

# Slicing Unbalanced Optimal Transport

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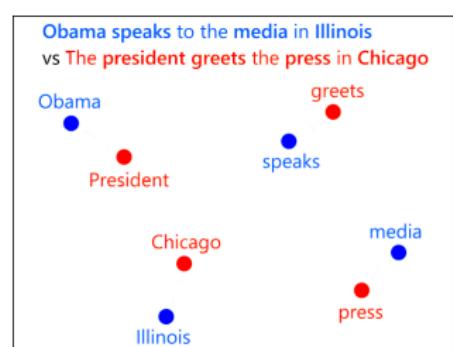
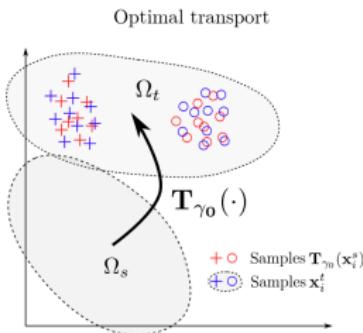
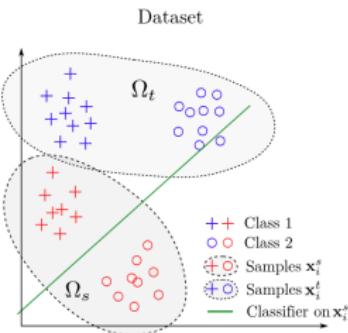
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# Motivations

**Optimal Transport:** Meaningful way to compare distributions

- Domain Adaptation (Courty et al., 2016)
- Generative Models (e.g. WGAN (Arjovsky et al., 2017))
- Document Classification (Kusner et al., 2015)



# Optimal Transport

## Definition (Wasserstein distance)

Let  $\mu, \nu \in \mathcal{P}_2(\mathbb{R}^d)$ ,

$$W_2^2(\mu, \nu) = \inf_{\gamma \in \Pi(\mu, \nu)} \int \|x - y\|_2^2 \, d\gamma(x, y),$$

$\Pi(\mu, \nu) = \{\gamma \in \mathcal{P}(\mathbb{R}^d \times \mathbb{R}^d), \pi_1^* \gamma = \mu, \pi_2^* \gamma = \nu\}$  and  $\pi^1(x, y) = x$ ,  
 $\pi^2(x, y) = y$ ,  $\pi_1^* \gamma = \gamma \circ (\pi^1)^{-1}$ .

### Properties:

- $W_2$  distance
- Metrizes the weak convergence
- Riemannian structure

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### Limitations:

- Computational cost
- Curse of dimensionality

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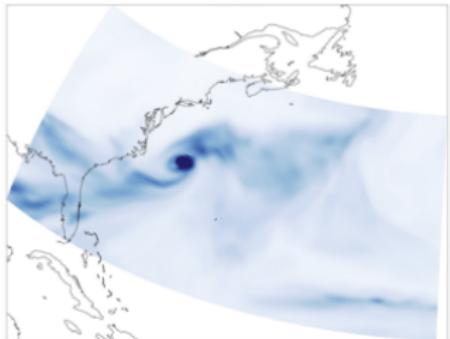
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- Restricted to **probability measures**



# Optimal Transport

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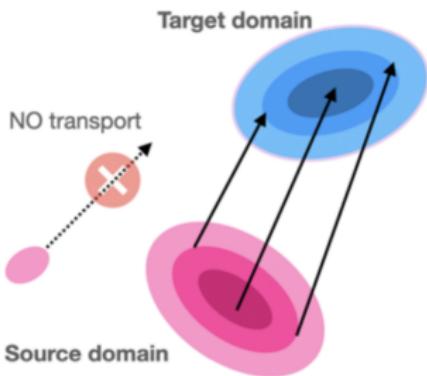
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 $\pi_2^*(x, y) = y$ ,  $\pi_1^* \gamma = \gamma \circ (\pi_1^*)^{-1}$ .

### Limitations:

- Computational cost
- Curse of dimensionality
- Restricted to **probability measures**
- Lack of robustness to **outliers**



## Solving the OT Problem

Let  $x_1, \dots, x_n, y_1, \dots, y_n \in \mathbb{R}^d$ ,  $\alpha, \beta \in \Sigma_n$ ,  $\mu = \sum_{i=1}^n \alpha_i \delta_{x_i}$ ,  $\nu = \sum_{i=1}^n \beta_i \delta_{y_i}$ ,

$$W_2^2(\mu, \nu) = \min_{P \in \mathbb{R}_+^{n \times n}, P\mathbf{1}_n = \alpha, P^T\mathbf{1}_n = \beta} \langle C, P \rangle_F \quad \text{with} \quad C = (d(x_i, y_j)^2)_{i,j}$$

Computational Complexity (Pele and Werman, 2009)

