

RÉNYI REGULARIZED OT—INTERPOLATING BETWEEN KL AND UNREGULARIZED OT



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V. NUMERICAL EXPERIMENTS

- **Contribution.** Regularize OT between probability distributions $\mu, \nu \in \mathcal{P}(\mathbb{X})$, $\mathbb{X} \subseteq \mathbb{R}^d$

$$\arg \min_{\pi \in \Pi(\mu, \nu)} \langle c, \pi \rangle := \int_{\mathbb{X} \times \mathbb{X}} c(x, y) \, d\pi(x, y), \quad \text{with cost } c: \mathbb{X} \times \mathbb{X} \rightarrow \mathbb{R}_+$$

using the α -Rényi-divergences R_α for $\alpha \in (0, 1)$.

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- **Prior work.** Regularization with $\text{KL} = \lim_{\alpha \nearrow 1} R_\alpha$ [3] and with q -Tsallis divergence $T_q = (q - 1)^{-1} [\exp((q - 1)R_q) - 1]$ for $q > 0$ [4].

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- **Result.** Rényi-regularized OT plans outperform KL / Tsallis regularized OT plans on real and synthetic data.
- **Novelty.** $R_\alpha \notin \{f\text{-divergence, Bregman divergence}\}$ and R_α not “separable” due to the logarithm.

- The transport polytope is

$$\Pi(\mu, \nu) := \{\pi \in \mathcal{P}(\mathbb{X} \times \mathbb{X}) : \pi(A \times \mathbb{X}) = \mu(A), \pi(\mathbb{X} \times B) = \nu(B) \quad \forall A, B \in \mathcal{B}(\mathbb{X})\}$$

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- $\mathcal{D}_p := \{c = d^p \mid d: \mathbb{X} \times \mathbb{X} \mapsto \mathbb{R}_+ \text{ is lower semicontinuous metric}\}$ the set of cost functions, where $p \in [1, \infty)$

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- $\mathcal{P}_p(\mathbb{X})$ is the set of probability measures with finite p -th moment.

- **Definition.** The α -Rényi-divergence of *order* $\alpha \in (0, 1)$ is

$$R_\alpha: \mathcal{P}(\mathbb{X}) \times \mathcal{P}(\mathbb{X}) \rightarrow \mathbb{R}_+, \quad (\mu \mid \nu) \mapsto \frac{1}{\alpha - 1} \ln \left(\int_{\mathbb{X}} \left(\frac{d\mu}{d\tau}(x) \right)^\alpha \left(\frac{d\nu}{d\tau}(x) \right)^{1-\alpha} d\tau(x) \right),$$

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- where τ is a finite *reference* measure, e.g. $\tau = \mu + \nu \in \mathcal{M}(\mathbb{X})_+$, is chosen such that $\mu, \nu \ll \tau$,
- and $\ln(0) := -\infty$.
- **Remark.** $R_\alpha(\cdot \mid \mu \otimes \nu)$ is well defined on $\Pi(\mu, \nu)$, i.e. $\pi \in \Pi(\mu, \nu)$ implies that $\pi \ll \mu \otimes \nu$.

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- For regularization parameter $\gamma \in [0, \infty]$ and $\alpha \in (0, 1)$, the *restricted transport polytope*,

$$\Pi_{\gamma}^{\alpha}(\mu, \nu) := \{\pi \in \Pi(\mu, \nu) : R_{\alpha}(\pi \mid \mu \otimes \nu) \leq \gamma\},$$

is weakly compact, since $R_{\alpha}(\cdot \mid \mu \otimes \nu)$ is weakly lsc. and $\Pi(\mu, \nu)$ is weakly compact.

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- **Definition.** The **Rényi-Sinkhorn distance** between $\mu, \nu \in \mathcal{P}_p(\mathbb{X})$ with cost $c \in \mathcal{D}_p$ is

$$d_{c, \gamma, \alpha} : \mathcal{P}_p(\mathbb{X}) \times \mathcal{P}_p(\mathbb{X}) \rightarrow \mathbb{R}, \quad (\mu, \nu) \mapsto \min \left\{ \langle c, \pi \rangle^{\frac{1}{p}} : \pi \in \Pi_{\gamma}^{\alpha}(\mu, \nu) \right\}. \quad (1)$$

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THEOREM 1 (B., STEIN [2])

$\mathcal{P}_p(\mathbb{X})^2 \ni (\mu, \nu) \mapsto \mathbf{1}_{[\mu \neq \nu]} d_{c,\gamma,\alpha}(\mu, \nu)$ is a metric for $\alpha \in (0, 1)$, $\gamma \in [0, \infty]$, $c \in \mathcal{D}_p$.

