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

Thesis defense of Tanguy KERDONCUFF

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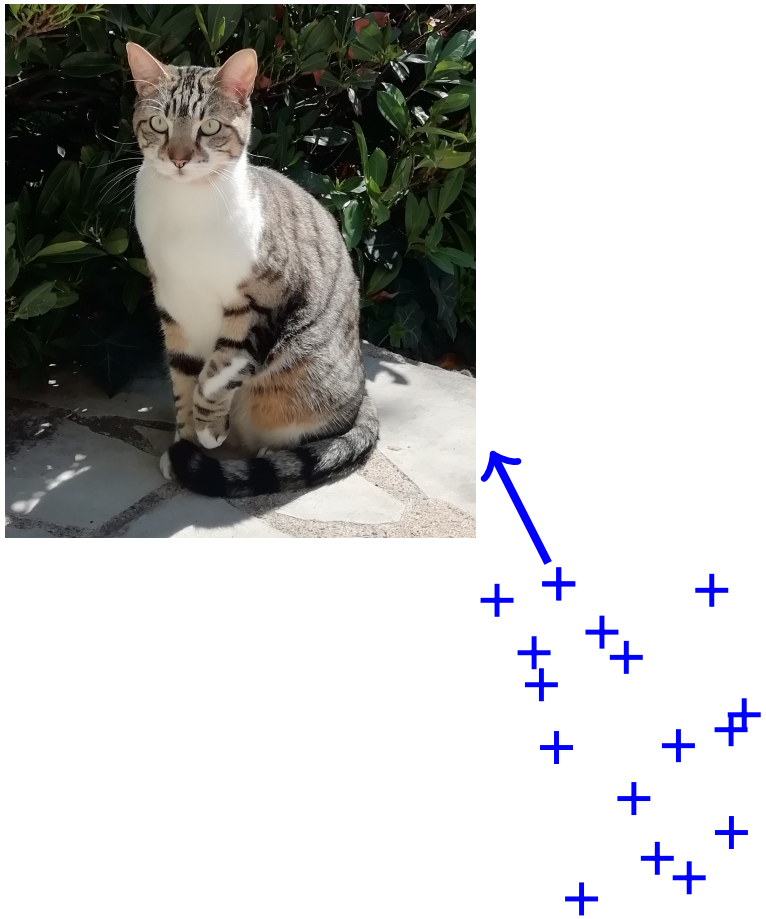
Marc SEBBAN	Professeur, Université de Saint-Étienne	Directeur
Rémi EMONET	Maître de conférences, Université de Saint-Étienne	Co-encadrant

December 9, 2021

Machine Learning: a classification example



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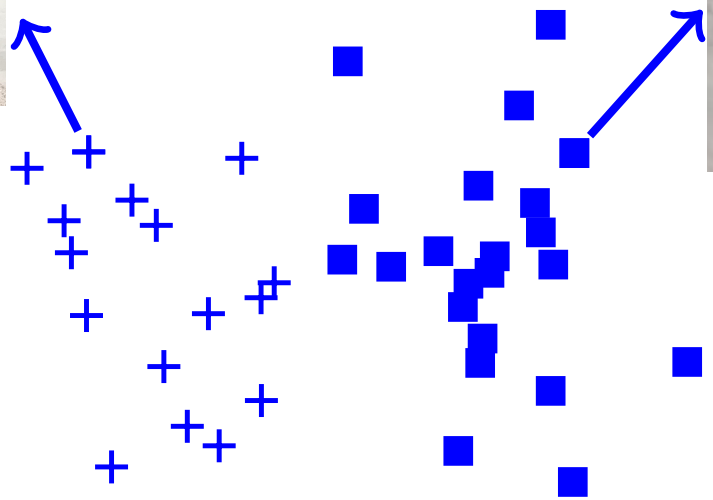

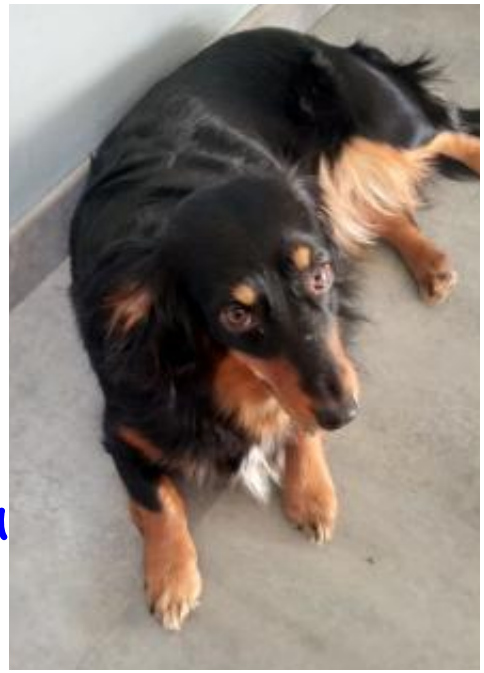

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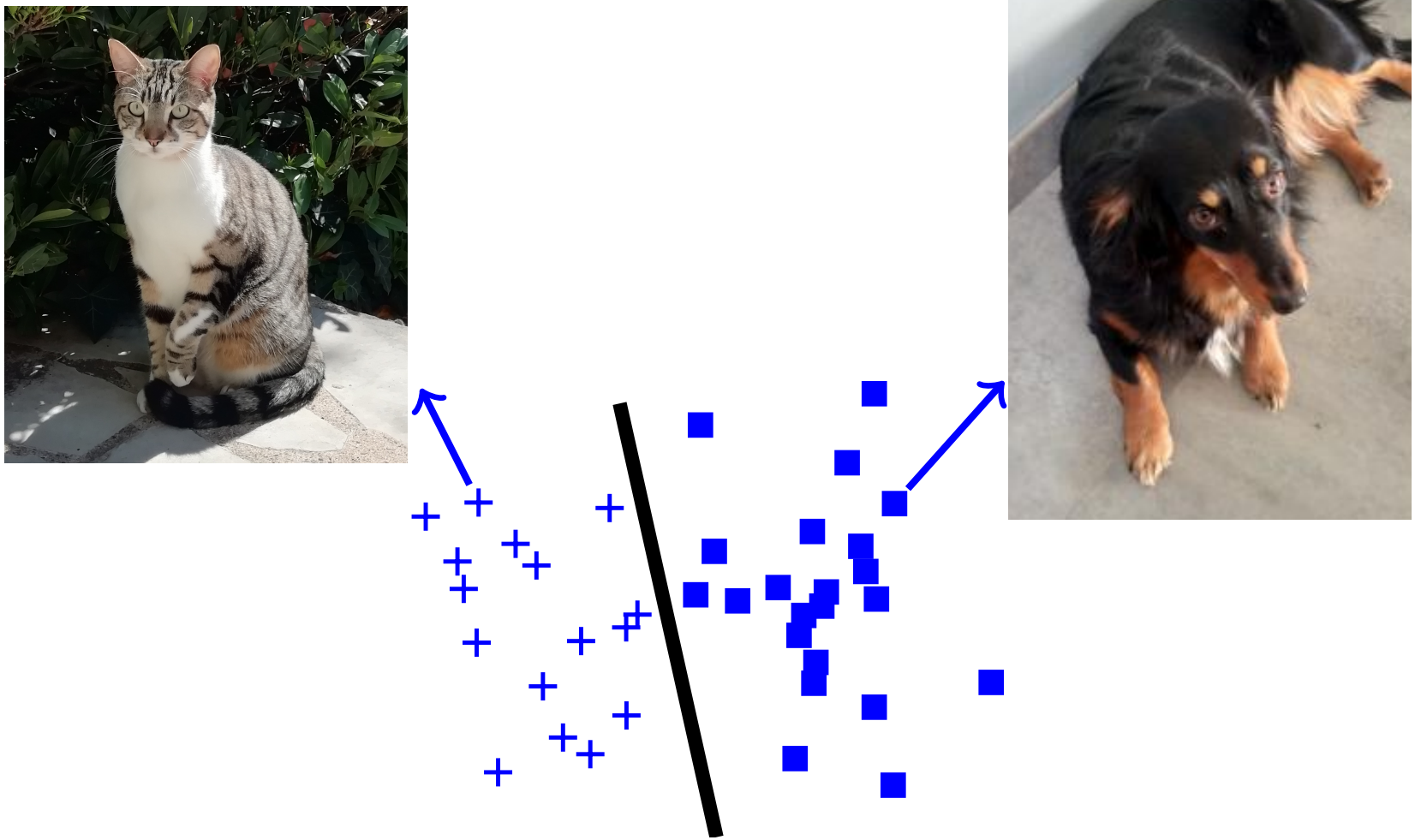

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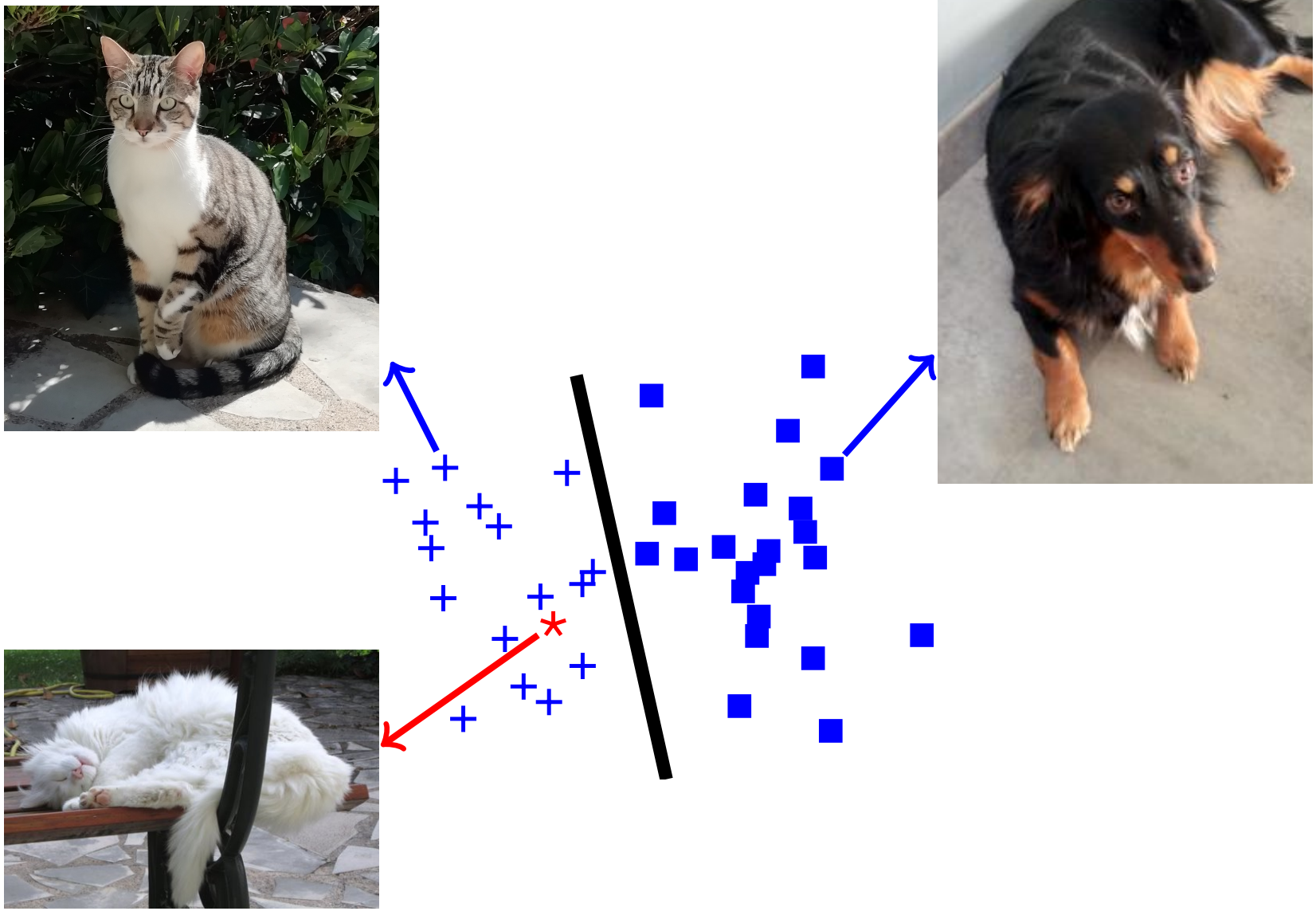

Intuition behind Optimal Transport

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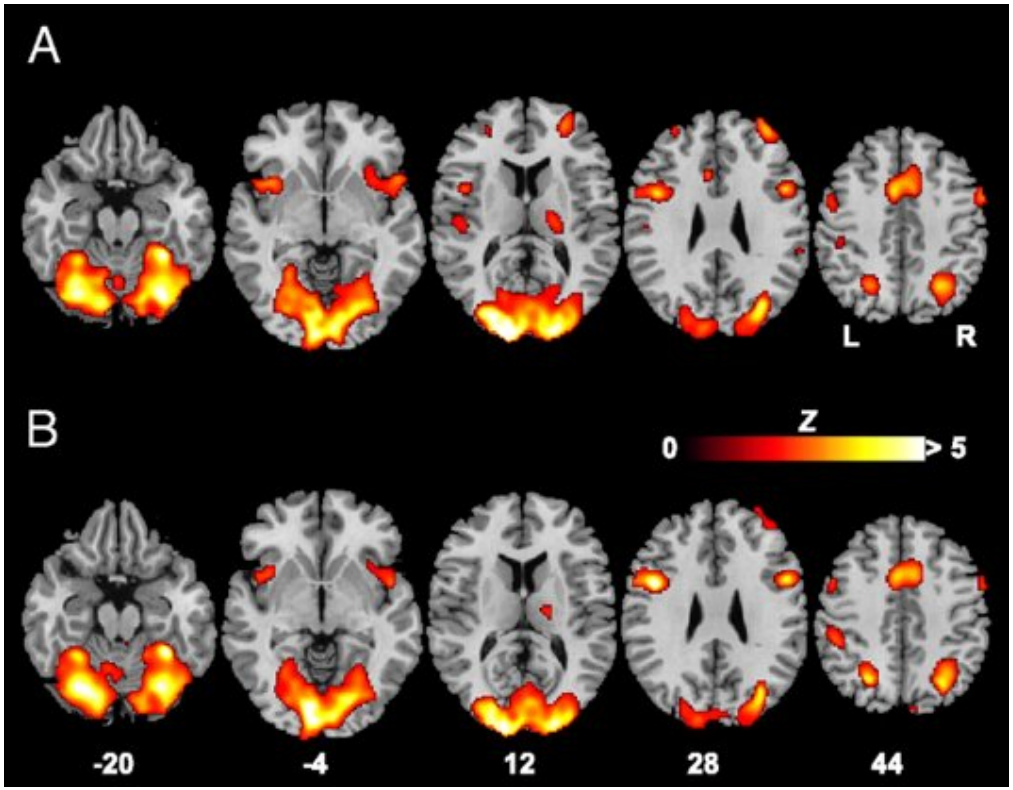
Optimal Transport in Machine Learning

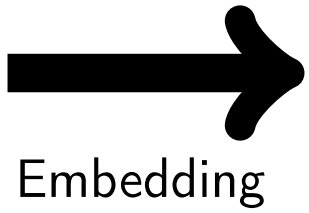
- We can use the Optimal Transport to compare two brain activation maps [Tan et al., 2008]