Numerical computation: **Linear program** in  $O(n^3 \log n)$

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## Computational Complexity (Pele and Werman, 2009)

Numerical computation: **Linear program** in  $O(n^3 \log n)$

## Sample Complexity (Boissard and Le Gouic, 2014)

For  $\mu, \nu \in \mathcal{P}_2(\mathbb{R}^d)$ ,  $x_1, \dots, x_n \sim \mu$ ,  $y_1, \dots, y_n \sim \nu$ ,  $\hat{\mu}_n = \frac{1}{n} \sum_{i=1}^n \delta_{x_i}$  and  $\hat{\nu}_n = \frac{1}{n} \sum_{i=1}^n \delta_{y_i}$ ,

$$\mathbb{E}[|W_2(\hat{\mu}_n, \hat{\nu}_n) - W_2(\mu, \nu)|] = O(n^{-1/d})$$

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$$\mathbb{E}[|W_2(\hat{\mu}_n, \hat{\nu}_n) - W_2(\mu, \nu)|] = O(n^{-1/d})$$

## Proposed solutions:

- Entropic regularization + Sinkhorn (Cuturi, 2013)
- Minibatch estimator (Fatras et al., 2020)
- Sliced-Wasserstein (Rabin et al., 2011; Bonnotte, 2013)

# 1D OT Problem

Let  $\mu, \nu \in \mathcal{P}_2(\mathbb{R})$ ,

- Cumulative distribution function:

$$\forall t \in \mathbb{R}, F_\mu(t) = \mu([-\infty, t]) = \int \mathbb{1}_{]-\infty, t]}(x) d\mu(x)$$

- Quantile function:

$$\forall u \in [0, 1], F_\mu^{-1}(u) = \inf \{x \in \mathbb{R}, F_\mu(x) \geq u\}$$

## 1D Wasserstein Distance

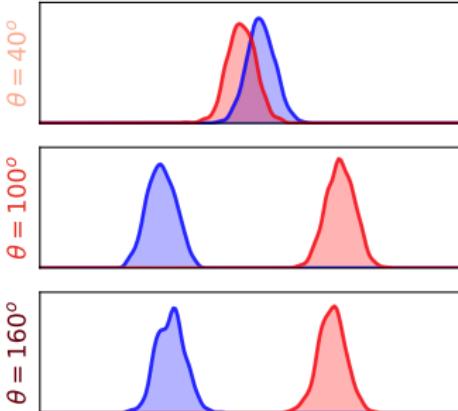
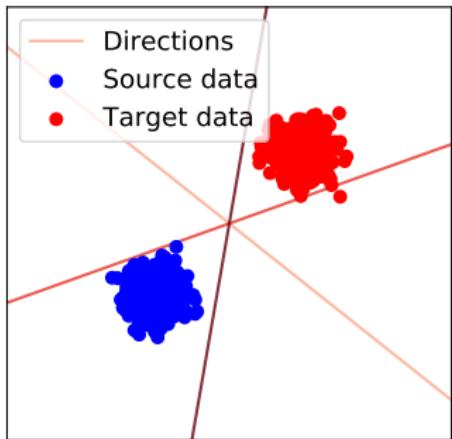
$$W_2^2(\mu, \nu) = \int_0^1 |F_\mu^{-1}(u) - F_\nu^{-1}(u)|^2 du = \|F_\mu^{-1} - F_\nu^{-1}\|_{L^2([0,1])}^2$$

Let  $x_1 < \dots < x_n, y_1 < \dots < y_n, \mu = \frac{1}{n} \sum_{i=1}^n \delta_{x_i}, \nu = \frac{1}{n} \sum_{i=1}^n \delta_{y_i}$ ,

$$W_2^2(\mu, \nu) = \frac{1}{n} \sum_{i=1}^n (x_i - y_i)^2$$

$\rightarrow O(n \log n)$

# Sliced-Wasserstein Distance



Definition (Sliced-Wasserstein (Rabin et al., 2011))

Let  $\mu, \nu \in \mathcal{P}_2(\mathbb{R}^d)$ ,

$$\text{SW}_2^2(\mu, \nu) = \int_{S^{d-1}} W_2^2(P_\#^\theta \mu, P_\#^\theta \nu) \, d\lambda(\theta),$$

where  $P^\theta(x) = \langle x, \theta \rangle$ ,  $\lambda$  uniform measure on  $S^{d-1}$ .

# Properties of the Sliced-Wasserstein Distance

Let  $x_1, \dots, x_n, y_1, \dots, y_n \in \mathbb{R}^d$ ,  $\alpha, \beta \in \Sigma_n$ ,  $\mu = \sum_{i=1}^n \alpha_i \delta_{x_i}$ ,  $\nu = \sum_{i=1}^n \beta_i \delta_{y_i}$ .

