Unbalanced minibatch Optimal Transport

Applications to Domain Adaptation

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Unbalanced Optimal Transport Introduction

Unbalanced Optimal Transport

Definition

Unbalanced Optimal Transport measures the distance between probablity distributions, but with relaxed marginals.

$$\mathrm{UOT}^{\tau,\varepsilon}(\alpha,\beta,c) = \min_{\pi \in \mathcal{M}_+(\mathcal{X}\times\mathcal{Y})} \int c d\pi + \varepsilon \mathtt{KL}(\pi|\alpha\otimes\beta) + \tau(\mathtt{KL}(\pi_1\|\alpha) + \mathtt{KL}(\pi_2\|\beta)),$$

where π is the transport plan, π_1 and π_2 the plan's marginals, $\tau \geq 0$ is the marginal penalization and $\varepsilon \geq 0$ is the regularization coefficient.

Robustness of UOT

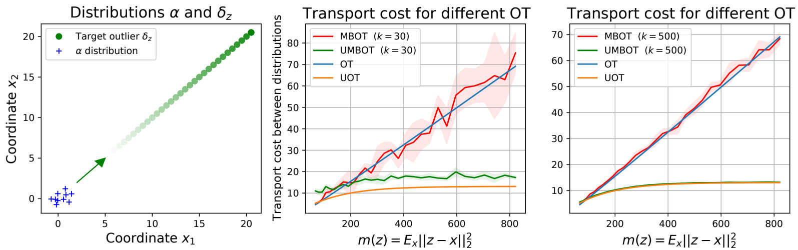
Lemma

Take (α, β) two probability distributions. For $\zeta \in [0,1]$, write $\tilde{\alpha} = \zeta\alpha + (1-\zeta)\delta_{\boldsymbol{z}}$. Write $m(\boldsymbol{z}) = \int C(\boldsymbol{z}, \boldsymbol{y}) d\beta(\boldsymbol{y})$.

$$\mathrm{UOT}^{\tau,0}(\tilde{\alpha}, \beta, C) \lesssim \zeta\, \mathrm{UOT}^{\tau,0}(\alpha, \beta, C) + 2\tau(1-\zeta)(1 - e^{-m(\boldsymbol{z})/2\tau})$$

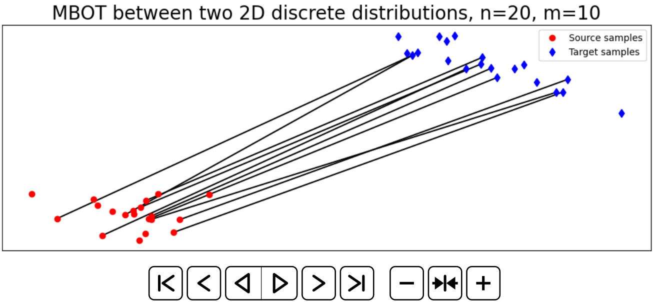
Let (f, g) be the optimal dual potentials of $\mathrm{OT}(\alpha, \beta)$, and y^* in β's support.

$$\mathrm{OT}(\tilde{\alpha}, \beta) \geq \zeta\, \mathrm{OT}(\alpha, \beta) + (1-\zeta)\Big(C(\boldsymbol{z}, y^*) - g(y^*) + \int g d\beta\Big)$$



Minibatch Optimal Transport

Minibatch Optimal Transport definition



Idea : Compute OT between the minibatches from domains

Expectation of minibatches

$$E_h(\alpha, \beta, C) := \mathbb{E}_{(X,Y)\sim\alpha^{\otimes m}\otimes\beta^{\otimes m}}[h(\mu_m, \mu_m, C(X, Y))]$$

- Can be defined for OT variants h
- Studied in [Fatras et al., 2020, Fatras et al., 2021]

Estimate minibatch OT distance

Definition (Estimators)

$$\overline{h}^m(X,Y) := \binom{n}{m}^{-2} \sum_{I,J \in \mathcal{P}_m} h(\mu_m, \mu_m, C_{I,J})$$

where $\mathcal{P}_m$ is the set of all m-tuples without replacement and ordered. Pick an integer $k > 0$ and let D_k be a set of cardinality k whose elements are minibatches drawn uniformly at random. Then,

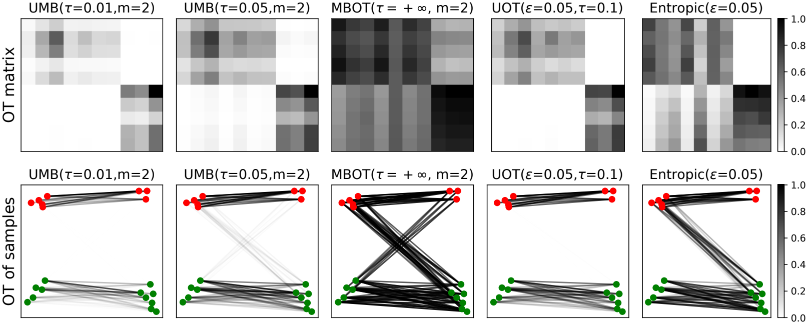
$$\widetilde{h}_k(X,Y) := k^{-1} \sum_{(I,J) \in D_k} h(\mu_m, \mu_m, C_{I,J})$$

Proposition

We have the following properties:

- $\widetilde{\mathrm{UOT}}_k, \overline{\mathrm{UOT}}^m$ *are unbiased estimators of* E_{UOT}
- *Strictly positive losses:* $\widetilde{\mathrm{UOT}}_k(X,Y) > 0$, $\overline{\mathrm{UOT}}^m(X,Y) > 0$

Unbalanced minibatch OT plan



Limits of unbalanced UOT

- Find the correct τ
- Lazy gradients for too small τ

Statistical and optimization properties

Theorem (Maximal deviation bound)

