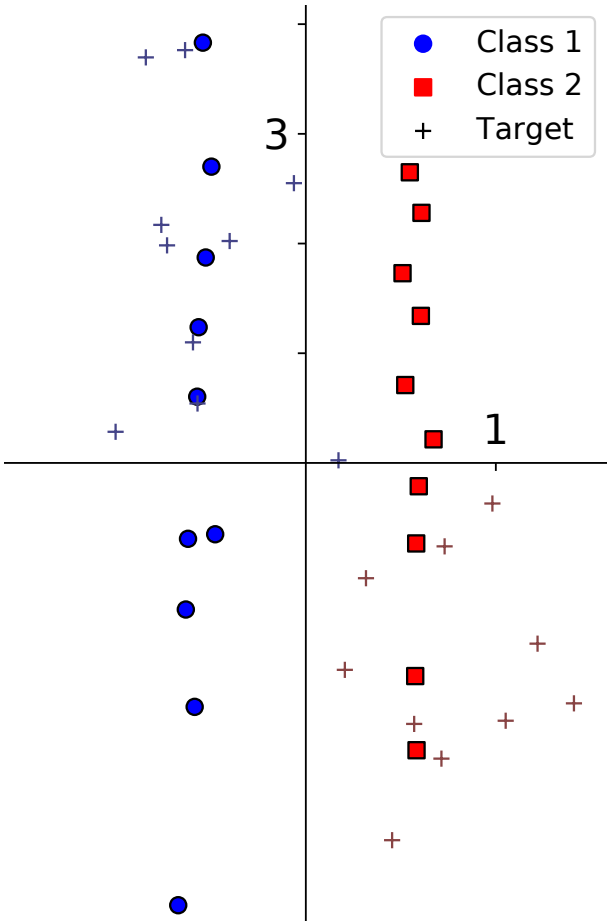
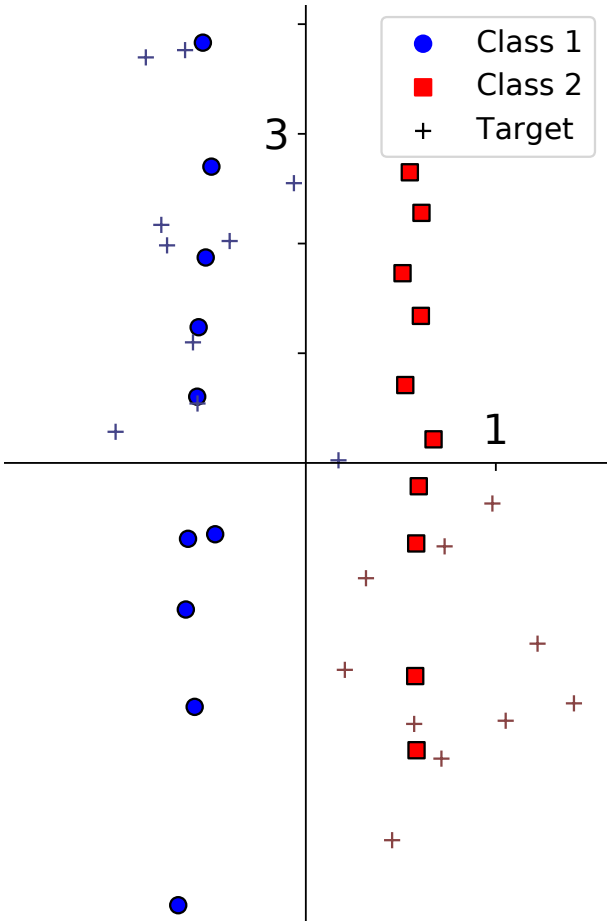


Figure 9: Dataset

Illustration of the usefulness of Metric Learning



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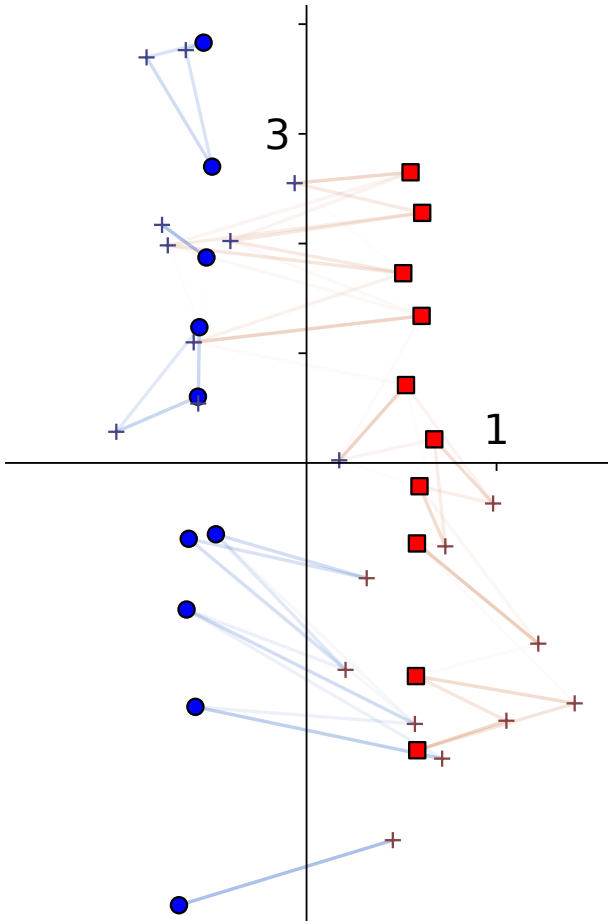

Figure 10: OTDA

Illustration of the usefulness of Metric Learning

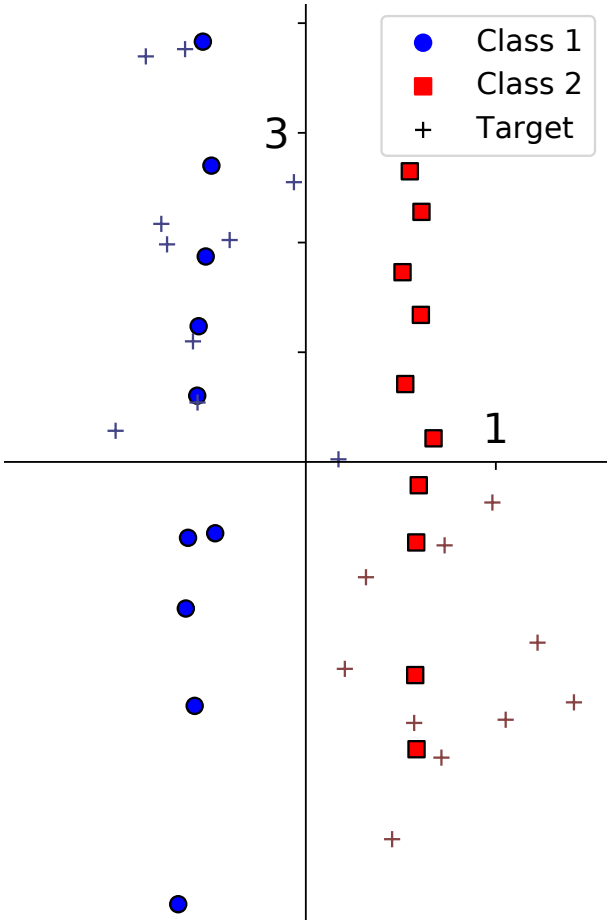

Figure 9: Dataset

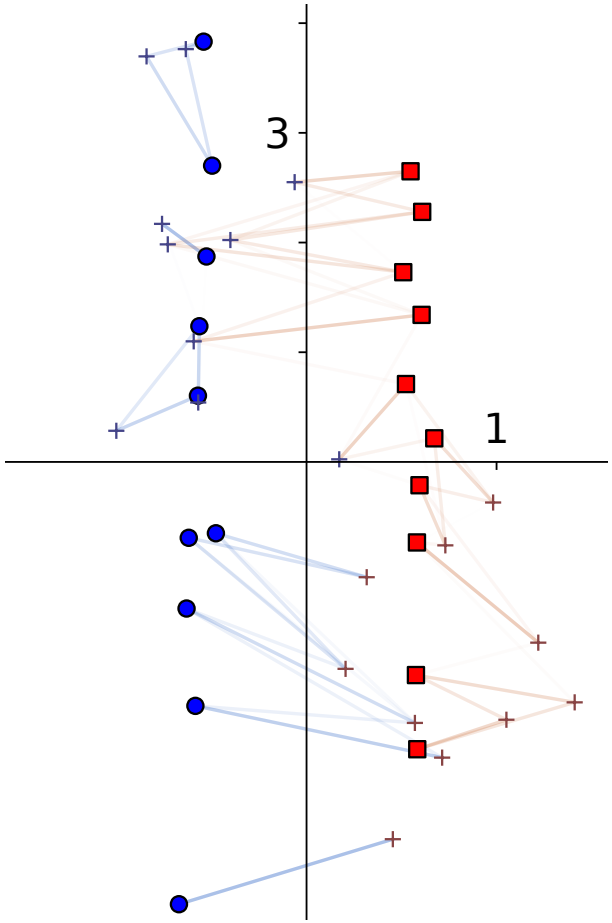

Figure 10: OTDA

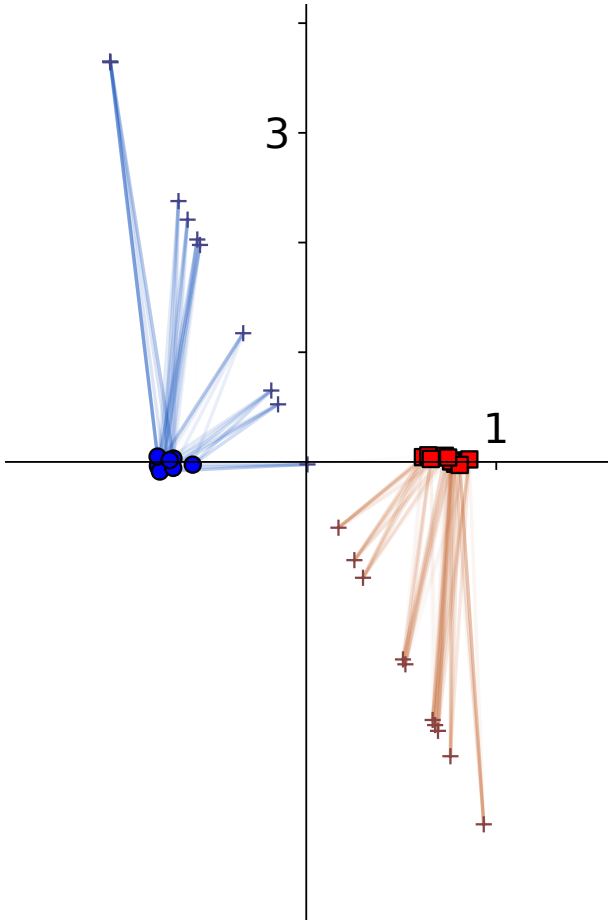

Figure 11: MLOT

Cross validation of hyperparameters

- In **Unsupervised** Domain Adaptation the target labels are **not available**
- We use the Reverse Validation of Zhong et al. [2010]

Method	OT	TCA	LMNN	SA	JDOT	OTDA	OTDA_p	MLOT
Classical Validation	45.3	45.3	47.9	47.4	48.5	52.8	54	**55.1**
Reverse Validation	42.2	44.5	44.8	45.8	47.0	48.2	48.8	**49.7**

Table 1: Accuracy on Office-Caltech dataset [Gong et al., 2012] with SURF features.