**Approximation via Monte-Carlo:**

$$\widehat{\text{SW}}_{2,L}^2(\mu, \nu) = \frac{1}{L} \sum_{\ell=1}^L W_2^2(P_{\#}^{\theta_\ell} \mu, P_{\#}^{\theta_\ell} \nu),$$

$\theta_1, \dots, \theta_L \sim \lambda$ .

**Properties:**

- Computational complexity:  $O(Ln \log n + Lnd)$
- Sample complexity: independent of the dimension ([Nadjahi et al., 2020](#))
- SW<sub>2</sub> distance ([Bonnotte, 2013](#))
- Topologically equivalent to the Wasserstein distance ([Nadjahi et al., 2019](#)), i.e.  
$$\lim_{n \rightarrow \infty} \text{SW}_2^2(\mu_n, \mu) = 0 \iff \lim_{n \rightarrow \infty} W_2^2(\mu_n, \mu) = 0.$$

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## Limitations

- Restricted to probability measures
- Not robust to outliers

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Computing Sliced UOT

Experiments

# Unbalanced Optimal Transport

$\mathcal{M}_+(\mathbb{R}^d)$ : set of positive Radon measures on  $\mathbb{R}^d$

## UOT Problem (static formulation) (Liero et al., 2018)

Let  $\alpha, \beta \in \mathcal{M}_+(\mathbb{R}^d)$ ,

$$\text{UOT}(\alpha, \beta) \triangleq \inf_{\gamma \in \mathcal{M}_+(\mathbb{R}^d \times \mathbb{R}^d)} \int \|x - y\|_2^2 d\gamma(x, y) + \rho_1 D_{\varphi_1}(\pi_\#^1 \gamma | \alpha) + \rho_2 D_{\varphi_2}(\pi_\#^2 \gamma | \beta)$$

**$\varphi$ -divergence:**

$$D_\varphi(\alpha | \beta) \triangleq \int_{\mathbb{R}^d} \varphi \left( \frac{d\alpha}{d\beta}(x) \right) d\beta(x) + \varphi'_\infty \int_{\mathbb{R}^d} d\alpha^\perp(x),$$

where  $\alpha^\perp$  is defined as  $\alpha = \frac{d\alpha}{d\beta}\beta + \alpha^\perp$ ,  $\varphi'_\infty = \lim_{t \rightarrow +\infty} \frac{\varphi(t)}{t}$ ,  $\varphi$ : “entropy function”.

### Example

- Kullback-Leibler divergence:  $\varphi(t) = t \log t - t + 1$
- Total Variation distance:  $\varphi(t) = |t - 1|$

# Unbalanced Optimal Transport

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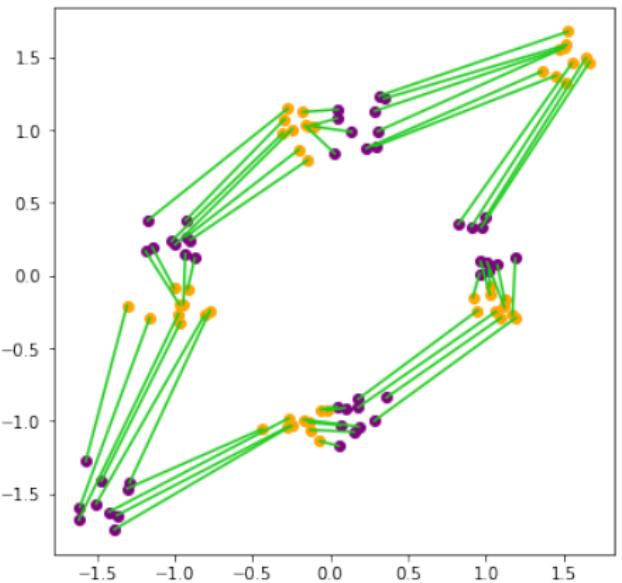
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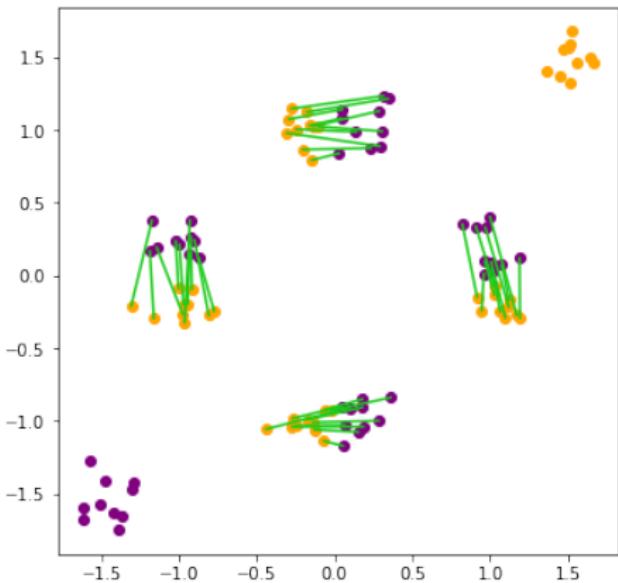
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# Balanced vs Unbalanced OT



