Rényi-regularized Optimal Transport

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

$$\operatorname*{argmin}_{\pi \in \Pi(\mu,\nu)} \langle c, \pi \rangle := \int_{\mathbb{X} \times \mathbb{X}} c(x,y) \, \mathrm{d}\pi(x,y), \qquad \text{with cost } c \colon \mathbb{X} \times \mathbb{X} \to \mathbb{R}_+$$

  using the α-Rényi-divergences R_α for $\alpha \in (0,1)$.
- **Prior work.** Regularization with $\mathrm{KL} = \lim_{\alpha \nearrow 1} R_\alpha$ [Cut13] and with q-Tsallis divergence $T_q = (q-1)^{-1} [\exp((q-1)R_q) - 1]$ for $q > 0$ [Muz+17].
- **Method.** Solve primal problem with mirror descent [BT03] and dual problem with subgradient descent.
- **Result.** Rényi-regularized OT plans outperform KL / Tsallis regularized OT plans on real and synthetic data.
- **Novelty.** $R_\alpha \notin \{f\text{-divergence}, \text{Bregman divergence}\}$ and R_α not "separable" due to ln.

Preliminaries: OT and Rényi divergence

The transport polytope is

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

and $\mathcal{D} := \{c \colon \mathbb{X} \times \mathbb{X} \mapsto \mathbb{R}_+ :\ c \text{ is lower semicontinuous metric}\}$ the set of cost functions.

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

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

where a finite reference measure τ, 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 $\pi \ll \mu \otimes \nu$.

Theorem. (Convex conjugate of $R_\alpha(\cdot \mid \theta)$)

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

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

Rényi-Regularized OT Problem

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

$$\Pi_\gamma^\alpha(\mu,\nu) := \{\pi \in \Pi(\mu,\nu) : R_\alpha(\pi \mid \mu \otimes \nu) \le \gamma\}, \tag{2}$$

is weakly compact, since $R_\alpha(\cdot \mid \mu \otimes \nu)$ is weakly lsc and $\Pi(\mu,\nu)$ is weakly compact.
The **Rényi-Sinkhorn distance** between $\mu, \nu \in \mathcal{P}(\mathbb{X})$ is

$$d_{c,\gamma,\alpha} \colon \mathcal{P}(\mathbb{X}) \times \mathcal{P}(\mathbb{X}) \to \mathbb{R}, \qquad (\mu,\nu) \mapsto \min\left\{\langle c, \pi \rangle : \pi \in \Pi_\gamma^\alpha(\mu,\nu)\right\}. \tag{3}$$

Remark. (3) is a convex problem, with unique minimizer.

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

The Dual Point of View - Penalizing the Constraint

Instead of restricted the domain of the optimization problem, one can penalize the Rényi divergence constraint in (3). The **dual Rényi-Divergence-Sinkhorn distance** for $\alpha \in (0,1)$, $\lambda \in (0,\infty]$ is

$$d_c^{\alpha,\lambda} \colon \mathcal{P}(\mathbb{X}) \times \mathcal{P}(\mathbb{X}) \to \mathbb{R}, \qquad (\mu,\nu) \mapsto \langle c, \pi_c^{\alpha,\lambda}(\mu,\nu) \rangle, \tag{4}$$

$$\text{where } \pi_c^{\alpha,\lambda}(\mu,\nu) \in \operatorname{argmin}\left\{\langle c, \pi \rangle + \frac{1}{\lambda} R_\alpha(\pi \mid \mu \otimes \nu) : \pi \in \Pi(\mu,\nu)\right\}. \tag{5}$$

Theorem. Problem (5) has a unique solution for every $\alpha \in (0,1)$, $\lambda > 0$ and $\mu, \nu \in \mathcal{P}(\mathbb{X})$.