OTDA vs MLOT

Figure 12: MLOT - OTDA

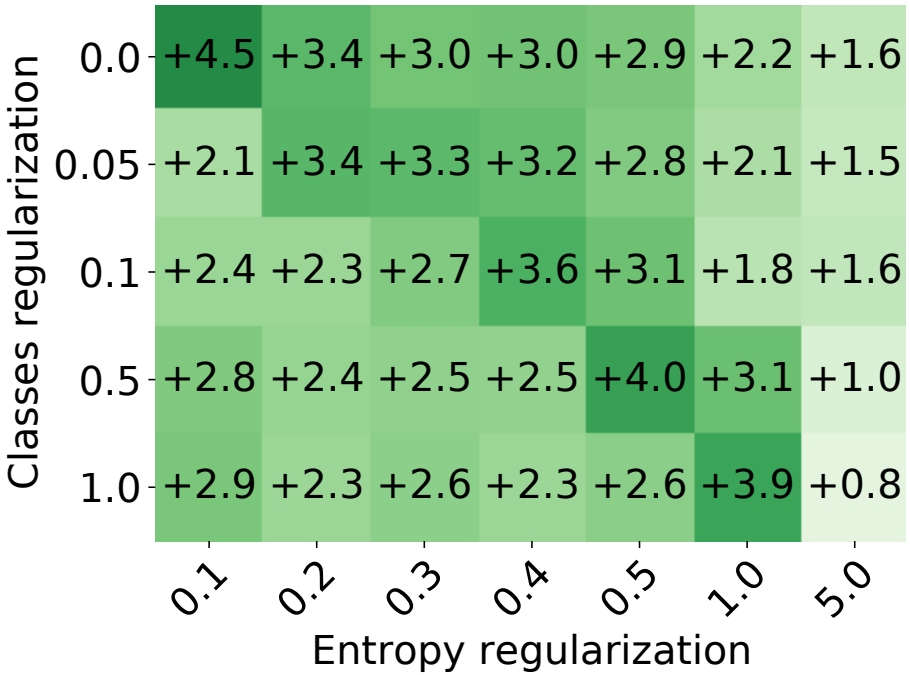

Figure 13: MLOT

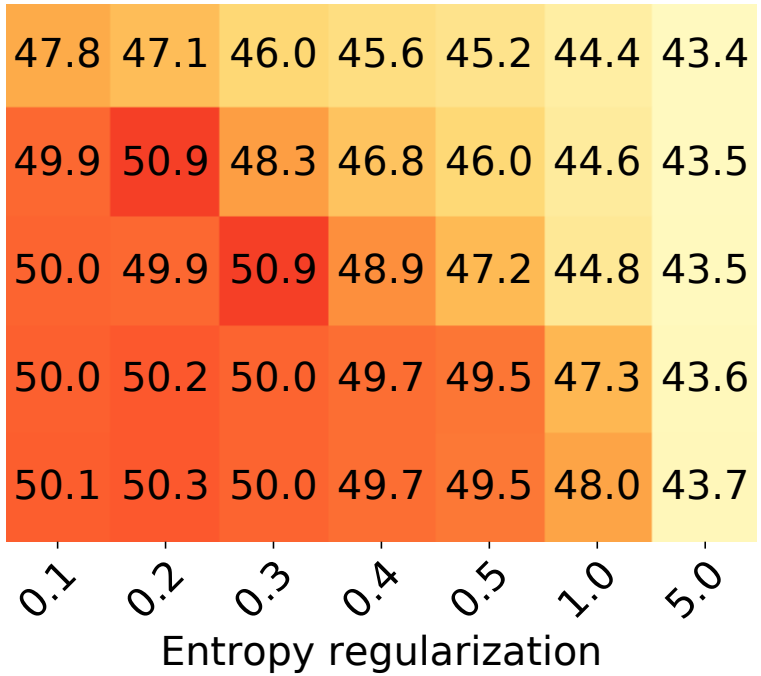

Figure 14: Accuracy of OTDA and MLOT on Office-Caltech dataset [Gong et al., 2012] with SURF features.

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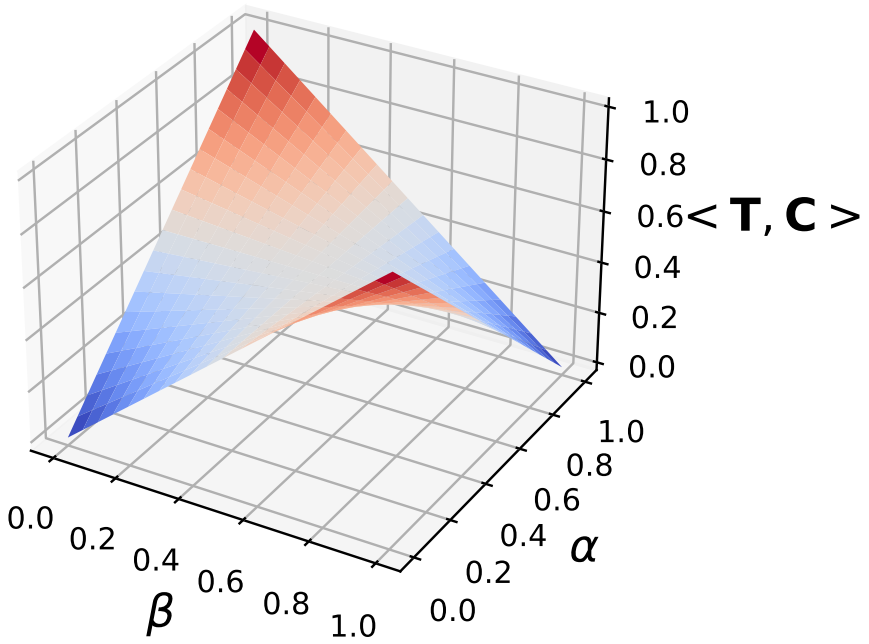
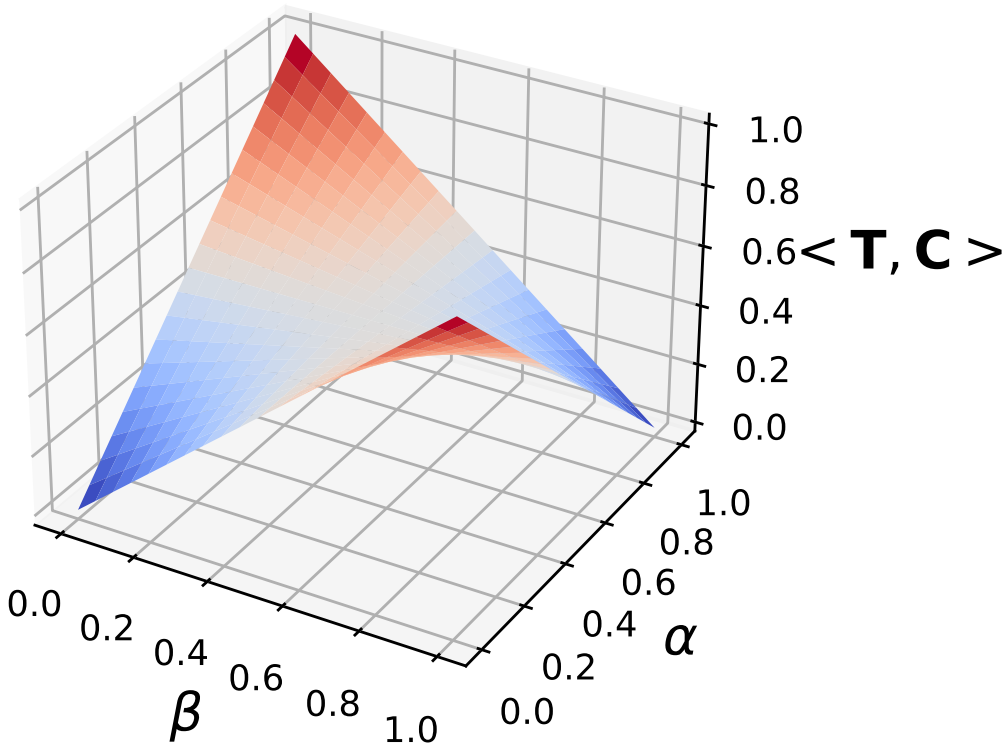
A Swiss Army Knife for Minimax Optimal Transport

Based on a published paper at International Conference on Machine Learning (ICML) 2020 [Dhouib et al., 2020]



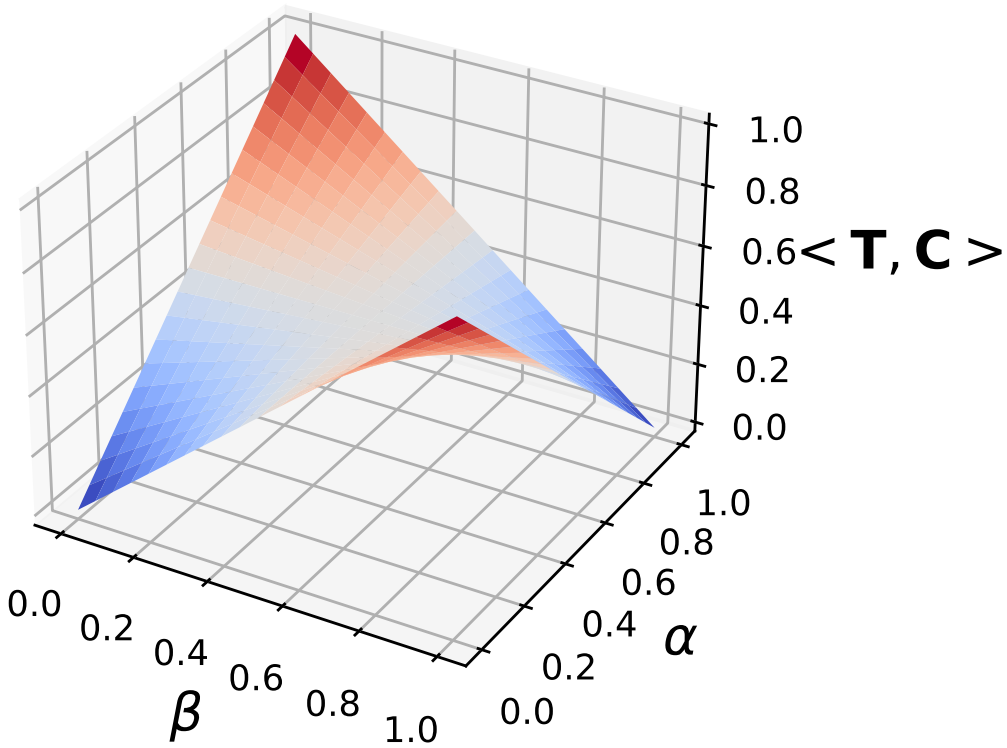
Intuition of the OT Minimax problem



Intuition of the OT Minimax problem

Cost matrices

- $C_1 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$
- $C_2 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$
- $C = \alpha C_1 + (1-\alpha) C_2$



