

Slicing Unbalanced Optimal Transport

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SIAM AN

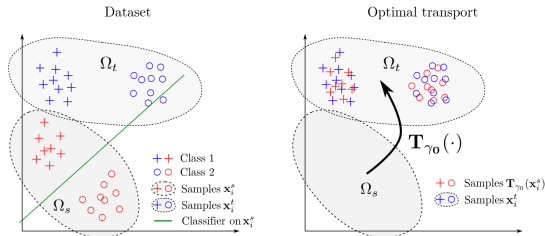
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Motivations

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

Optimal Transport

Definition (Wasserstein distance)

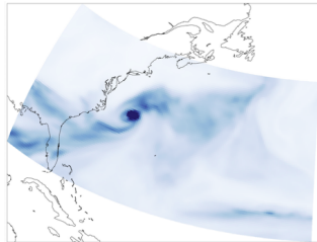
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Limitations:

- Computational cost
- Curse of dimensionality
- Restricted to **probability measures**



Optimal Transport

Definition (Wasserstein distance)

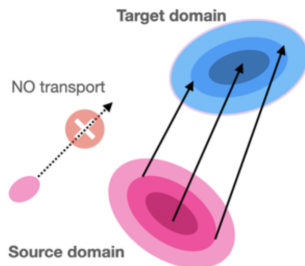
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 $\pi^2(x, y) = y, \pi_{\#}^1 \gamma = \gamma \circ (\pi^1)^{-1}$.

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 $O(n^3 \log n)$

Solving the OT Problem

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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 $\hat{\nu}_n = \frac{1}{n} \sum_{i=1}^n \delta_{y_i}$,

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

Solving the OT Problem

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

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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 ([Fratras 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

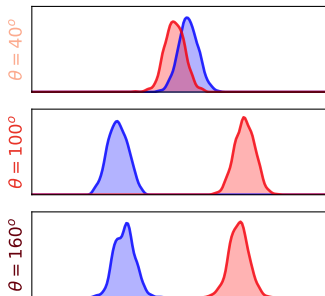
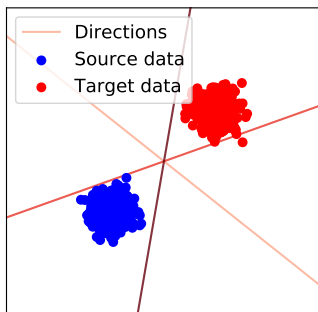
$$W_2^2(\mu, \nu) = \int_0^1 |F_\mu^{-1}(u) - F_\nu^{-1}(u)|^2 \, du = \|F_\mu^{-1} - F_\nu^{-1}\|_{L^2([0,1])}^2$$

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 $P^{\theta}(x) = \langle x, \theta \rangle$, λ 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_2 distance ([Bonnotte, 2013](#))
- Topologically equivalent to the Wasserstein distance ([Nadjahi et al., 2019](#)), i.e.
 $\lim_{n \rightarrow \infty} \text{SW}_2^2(\mu_n, \mu) = 0 \iff \lim_{n \rightarrow \infty} W_2^2(\mu_n, \mu) = 0$.

Properties of the Sliced-Wasserstein Distance

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

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Limitations

- Restricted to probability measures
- Not robust to outliers

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Sliced UOT

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

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

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

Example

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

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

$$\text{UOT}(\alpha, \beta) = \inf_{(\pi_1, \pi_2) \in \mathcal{M}_+(\mathbb{R}^d) \times \mathcal{M}_+(\mathbb{R}^d)} \text{OT}(\pi_1, \pi_2) + \rho_1 D_{\varphi_1}(\pi_1 | \alpha) + \rho_2 D_{\varphi_2}(\pi_2 | \beta)$$

φ -divergence:

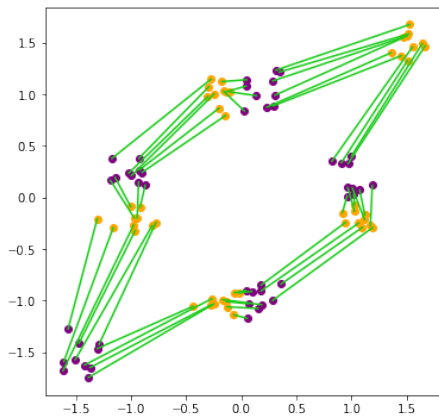
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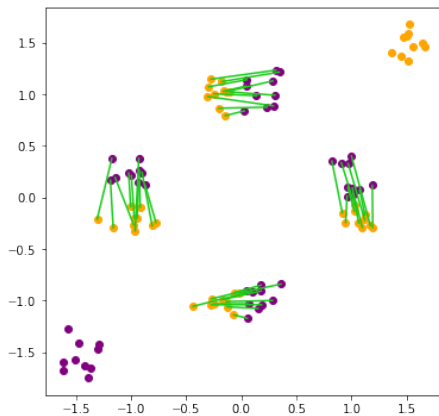
Example

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- Total Variation distance: $\varphi(t) = |t - 1|$

Balanced vs Unbalanced OT



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



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

From (Séjourné et al., 2023)

Solving the UOT Problem

Various solutions in particular cases:

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

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](#))

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](#))
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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](#))

Slicing and Unbalancing OT

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Unbalanced Sliced OT

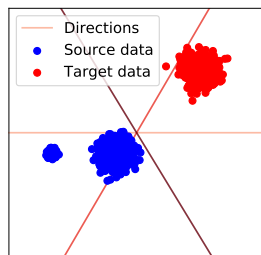
Let $\alpha, \beta \in \mathcal{M}_+(\mathbb{R}^d)$,

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

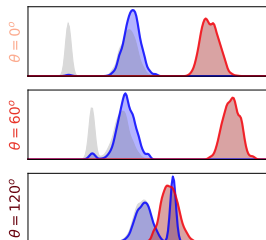
→ new!

SUOT vs USOT

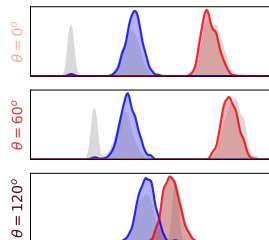
In the rest of the talk: $\mathcal{D}_\varphi = \text{KL}$



Samples and directions



SUOT ($\rho_1 = 0.01$, $\rho_2 = 1$)



USOT ($\rho_1 = 1$, $\rho_2 = 1$)

- 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. $f \oplus g \leq c \implies f + \lambda \oplus g - \lambda \leq c$

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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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- 1D UOT by Frank-Wolfe algorithm (for $D_\varphi = \text{KL}$)
→ complexity $O(Tn \log n)$ with T number of Frank-Wolfe iterations

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- 1D UOT by Frank-Wolfe algorithm (for $D_\varphi = \text{KL}$)
→ 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

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

end for

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

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

→ Complexity in $O(TLn \log n)$

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Unbalanced Optimal Transport