THE DUAL POINT OF VIEW - PENALIZING THE CONSTRAINT

- Instead of restricting the domain of the optimization problem, one can penalize the Rényi divergence constraint in (1).

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- **Definition.** The **dual Rényi-Divergence-Sinkhorn distance** for $\alpha \in (0, 1)$, $\lambda \in (0, \infty]$ is

$$d_c^{\alpha, \lambda}: \mathcal{P}_p(\mathbb{X}) \times \mathcal{P}_p(\mathbb{X}) \rightarrow \mathbb{R}, \quad (\mu, \nu) \mapsto \langle c, \pi_c^{\alpha, \lambda}(\mu, \nu) \rangle^{\frac{1}{p}},$$

where $\pi_c^{\alpha, \lambda}(\mu, \nu) \in \arg \min \left\{ \langle c, \pi \rangle + \frac{1}{\lambda} R_\alpha(\pi \mid \mu \otimes \nu) : \pi \in \Pi(\mu, \nu) \right\}.$ (2)

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THEOREM 2 (B., STEIN [2])

Problem (2) has a unique solution for every $\alpha \in (0, 1)$, $\lambda > 0$ and $\mu, \nu \in \mathcal{P}_p(\mathbb{X})$.

- **Rényi-Sinkhorn distance** $d_{c,\gamma,\alpha}(\mu, \nu)$ and **dual Rényi-Sinkhorn distance** $d_c^{\alpha,\lambda}(\mu, \nu)$ are equivalent:

for $\mu, \nu \in \mathcal{P}_p(\mathbb{X})$ and $\gamma > 0$, there exists $\lambda \in [0, \infty]$, such that

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- The problem (2) yields the regularized OT problem

$$\text{OT}_{\frac{1}{\lambda},\alpha}: \mathcal{P}_p(\mathbb{X}) \times \mathcal{P}_p(\mathbb{X}) \rightarrow [0, \infty), (\mu, \nu) \mapsto \min_{\pi \in \Pi(\mu, \nu)} \langle c, \pi \rangle + \frac{1}{\lambda} R_\alpha(\pi \mid \mu \otimes \nu). \quad (3)$$

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THEOREM 4 (B., STEIN [2] — PRE-CONVEX CONJUGATE OF $R_\alpha(\cdot \mid \theta)$)

For $\theta \in \mathcal{M}(\mathbb{X})$ we have

$$[R_\alpha(\cdot \mid \theta)]_*(g) = \begin{cases} \ln \left(\langle |g|^{\frac{\alpha}{\alpha-1}}, \theta \rangle \right) + \text{const}_\alpha, & \text{if } g \in \mathcal{C}_0(\mathbb{X}), \ g < 0, \\ +\infty & \text{else.} \end{cases}$$

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- **Remark.** The latter theorem holds not only for compact $\mathbb{X}$ but also for $\mathbb{X} = \mathbb{R}^d$.

THEOREM 5 (B., STEIN [2] — DUAL PROBLEM)

If $\mathbb{X} \subset \mathbb{R}^d$ **compact**, then the Fenchel-Rockafellar theorem yields the strong duality

$$(3) = \max_{\substack{f, g \in \mathcal{C}(\mathbb{X}) \\ f \oplus g < c}} \langle f \oplus g, \mu \otimes \nu \rangle - \frac{1}{\lambda} \ln \left(\langle (c - f \oplus g)^{\frac{\alpha}{\alpha-1}}, \mu \otimes \nu \rangle \right) + \text{const}_{\alpha, \lambda}. \quad (4)$$

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COROLLARY 6 (B., STEIN [2] — REPRESENTATION OF $\pi_c^{\alpha, \lambda}$)

For unique solution $\pi_c^{\alpha, \lambda}(\mu, \nu)$ of (2), and optimal dual potentials $\hat{f}, \hat{g} \in \mathcal{C}(\mathbb{X})$ from (4):

$$\pi_c^{\alpha, \lambda} = \frac{(c - \hat{f} \oplus \hat{g})^{\frac{1}{\alpha-1}}}{\langle (c - \hat{f} \oplus \hat{g})^{\frac{1}{\alpha-1}}, \mu \otimes \nu \rangle} \mu \otimes \nu.$$

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- **Remark.** We have: $\text{supp}(\pi_c^{\alpha, \lambda}(\mu, \nu)) = \text{supp}(\mu \otimes \nu)$ and uniqueness of $(\hat{f}, \hat{g})$ up to additive constants.