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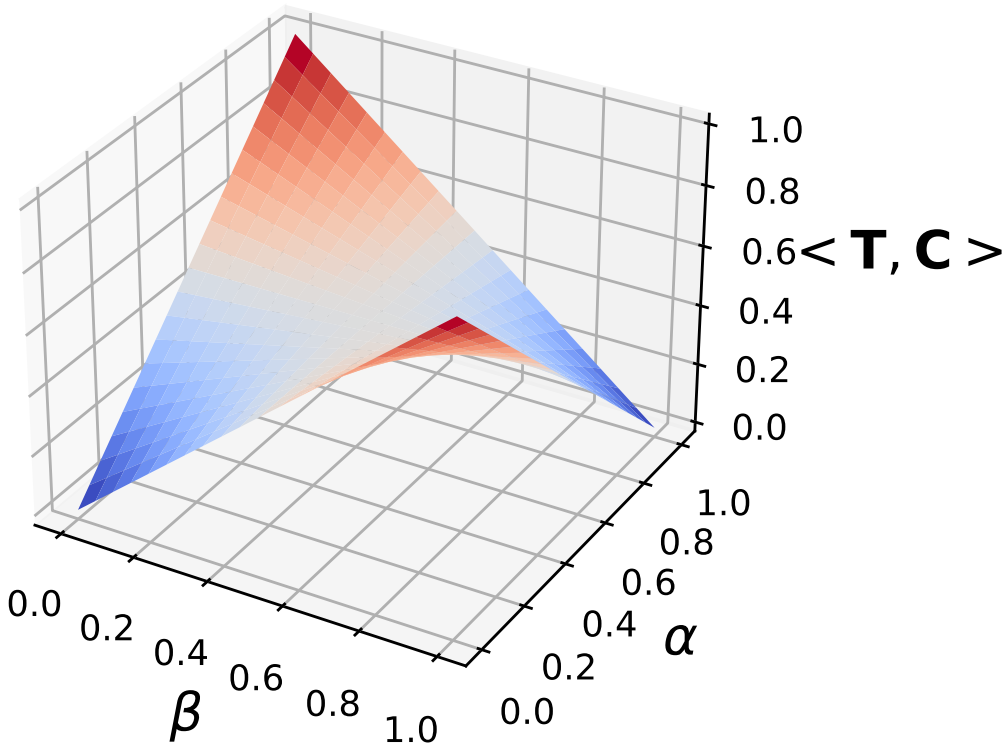
- $C_2 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$
- $C = \alpha C_1 + (1-\alpha) C_2$

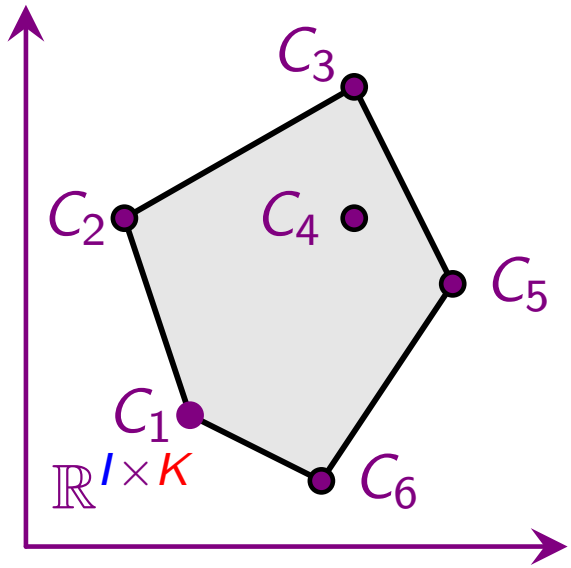
Associated Transport Plan

- $T_1^* = \begin{pmatrix} 0 & 0.5 \\ 0.5 & 0 \end{pmatrix}$
- $T_2^* = \begin{pmatrix} 0.5 & 0 \\ 0 & 0.5 \end{pmatrix}$
- $T = \beta T_1^* + (1-\beta) T_2^*$



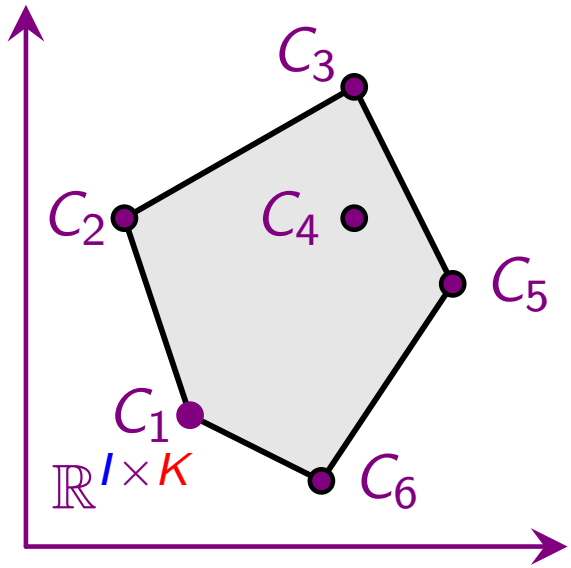
Different type of set

- Convex hull of finite set of cost matrices:

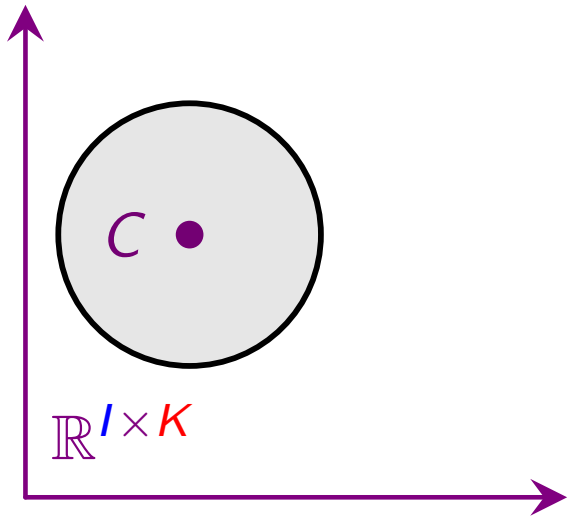


Different type of set

- Convex hull of finite set of cost matrices:



- Mahalanobis ball centered at a matrix C :



Cutting set algorithm [Mutapcic and Boyd, 2009]

Proper definition of the Minimax problem

$$\mathcal{W}_{\mathcal{C}} = \min_{T \in Conv(\mathcal{P})} \max_{C \in \mathcal{C}} \langle T, C \rangle$$

Cutting set algorithm [Mutapcic and Boyd, 2009]

Proper definition of the Minimax problem

$$\mathcal{W}_{\mathcal{C}} = \min_{T \in Conv(\mathcal{P})} \max_{C \in \mathcal{C}} \langle T, C \rangle \quad \Longleftrightarrow \quad \operatorname*{argmax}_{C \in \mathcal{C}, \omega \geq 0} \ \omega \tag{5}$$
$$\text{s.t.} \ \langle T, C \rangle \geq \ \omega, \ \forall T \in \mathcal{P}$$

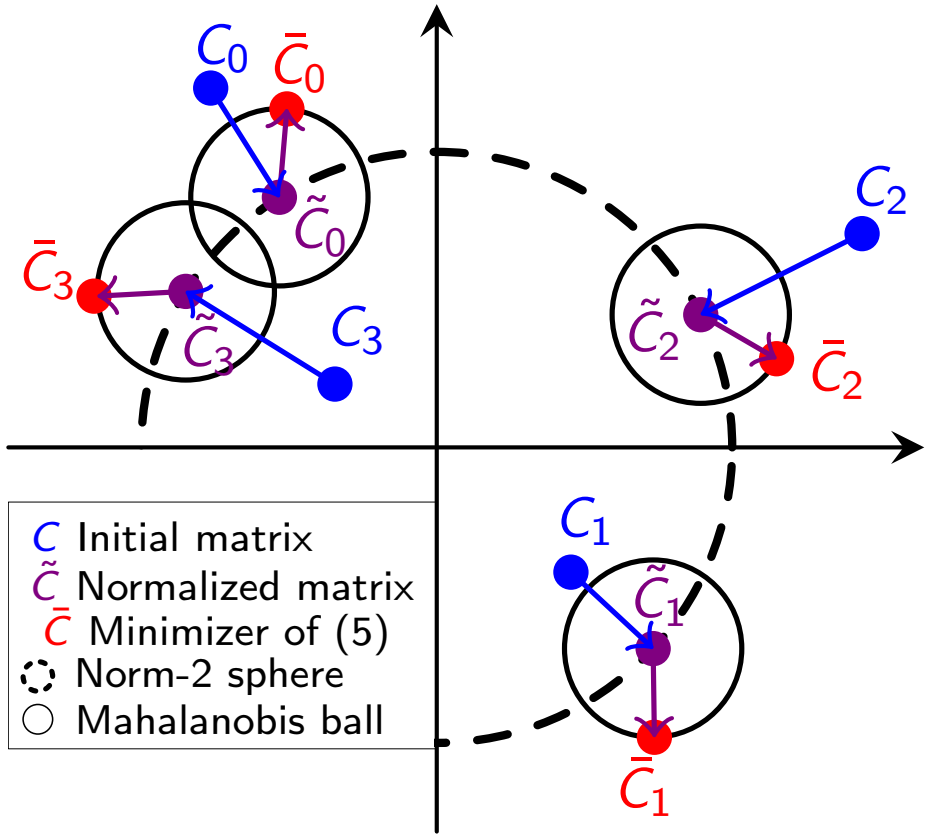
Algorithm 3 Cutting set method for RKP$(\Pi, \mathcal{C})$