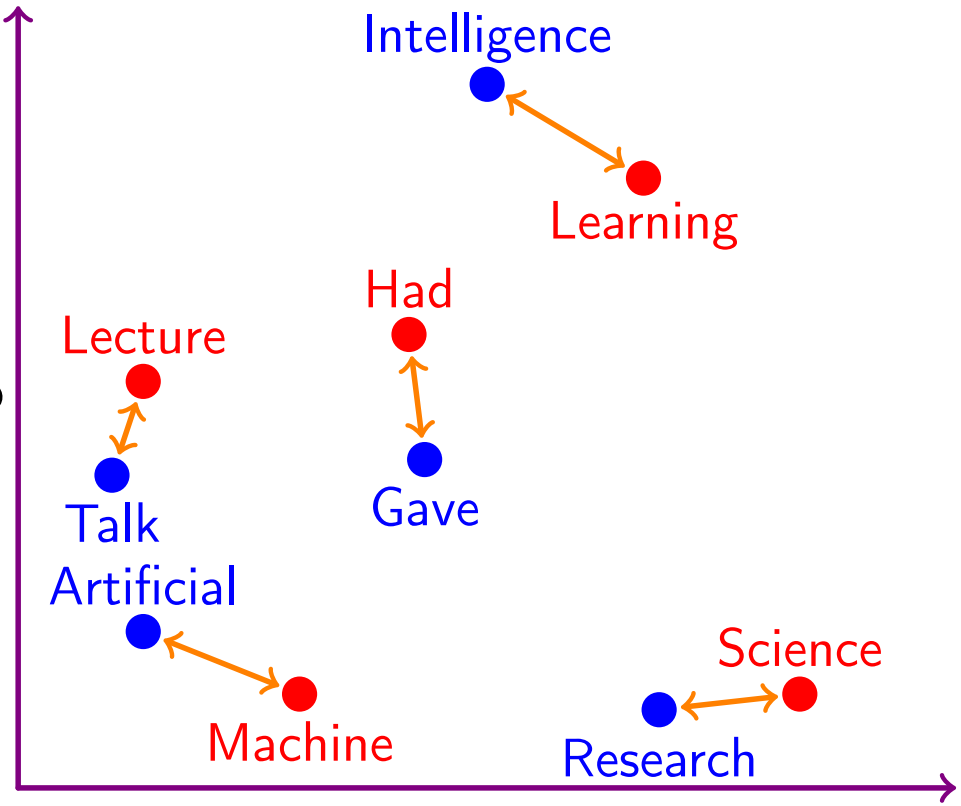


Optimal Transport in Machine Learning

- We can use the Optimal Transport to compare two sentences

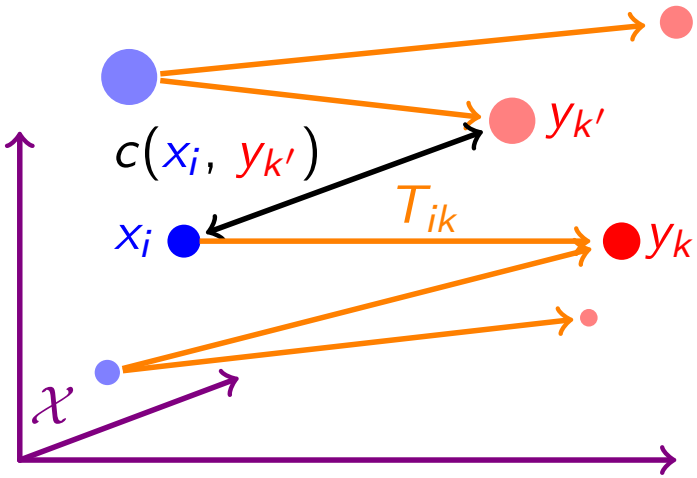
he	she
Gave	Had
a	a
Research	Science
Talk	Lecture
on	in
Artificial	Machine
Intelligence	Learning





Overview

- Ground Metric



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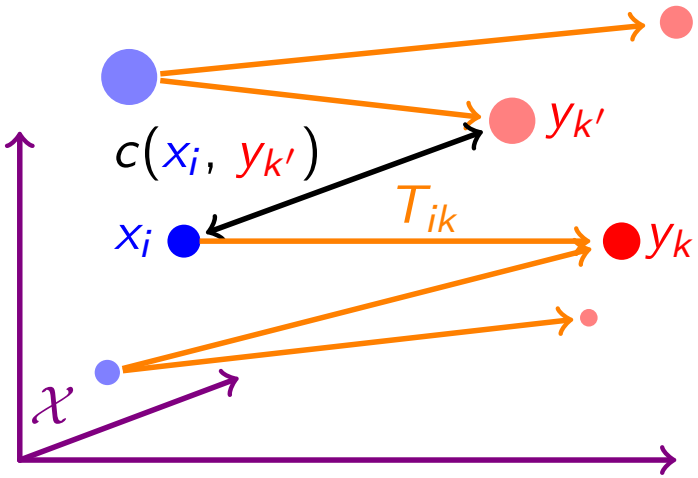
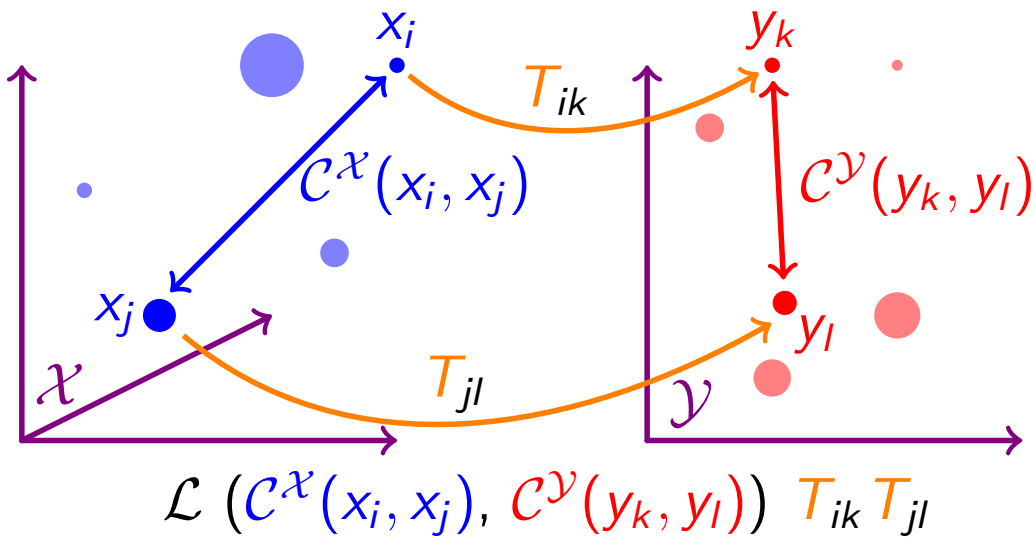


- Gromov Wasserstein



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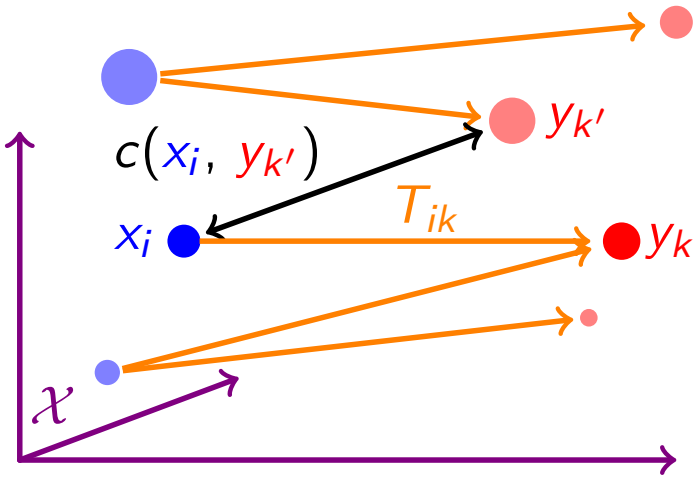

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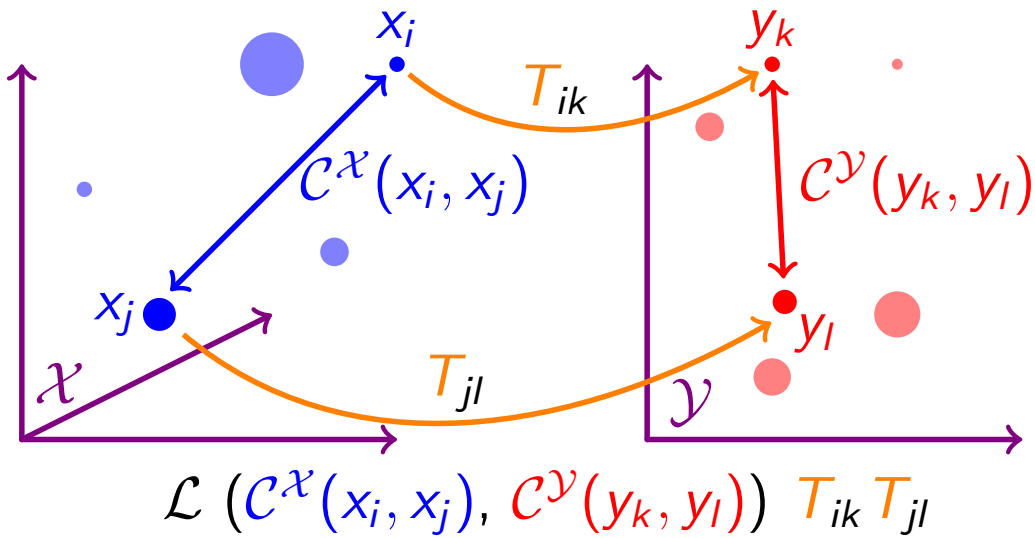
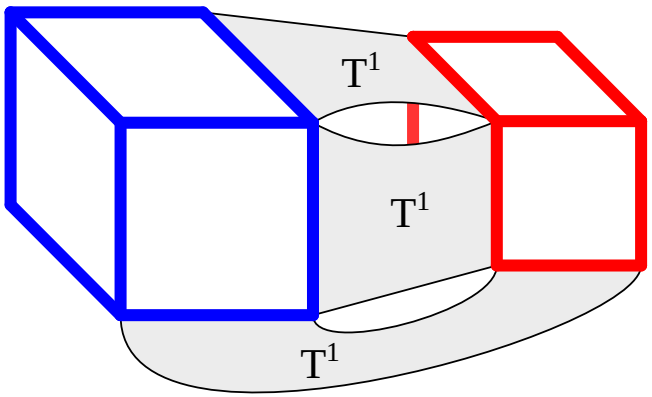


- Generalized OT



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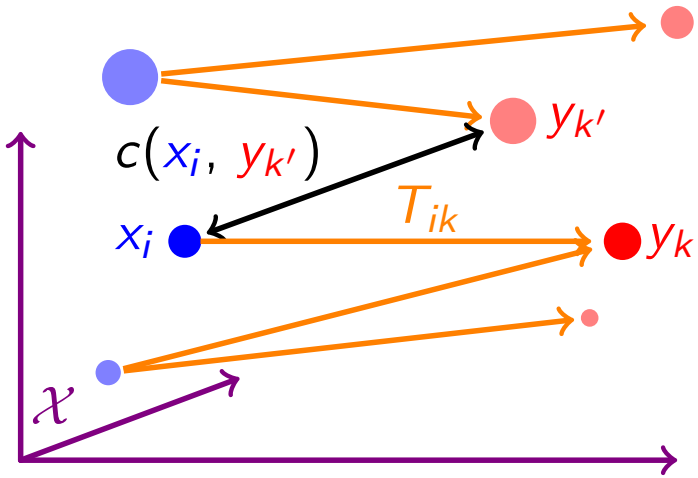
Discrete Optimal Transport (OT) and Wasserstein distance



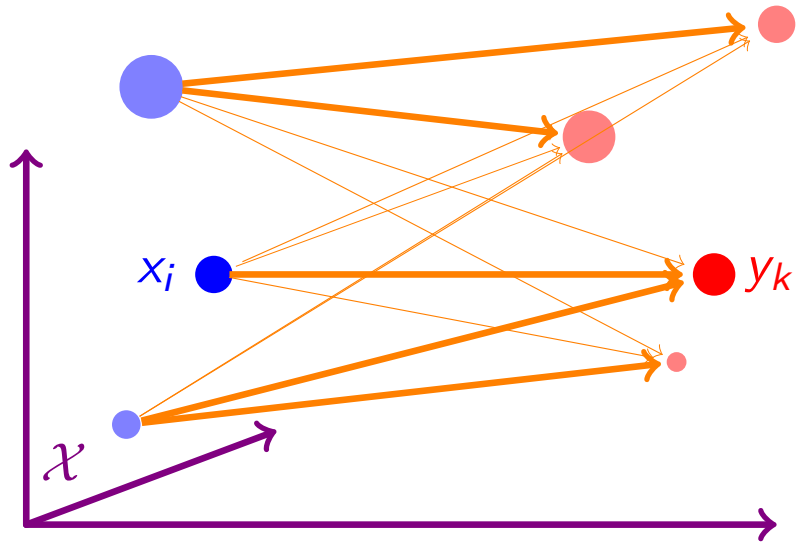
- The ground cost c is used to compare points.