OT matching  
 $(\pi_{\#}^1 \gamma, \pi_{\#}^2 \gamma) = (\alpha, \beta)$

From (Séjourné et al., 2023)



UOT matching  
 $\text{TV}(\pi_{\#}^1 \gamma | \alpha) + \text{TV}(\pi_{\#}^2 \gamma | \beta)$

# Solving the UOT Problem

## Various solutions in particular cases:

- Entropic regularization (Chizat et al., 2018)  
→  $O(n^2/\varepsilon)$  (Pham et al., 2020)
- Translation-invariant Sinkhorn (Séjourné et al., 2022)
- Translation-invariant + Frank-Wolfe in 1D (Séjourné et al., 2022)  
→  $O(n \log n)$
- Maximization-Minimization algorithm for Bregman divergences (Chapel et al., 2021) →  $O(n^3)$

## Slicing approaches: only in the case TV

- No mass destruction in the source measure (Bonneel and Coeurjolly, 2019)
- Restricted to equal weights (Bai et al., 2023)

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## Contributions

- Slicing UOT
- Unbalancing SOT

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# Slicing and Unbalancing OT

2 strategies:

## Sliced Unbalanced OT

Let  $\alpha, \beta \in \mathcal{M}_+(\mathbb{R}^d)$ ,

$$\text{SUOT}(\alpha, \beta) = \int_{S^{d-1}} \text{UOT}(P_\#^\theta \alpha, P_\#^\theta \beta) \, d\lambda(\theta)$$

- generalization of sliced partial OT (Bai et al., 2023) (in the case  $\mathcal{D}_\varphi = \text{TV}$ )
- particular case of sliced divergence (Nadjahi et al., 2020)

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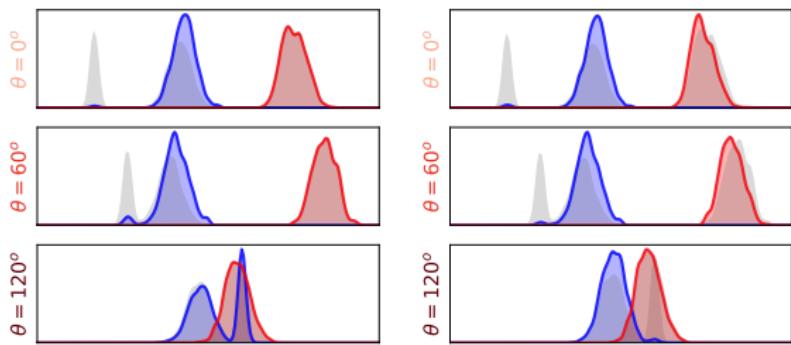
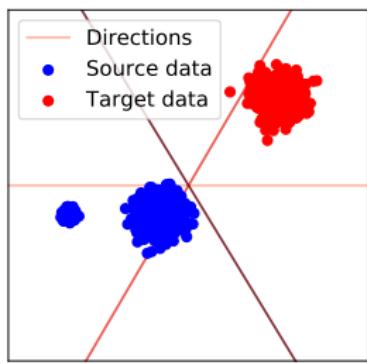
Let  $\alpha, \beta \in \mathcal{M}_+(\mathbb{R}^d)$ ,

$$\text{USW}_2^2(\alpha, \beta) = \inf_{\pi_1, \pi_2 \in \mathcal{M}_+(\mathbb{R}^d)} \text{SW}_2^2(\pi_1, \pi_2) + D_{\varphi_1}(\pi_1 | \alpha) + D_{\varphi_2}(\pi_2 | \beta)$$

→ new!

# SUOT vs USOT

In the rest of the talk:  $\mathcal{D}_\varphi = \text{KL}$



- SUOT: penalize the marginals of  $\pi_\theta \in \Pi(P_\#^\theta \alpha, P_\#^\theta \beta)$
- USOT: penalize the marginals of  $\gamma \in \Pi(\alpha, \beta)$

# Theoretical Properties

- Under mild assumptions, solutions of USOT, SUOT exist
- SUOT and USOT metrize the weak convergence

## Metric properties

- UOT (pseudo) metric on  $\mathbb{R} \implies$  SUOT (pseudo) metric on  $\mathbb{R}^d$
- USOT pseudo-metric
- Sample complexity independent of the dimension (shown theoretically for SUOT and empirically for USOT)

$$\text{SUOT}(\alpha, \beta) \leq \text{USOT}(\alpha, \beta) \leq \text{UOT}(\alpha, \beta)$$

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# Frank-Wolfe Algorithm

**Frank-Wolfe algorithm:**

$$\min_{x \in X} h(x),$$

$X \subset \mathbb{R}^d$  **compact** and convex,  $h : X \rightarrow \mathbb{R}$  convex and differentiable