1: **Input:** $\mathcal{C}$, $\mathcal{P}_0 \subset \Pi$, thd
2: **while** $err >$ thd **do**
3: Solve (5) to obtain (ω_t, C_t) and $(q_0, ..., q_{|\mathcal{P}_t|-1})$
4: Find $T_t \in \underset{T \in \Pi}{argmin} \langle T, C_t \rangle$
5: $err \leftarrow (\omega_t - \langle T_t, C_t \rangle) / \langle T_t, C_t \rangle$
6: $\mathcal{P}_{t+1} = \mathcal{P}_t \cup \{T_t\}$
7: $t \leftarrow t + 1$
8: **end while**
9: **return** $\sum_{l=0}^{|\mathcal{P}_t|-1} q_l T_l, \ C_t$

Wasserstein stability

Wasserstein stability of a matrix C induce by μ and ν

$$\mathcal{WS}_C = \mathcal{W}_{\mathcal{C}_C}(\mu, \nu) - \mathcal{W}_C(\mu, \nu)$$



Usefulness of the Wasserstein stability (Color transfer)

Usefulness of the Wasserstein stability (Color transfer)

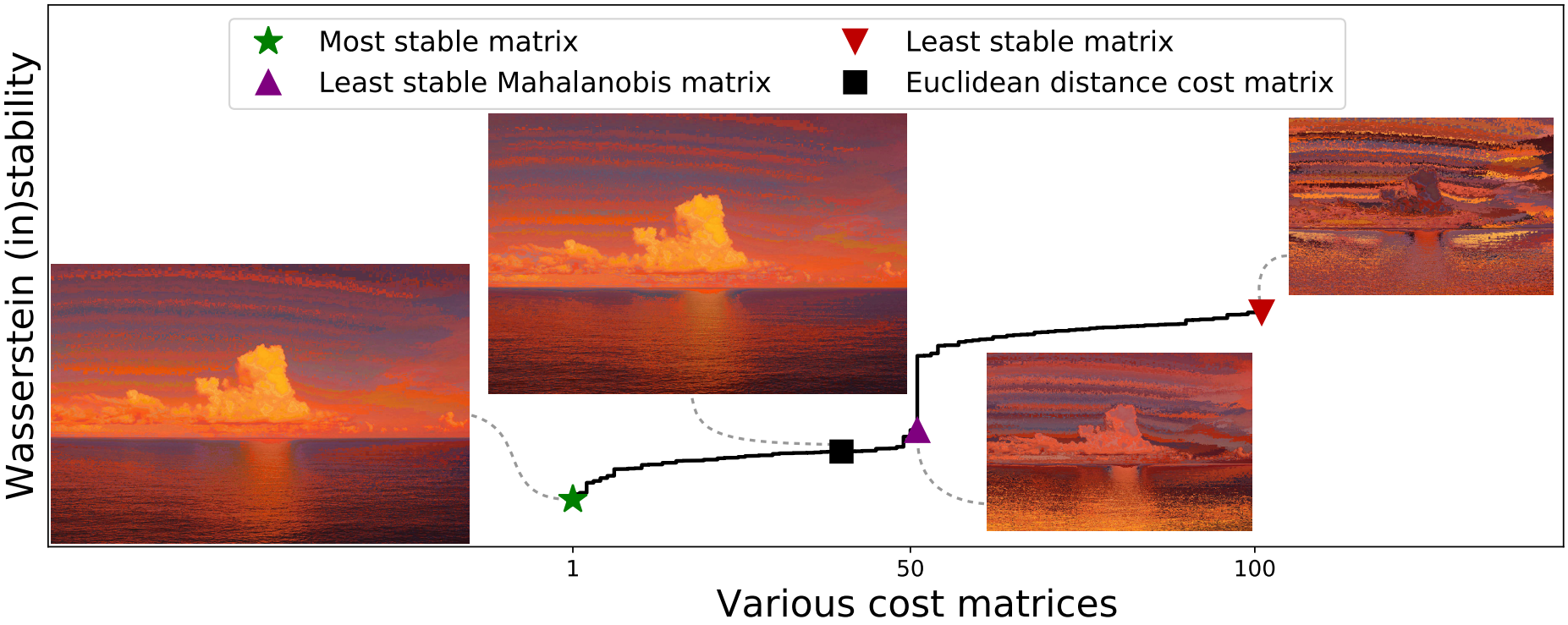
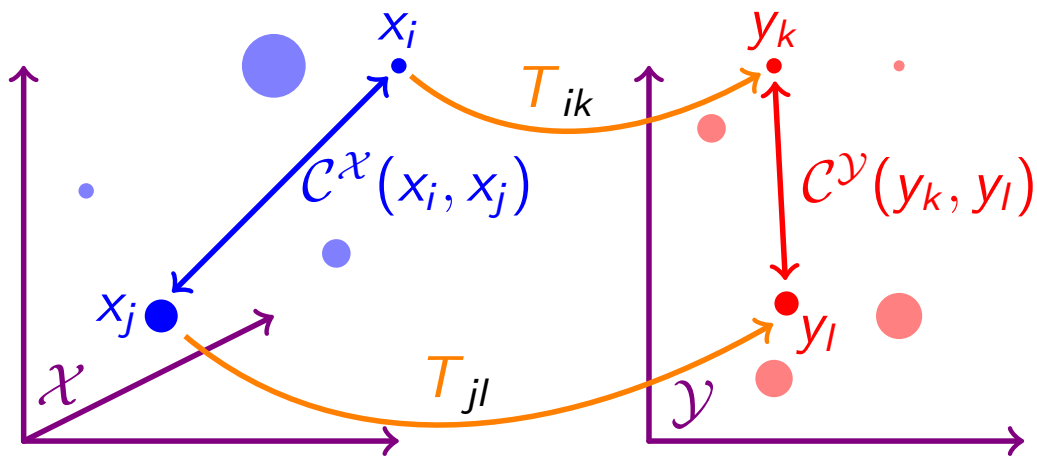


Table of Contents

Sampled Gromov Wasserstein

Based on a published paper in the Machine Learning Journal (MLJ) [Kerdoncuff et al., 2021] and presented at the ECML-PKDD 2021 conference.



The Gromov Wasserstein problem

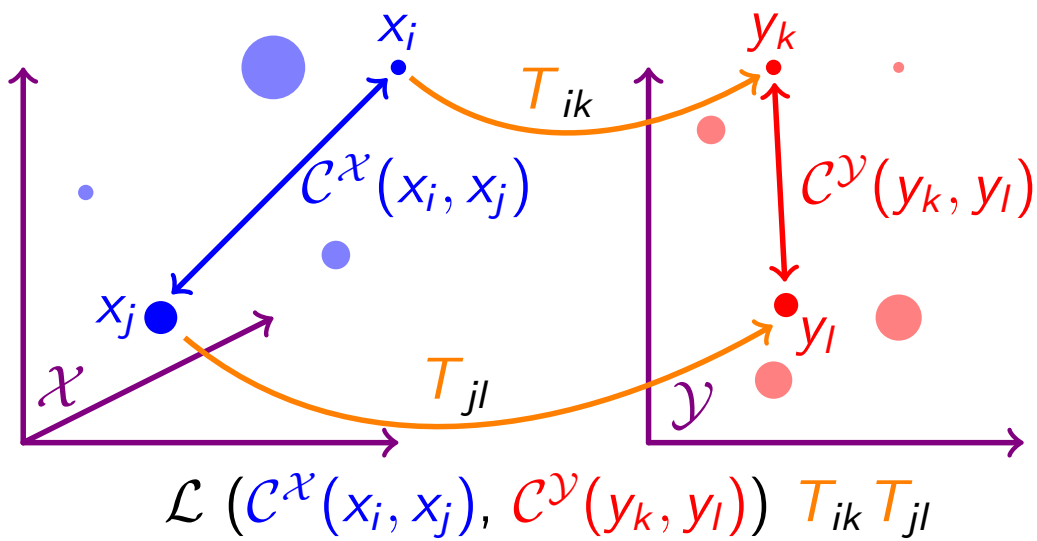


Figure 15: Gromov Wasserstein between two distributions in two vector spaces $\mathcal{X}$ and $\mathcal{Y}$, with one term from Equation (6).

Gromov Wasserstein (GW) [Memoli, 2007; Peyré et al., 2016]

- The GW distance rely only on intra-pairwise distance,

$$\min_{T \in \Pi(\mu,\nu)} \mathcal{E}(T, T) = \min_{T \in \Pi(\mu,\nu)} \sum_{ijkl=1}^{I,I,K,K} \mathcal{L}\left(\mathcal{C}^{\mathcal{X}}(x_i, x_j), \mathcal{C}^{\mathcal{Y}}(y_k, y_l)\right) T_{ik} T_{jl} \quad (6)$$

The mostly used solver: Entropy Gromov Wasserstein

Algorithm 4 Entropy Gromov Wasserstein (EGW) [Peyré et al., 2016]

Require: $a, b, \mathcal{C}^{\mathcal{X}}, \mathcal{C}^{\mathcal{Y}}, \mathcal{L}, \epsilon$

$T_0 = ab^\top$

for s= 0 **to** S-1 **do**

$\Lambda = \nabla_T \mathcal{E}(T, T) = \sum_{jl=1}^{I,K} \mathcal{L}\left(\mathcal{C}^{\mathcal{X}}(\cdot, x_j), \mathcal{C}^{\mathcal{Y}}(\cdot, y_l)\right) T_{jl}$

$T'_s = \min_{T' \in \Pi(\mu,\nu)} \langle \Lambda, T' \rangle + \epsilon KL(T' || ab^\top)$

$T_{s+1} = (1-1)T_s + 1\,T'_s$

end for

The mostly used solver: Entropy Gromov Wasserstein

Algorithm 5 Entropy Gromov Wasserstein (EGW) [Peyré et al., 2016]

Require: $a, b, \mathcal{C}^{\mathcal{X}}, \mathcal{C}^{\mathcal{Y}}, \mathcal{L}, \epsilon$

$T_0 = ab^\top$

for s= 0 **to** S-1 **do**

$\Lambda = \nabla_T \mathcal{E}(T, T) = \sum_{jl=1}^{I,K} \mathcal{L}\left(\mathcal{C}^{\mathcal{X}}(\cdot, x_j), \mathcal{C}^{\mathcal{Y}}(\cdot, y_l)\right) T_{jl}$

$T'_s = \min_{T' \in \Pi(\mu,\nu)} \langle \Lambda, T' \rangle + \epsilon KL(T' || ab^\top)$

$T_{s+1} = (1-1)T_s + 1\,T'_s$

end for

Relation with the Frank-Wolfe (FW) algorithm [Frank et al., 1956]

- EGW with no entropy ($\epsilon = 0$) $\iff$ FW with full step size ($\alpha = 1$).