Lagrangian Reformulation for $\Pi_\gamma^\alpha(\mu,\nu)$

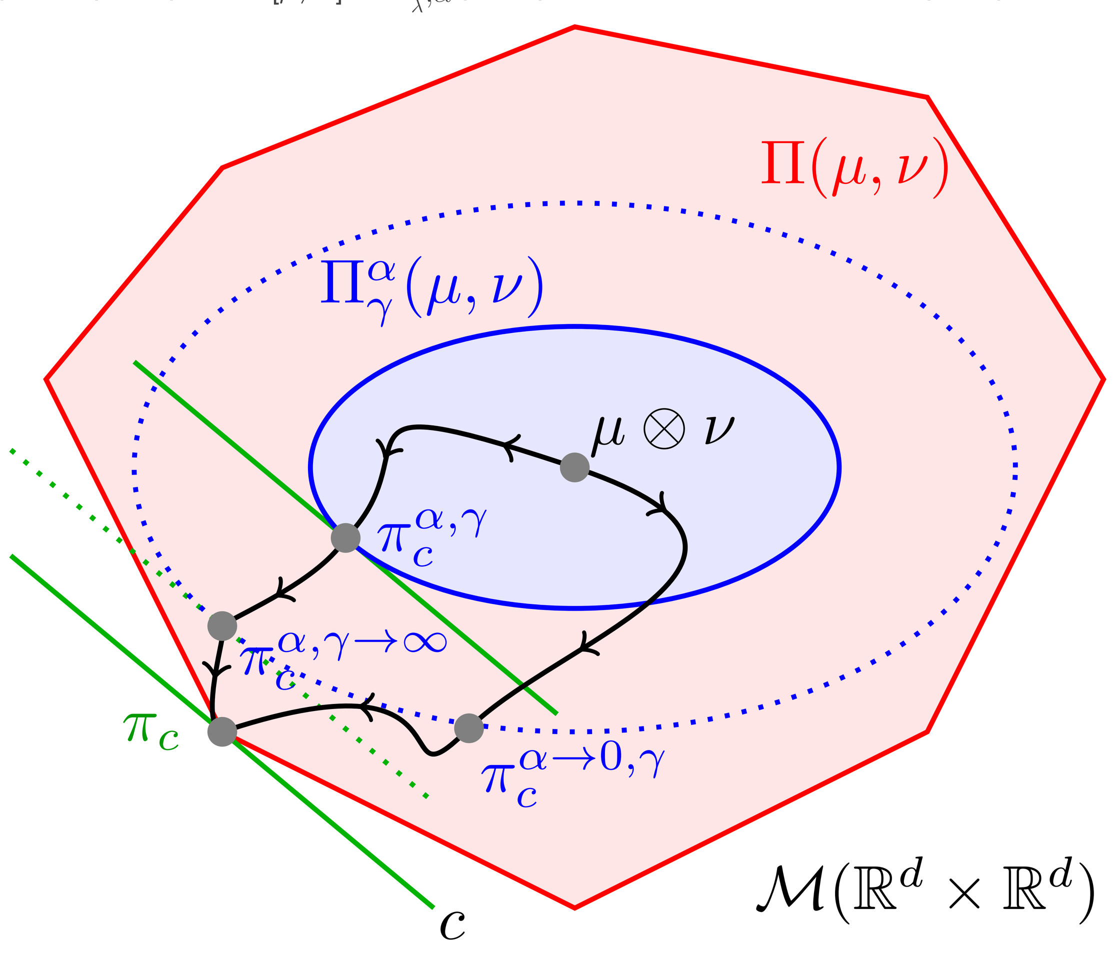
Rényi-Sinkhorn distance $d_{c,\gamma,\alpha}(\mu,\nu)$ and **dual Rényi-Sinkhorn distance** are equivalent: for $\mu, \nu \in \mathcal{P}(\mathbb{X})$ and $\gamma > 0$, there exists $\lambda \in [0,\infty]$, such that $\langle c, \pi_c^{\alpha,\lambda}(\mu,\nu) \rangle = d_{c,\gamma,\alpha}(\mu,\nu)$.

Rényi-regularized OT pre-metric

The problem (5) yields the regularized OT problem

$$\mathrm{OT}_{\frac{1}{\lambda},\alpha} \colon \mathcal{P}(\mathbb{X}) \times \mathcal{P}(\mathbb{X}) \to [0,\infty), \qquad (\mu,\nu) \mapsto \min\left\{\langle c, \pi \rangle + \frac{1}{\lambda} R_\alpha(\pi \mid \mu \otimes \nu) : \pi \in \Pi(\mu,\nu)\right\}. \tag{6}$$

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



Transport polytope $\Pi(\mu,\nu)$ with the restricted transport polytope $\Pi_\gamma^\alpha(\mu,\nu)$. Convergence of $\pi_c^{\alpha,\gamma} \to \pi_c$ to the unregularized OT plan with $\alpha \to 0$ and $\gamma \to \infty$. (Plot inspired by [Cut13].)

Dual formulation of the Rényi-Sinkhorn distance

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

$$(6) = \max\left\{\langle f \oplus g, \mu \otimes \nu \rangle - \frac{1}{\lambda} \ln\left(\langle (c - f \oplus g)^{\frac{\alpha}{\alpha-1}}, \mu \otimes \nu \rangle\right) : \begin{matrix} f, g \in \mathcal{C}(\mathbb{X}) \\ f \oplus g < c \end{matrix}\right\} + \text{const}_{\alpha,\lambda}, \tag{7}$$

where $(f \oplus g)(x,y) := f(x) + g(y)$.