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: $\Pi(\mu,\nu) = \{T \in \mathbb{R}_+^{I \times K} \,|\, T^\top \mathbb{1}_I = b, T\mathbb{1}_K = a\}$

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

Kullback-Leibler regularization

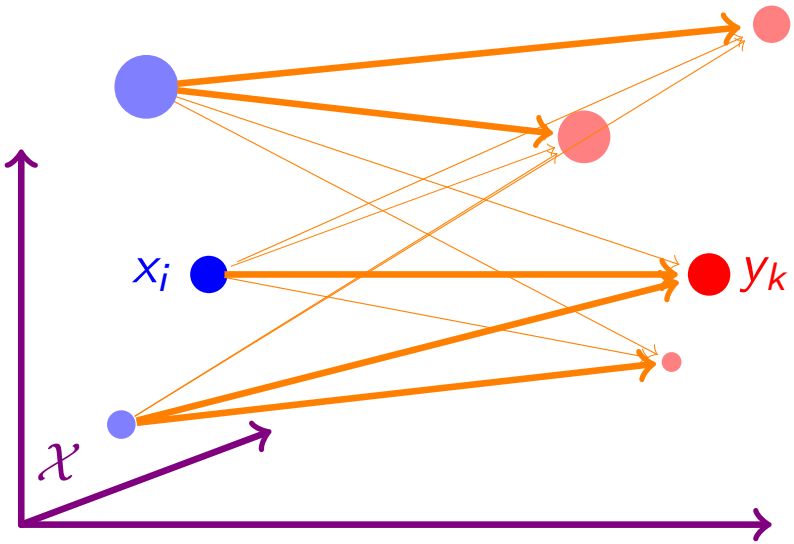


Entropy regularized OT [Cuturi, 2013; Sinkhorn and Knopp, 1967]

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

$$\min_{T \in \Pi(\mu,\nu)} \sum_{i,k=1}^{I,K} c(x_i, y_k) T_{ik} + \epsilon KL(T||ab^\top) \tag{2}$$

Kullback-Leibler regularization



- The OT plan is not sparse anymore

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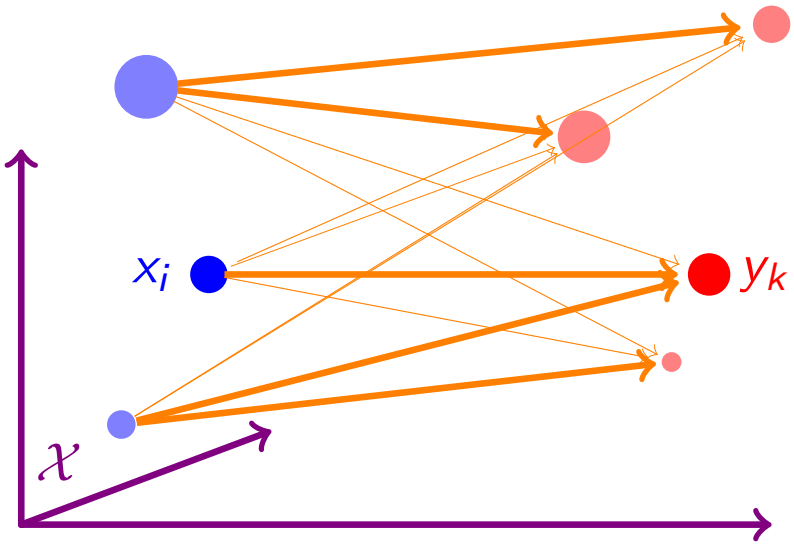

- The OT plan is not sparse anymore
- Unique solution

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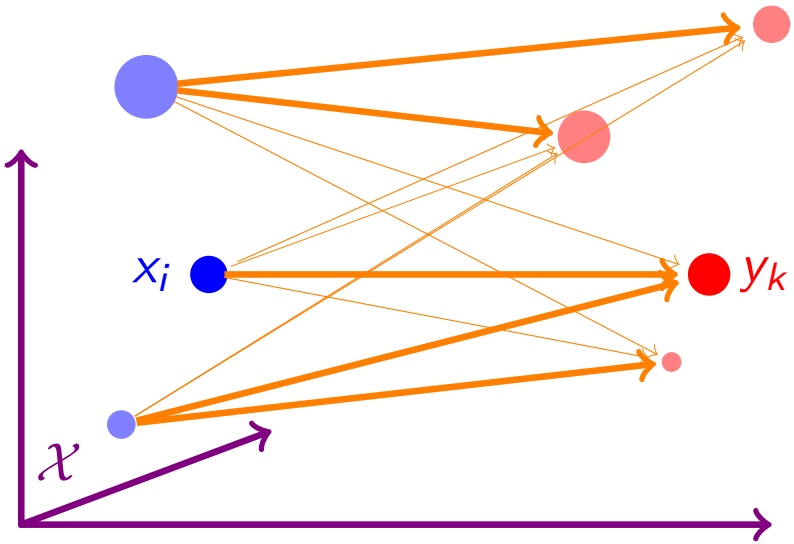

- The OT plan is not sparse anymore
- Unique solution
- The OT plan changes continuously

Entropy regularized OT [Cuturi, 2013; Sinkhorn and Knopp, 1967]

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

$$\min_{T \in \Pi(\mu,\nu)} \sum_{i,k=1}^{I,K} c(x_i, y_k) T_{ik} + \epsilon KL(T||ab^\top) \tag{2}$$

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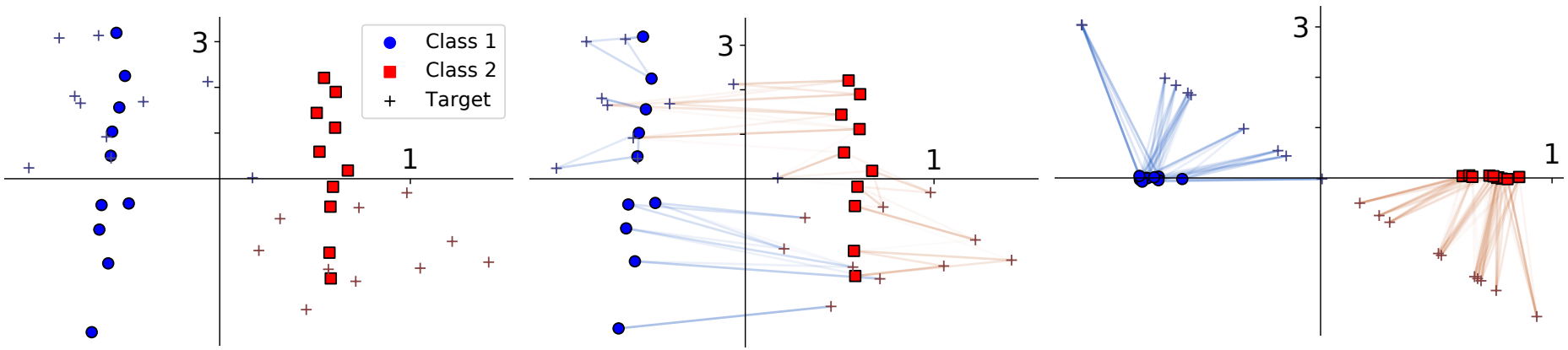
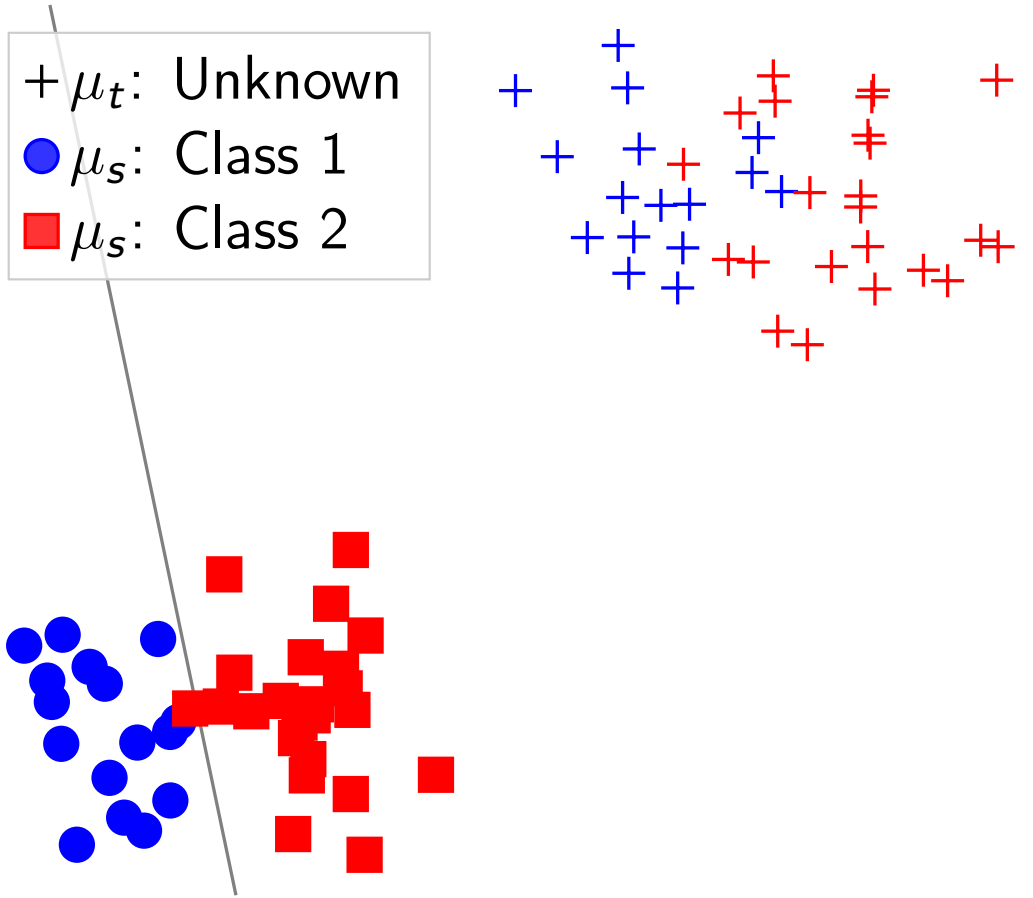
Metric Learning for Optimal Transport

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



Intuition of Optimal Transport for Domain Adaptation

DIRECTION GÉNÉRALE DES
FINANCES PUBLIQUES



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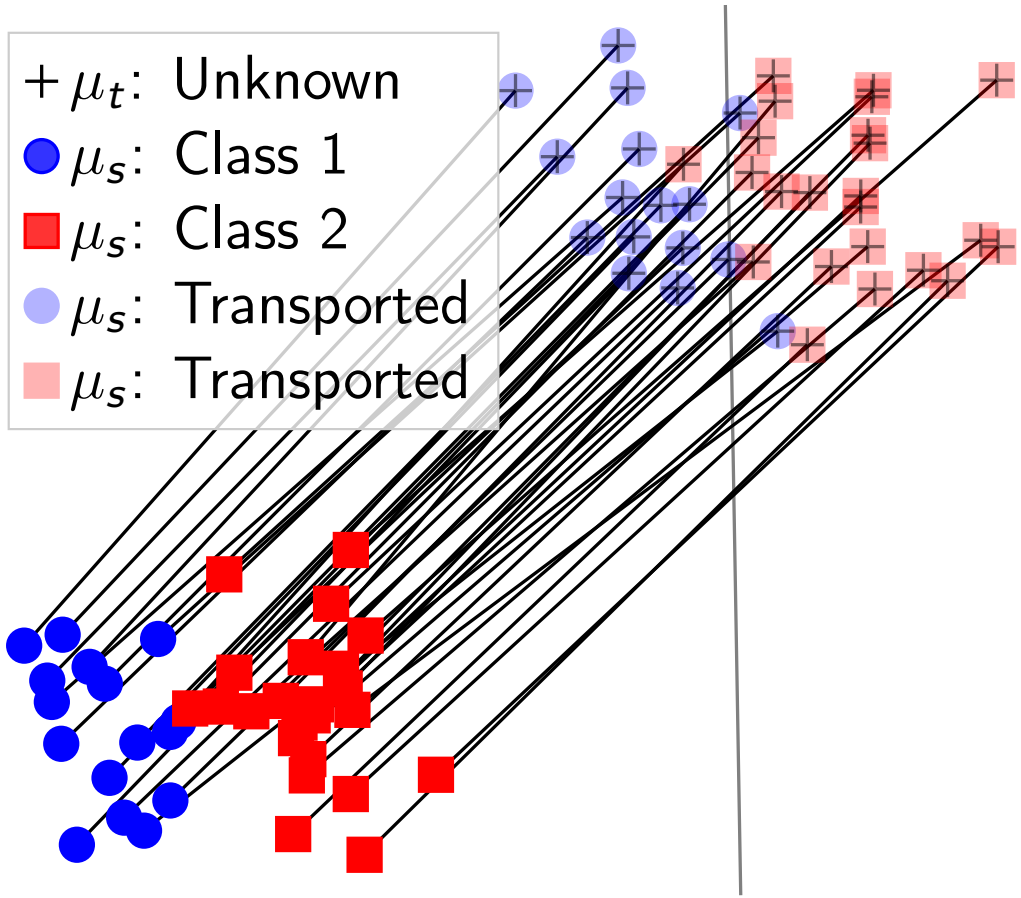

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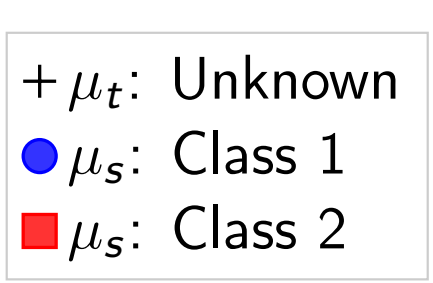

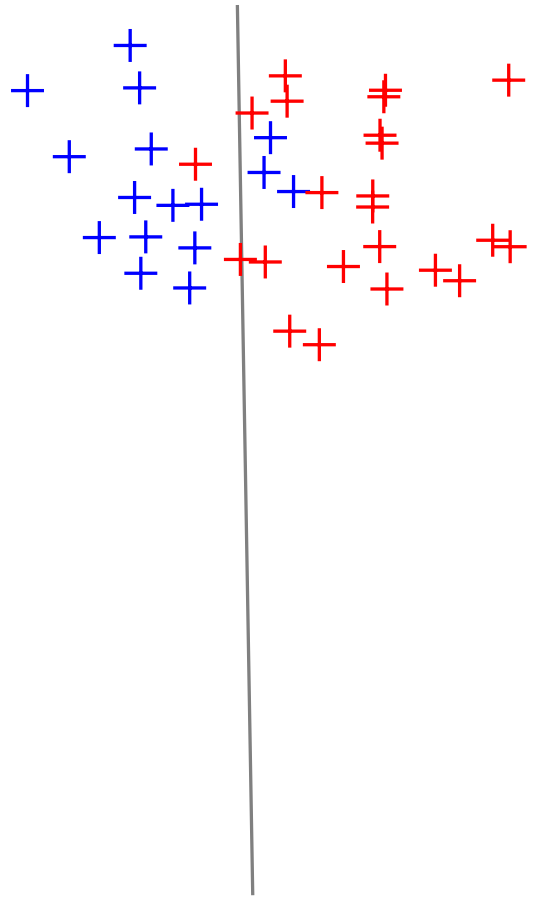

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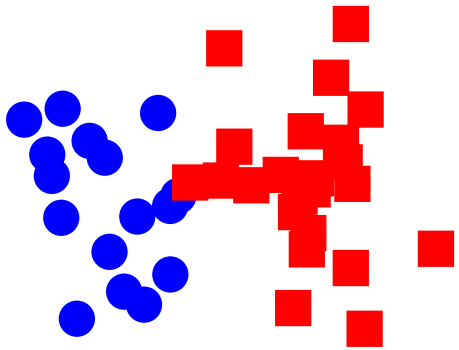


Optimal Transport for Domain Adaptation (OTDA)

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

$$\min_{T \in \Pi(\hat{\mu}_s, \hat{\mu}_t)} \langle T, C \rangle + \epsilon KL(T || ab^\top) + \lambda_c \underbrace{\left(\sum_{k=1}^{K} \sum_{cl=1}^{\#classes} \| T(\mathcal{I}_{cl}, k) \|_2 \right)}_{\Omega_c} \quad (3)$$