Motivations and contributions

Existing limitations

- Time complexity for computing the gradient $\nabla_T \mathcal{E}(T, T)$ is $O\left(N^4\right)$
- Time complexity can be reduce to $O\left(N^3\right)$ but only for specific loss functions $\mathcal{L}(x, y) = f_1(x) + h_1(x)h_2(y) + f_2(y)$
- The existing convergence proof of EGW are valid only for high value of ϵ.

Contributions

- ✓ Approximate the gradient $\nabla_T \mathcal{E}(T, T)$ in $O\left(M \times N^2\right)$
- ✓ Propose a convergence bound to stationary points
- ✓ Explore a very fast variant with $M = 1$ using the 1D OT solver

Sampled Gromov Wasserstein idea (SaGroW)

$$\min_{T' \in \Pi(\mu,\nu)} \langle \nabla_T \mathcal{E}(T, T), T' \rangle = \min_{T' \in \Pi(\mu,\nu)} \left\langle \sum_{j,l} T_{jl} \boldsymbol{L}_{.j.l}, T' \right\rangle$$

Sampled Gromov Wasserstein idea (SaGroW)

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$$= \min_{T' \in \Pi_{\mu\nu}} \langle \mathbb{E}(\Lambda), T' \rangle$$

Sampled Gromov Wasserstein idea (SaGroW)

$$\min_{T' \in \Pi(\mu,\nu)} \langle \nabla_T \mathcal{E}(T, T), T' \rangle = \min_{T' \in \Pi(\mu,\nu)} \left\langle \sum_{j,l} T_{jl} \boldsymbol{L}_{.j.l}, T' \right\rangle$$

$$= \min_{T' \in \Pi_{\mu\nu}} \langle \mathbb{E}(\Lambda), T' \rangle$$

$$\approx \min_{T' \in \Pi_{\mu\nu}} \left\langle \frac{1}{M} \sum_{m=1}^{M} \boldsymbol{C}^m, T' \right\rangle$$

Summary of SaGroW algorithm.

Algorithm 6 SaGroW

Require: $a, b, \mathcal{C}^{\mathcal{X}}, \mathcal{C}^{\mathcal{Y}}, \mathcal{L}, M, \epsilon, \alpha$

$T_0 = ab^\top$

for s= 0 **to** S-1 **do**

  $(j_m, l_m) \sim \text{Sample}(T_s)\ \forall m \in [\![1, M]\!]$

  $\widehat{\mathbf{\Lambda}} = \frac{1}{M} \sum_{m=1}^{M} \mathcal{L}\left(\mathcal{C}^{\mathcal{X}}(\cdot, x_{j_m}), \mathcal{C}^{\mathcal{Y}}(\cdot, y_{l_m})\right)$

  $T'_s = \min_{T' \in \Pi(\mu,\nu)} \left\langle \widehat{\mathbf{\Lambda}}, T' \right\rangle + \epsilon KL(T' || ab^\top)$

  $T_{s+1} = (1-\alpha) T_s + \alpha T'_s$

end for

Bound for convergence to a stationary point

- The FW gap: $G(T) = \mathcal{E}(T, T) - \min_{T' \in \Pi(\mu,\nu)} \mathcal{E}(T, T')$.
- $G(T) = 0 \iff T$ is a stationary point of GW.

Bound for convergence to a stationary point

- The FW gap: $G(T) = \mathcal{E}(T, T) - \min_{T' \in \Pi(\mu,\nu)} \mathcal{E}(T, T')$.
- $G(T) = 0 \iff T$ is a stationary point of GW.

Theorem (Based on Reddi et al. [2016])

For any $\boldsymbol{L}_{ijkl} \in [0, B]$, for any distributions μ and ν with uniform weights a and b respectively, for any optimal solution T^* of Problem (6), on average for the transport plan $\overline{T}$ uniformly sampled from $(T_s)_{s \in [\![0, S-1]\!]}$, on average over all the samplings, the following bound holds:

$$\mathbb{E}\left(G\left(\overline{T}\right)\right) \leq \sqrt{\frac{2B\left(\mathcal{E}(T_0) - \mathcal{E}(T^*)\right)N}{S}} + B\sqrt{\frac{2N}{M}} + \epsilon \log(N).$$

Mirror Descent

Kullback Leiber regularization with previous iteration [Xu et al., 2019]

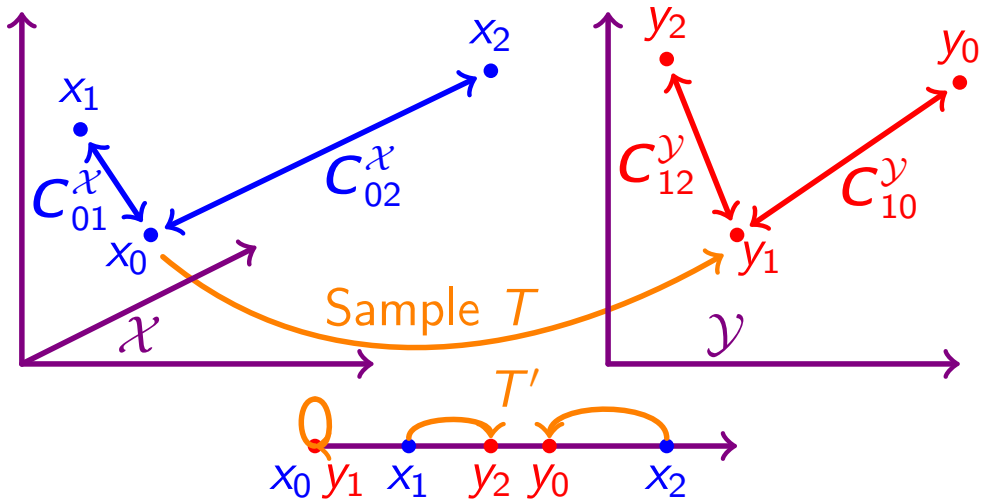
$$\left\langle \widehat{\mathbf{\Lambda}}, T' \right\rangle + \epsilon KL(T'||T) = \left\langle \widehat{\mathbf{\Lambda}} - \epsilon log(T), T' \right\rangle + \epsilon \sum_{ik} T'_{ik} log(T'_{ik}) \quad (7)$$

Algorithm 7 SaGroW with KL regularization

Require: $a, b, \mathcal{C}^{\mathcal{X}}, \mathcal{C}^{\mathcal{Y}}, \mathcal{L}, M, \epsilon, \alpha$

1: $T_0 = ab^\top$
2: **for** s= 0 **to** S-1 **do**
3: $(j_m, l_m) \sim \text{Sample}(T_s)\ \forall m \in [\![1, M]\!]$
4: $\widehat{\mathbf{\Lambda}} = \frac{1}{M} \sum_{m=1}^{M} \mathcal{L}\left(\mathcal{C}^{\mathcal{X}}(\cdot, x_{j_m}), \mathcal{C}^{\mathcal{Y}}(\cdot, y_{l_m})\right)$
5: $T_{s+1} = \min_{T' \in \Pi(\mu,\nu)} \left\langle \widehat{\mathbf{\Lambda}} - \epsilon log(T_s), T' \right\rangle - \epsilon \mathcal{H}(T')$
6: **end for**

Pointwise Gromov Wasserstein (PoGroW): sample $M = 1$



Speed and performances (SaGrow and PoGroW are implemented in POT)

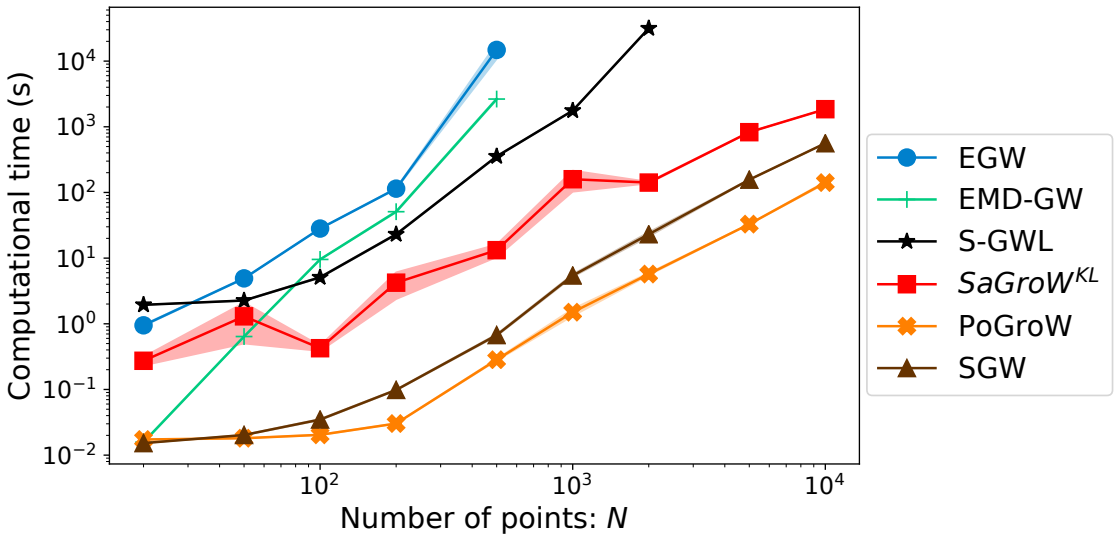


Figure 16: Computational time of various methods to compute the distance between samples from two mixtures of gaussians. The mean and the standard deviation over 10 runs are reported.