---

**Algorithm – Frank-Wolfe**

---

**Input:**  $x^{(0)}, (\gamma_t)_t$

**Output:**  $h(x^{(T)})$

**for**  $t = 1, \dots, T$  **do**

$$y^{(t)} \leftarrow \operatorname{argmin}_{y \in X} \langle y, \nabla h(x^{(t)}) \rangle$$

$$x^{(t+1)} \leftarrow (1 - \gamma_t)x^{(t)} + \gamma_t y^{(t)}$$

**end for**

---

# UOT Problem in 1D

For  $\varphi : \mathbb{R} \rightarrow \mathbb{R}$  convex, note  $\varphi^*(t) = \sup_{s \in \mathbb{R}} st - \varphi(s)$

## Dual of UOT problem (Liero et al., 2018)

Let  $\alpha, \beta \in \mathcal{M}_+(\mathbb{R})$ ,

$$\text{UOT}(\alpha, \beta) = \sup_{f \oplus g \leq c} \mathcal{D}(f, g; \alpha, \beta)$$

with  $\mathcal{D}(f, g; \alpha, \beta) \triangleq - \int \varphi_1^*(-f(x)) d\alpha(x) - \int \varphi_2^*(-g(y)) d\beta(y)$ .

- Dual of UOT not translation invariant (Séjourné et al., 2022), i.e. there exists  $\lambda \in \mathbb{R}$  s.t.

$$\mathcal{D}(f + \lambda, g - \lambda) \neq \mathcal{D}(f, g)$$

- Can't apply Frank-Wolfe as constraint set is unbounded (Séjourné et al., 2022), i.e.  $f \oplus g \leq c \implies f + \lambda \oplus g - \lambda \leq c$

# UOT Problem in 1D

For  $\varphi : \mathbb{R} \rightarrow \mathbb{R}$  convex, note  $\varphi^*(t) = \sup_{s \in \mathbb{R}} st - \varphi(s)$

Translation-Invariant Dual of UOT problem (Séjourné et al., 2022)

Let  $\alpha, \beta \in \mathcal{M}_+(\mathbb{R})$ ,

$$\text{UOT}(\alpha, \beta) = \sup_{f \oplus g \leq c} \mathcal{H}(f, g; \alpha, \beta)$$

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→ complexity  $O(Tn \log n)$  with  $T$  number of Frank-Wolfe iterations

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→ complexity  $O(Tn \log n)$  with  $T$  number of Frank-Wolfe iterations
- SUOT solved in  $O(LTn \log n)$  by doing  $L$  Frank-Wolfe in parallel

# Solving USOT

## Dual of USOT

$$\text{USOT}(\alpha, \beta) = \sup_{\forall \ell, f_{\theta_\ell} \oplus g_{\theta_\ell} \leq c} \mathcal{D} \left( \frac{1}{L} \sum_{\ell=1}^L f_{\theta_\ell} \circ P^{\theta_\ell}, \frac{1}{L} \sum_{\ell=1}^L g_{\theta_\ell} \circ P^{\theta_\ell}; \alpha, \beta \right)$$

→ solve  $\max_{\bar{f} = \frac{1}{L} \sum_{\ell=1}^L f_\ell, \bar{g} = \frac{1}{L} \sum_{\ell=1}^L g_\ell, f_\ell \oplus g_\ell \leq c} \mathcal{H}(\bar{f}, \bar{g}; \alpha, \beta)$

---

### Algorithm – Frank-Wolfe

---

**Input:**  $(f_\ell^{(0)}, g_\ell^{(0)})_\ell, (\gamma_t)_t$

**Output:**  $\mathcal{H}(\bar{f}^{(T)}, \bar{g}^{(T)})$

**for**  $t = 1, \dots, T$  **do**

$(\bar{r}^{(t)}, \bar{s}^{(t)}) \leftarrow \operatorname{argmax}_{\bar{r}, \bar{s}, r_\ell \oplus s_\ell \leq c} \langle (\bar{r}, \bar{s}), \nabla \mathcal{H}(\bar{f}^{(t)}, \bar{g}^{(t)}) \rangle$

$(\bar{f}^{(t+1)}, \bar{g}^{(t+1)}) \leftarrow (1 - \gamma_t)(\bar{f}^{(t)}, \bar{g}^{(t)}) + \gamma_t(\bar{r}^{(t)}, \bar{s}^{(t)})$