Theorem. (Representation of $\pi_c^{\alpha,\lambda}$)

For unique solution $\pi_c^{\alpha,\lambda}(\mu,\nu)$ of (5), and optimal dual potentials $\hat{f}, \hat{g} \in \mathcal{C}(\mathbb{X})$ from (7):

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

Corollary. We have $\operatorname{supp}(\pi_c^{\alpha,\lambda}(\mu,\nu)) = \operatorname{supp}(\mu \otimes \nu)$.

- $R_\alpha(\mu \mid \nu) \to \mathrm{KL}(\mu \mid \nu)$ for $\alpha \nearrow 1$ and $R_\alpha(\mu \mid \nu) \to -\ln(\nu(\operatorname{supp}(\mu)))$ for $\alpha \searrow 0$ [EH14].

$$\mathrm{OT}_{\frac{1}{\lambda},\alpha}(\mu,\nu) \to \mathrm{OT}_{\frac{1}{\lambda}}^{\mathrm{KL}}(\mu,\nu) \quad \text{for} \quad \alpha \nearrow 1 \quad \text{and} \quad \mathrm{OT}_{\frac{1}{\lambda},\alpha}(\mu,\nu) \to \mathrm{OT}(\mu,\nu) \quad \text{for} \quad \alpha \searrow 0.$$

Lemma. (Uniqueness of the optimal dual potentials up to additive const)

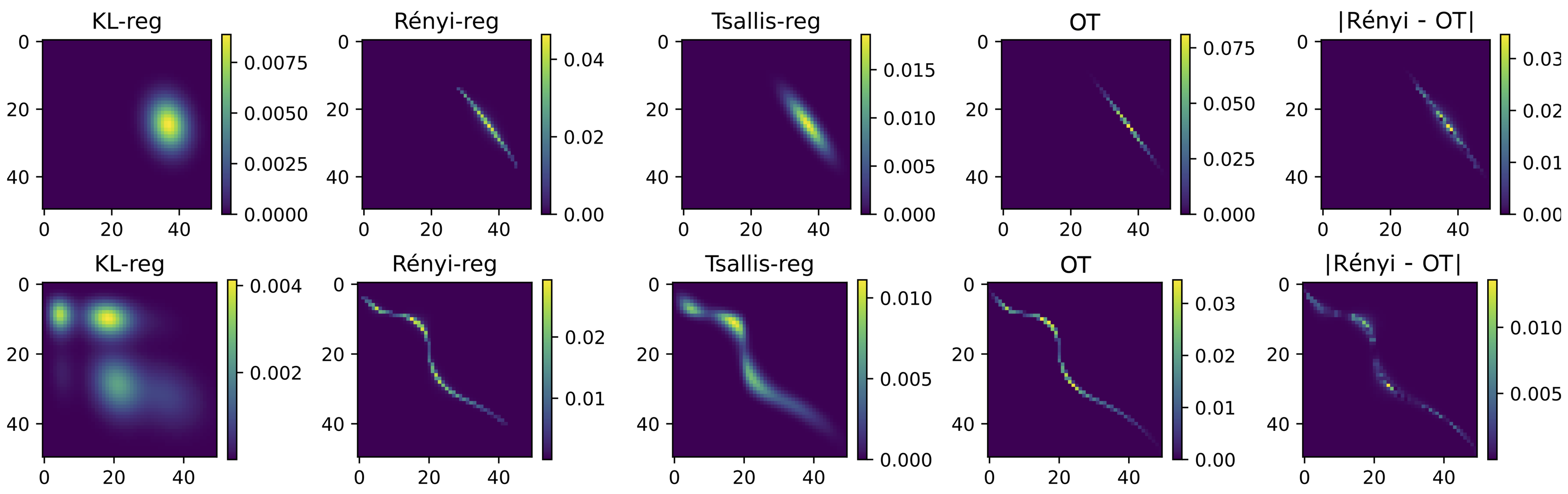
The optimal dual solution $(\hat{f}, \hat{g}) \in \mathcal{C}(\mathbb{X})^2$ is unique up to additive constants: for two optimal pairs $(\hat{f}, \hat{g}), (\tilde{f}, \tilde{g}) \in \mathcal{C}(\mathbb{X})^2$ there exists $\gamma \in \mathbb{R}$ such that $\hat{f} - \tilde{f} \equiv \gamma \equiv \tilde{g} - \hat{g}$.