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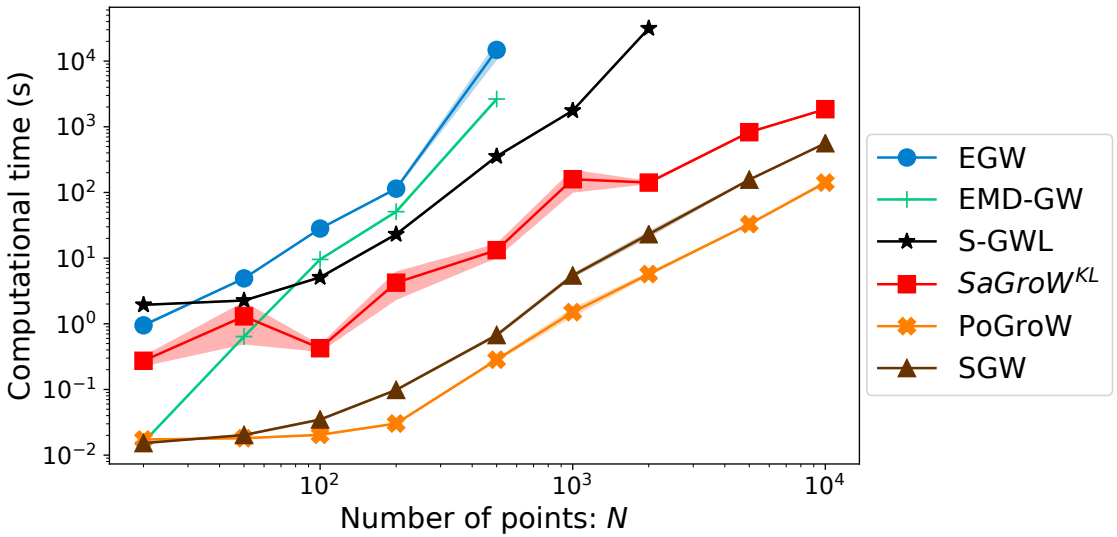

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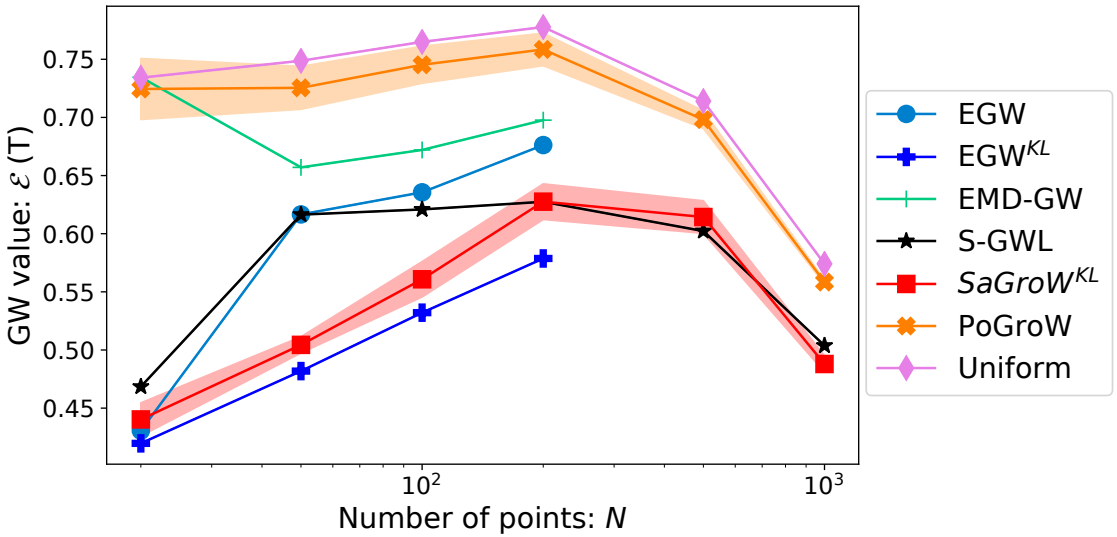

Figure 17: W distance estimation between synthetic graphs Brandes et al. [2003]. The mean and standard deviation over 10 runs are reported for the stochastic methods.

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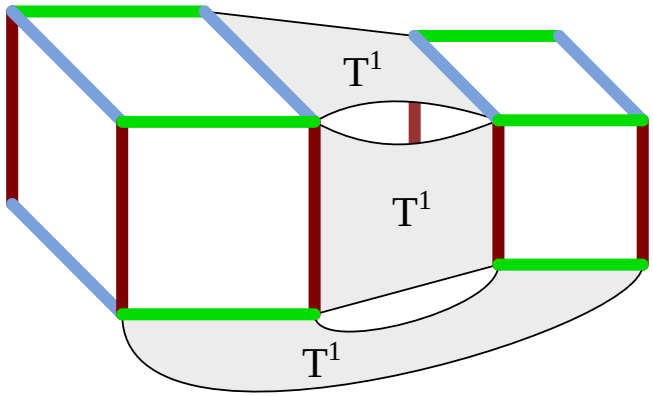
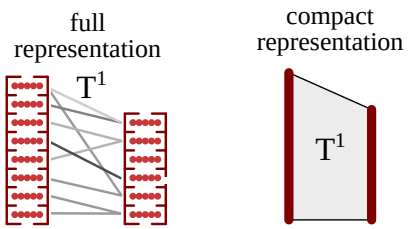
Optimal Tensor Transport

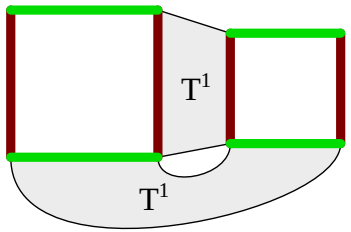
Based on an unpublished paper under submission at the AAAI conference.



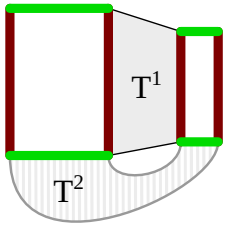
Motivation of Optimal Tensor Transport



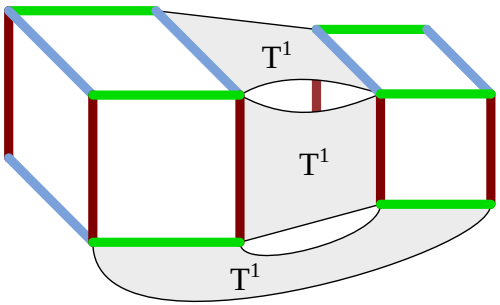
a) **OTT$_1$** (OT) *(F=5 features)*



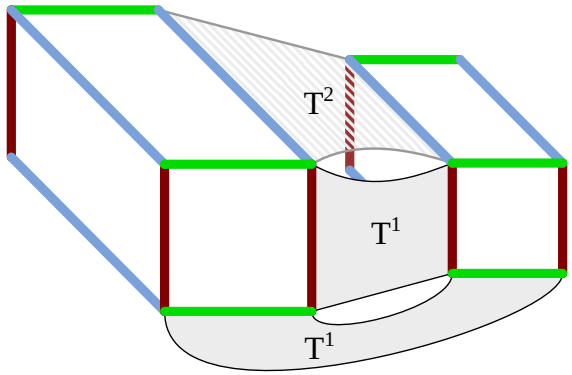
b) **OTT$_{11}$** (GW)



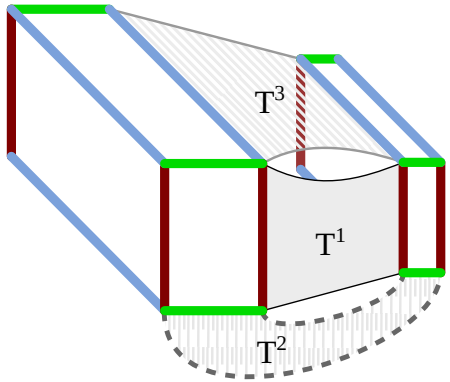
c) **OTT$_{12}$** (Co-OT)



d) **OTT$_{111}$** (triplets)

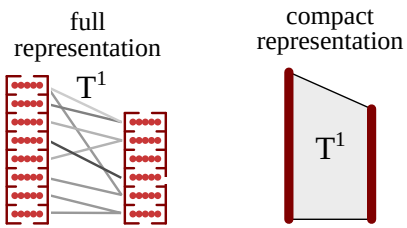


e) **OTT$_{112}$** (GW collections)

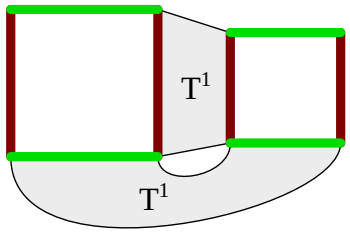


f) **OTT$_{123}$** (triCo-OT)

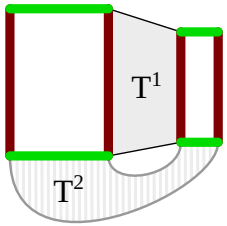
Motivation of Optimal Tensor Transport



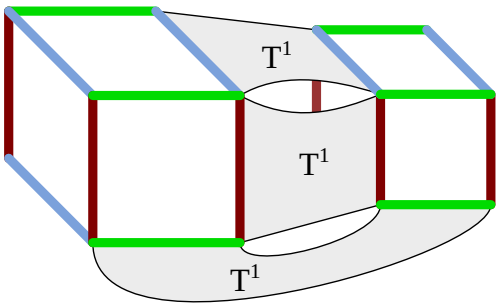
a) **OTT$_1$** (OT) *(F=5 features)*



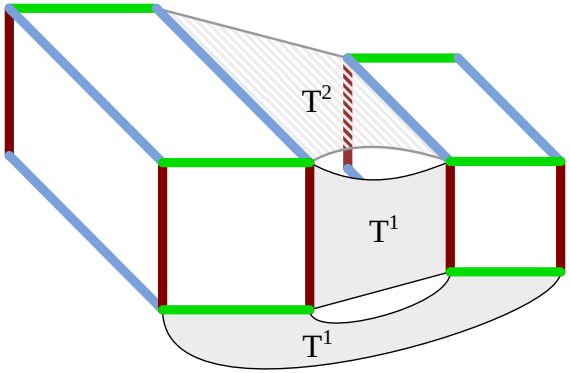
b) **OTT$_{11}$** (GW)



c) **OTT$_{12}$** (Co-OT)



d) **OTT$_{111}$** (triplets)



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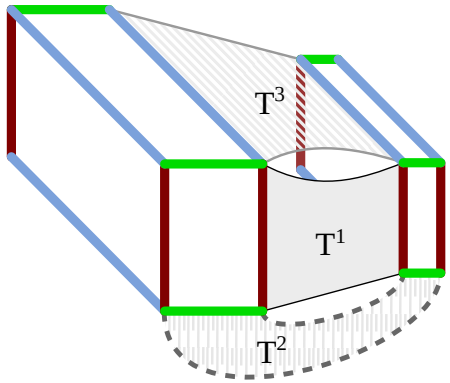
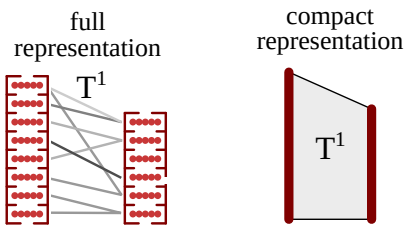


f) **OTT$_{123}$** (triCo-OT)

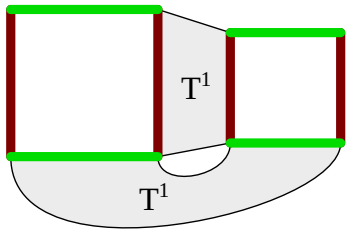
Optimal Transport

$$\mathrm{OT} = \min_{T^1 \in \Pi_{a^1 b^1}} \sum_{i_1=1}^{I_1} \sum_{k_1=1}^{K_1} \mathcal{L}(X_{i_1}, Y_{k_1})\, T^1_{i_1 k_1} \tag{8}$$