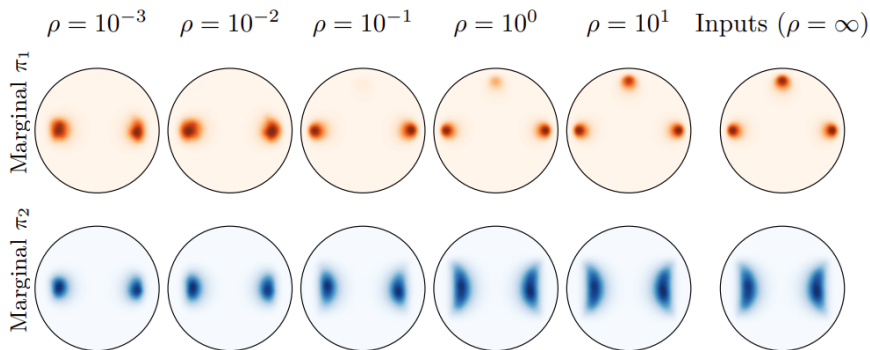
Sliced UOT

Computing Sliced UOT

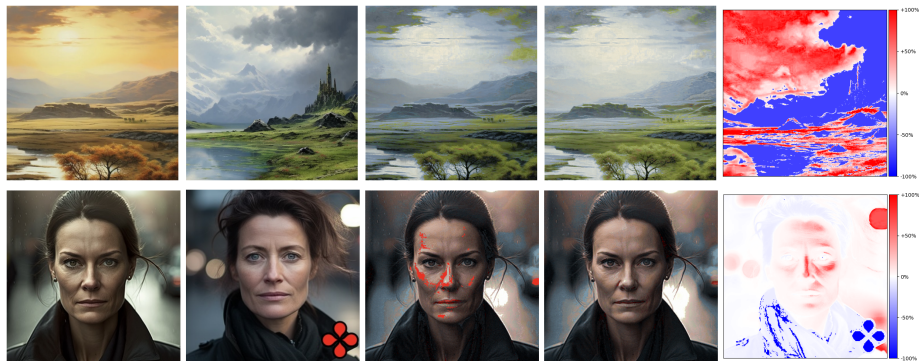
Experiments

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 (π_1, π_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 ρ

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Thank you!

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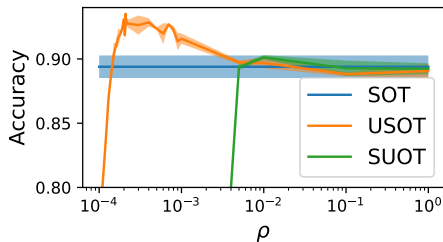
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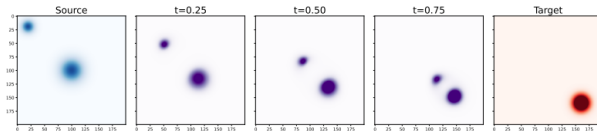
Document Classification

- 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

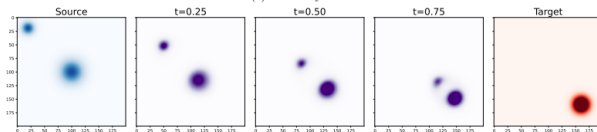
	BBCSport		Goodreads		
	Acc	t ($\cdot 10^{-3}s$)	Acc (genre)	Acc (like)	t ($\cdot 10^{-3}s$)
OT	94.55	3.12 ± 1.61	55.22	71.00	440.30 ± 250
UOT	96.73	243.39 ± 9.24	-	-	-
SinkhUOT	95.45	46.22 ± 2.17	53.55	67.81	2021.68 ± 356
SOT	89.39 ± 0.76	1.80 ± 0.22	50.09 ± 0.51	65.60 ± 0.20	4.49 ± 1.44
SUOT	90.12 ±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



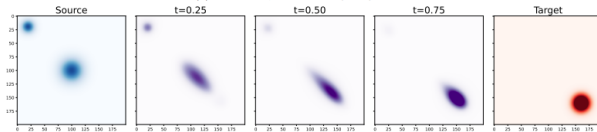
Barycenters



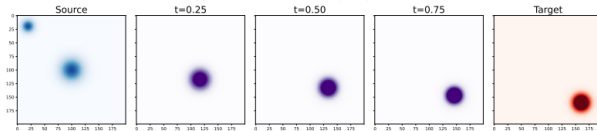
(a) SOT barycenters



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

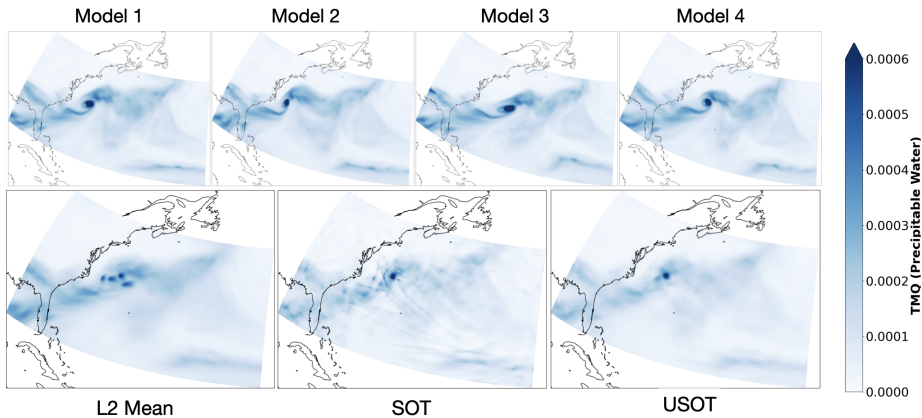


(c) USOT barycenters with $\rho_1 = \rho_2 = 0.01$



(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 100×200