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

Metric learning

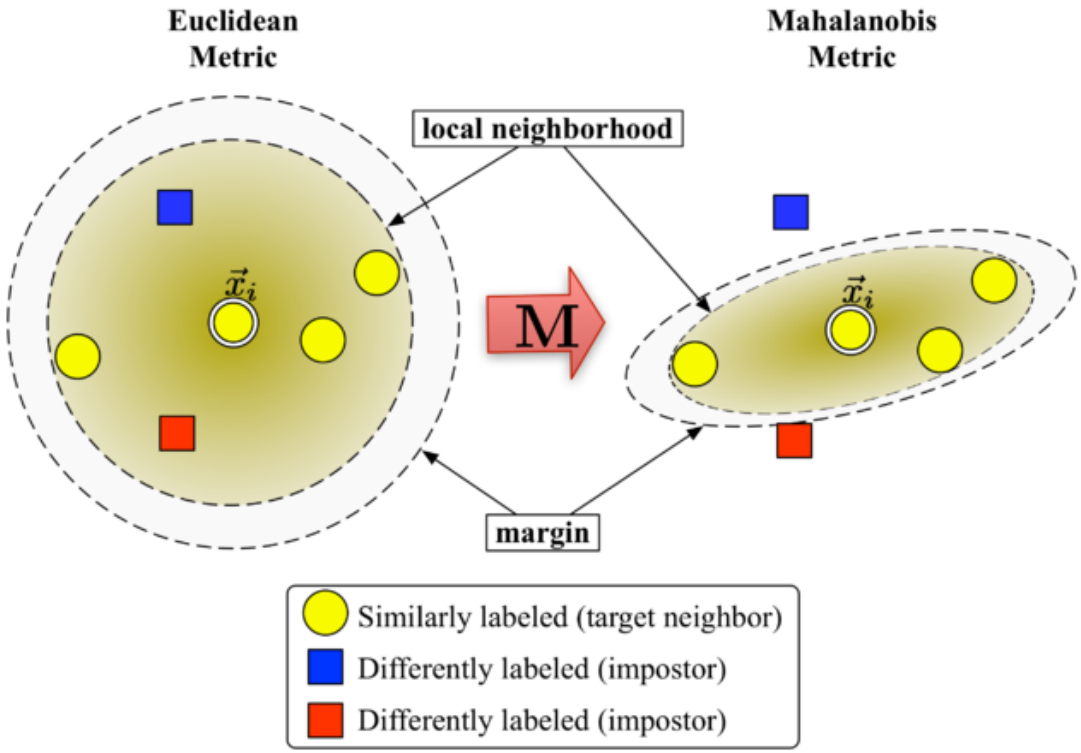


Figure 1: LMNN [Weinberger and Saul, 2009] CC-BY Mlguy (wikipedia)

Mahalanobis metric

- $C_M^2(x, x') = (x - x')^\top M(x - x') = \|Lx - Lx'\|_2^2$ with $L^\top L = M$

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

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 = learning classifier($\tilde{\boldsymbol{X}}^s$, $\boldsymbol{Y}^s$)

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

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

OTDA vs MLOT

Figure 2: MLOT - OTDA

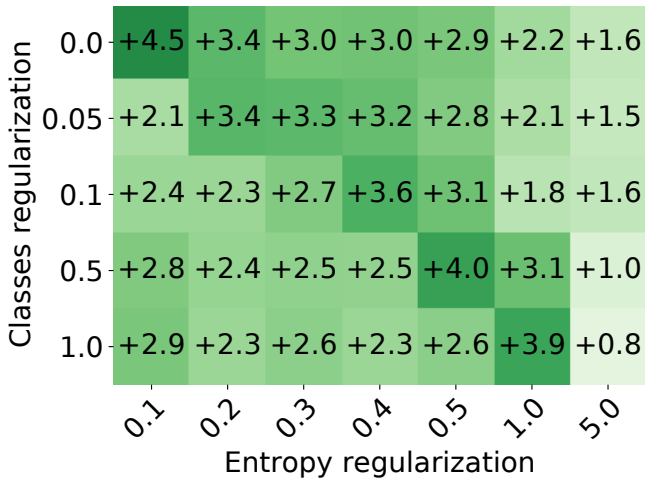
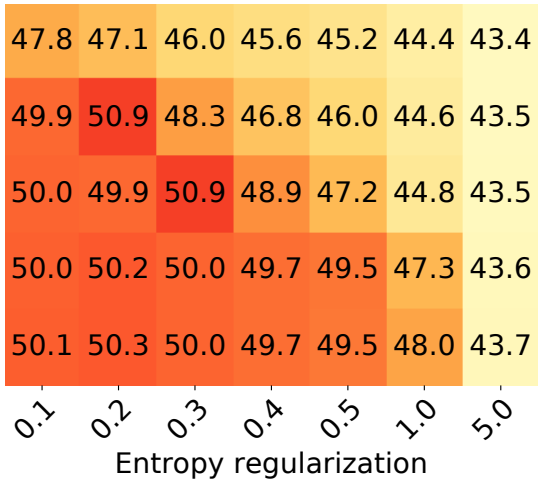


Figure 3: MLOT



OTDA and MLOT on Office-Caltech dataset [Gong et al., 2012] with SURF features

OTDA vs MLOT

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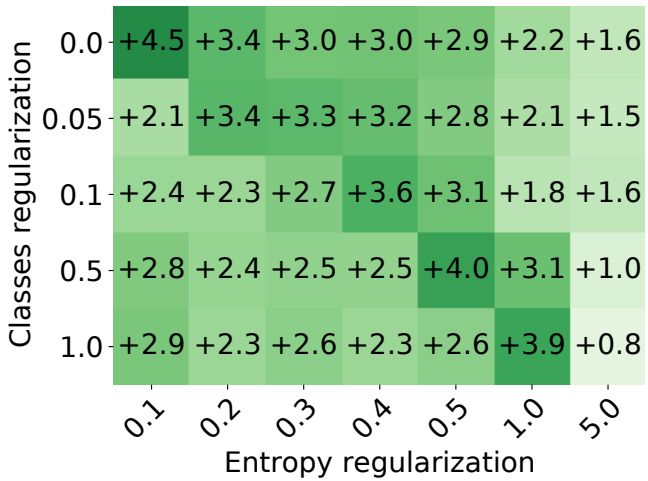

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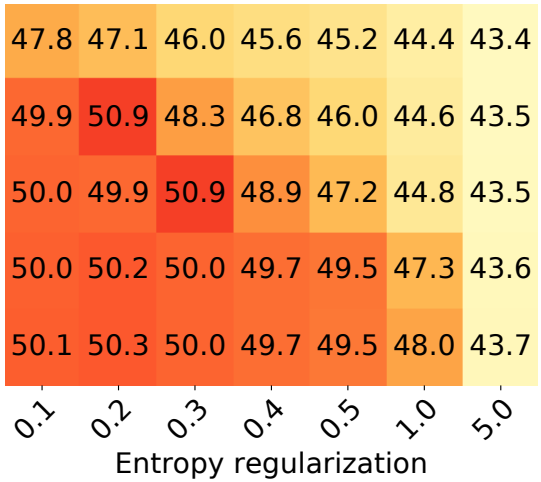

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- It is always good to learn a metric

OTDA vs MLOT

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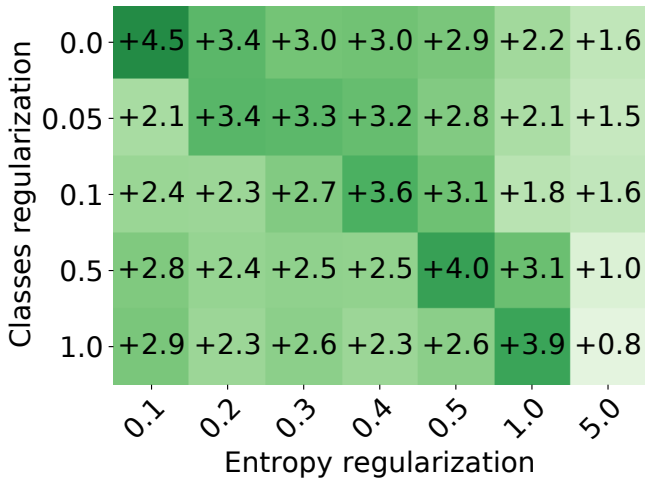

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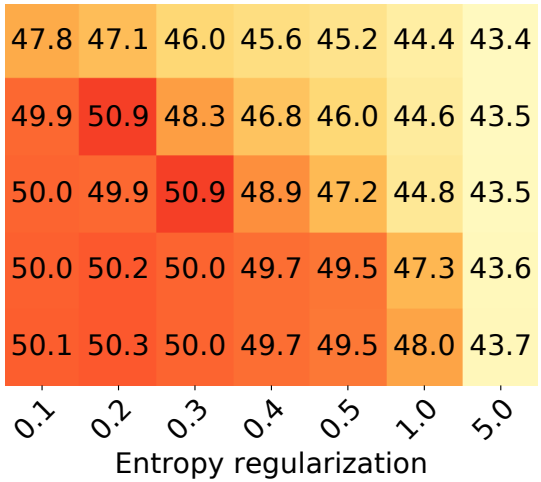

OTDA and MLOT on Office-Caltech dataset [Gong et al., 2012] with SURF features

- It is always good to learn a metric
- It is always good to use the OTDA class regularization

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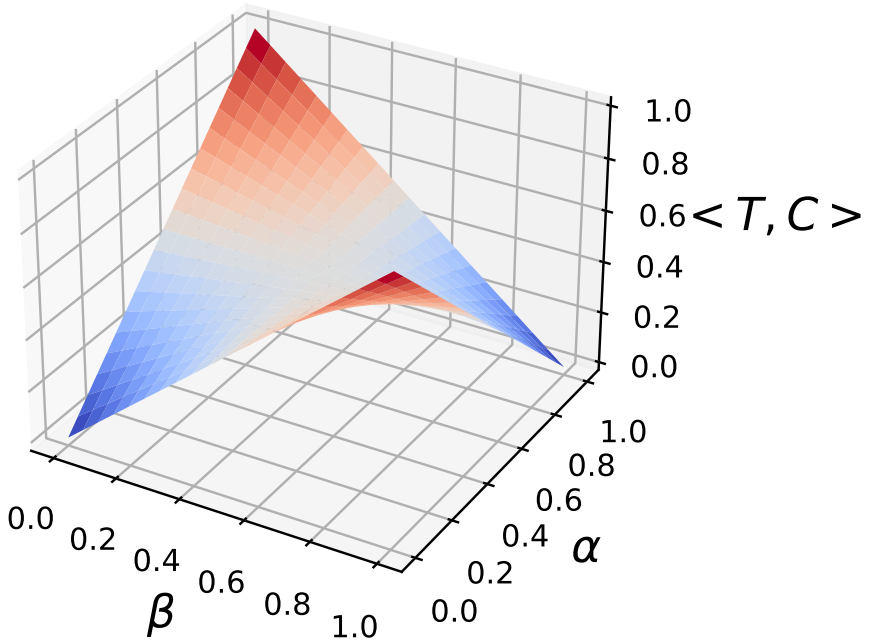
A Swiss Army Knife for Minimax Optimal Transport

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



Different type of set

Robust Kantorovich Problem (RKP)

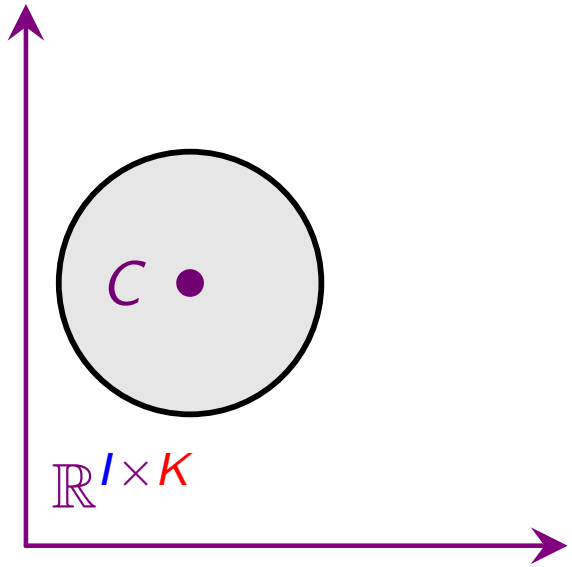
$$\mathcal{W}_{\mathcal{C}} = \min_{T \in \Pi} \max_{C \in \mathcal{C}} \langle T, C \rangle \tag{4}$$

Different type of set

Robust Kantorovich Problem (RKP)

$$\mathcal{W}_{\mathcal{C}} = \min_{T \in \Pi} \max_{C \in \mathcal{C}} \langle T, C \rangle \tag{4}$$

- Mahalanobis ball centered at a matrix C :



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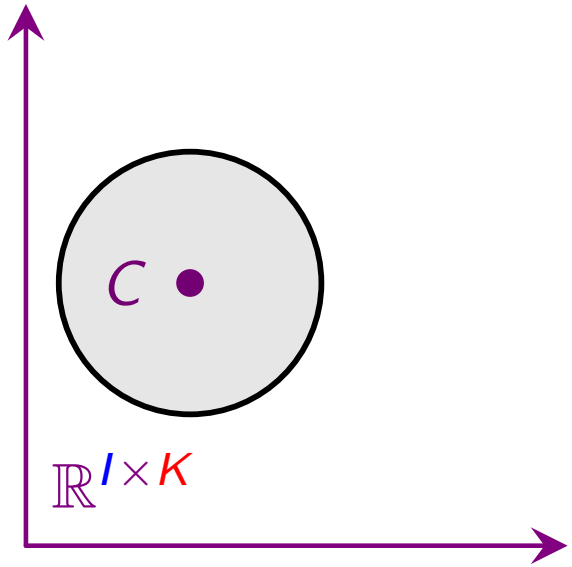
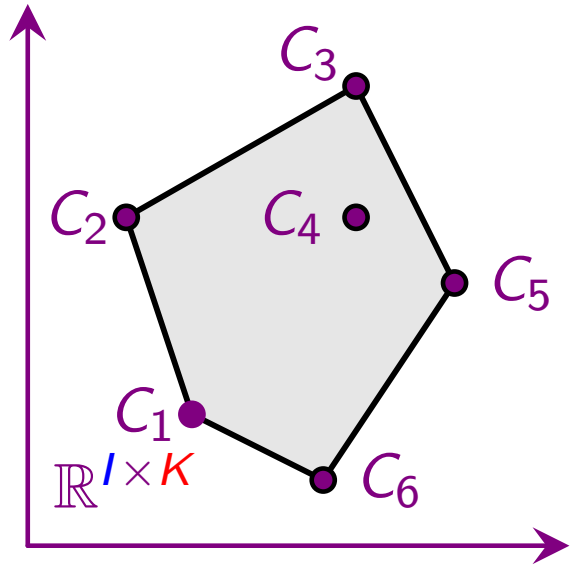


- Convex hull of finite set of cost matrices:



Cutting set algorithm [Mutapcic and Boyd, 2009]

Algorithm 2 Cutting set method for the Robust Kantorovich Problem (RKP)

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

Cutting set algorithm [Mutapcic and Boyd, 2009]

Algorithm 3 Cutting set method for the Robust Kantorovich Problem (RKP)

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

Robust Kantorovich Problem (RKP)

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

Cutting set algorithm [Mutapcic and Boyd, 2009]

Algorithm 4 Cutting set method for the Robust Kantorovich Problem (RKP)

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 $T_t \in \underset{T \in \Pi}{\operatorname{argmin}} \langle T, C_t \rangle$
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