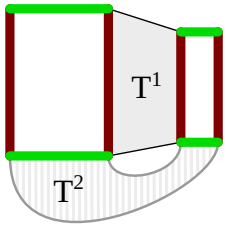
Motivation of Optimal Tensor Transport



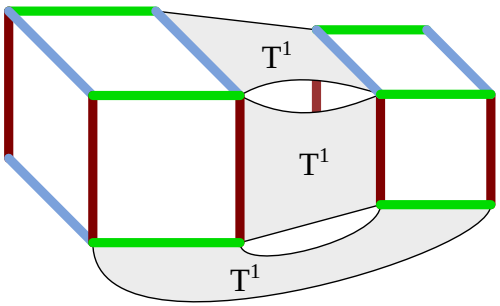
a) **OTT$_1$** (OT) *(F=5 features)*



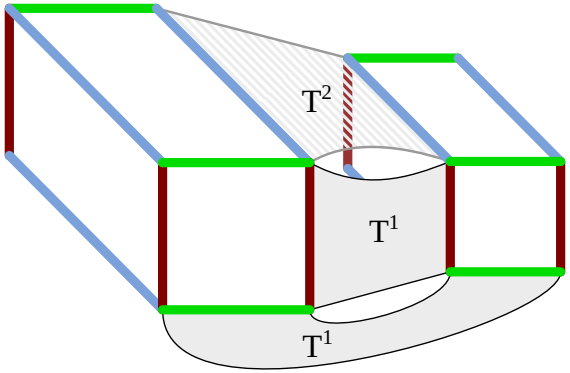
b) **OTT$_{11}$** (GW)



c) **OTT$_{12}$** (Co-OT)



d) **OTT$_{111}$** (triplets)



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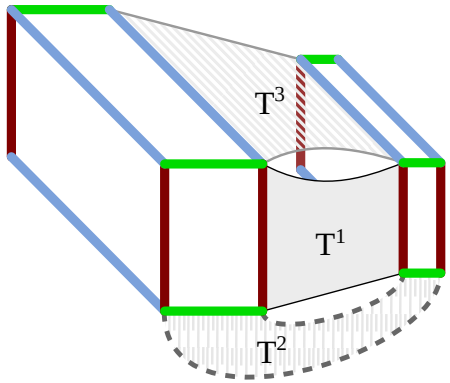
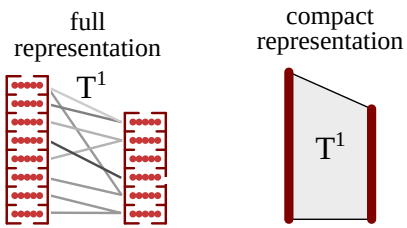


f) **OTT$_{123}$** (triCo-OT)

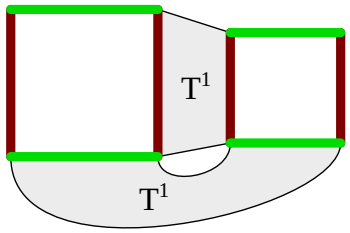
Gromov Wasserstein

$$\mathrm{GW} = \min_{T^1 \in \Pi_{a^1 b^1}} \sum_{i_1, i_2 = 1}^{I_1, I_2} \sum_{k_1, k_2 = 1}^{K_1, K_2} \mathcal{L}(X_{i_1 i_2}, Y_{k_1 k_2})\, T^1_{i_1 k_1}\, T^1_{i_2 k_2} \tag{8}$$

Motivation of Optimal Tensor Transport



a) **OTT$_1$** (OT) *(F=5 features)*



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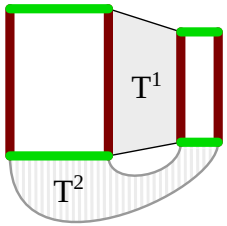

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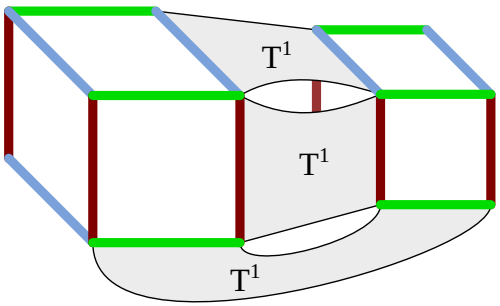

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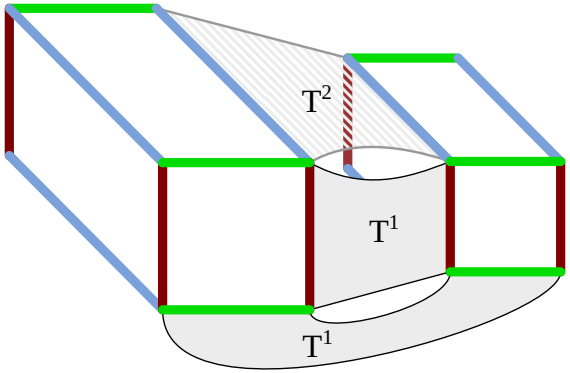
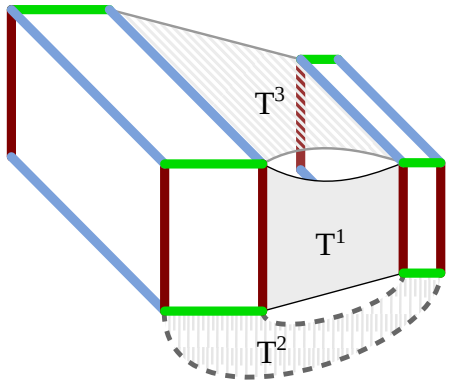


e) **OTT$_{112}$** (GW collections)

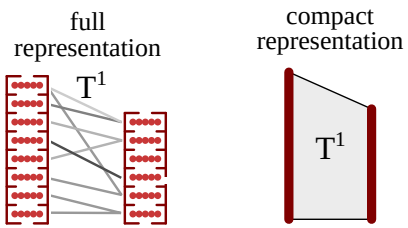


f) **OTT$_{123}$** (triCo-OT)

Co-Optimal Transport [Redko et al., 2020]

$$\text{Co-OT} = \min_{T^1 \in \Pi_{a^1 b^1}\, T^2 \in \Pi_{a^2 b^2}} \sum_{i_1, i_2 = 1}^{I_1, I_2} \sum_{k_1, k_2 = 1}^{K_1, K_2} \mathcal{L}(X_{i_1 i_2}, Y_{k_1 k_2})\, T^1_{i_1 k_1}\, T^2_{i_2 k_2} \qquad (8)$$

Motivation of Optimal Tensor Transport



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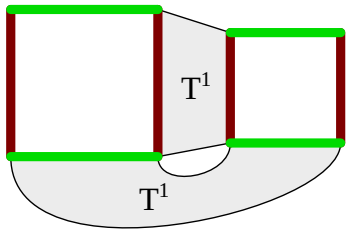

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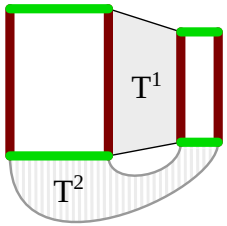

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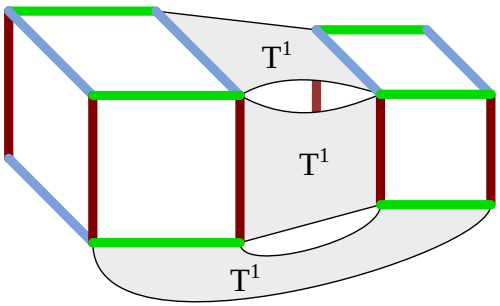

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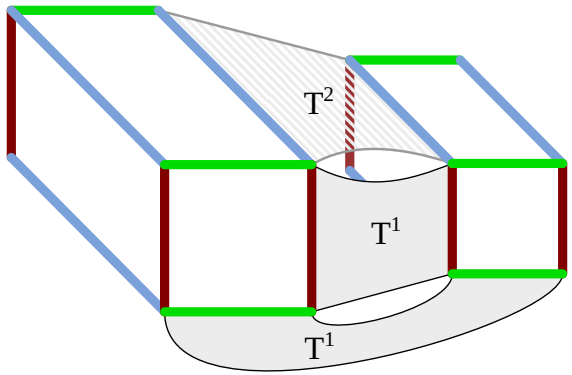
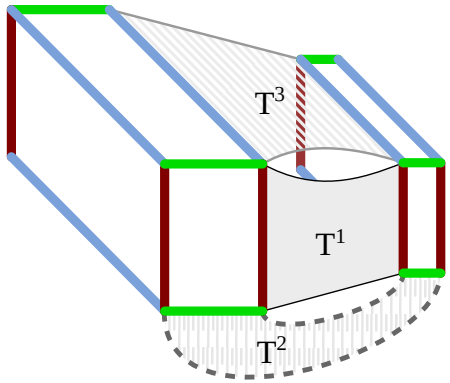


e) **OTT$_{112}$** (GW collections)



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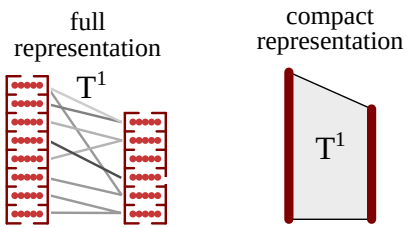
Optimal Tensor Transport with $(1, 1, 1)$

$$\min_{T^1 \in \Pi_{a^1 b^1}} \sum_{i_1,i_2,i_3=1}^{I_1,I_1,I_1} \sum_{k_1,k_2,k_3=1}^{K_1,K_1,K_1} \mathcal{L}(X_{i_1 i_2 i_3}, Y_{k_1 k_2 k_3})\, T^1_{i_1 k_1}\, T^1_{i_2 k_2}\, T^1_{i_3 k_3}$$

Motivation of Optimal Tensor Transport



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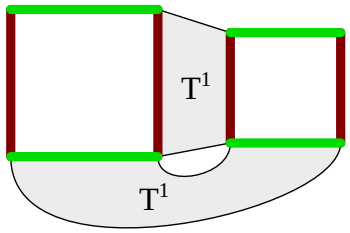

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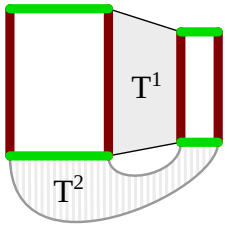