**end for**

# Solving USOT

---

## Algorithm – Frank-Wolfe

---

**Input:**  $(f_\ell^{(0)}, g_\ell^{(0)})_\ell, (\gamma_t)_t$

**Output:**  $\mathcal{H}(\bar{f}^{(T)}, \bar{g}^{(T)})$

**for**  $t = 1, \dots, T$  **do**

$$(\bar{r}^{(t)}, \bar{s}^{(t)}) \leftarrow \operatorname{argmax}_{\bar{r}, \bar{s}, r_\ell \oplus s_\ell \leq c} \langle (\bar{r}, \bar{s}), \nabla \mathcal{H}(\bar{f}^{(t)}, \bar{g}^{(t)}) \rangle$$

$$(\bar{f}^{(t+1)}, \bar{g}^{(t+1)}) \leftarrow (1 - \gamma_t)(\bar{f}^{(t)}, \bar{g}^{(t)}) + \gamma_t(\bar{r}^{(t)}, \bar{s}^{(t)})$$

**end for**

---

If  $D_{\varphi_1} = \rho_1 \text{KL}$ ,  $D_{\varphi_2} = \rho_2 \text{KL}$ :

- $\lambda^* = \operatorname{argmax}_{\lambda \in \mathbb{R}} D(\bar{f} + \lambda, \bar{g} - \lambda) = \frac{\rho_1 \rho_2}{\rho_1 + \rho_2} \log \left( \frac{\int e^{-\bar{f}(x)/\rho_1} d\alpha(x)}{\int e^{-\bar{g}(y)/\rho_2} d\beta(y)} \right)$
- $\nabla \mathcal{H}(\bar{f}, \bar{g}) = (\tilde{\alpha}, \tilde{\beta})$  with  $\tilde{\alpha} = \nabla \varphi_1^*(-\bar{f} - \lambda^*)\alpha$  and  $\tilde{\beta} = \nabla \varphi_2^*(-\bar{g} + \lambda^*)\beta$

$$(\bar{r}^{(t)}, \bar{s}^{(t)}) = \operatorname{argmax}_{r_\ell \oplus s_\ell \leq c} \langle \bar{r}, \tilde{\alpha} \rangle + \langle \bar{s}, \tilde{\beta} \rangle$$

→ FW step: solve OT( $P_{\#}^{\theta_\ell} \tilde{\alpha}, P_{\#}^{\theta_\ell} \tilde{\beta}$ )