Numerical Experiments - Better transport plans and voter migration

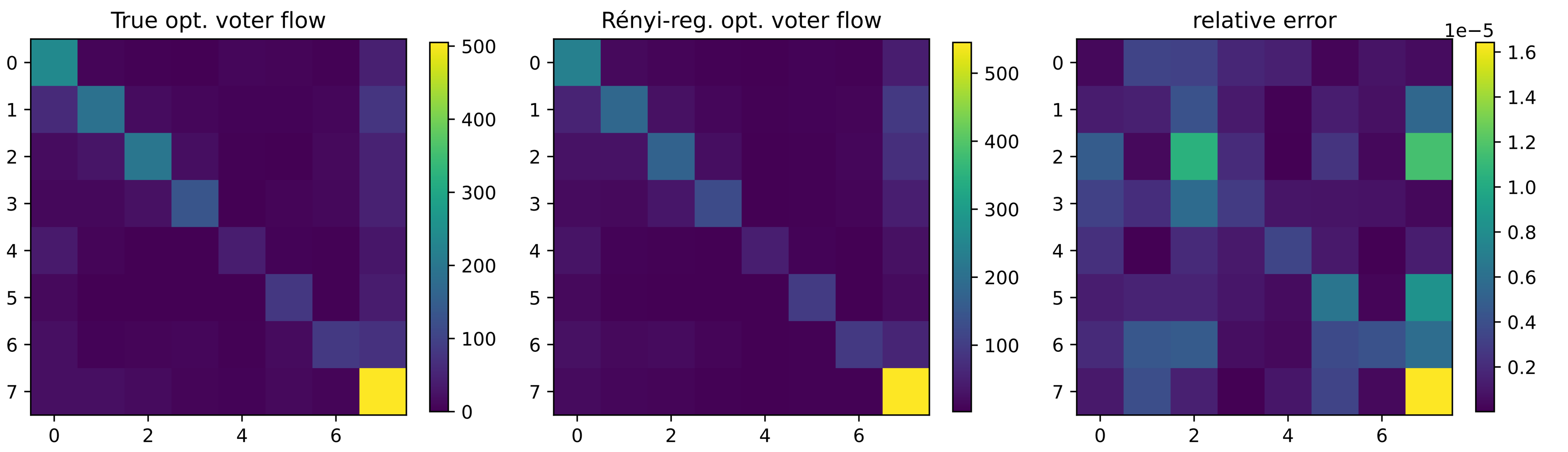
$\Phi_c^{\alpha,\lambda}$ is not Lipschitz continuous in zero, but locally Lipschitz in

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

where h generates KL divergence $\implies$ modified mirror descent algorithm with Polyak step size converges [YL22]. In each iteration one Sinkhorn-Knopp projection is performed.



Regularized OT plans for Gaussian *(top)* and Poisson *(bottom)* marginals with regularization parameter $\lambda = 10$, Rényi order $\alpha = 0.01$, Tsallis order: $q = 2$



The true voter migration (left) evaluated by "Infratest dimap"[a]. The Rényi-regularized OT plan $\pi_c^{\alpha,\lambda}(\mu,\nu)$ with squared cost $c(x,y) = |x-y|^2$, $\lambda = 1$, $\alpha = 0.3$ (middle). μ, ν are the Berlin elections results in 2021 and 2023 (source: "Federal Statistical Office"[bc]).

regularizer	absolute error ± std	KL error	MSE
KL, $\lambda = 1$	$2.4221 \times 10^1 \pm 2.848 \times 10^1$	8.422×10^2	9.008×10^4
Tsallis, $\lambda = 1, q = 1.4$	$9.112 \pm 1.368 \times 10^1$	3.173×10^2	1.724×10^4
None	$1.845 \times 10^1 \pm 2.358 \times 10^1$	7.655×10^2	5.738×10^4
Rényi, $\lambda = 1, \alpha = 0.3$	$\mathbf{6.611 \pm 7.868}$	$\mathbf{2.128 \times 10^2}$	$\mathbf{6.759 \times 10^3}$

{ KL, Tsallis, Rényi } regularizers for the optimal $\alpha \in \{k \cdot 10^{-1} : 1 \le k \le 9\}$ or $q \in \{k \cdot 10^{-1} : k \in \mathbb{N}\}$ each.

Conclusion

- Generalization of KL-regularized OT.
- Hard constraint from primal formulation stays hard constraint in dual problem, unlike in KL-regularized OT
- $\alpha \ll 1$ small yields thin regularized OT plans, where $\alpha \searrow 0$ yields the unregularized OT plan (new convergence property).
- Fast computation via mirror descent.

Further work. Rényi-regularized OT barycenters, debiased Rényi-regularized transport (like Sinkhorn divergences [Fey+19]), convergence rates for $\lambda \to \{0,\infty\}$ and $\alpha \to \{0,1\}$

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[b] https://www.wahlen-berlin.de/wahlen/BE2023/AFSPRAES/ergebnisse.html
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