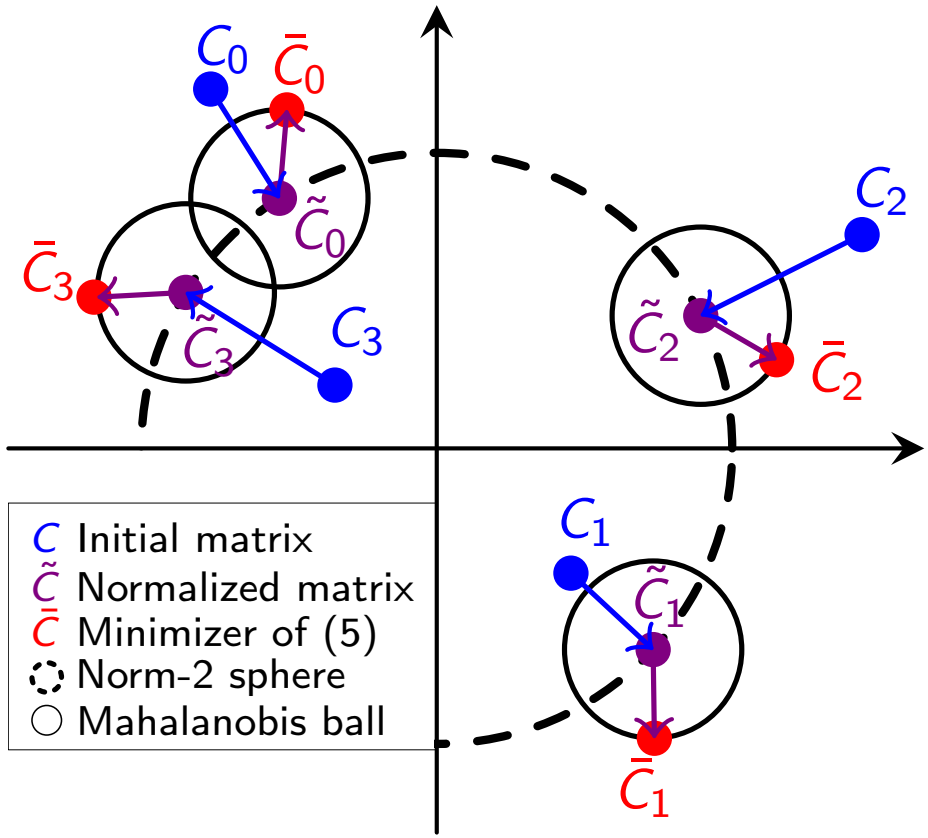
Robust Kantorovich Problem (RKP)

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

Wasserstein stability

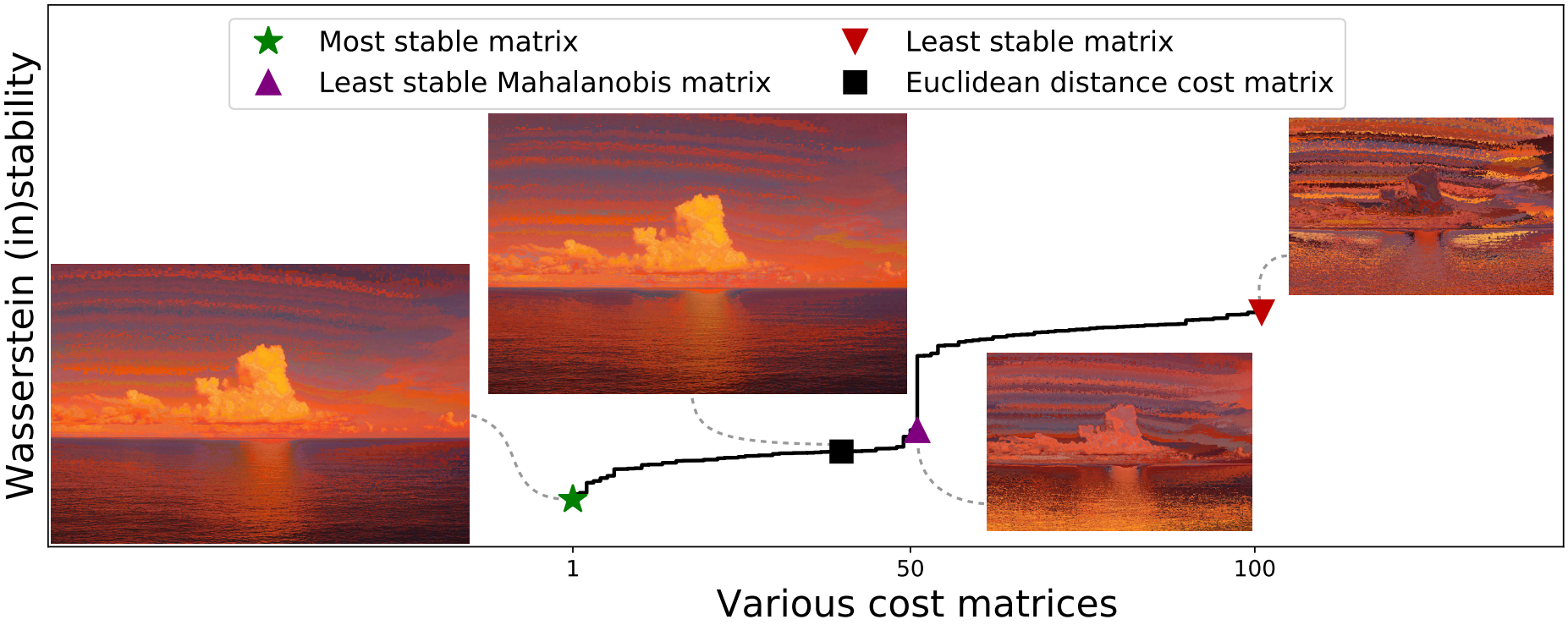
Wasserstein stability of a matrix C induced by μ and ν

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



Usefulness of the Wasserstein stability (Color transfer)

Usefulness of the Wasserstein stability (Color transfer)



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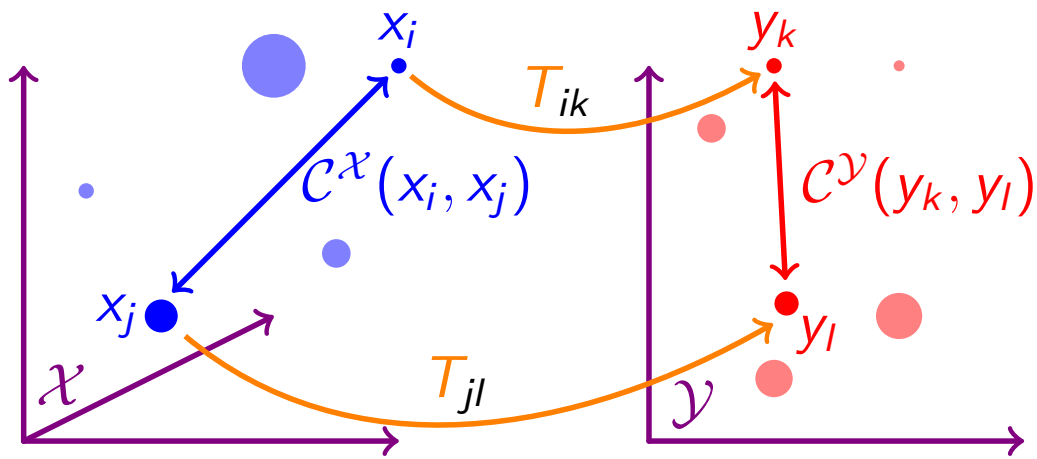
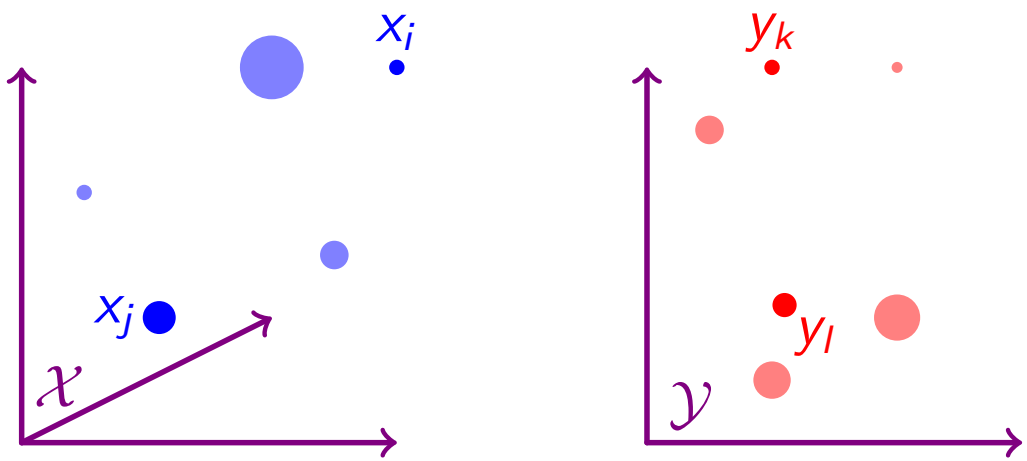
Sampled Gromov Wasserstein

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

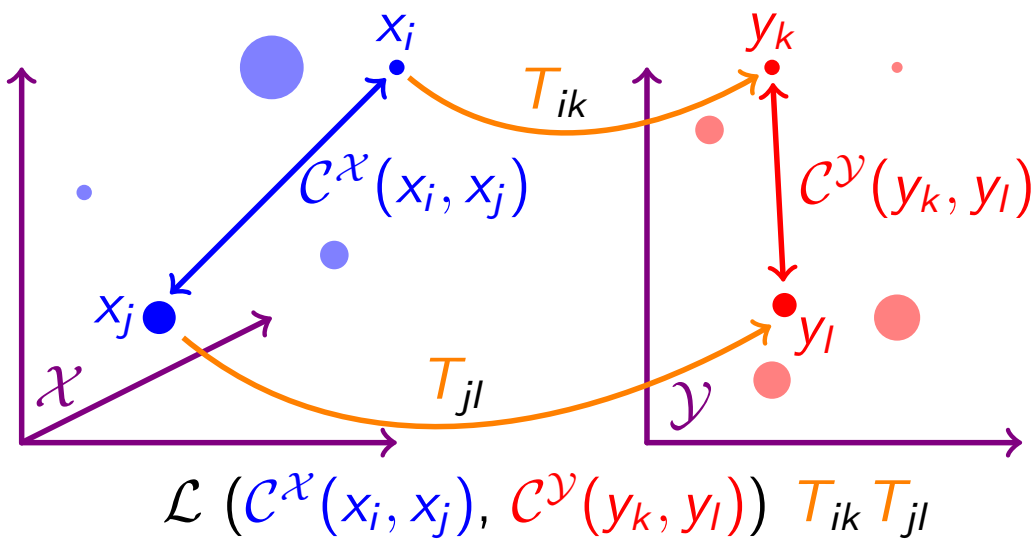


Gromov Wasserstein (GW) [Memoli, 2007; Peyré et al., 2016]

- The GW distance relies only on intra-pairwise distances,

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

The Gromov Wasserstein problem



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The most used solver: Entropy Gromov Wasserstein

Algorithm 5 Entropy Gromov Wasserstein (EGW)
[Peyré et al., 2016; Rangarajan et al., 1999]

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

1: $T_0 = ab^\top$

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

3: $\Lambda = \nabla_{T_s} \mathcal{E}(T_s, T_s) = \sum_{j,l=1}^{I,K} \mathcal{L}\left(\mathcal{C}^{\mathcal{X}}(\cdot, x_j), \mathcal{C}^{\mathcal{Y}}(\cdot, y_l)\right)(T_s)_{jl}$

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

5: **end for**

Motivations and contributions

Limitation of EGW

- Time complexity for computing the gradient $\nabla_T \mathcal{E}(T, T)$ is $O\left(N^4\right)$
- Time complexity can be reduced to $O\left(N^3\right)$ but only for specific loss functions $\mathcal{L}(x, y) = f_1(x) + h_1(x)h_2(y) + f_2(y)$

Motivations and contributions

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- Time complexity for computing the gradient $\nabla_T \mathcal{E}(T, T)$ is $O\left(N^4\right)$
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Contributions

- ✓ Approximate the gradient $\nabla_T \mathcal{E}(T, T)$ in $O\left(M \times N^2\right)$ for any loss
- ✓ 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)

$$\min_{T' \in \Pi(\mu,\nu)} \left\langle \nabla_T \mathcal{E}(T, T), T' \right\rangle = \min_{T' \in \Pi(\mu,\nu)} \left\langle \sum_{j,l=1}^{I,K} \mathcal{L}\left(\mathcal{C}^{\mathcal{X}}(\cdot, x_j), \mathcal{C}^{\mathcal{Y}}(\cdot, y_l)\right) T_{jl}, T' \right\rangle$$

Sampled Gromov Wasserstein idea (SaGroW)

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Sampled Gromov Wasserstein idea (SaGroW)

$$\min_{T' \in \Pi(\mu,\nu)} \langle \nabla_T \mathcal{E}(T, T), T' \rangle = \min_{T' \in \Pi(\mu,\nu)} \left\langle \sum_{j,l=1}^{I,K} \mathcal{L}\left(\mathcal{C}^{\mathcal{X}}(\cdot, x_j), \mathcal{C}^{\mathcal{Y}}(\cdot, y_l)\right) T_{jl}, T' \right\rangle$$

$$= \min_{T' \in \Pi(\mu,\nu)} \left\langle \sum_{j,l=1}^{I,K} \boldsymbol{L}_{.j.l}\, T_{jl}, T' \right\rangle$$

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

Sampled Gromov Wasserstein idea (SaGroW)

$$\min_{T' \in \Pi(\mu,\nu)} \langle \nabla_T \mathcal{E}(T, T), T' \rangle = \min_{T' \in \Pi(\mu,\nu)} \left\langle \sum_{j,l=1}^{I,K} \mathcal{L}\left(\mathcal{C}^{\mathcal{X}}(\cdot, x_j), \mathcal{C}^{\mathcal{Y}}(\cdot, y_l)\right) T_{jl}, T' \right\rangle$$

$$= \min_{T' \in \Pi(\mu,\nu)} \left\langle \sum_{j,l=1}^{I,K} \boldsymbol{L}_{.j.l}\, T_{jl}, T' \right\rangle$$

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

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

SaGroW algorithm

- SaGrow has been implemented in POT [Flamary and Courty, 2017]

Algorithm 6 SaGroW

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

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

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

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

7: **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

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- $G(T) = 0 \iff T$ 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:

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

Stochastic Mirror Descent

Kullback Leibler regularization [Xu et al., 2019]

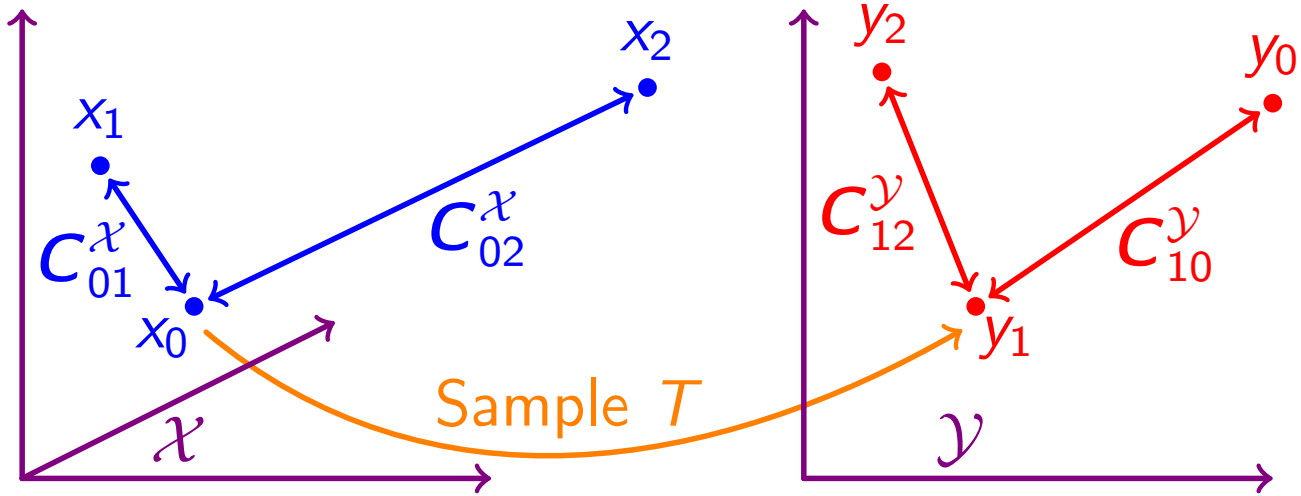
$$\left\langle \widehat{\mathbf{\Lambda}}, T' \right\rangle + \epsilon KL(T' || T) = \left\langle \widehat{\mathbf{\Lambda}} - \epsilon log(T), T' \right\rangle + \epsilon \sum_{ik} T'_{ik} log(T'_{ik}) \quad (7)$$