→ Complexity in  $O(TLn \log n)$

# Table of Contents

Unbalanced Optimal Transport

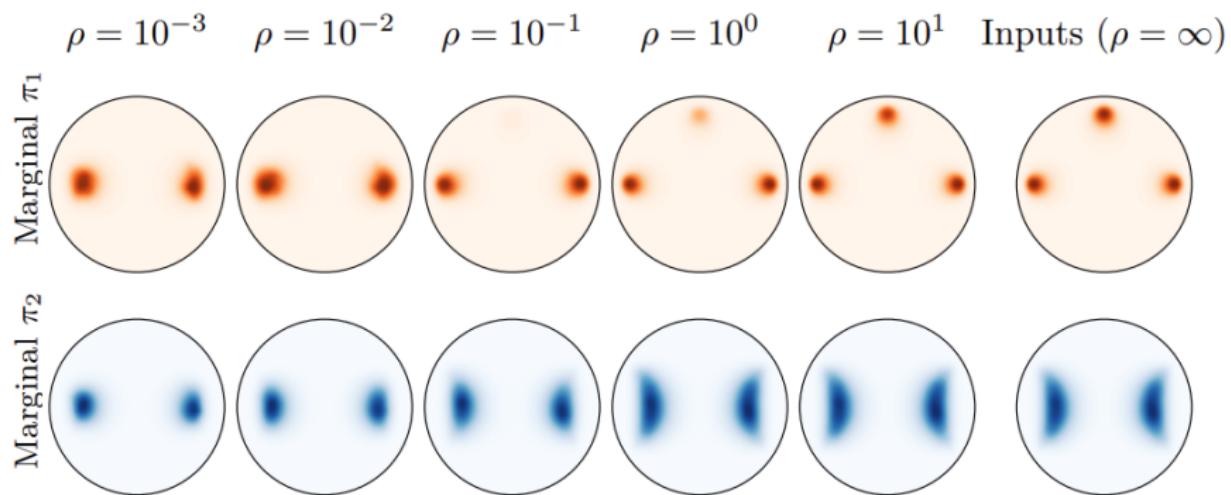
Sliced UOT

Computing Sliced UOT

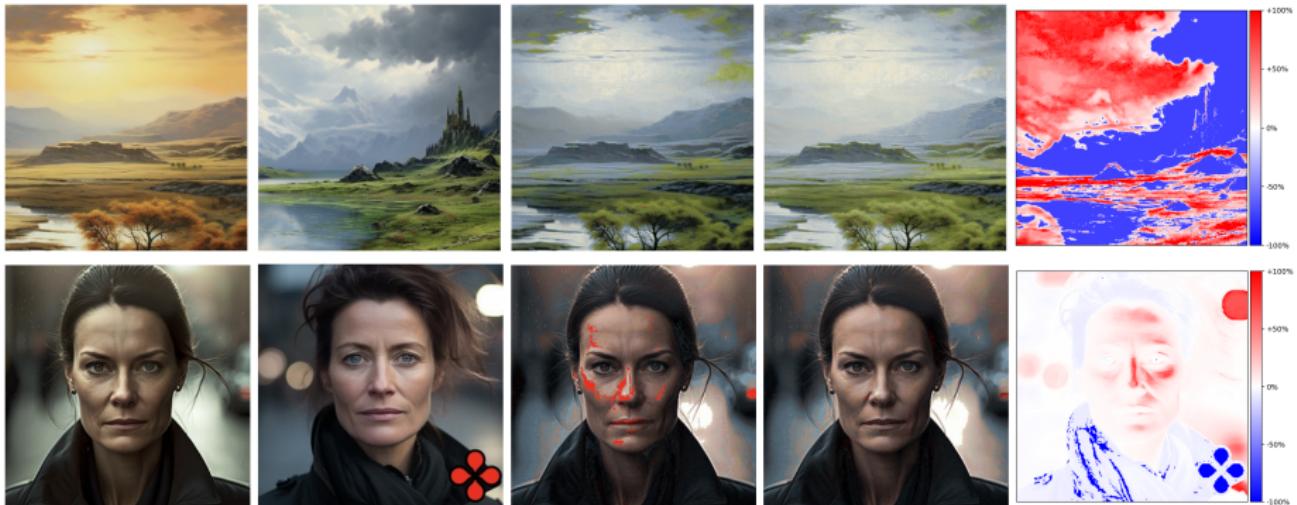
Experiments

# Hyperbolic Space

Can use any projection on  $\mathbb{R}$ : e.g. projection on geodesics on hyperbolic spaces  
(Bonet et al., 2023)



# Color Transfer



1st column: sources, 2nd column: targets, 3rd column: SOT gradient flow, 4th column: USOT + SOT gradient flow, 5th column: % of mass change by USOT (red: mass creation, blue: mass destruction)

- 300x300 images:  $n = 90K$
- Step 1: solve USOT to obtain marginals  $(\pi_1, \pi_2)$
- Step 2: gradient flow of SOT

# Conclusion

## Conclusion

- Introduction 2 new losses merging UOT and SOT
- Theoretical Analysis
- Efficient and modular Frank-Wolfe algorithm
- Encouraging empirical results

## Some perspectives:

- Open theoretical questions: sample complexity of USOT, strong duality for  $\lambda = \text{Unif}(S^{d-1})$
- New large scale applications
- Challenge: choice of  $\rho$

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Thank you!

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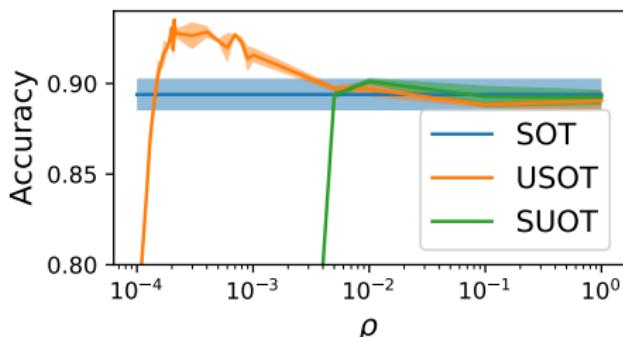
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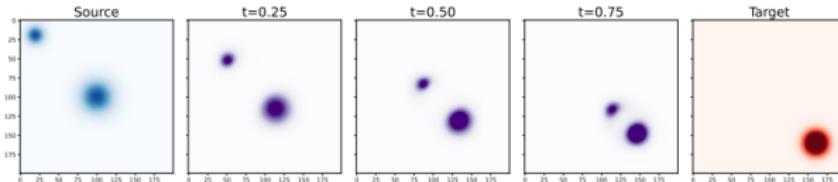
# Document Classification

- Document  $D_k = \sum_{i=1}^{n_k} w_i^k \delta_{x_i^k}$
- Compute  $(L(D_k, D_\ell))_{k,\ell}$
- k-nearest neighbor classifier