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THEOREM 7 (B., STEIN [2] — INTERPOLATION PROPERTIES I)

For fixed $\alpha \in (0, 1)$, we have

$$\text{OT}_{\frac{1}{\lambda}, \alpha}(\mu, \nu) \rightarrow \text{OT}(\mu, \nu) \quad \text{for } \lambda \rightarrow \infty$$

and

$$\text{OT}_{\frac{1}{\lambda}, \alpha}(\mu, \nu) \rightarrow \langle c, \mu \otimes \nu \rangle \quad \text{for } \lambda \rightarrow 0.$$

with

$$\begin{aligned} \pi_c^{\alpha, \lambda}(\mu, \nu) &\rightharpoonup \arg \min \{ R_\alpha(\pi \mid \mu \otimes \nu) : \pi \in \Pi(\mu, \nu), \langle c, \pi \rangle = \text{OT}(\mu, \nu) \}, & \lambda \rightarrow \infty, \\ \pi_c^{\alpha, \lambda}(\mu, \nu) &\rightharpoonup \mu \otimes \nu, & \lambda \rightarrow 0. \end{aligned}$$

THEOREM 8 (B., STEIN [2] — INTERPOLATION PROPERTIES II)

For fixed $\lambda > 0$, we have

$$\mathrm{OT}_{\frac{1}{\lambda}, \alpha}(\mu, \nu) \rightarrow \mathrm{OT}(\mu, \nu) \quad \text{for } \alpha \searrow 0$$

and

$$\mathrm{OT}_{\frac{1}{\lambda}, \alpha}(\mu, \nu) \rightarrow \mathrm{OT}_{\frac{1}{\lambda}, \alpha'}(\mu, \nu) \quad \text{for } \alpha \nearrow \alpha' \in (0, 1].$$

and

$$\pi_c^{\alpha, \lambda}(\mu, \nu) \rightharpoonup \pi \in \Pi(\mu, \nu) \quad \text{with} \quad \langle c, \pi \rangle = \mathrm{OT}(\mu, \nu) \quad \alpha \searrow 0, \quad (5)$$

$$\pi_c^{\alpha, \lambda}(\mu, \nu) \rightharpoonup \pi_c^{\alpha', \lambda}(\mu, \nu), \quad \alpha \nearrow \alpha' \in (0, 1]. \quad (6)$$

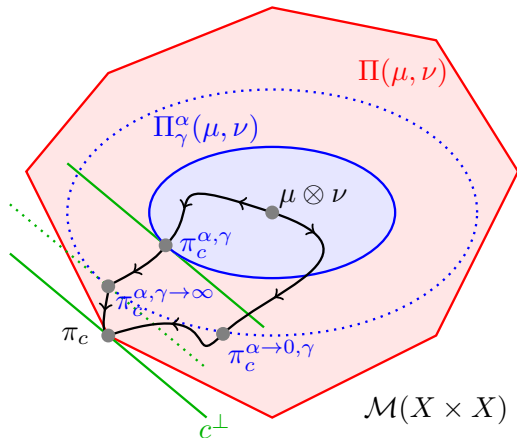


FIGURE 1: Transport polytope $\Pi(\mu, \nu)$ with the restricted transport polytope $\Pi_\gamma^\alpha(\mu, \nu)$. Convergence of $\pi_c^{\alpha, \gamma} \rightarrow \pi_c$ to the unregularized OT plan with $\alpha \rightarrow 0$ and $\gamma \rightarrow \infty$. (Plot inspired by Cuturi [3].)