With probability at least $1-\delta$ on the draw of X, Y and D_k we have:

$$|\widetilde{\mathrm{UOT}^{\tau,\varepsilon}}_k^m(X,Y) - E_{\mathrm{UOT}}| \leq \mathcal{O}\left(\sqrt{\frac{\log(\frac{2}{\delta})}{2\lfloor\frac{n}{m}\rfloor}} + \sqrt{\frac{2\log(\frac{2}{\delta})}{k}}\right),$$

SGD converges [Majewski et al., 2018, Davis et al., 2020] if:

- $\overline{UOT}^m$ is an unbiased estimator of E_{UOT}
- Exchange Clarke gradients and expectations

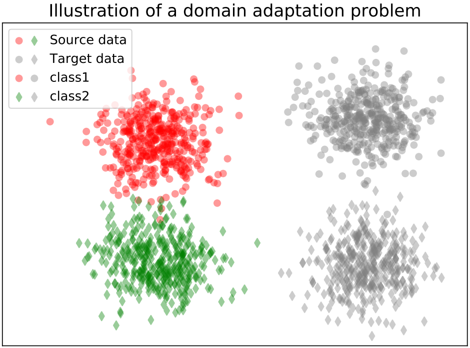
Theorem

Let $\hat{X}, \{\hat{Y}_\theta\}_{\theta\in\Theta}$ be two m-tuples of random vectors compactly supported and C^m a $\mathbf{C}^1$ cost. We have:

$$\partial_\theta\, \mathbb{E}[\mathrm{UOT}^{\tau,\varepsilon}(\mu_m, \mu_m, C^m(\hat{X}, \hat{Y}_\theta))] = \mathbb{E}[\partial_\theta\, \mathrm{UOT}^{\tau,\varepsilon}(\mu_m, \mu_m, C^m(\hat{X}, \hat{Y}_\theta))],$$

Experiments

Domain adaptation



Domain adaptation (DA) setting

- Two domains, only one with labels
- Share the same label distribution
- Goal: Classify unlabelled target data with source labelled data

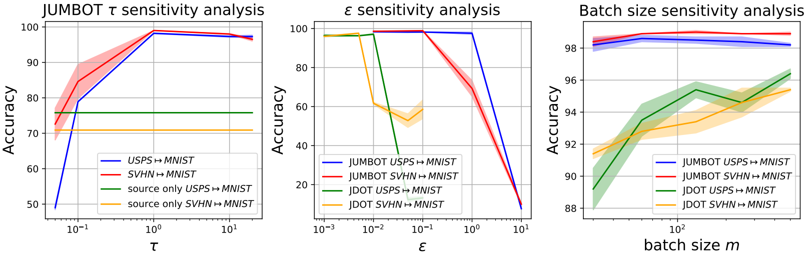
Office Home experiments

We replace minibatch OT by unbalanced minibatch OT in the state of the art DEEPJDOT algorithm [Damodaran et al., 2018]. This allows to reduce the weight of non optimal connections between samples. Our method is called JUMBOT.

	Method	A-C	A-P	A-R	C-A	C-P	C-R	P-A	P-C	P-R	R-A	R-C	R-P	avg
DA	RESNET-50	34.9	50.0	58.0	37.4	41.9	46.2	38.5	31.2	60.4	53.9	41.2	59.9	46.1
	DANN (*)	44.3	59.8	69.8	48.0	58.3	63.0	49.7	42.7	70.6	64.0	51.7	78.3	58.3
	CDAN-E(*)	52.5	71.4	76.1	59.7	69.9	71.5	58.7	50.3	77.5	70.5	57.9	**83.5**	66.6
	DEEPJDOT (*)	50.7	68.6	74.4	59.9	65.8	68.1	55.2	46.3	73.8	66.0	54.9	78.3	63.5
	ALDA (*)	52.2	69.3	76.4	58.7	68.2	71.1	57.4	49.6	76.8	70.6	57.3	82.5	65.8
	ROT (*)	47.2	71.8	76.4	58.6	68.1	70.2	56.5	45.0	75.8	69.4	52.1	80.6	64.3
	JUMBOT	**55.2**	**75.5**	**80.8**	**65.5**	**74.4**	**74.9**	**65.2**	**52.7**	**79.2**	**73.0**	**59.9**	83.4	**70.0**
PDA	RESNET-50	46.3	67.5	75.9	59.1	59.9	62.7	58.2	41.8	74.9	67.4	48.2	74.2	61.4
	DEEPJDOT(*)	48.2	66.2	76.6	56.1	57.8	64.5	58.3	42.7	73.5	65.7	48.2	73.7	60.9
	PADA	51.9	67.0	78.7	52.2	53.8	59.0	52.6	43.2	78.8	73.7	56.6	77.1	62.1
	ETN	59.2	77.0	79.5	62.9	65.7	75.0	68.3	55.4	84.4	75.7	57.7	**84.5**	70.4
	BA3US(*)	56.7	76.0	**84.8**	73.9	67.8	**83.7**	72.7	56.5	84.9	77.8	64.5	83.8	73.6
	JUMBOT	**62.7**	**77.5**	84.4	**76.0**	**73.3**	80.5	**74.7**	**60.8**	**85.1**	**80.2**	**66.5**	83.9	**75.5**

Analysis: Ablation and sensitivity

Methods	U → M	S → M
DEEPJDOT	96.4 ± 0.3	95.4 ± 0.1
ENTROPIC DEEPJDOT	97.1 ± 0.3	97.6 ± 0.1
JUMBOT	$\mathbf{98.2 \pm 0.1}$	$\mathbf{98.9 \pm 0.1}$



Paper

Full details in the paper !

Check it out : https://arxiv.org/abs/2103.03606

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