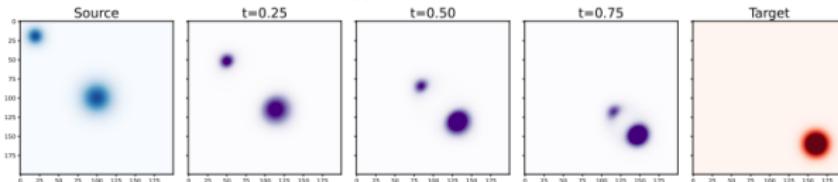
	BBCSport		Goodreads		
	Acc	t ( $\cdot 10^{-3}s$ )	Acc (genre)	Acc (like)	t ( $\cdot 10^{-3}s$ )
OT	94.55	$3.12 \pm 1.61$	55.22	71.00	$440.30 \pm 250$
UOT	96.73	$243.39 \pm 9.24$	-	-	-
SinkhUOT	95.45	$46.22 \pm 2.17$	53.55	67.81	$2021.68 \pm 356$
SOT	$89.39 \pm 0.76$	$1.80 \pm 0.22$	$50.09 \pm 0.51$	$65.60 \pm 0.20$	$4.49 \pm 1.44$
SUOT	$90.12 \pm 0.15$	$13.9 \pm 1.21$	$50.15 \pm 0.04$	$66.72 \pm 0.38$	$14.32 \pm 0.95$
USOT	$93.52 \pm 0.04$	$14.37 \pm 1.29$	$52.67 \pm 0.62$	$67.78 \pm 0.39$	$14.45 \pm 0.88$



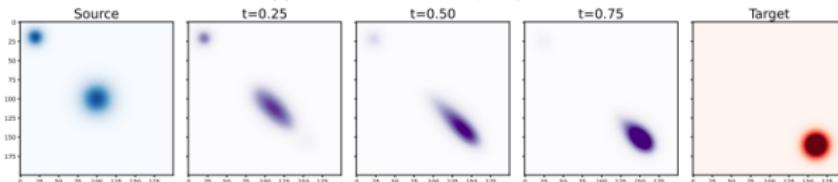
# Barycenters



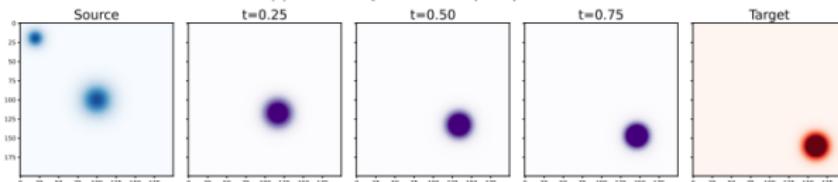
(a) SOT barycenters



(b) USOT barycenters with  $\rho_1 = \rho_2 = 100$

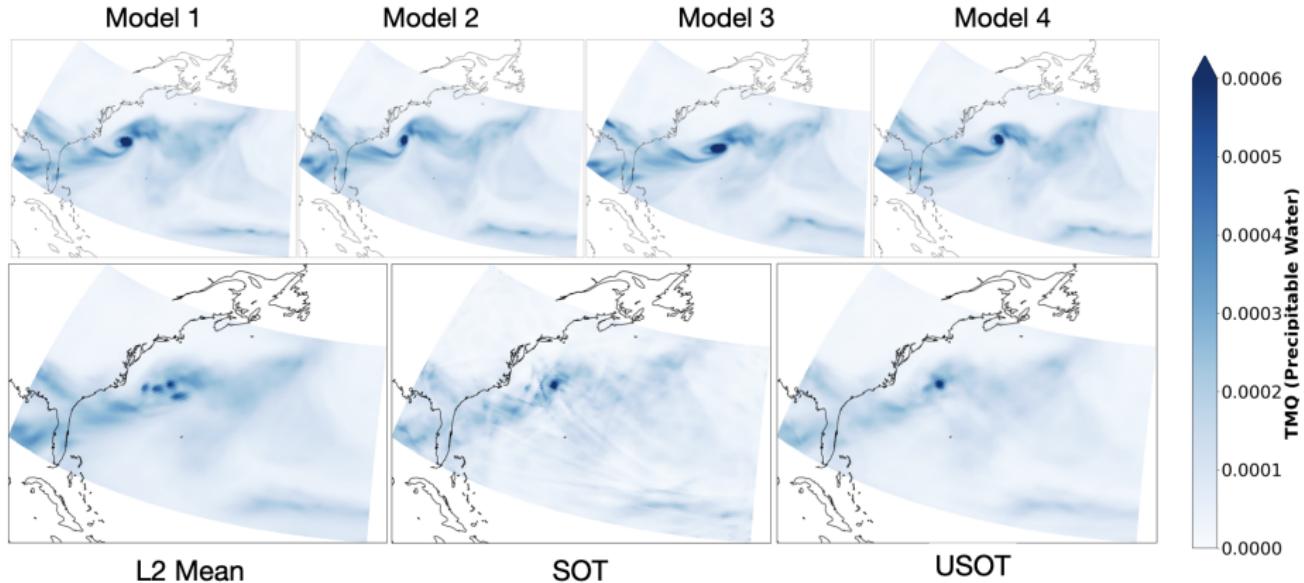


(c) USOT barycenters with  $\rho_1 = \rho_2 = 0.01$



(d) USOT barycenters with  $\rho_1 = 0.01$  and  $\rho_2 = 100$

# Barycenter on Geophysical Data



- First row: 4 climate models
- Second row: Different barycenters
- Measures of size  $100 \times 200$