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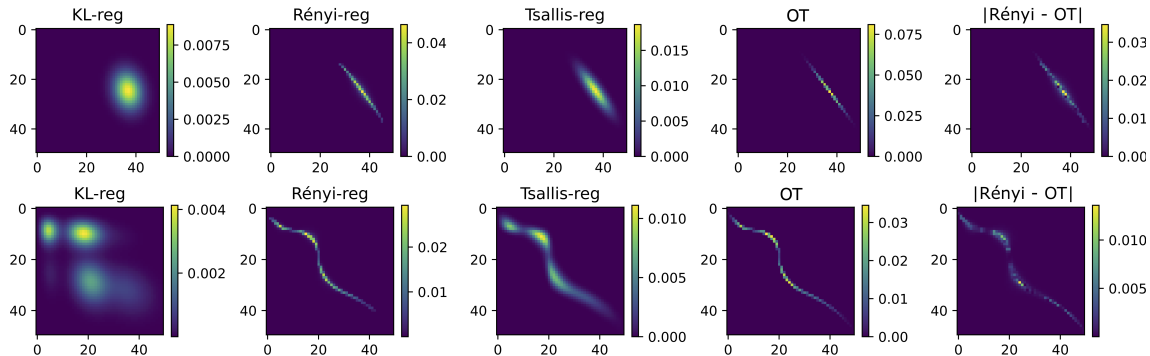
V. NUMERICAL EXPERIMENTS

NUMERICAL EXPERIMENTS - BETTER TRANSPORT PLANS

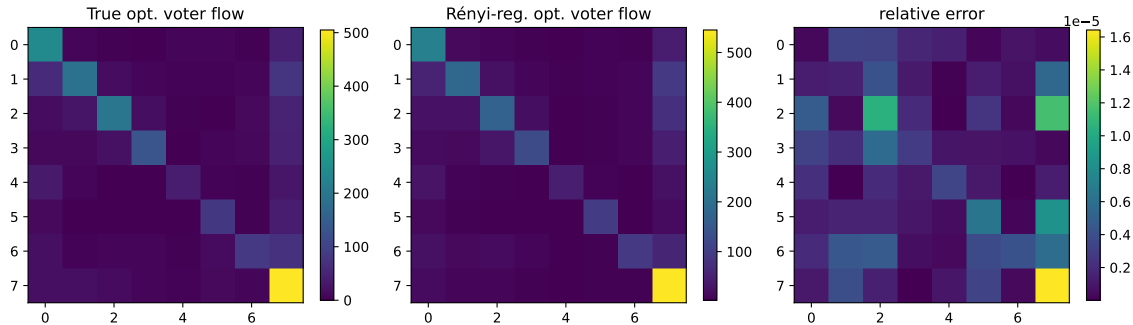
- $\Phi_c^{\alpha,\lambda}$ is not Lipschitz continuous in zero, but locally Lipschitz in

$$\{\pi \in \Pi(\mu, \nu) : \pi|_{\text{supp}(\mu \otimes \nu)} > 0\} = \Pi(\mu, \nu) \cap \text{int}(\text{dom } h),$$

where h generates KL divergence $\Rightarrow$ modified mirror descent algorithm with Polyak step size converges [5]. In each iteration one Sinkhorn projection is performed.



NUMERICAL EXPERIMENTS - PREDICTING VOTER MIGRATION



distance matrix	regularizer	abs error $\pm$ std	KL error	mean squared error	scalar
M^{Eucl}	$\text{KL}_{\lambda=1}$	$2.4221 \times 10^1 \pm 2.848 \times 10^1$	8.422×10^2	9.008×10^4	10
	$T_{\lambda=1,q=10}^\dagger$	$9.409 \pm 1.529 \times 10^1$	3.173×10^2	2.063×10^4	
	OT	$1.845 \times 10^1 \pm 2.358 \times 10^1$	7.655×10^2	5.738×10^4	
	$R_{\lambda=1,\alpha=0.3}$	6.611 ± 7.868	2.128×10^2	6.759×10^3	

Thank you for your attention!

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- [2] Jonas Bresch and Viktor Stein. *Interpolating between Optimal Transport and KL regularized Optimal Transport using Rényi Divergences*. 2024. arXiv: 2404.18834 [math.OC]. URL: <https://arxiv.org/abs/2404.18834>.
- [3] Marco Cuturi. “Sinkhorn Distances: Lightspeed Computation of Optimal Transportation Distances”. In: *Advances in Neural Information Processing Systems* 26 (2013).
- [4] Boris Muzellec et al. “Tsallis regularized optimal transport and ecological inference”. In: *Proceedings of the AAAI conference on artificial intelligence*. Vol. 31. 2017.

- [5] Jun-Kai You and Yen-Huan Li. *Two Polyak-Type Step Sizes for Mirror Descent*. 2022. arXiv: 2210.01532 [math.OC].

OUTLOOK—RÉNYI-SINKHORN DIVERGENCE