Algorithm 7 SaGroW with KL regularization

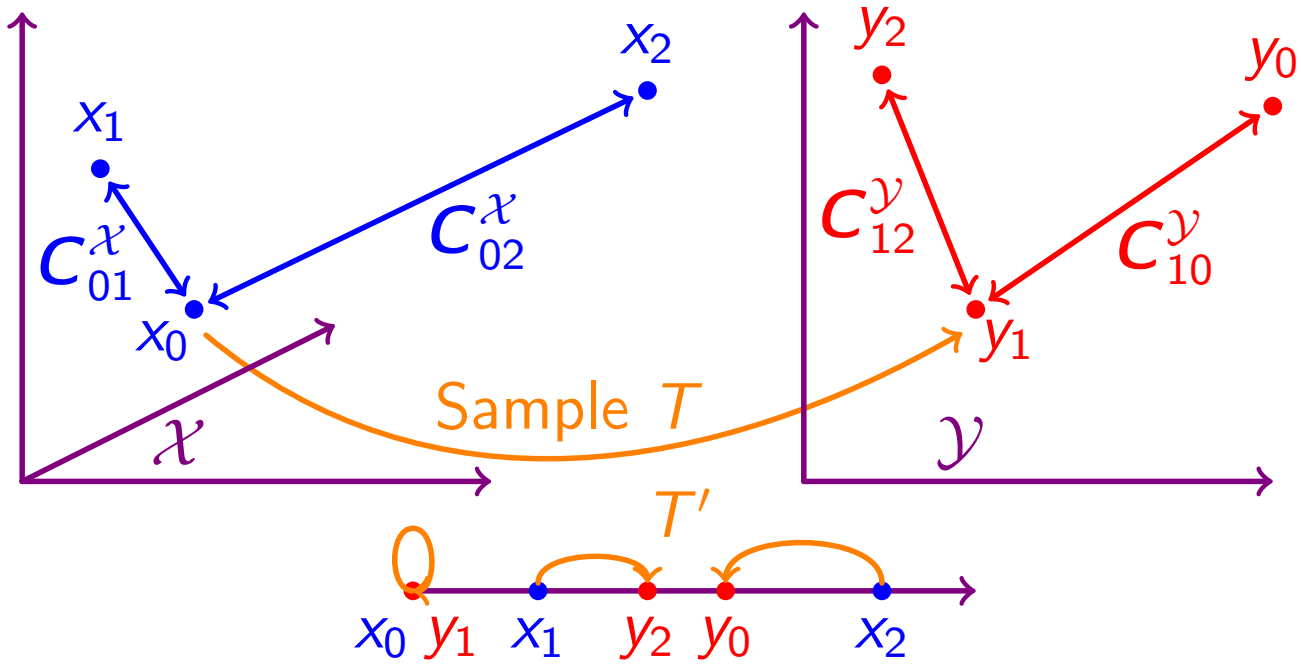
Require: $a, b, \mathcal{C}^{\mathcal{X}}, \mathcal{C}^{\mathcal{Y}}, \mathcal{L}, M, \epsilon, \alpha$

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**

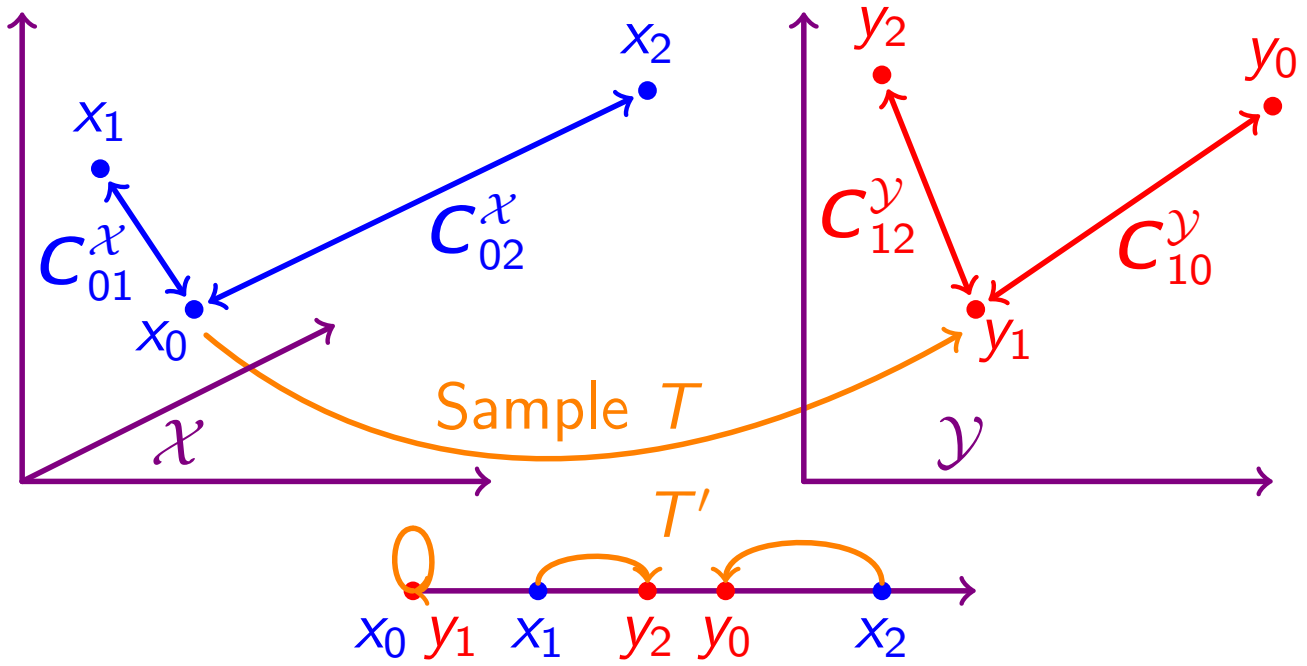
Pointwise Gromov Wasserstein (PoGroW): $M = 1$



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



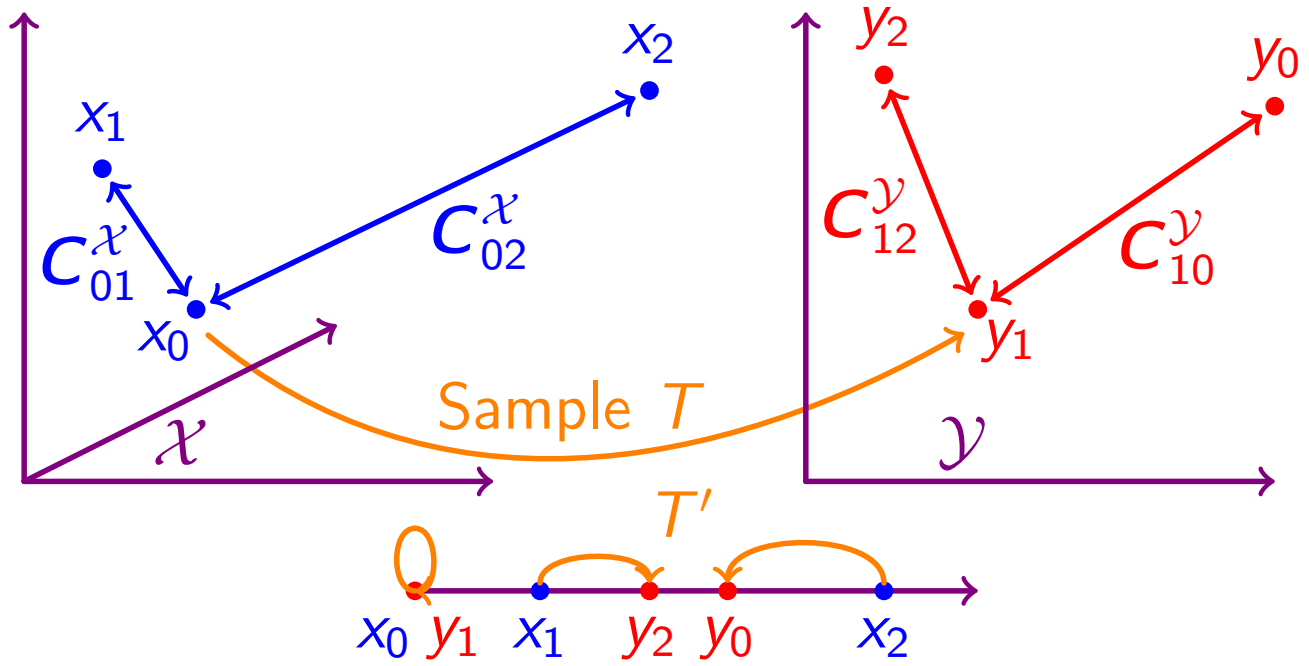
Pointwise Gromov Wasserstein (PoGroW): $M = 1$



Sliced Gromov Wasserstein (SGW) [Vayer et al., 2019]

- Approximate a distance related to the GW distance

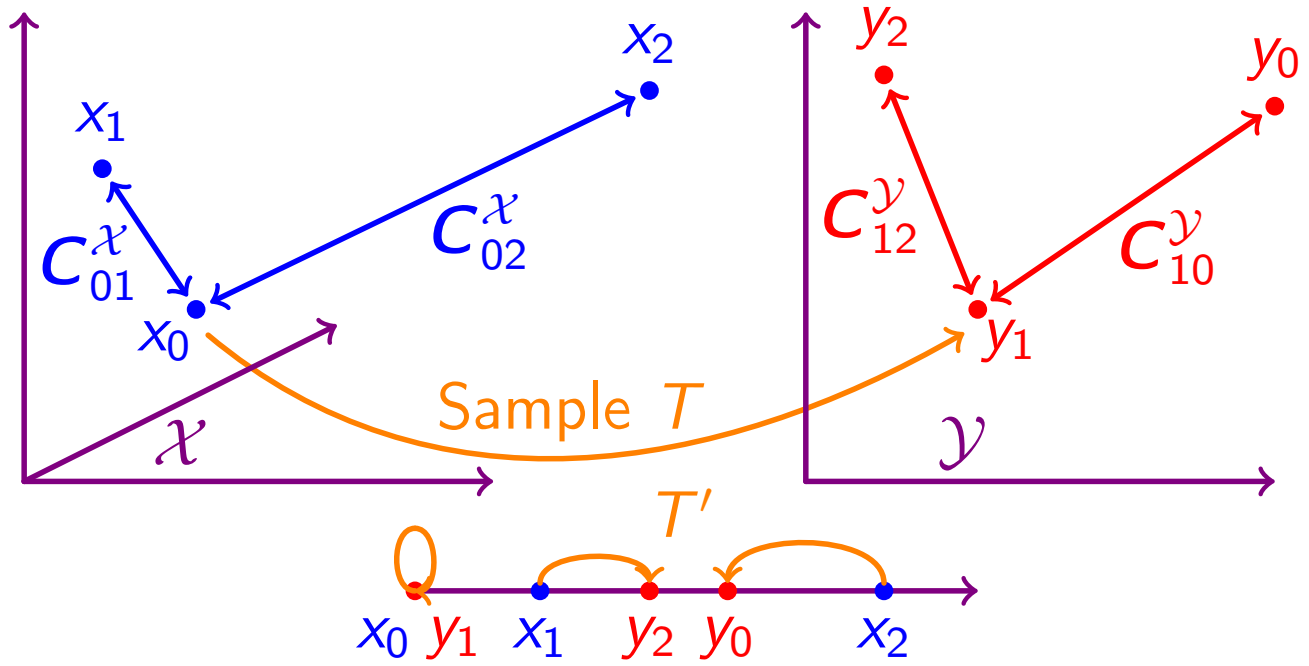
Pointwise Gromov Wasserstein (PoGroW): $M = 1$



Sliced Gromov Wasserstein (SGW) [Vayer et al., 2019]

- Approximate a distance related to the GW distance
- Does not provide a transport plan

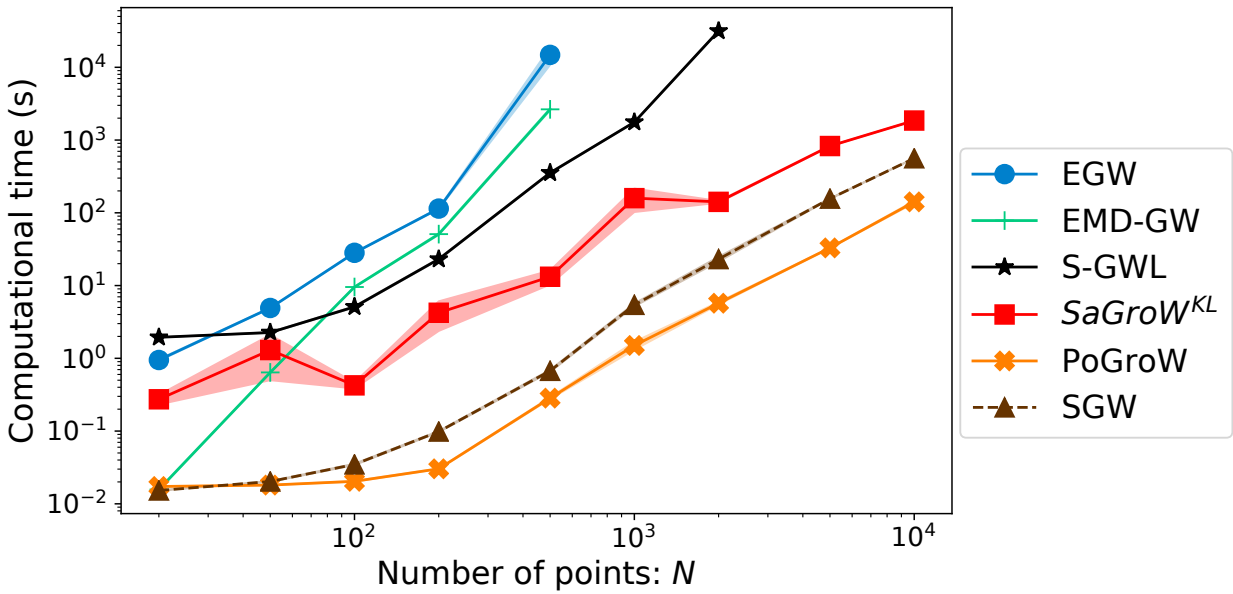
Pointwise Gromov Wasserstein (PoGroW): $M = 1$