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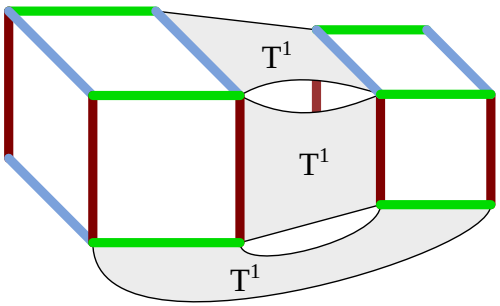

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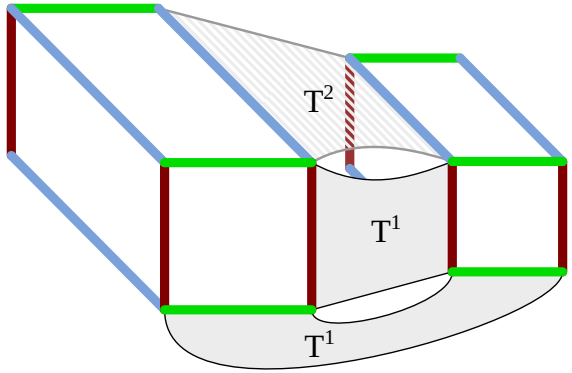

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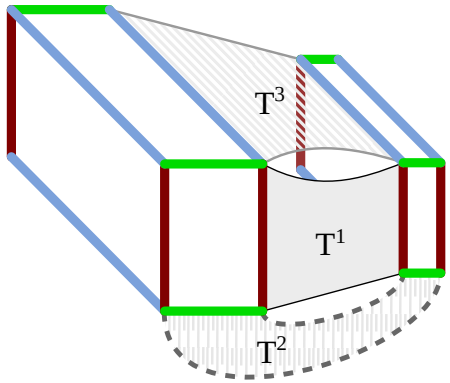
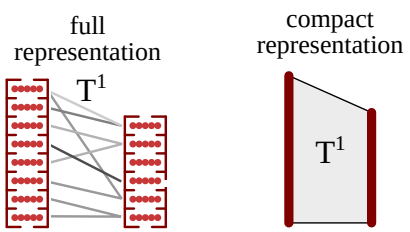


f) **OTT$_{123}$** (triCo-OT)

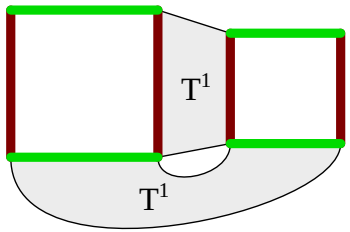
Optimal Tensor Transport with $(1, 1, 2)$

$$\min_{T^1 \in \Pi_{a^1 b^1}\, T^2 \in \Pi_{a^2 b^2}} \sum_{i_1, i_2, i_3 = 1}^{I_1, I_1, I_2} \sum_{k_1, k_2, k_3 = 1}^{K_1, K_1, K_2} \mathcal{L}(X_{i_1 i_2 i_3}, Y_{k_1 k_2 k_3})\, T^1_{i_1 k_1}\, T^1_{i_2 k_2}\, T^2_{i_3 k_3}$$

Motivation of Optimal Tensor Transport



a) **OTT$_1$** (OT) *(F=5 features)*



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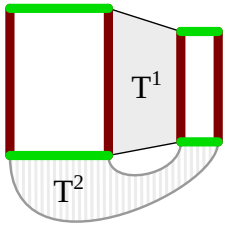

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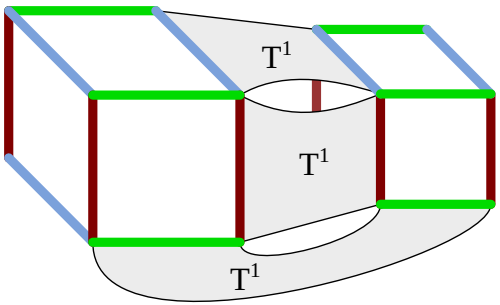

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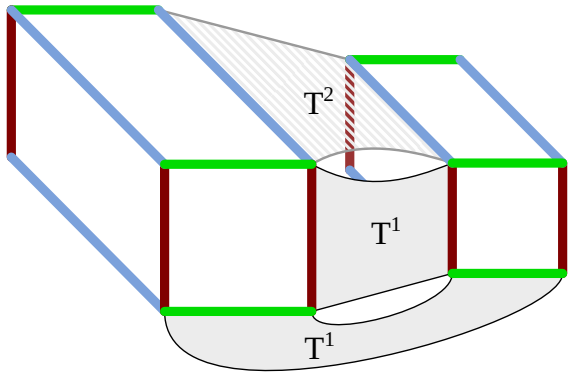

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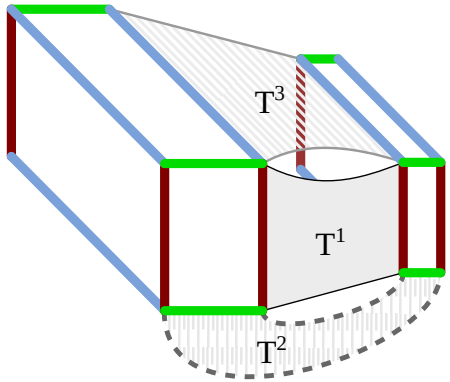

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Optimal Tensor Transport with $(1, 2, 3)$

$$\forall e \min_{T^e \in \Pi_{a^e b^e}} \sum_{i_1,i_2,i_3=1}^{I_1,I_2,I_3} \sum_{k_1,k_2,k_3=1}^{K_1,K_2,K_3} \mathcal{L}(X_{i_1 i_2 i_3}, Y_{k_1 k_2 k_3})\, T^1_{i_1 k_1}\, T^2_{i_2 k_2}\, T^3_{i_3 k_3}$$

Mathematical formulations

Optimal Tensor Transport

$$\mathrm{OTT}_f(X, Y, (a^e)_{e\in[\![1,E]\!]}, (b^e)_{e\in[\![1,E]\!]}) = \min_{\forall e\ T^e\in\Pi_{a^e b^e}} \mathcal{E}_f\left(X, Y, (T^e)_{e\in[\![1,E]\!]}\right)$$

$$\mathcal{E}_f\left(X, Y, (T^e)_{e\in[\![1,E]\!]}\right) = \sum_{i_1,\dots,i_D=1}^{I_{f(1)},\dots,I_{f(D)}} \sum_{k_1,\dots,k_D=1}^{K_{f(1)},\dots,K_{f(D)}} \mathcal{L}(X_{i_1\dots i_D}, Y_{k_1\dots k_D}) \prod_{d=1}^{D} T^{f(d)}_{i_d k_d}$$

Stochastic Mirror Descent to solve the OTT problem

The gradient require N^{2D} operation

$$\nabla_{T^e}\mathcal{E}_f = \sum_{\{d'|f(d')=e\}} \mathbb{E}\left(\Lambda^{d'}\right)$$

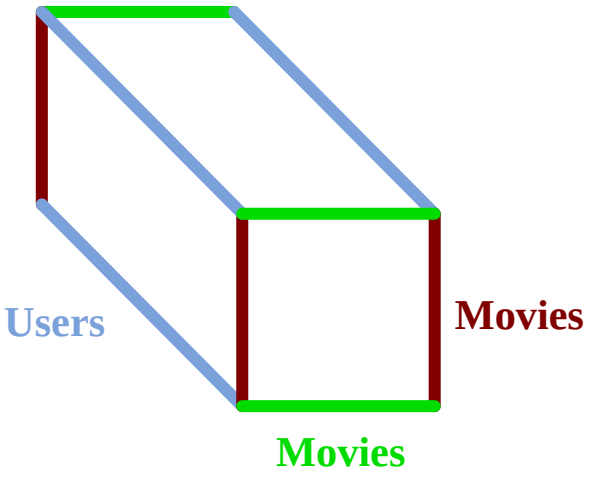
Algorithm 8 Alternated Stochastic Mirror Descent algorithm

Require: $(a^e)_{e\in[\![1,E]\!]}$, $(b^e)_{e\in[\![1,E]\!]}$, X, Y, $\mathcal{L}$, M, ϵ

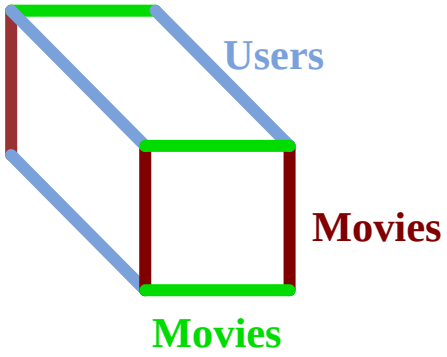
1: $\forall e \in [\![1, E]\!]$, $T^e = a^e b^{e\top}$
2: **for** s = 0 **to** S-1 **do**
3: **for** e = 1 **to** E **do**
4: $\widehat{\nabla_{T^e}\mathcal{E}_f} = M$ samples of the gradient
5: $T^e = \underset{T'\in\Pi(a^e,b^e)}{min} \left\langle \widehat{\nabla_{T^e}\mathcal{E}_f}, T' \right\rangle + \epsilon KL(T'||T^e)$
6: **end for**
7: **end for**

Interest of such formulation: Domain Adaptation

Domain Adaptation: predict the type of movies



Old movies



New movies

Datasets	Rdm	SVM	S-GWL	GW	Co-OT	OTT
AVG	50.0±3.3	58.6	63.8	64.9	68.2	**77.3**±3.1
AVG (best)	50.0±3.3	58.6	66.3	71.0	70.7	**78.9**±2.9

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   - ✓ Interest of **learning a ground metric** for a DA task.

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   - ✓ Fast approximation of the GW distance with **any losses**
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4. OTT
   - ✓ New OT formulation to handle **tensors** of arbitrary orders
   - ✓ Adaptation of the previous solver to solve it in a reasonable time

Further works

Related to the contributions

1. Deep version of MLOT
2. Extend the use of the Wasserstein stability with a min minimax formulation
3. Convergence bound of SaGroW^{KL} to stationary points
4. Fused OTT

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Some perspectives for the OT's application to ML

1. GW $\Leftrightarrow$ Linear GAN
2. Under which condition on $\mathcal{L}$, GW has a sparse solution ?

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Conclusions

- Problem:
  - We tackle the challenging unsupervised DA problem
  - OT for DA always relies on the euclidean distance
- ✓ Solutions:
  - We provide a metric dependent bound on the target error
  - We use labeled sources to learn a class-informed metric
  - We project, independently, the source and target point into subspaces
  - We show a relation between OT and PCA, and use PCA as initialization
- ✓ Results:
  - Competitive against various baselines with a Reverse Validation method
  - Improve the performance of OTDA for different set of hyperparameters

Continuous GW