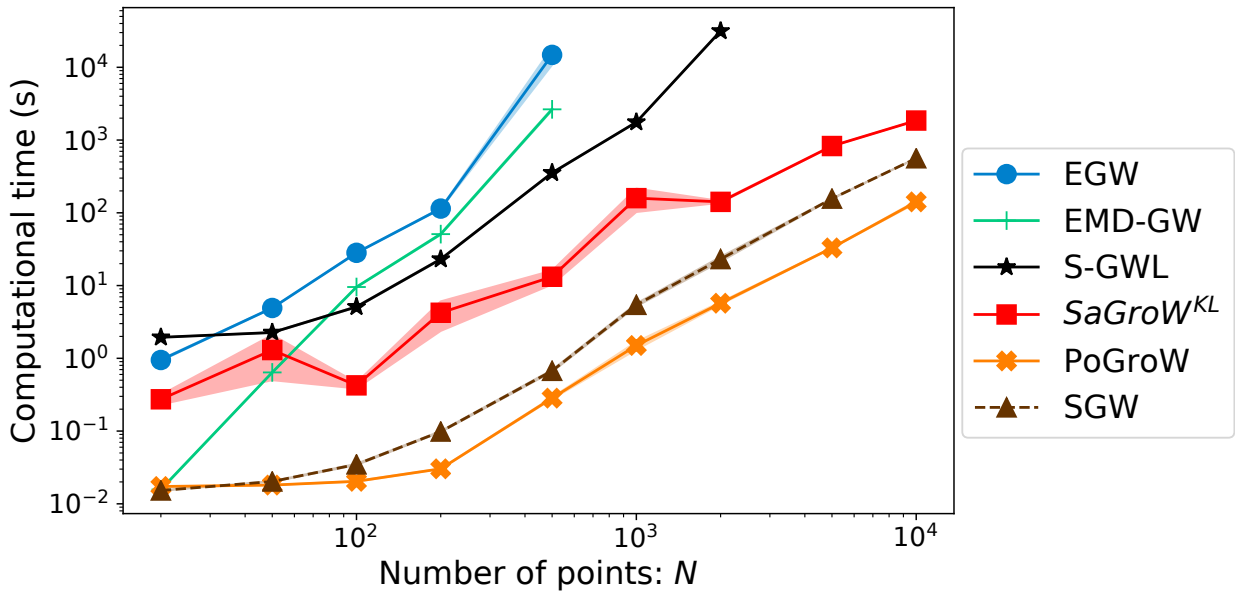
Sliced Gromov Wasserstein (SGW) [Vayer et al., 2019]

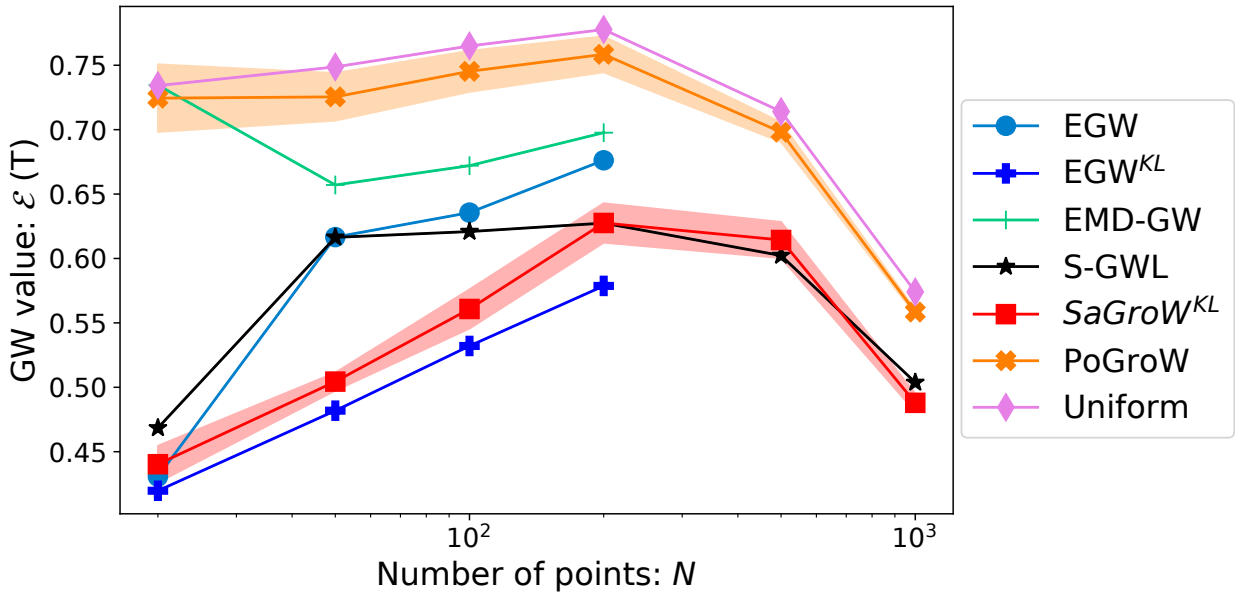
- Approximate a distance related to the GW distance
- Does not provide a transport plan
- Does not work on graphs

Speed and performances



Speed and performances





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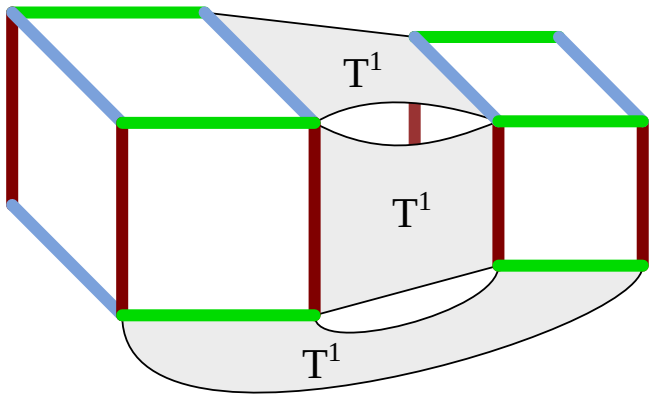
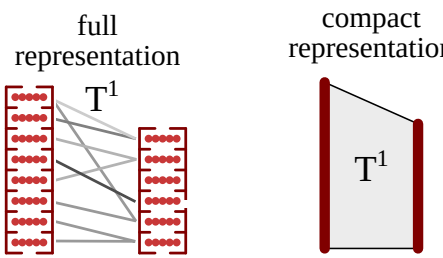
Optimal Tensor Transport

Based on a published paper at the Association for the Advancement of Artificial Intelligence (AAAI) [Kerdoncuff et al., 2022].



Motivation of Optimal Tensor Transport (OTT)

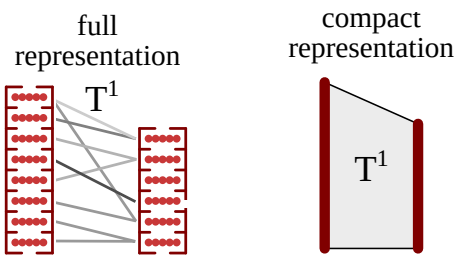


a) **OTT$_1$** (OT) *(F=5 features)*

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 (OTT)



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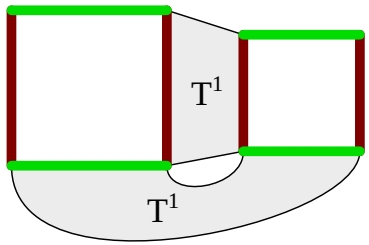
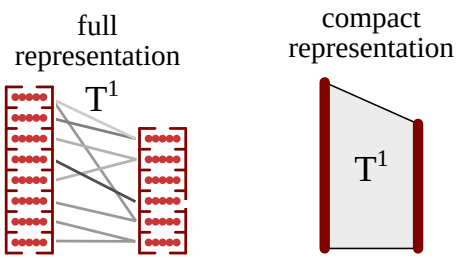


b) **OTT$_{11}$** (GW)

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 (OTT)



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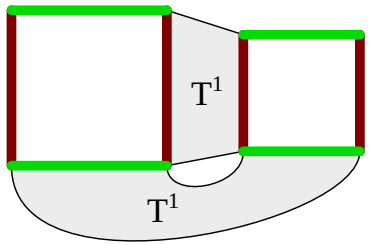

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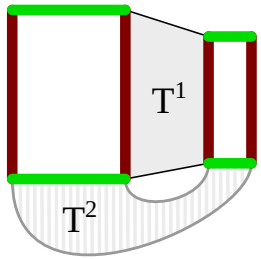
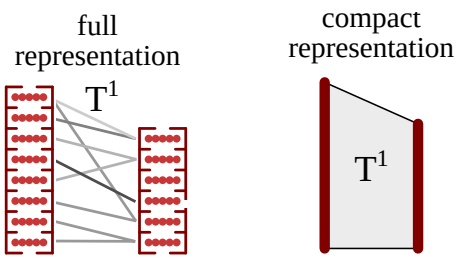


c) **OTT$_{12}$** (Co-OT)

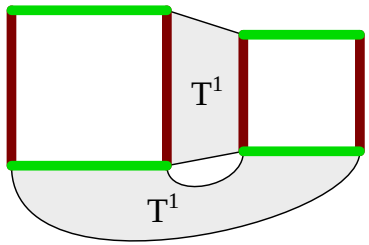
Co-Optimal Transport [Redko et al., 2020]

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

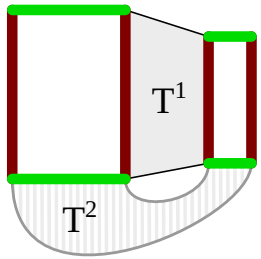
Motivation of Optimal Tensor Transport (OTT)



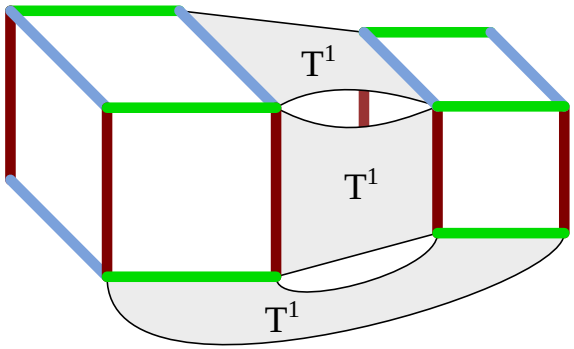
a) **OTT$_1$** (OT) *(F=5 features)*



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



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

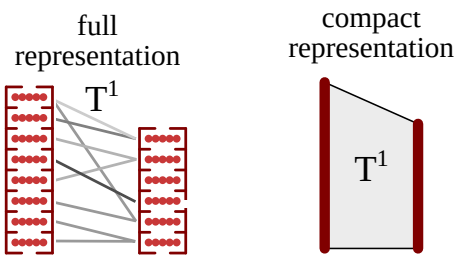


d) **OTT$_{111}$** (triplets)

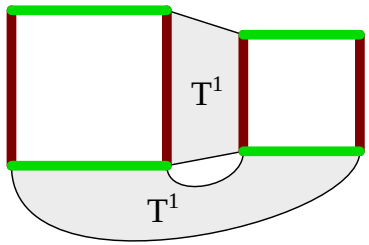
Optimal Tensor Transport with $(1, 1, 1)$

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

Motivation of Optimal Tensor Transport (OTT)



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



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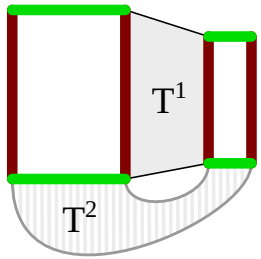
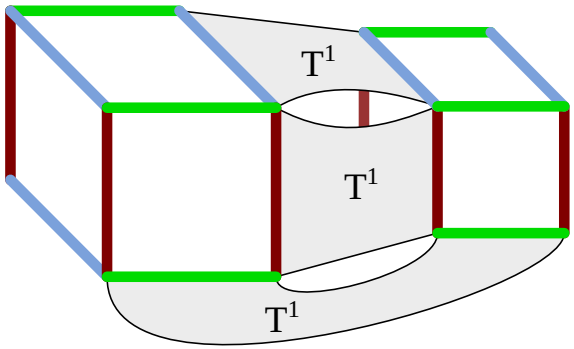
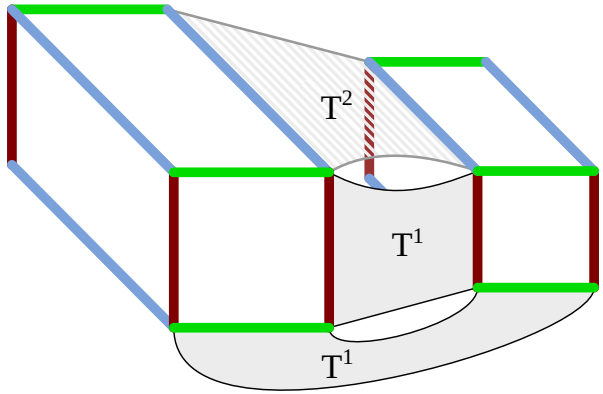


c) **OTT$_{12}$** (Co-OT)



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



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

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

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

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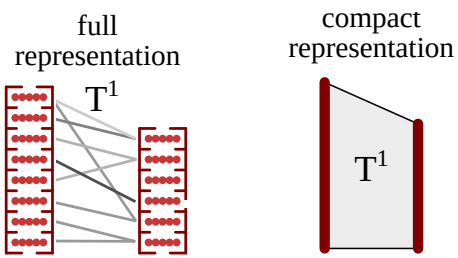

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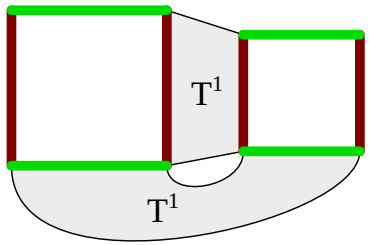

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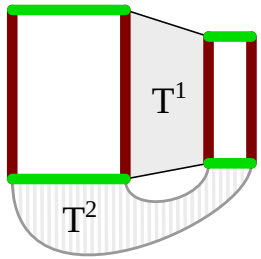

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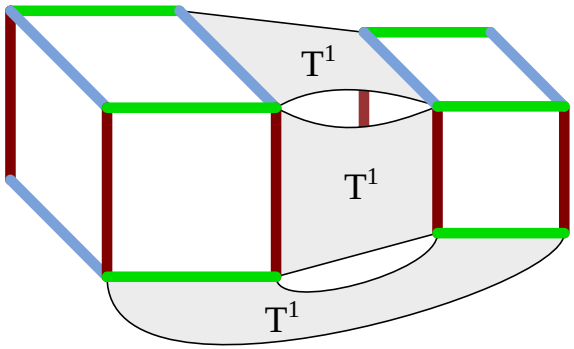

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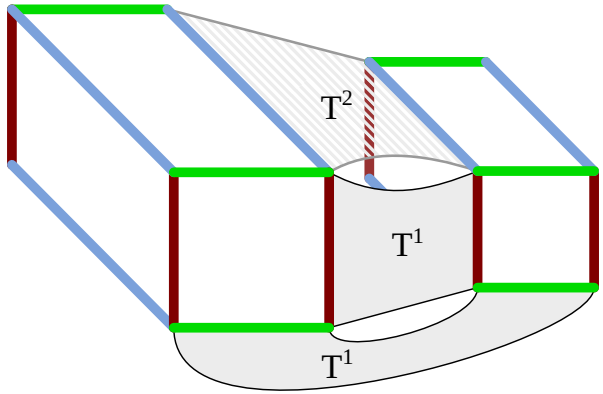

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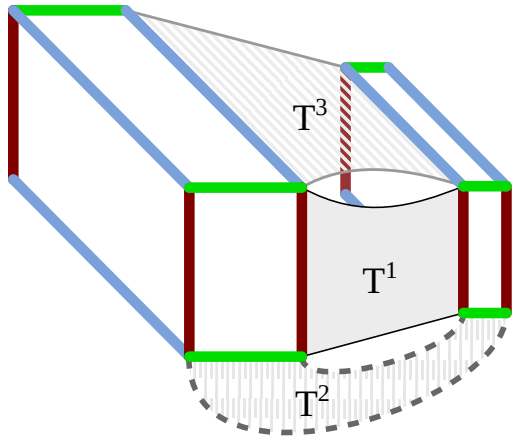


f) **OTT$_{123}$** (triCo-OT)

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

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

Stochastic Mirror Descent to solve the OTT problem

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

$\forall e \in [\![1, E]\!],\ T^e = a^e b^{e\top}$

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

  for e = 1 **to** E **do**

    $\widehat{\nabla_{T^e}\mathcal{E}_f}$ = M samples of the gradient

    $T^e = \min_{T'\in\Pi(a^e,b^e)} \left\langle \widehat{\nabla_{T^e}\mathcal{E}_f}, T' \right\rangle + \epsilon KL(T'||T^e)$

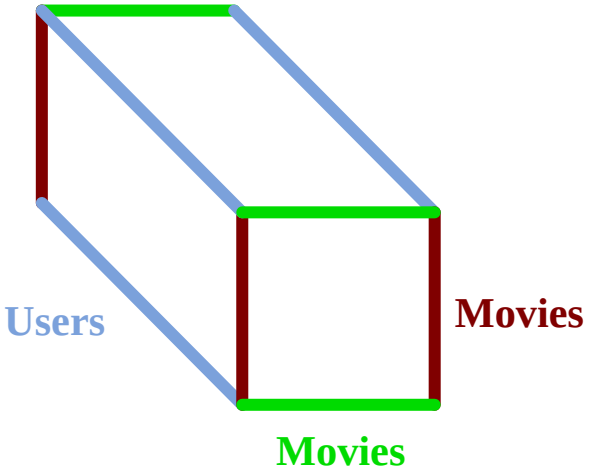
  end for

end for

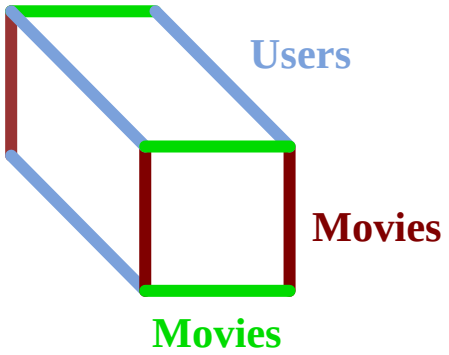
Application to Domain Adaptation

Domain Adaptation: predict the type of movies

Movielens dataset [Harper and Konstan, 2015]



Old movies



New movies

	SVM	S-GWL	GW	Co-OT	OTT
AVG	58.6	63.8	64.9	68.2	**77.3**±3.1

Table of Contents

Conclusion

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   - ✓ Adaptation of the previous solver to solve it in a reasonable time

Further works related to the contributions

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Fused-Gromov Wasserstein:

$$\min_{T \in \Pi(\mu,\nu)} \alpha \sum_{i,k=1}^{I,K} C_{ik}\, T_{ik} + (1-\alpha) \sum_{i,j,k,l=1}^{I,I,K,K} L_{ijkl}\, T_{ik}\, T_{jl} \tag{9}$$

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$$\min_{T \in \Pi(\mu,\nu)} \alpha_1 \sum_{i_1,k_1=1}^{I,K} L^1_{i_1 k_1} T_{i_1 k_1} + \alpha_2 \sum_{i_1,i_2,k_1,k_2=1}^{I,I,K,K} L^2_{i_1 i_2 k_1 k_2} T_{i_1 k_1} T_{i_2 k_2} \tag{8}$$

$$+\alpha_3 \sum_{i_1,i_2,i_3,k_1,k_2,k_3=1}^{I,I,I,K,K,K} L^3_{i_1 i_2 i_3 k_1 k_2 k_3} T_{i_1 k_1} T_{i_2 k_2} T_{i_3 k_3}$$

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4. Relation of OT formulation to visualization and clustering methods
   - ✓ Strong link between PCA and Wasserstein barycenter
   - ✓ UMAP/t-STE and Gromov barycenter
   - ✓ Kmeans and Wasserstein barycenter
     - TAUDoS project: Fused-Kmeans for the distillation of Recurrent Neural Networks

Thank you for your attention

Published papers

- KERDONCUFF Tanguy, EMONET Rémi and SEBBAN Marc
  Metric Learning in Optimal Transport for Domain Adaptation
  IJCAI 2020
- DHOUIB Sofien, REDKO Ievgen, KERDONCUFF Tanguy, EMONET, Rémi, and SEBBAN Marc
  A Swiss Army Knife for Minimax Optimal Transport
  ICML 2021
- KERDONCUFF Tanguy, EMONET Rémi, and SEBBAN Marc
  Sampled Gromov Wasserstein
  MLJ 2021
- KERDONCUFF Tanguy, PERROT Michael, EMONET Rémi, and SEBBAN Marc
  Optimal Tensor Transport
  AAAI 2022

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Courty, N., Flamary, R., Tuia, D., and Rakotomamonjy, A. (2017). Optimal transport for domain adaptation. *PAMI*.

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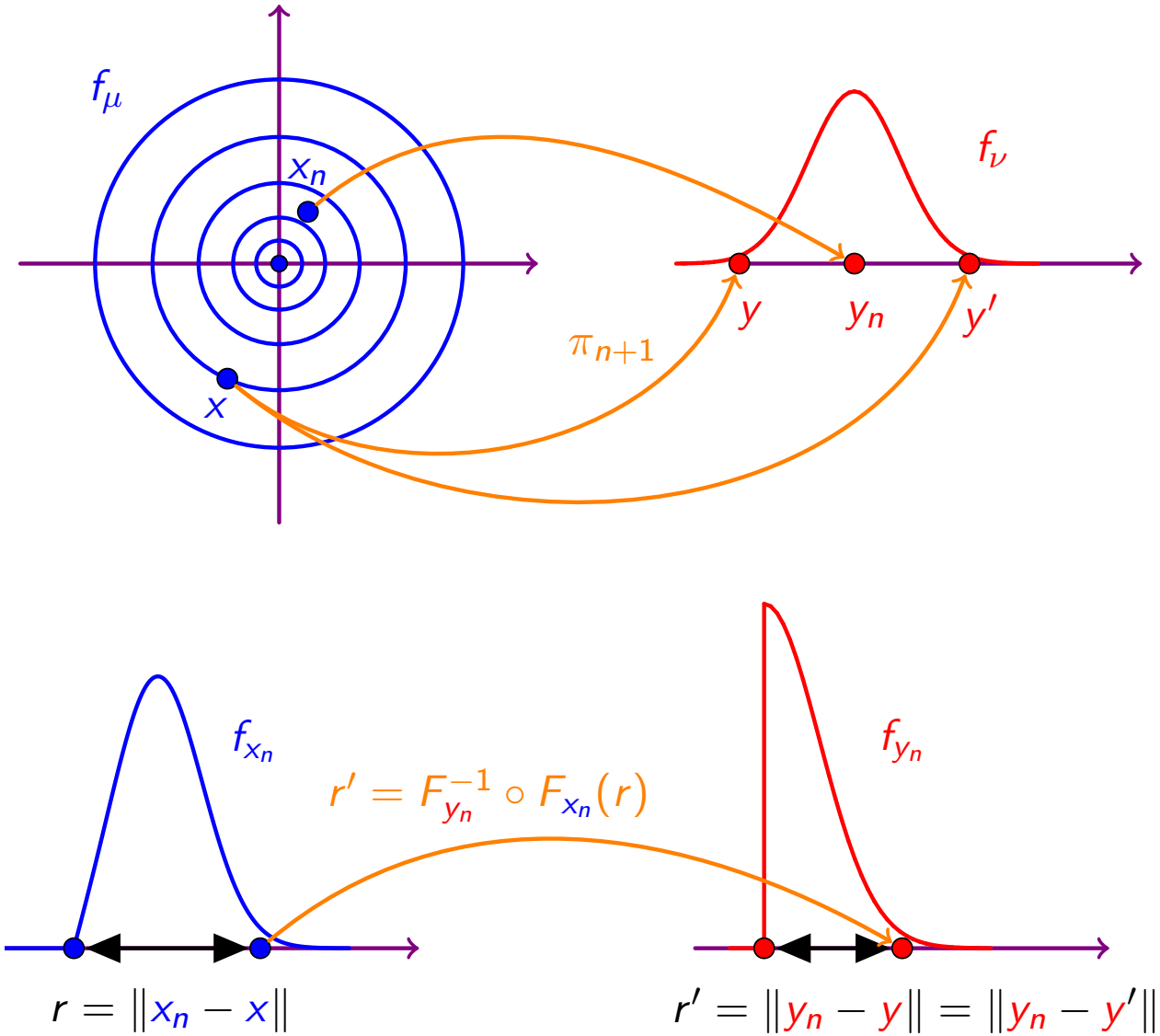
Continuous GW



Bound for convergence: concave case

- The problem is concave notably when T when $\mathcal{L}(x, y) = (x - y)^2$, $\mathcal{C}^{\mathcal{X}}$ and $\mathcal{C}^{\mathcal{Y}}$ are the euclidean distance.

Theorem (Concave case)

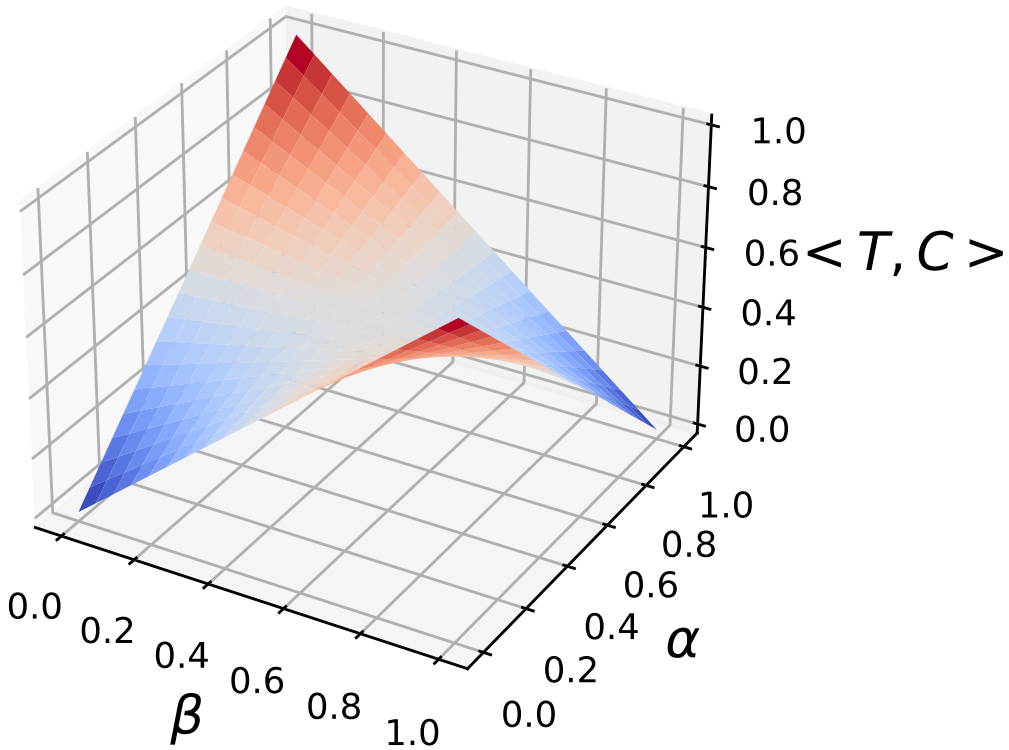
With the same notations as in the previous Theorem with the entropy regularization parameter ϵ_s that may now change along the iterations s, when L yields a concave GW problem, the following bound holds:

$$\mathbb{E}\left(G\left(\overline{T}\right)\right) \leq \frac{\mathcal{E}(T_0) - \mathcal{E}(T^*)}{2S} + B\sqrt{\frac{2N}{M}} + \frac{1}{S}\sum_{s=0}^{S-1} \epsilon_s log(N).$$

Intuition of the OT Minimax problem

The Minimax problem

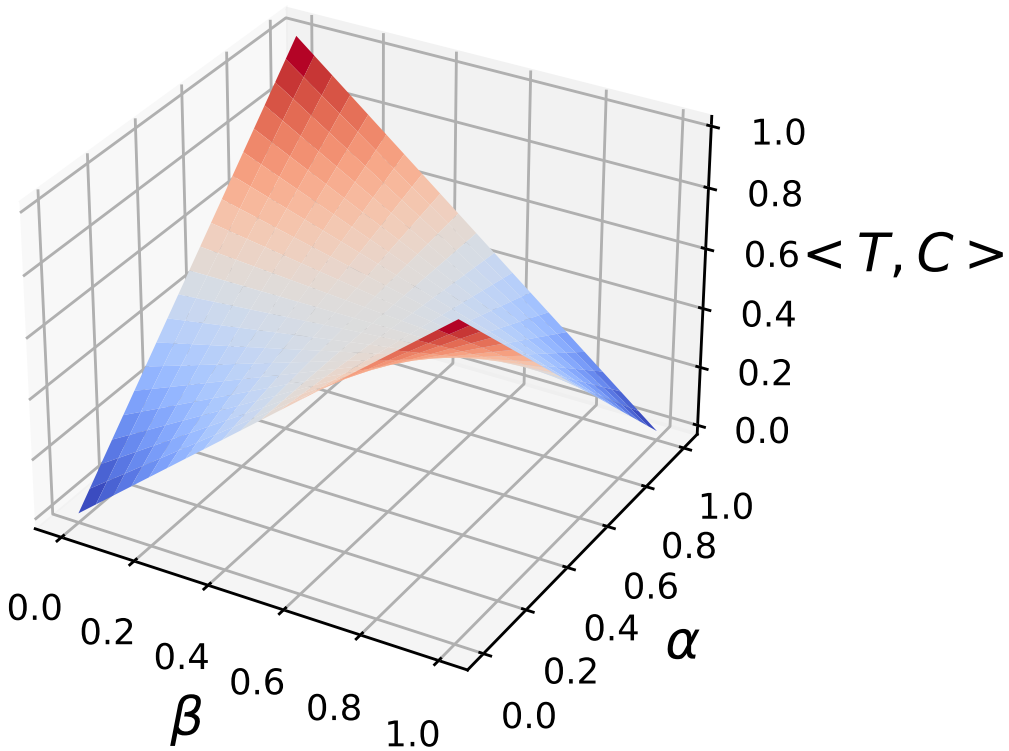
$$\mathcal{W}_{\mathcal{C}} = \min_{T \in \Pi} \max_{C \in \mathcal{C}} \langle T, C \rangle \quad (10)$$



Intuition of the OT Minimax problem

Cost matrices

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



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Associated Transport Plan

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