

Nearly Tight Convergence Bounds for Semi-discrete Entropic Optimal Transport

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Introduction

Quadratic Optimal Transport with Entropic Regularization

- ▶ Let \mathcal{X}, \mathcal{Y} be compact subsets of \mathbb{R}^d and $\rho \in \mathcal{P}(\mathcal{X}), \mu \in \mathcal{P}(\mathcal{Y})$.
- ▶ For $\varepsilon \geq 0$, Quadratic OT problem between ρ and μ with entropic regularization:

$$\min_{\pi \in \Pi(\rho, \mu)} \int_{\mathcal{X} \times \mathcal{Y}} \|x - y\|^2 d\pi(x, y) + \varepsilon \text{KL}(\pi | \rho \otimes \mu), \quad (\text{P}_\varepsilon)$$

where

$$\text{KL}(\pi | \rho \otimes \mu) = \begin{cases} \int_{\mathcal{X} \times \mathcal{Y}} \left(\log \left(\frac{d\pi}{d\rho \otimes \mu}(x, y) \right) - 1 \right) d\pi(x, y) + 1 & \text{if } \pi \ll \rho \otimes \mu, \\ +\infty & \text{else.} \end{cases}$$

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- ▶ **If $\varepsilon = 0$:** value of (P_ε) defines $W_2^2(\rho, \mu)$.
Possibly hard to solve numerically, bad sample complexity.

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- ▶ **If $\varepsilon = 0$:** value of (P_ε) defines $W_2^2(\rho, \mu)$.
Possibly hard to compute, bad sample complexity.
- ▶ **If $\varepsilon > 0$:**
 - ▶ (P_ε) is a ε -strongly-convex min. problem \implies **fast optimization algorithms** (see e.g. Cuturi (2013); Altschuler et al. (2017); Dvurechensky et al. (2018); Peyré and Cuturi (2019); Schmitzer (2019); Genevay et al. (2016); Bercu and Bigot (2020)).
 - ▶ **improved sample complexity** for the value of (P_ε) (Genevay et al. (2019); Mena and Niles-Weed (2019)).

Introduction

Quadratic Optimal Transport with Entropic Regularization

$$\min_{\pi \in \Pi(\rho, \mu)} \int_{\mathcal{X} \times \mathcal{Y}} \|x - y\|^2 d\pi(x, y) + \varepsilon \text{KL}(\pi | \rho \otimes \mu). \quad (\text{P}_\varepsilon)$$

- ▶ The case $\varepsilon > 0$ is generally easier to solve than the case $\varepsilon = 0$.
- ▶ For $\varepsilon > 0$ and a solution $\pi^{(\text{P}_\varepsilon)}$ to (P_ε) , introduce

$$W_{2,\varepsilon}(\rho, \mu) := \left(\int_{\mathcal{X} \times \mathcal{Y}} \|x - y\|^2 d\pi^{(\text{P}_\varepsilon)}(x, y) \right)^{1/2}.$$

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Quadratic Optimal Transport with Entropic Regularization

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$$W_{2,\varepsilon}(\rho, \mu) := \left(\int_{\mathcal{X} \times \mathcal{Y}} \|x - y\|^2 d\pi^{(\text{P}_\varepsilon)}(x, y) \right)^{1/2}.$$

- ▶ Hope that:

$$W_{2,\varepsilon}(\rho, \mu) \approx W_{2,0}(\rho, \mu) = W_2(\rho, \mu).$$

How good is this approximation?

Introduction

Quadratic Optimal Transport with Entropic Regularization

- ▶ $W_{2,\varepsilon} \xrightarrow{\varepsilon \rightarrow 0} W_2$ is established in general settings (see e.g. Mikami (2004); Léonard (2012); Bernton et al. (2021); Nutz and Wiesel (2021)).

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- ▶ **In the continuous setting** (where ρ, μ are a.c.): Adams et al. (2011); Duong et al. (2013); Erbar et al. (2015); Pal (2019); Conforti and Tamanini (2021) gave **1st/2nd order asymptotics**:

If the densities of ρ, μ are bounded, then

$$W_{2,\varepsilon}^2(\rho, \mu) + \varepsilon \text{KL}(\pi^{(P_\varepsilon)} | \rho \otimes \mu) = W_2^2(\rho, \mu) - \frac{\varepsilon}{2} (\text{KL}(\rho | \lambda) + \text{KL}(\mu | \lambda)) \\ - \frac{\varepsilon}{2} d \log(\pi \varepsilon) + \frac{\varepsilon^2}{16} I(\rho, \mu) + o(\varepsilon^2),$$

where

- ▶ λ is the Lebesgue measure on \mathbb{R}^d .
- ▶ $I(\rho, \mu)$ is the integrated Fisher information along the 2-Wasserstein geodesic connecting ρ and μ .

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- ▶ **In the discrete setting** (where ρ, μ are discrete): Cominetti and Martín (1994); Weed (2018) showed an **exponential convergence rate**:

$$0 \leq W_{2,\varepsilon}^2(\rho, \mu) - W_2^2(\rho, \mu) \leq C_1(\rho, \mu) \exp\left(-\frac{C_2(\rho, \mu)}{\varepsilon}\right),$$

where $C_1(\rho, \mu), C_2(\rho, \mu)$ are explicit positive constants that depend on ρ and μ .

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Quadratic Optimal Transport with Entropic Regularization

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- ▶ **In the continuous setting** (where ρ, μ are a.c.): Adams et al. (2011); Duong et al. (2013); Erbar et al. (2015); Pal (2019); Conforti and Tamanini (2021) gave $1^{\text{st}}/2^{\text{nd}}$ **order asymptotics**.
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What about the intermediate semi-discrete setting (where ρ is a.c. and μ is discrete)?

Convergence Bounds for Entropic SDOT

Entropic Semi-discrete Optimal Transport

▶ **Semi-discrete setting:**

- ▶ Let $\mathcal{X} \subset \mathbb{R}^d$ compact and $\rho \in \mathcal{P}_{a.c.}(\mathcal{X})$ absolutely continuous.
- ▶ Let $\mathcal{Y} = \{y_1, \dots, y_N\} \subset \mathbb{R}^d$ and $\mu = \sum_{i=1}^N \mu_i \delta_{y_i} \in \mathcal{P}(\mathcal{Y})$.

- ▶ Note that (P_ε) is equivalent to a regularized "maximum covariance" problem:

$$\boxed{\max_{\pi \in \Pi(\rho, \mu)} \int_{\mathcal{X} \times \mathcal{Y}} \langle x | y \rangle d\pi(x, y) - \varepsilon \text{KL}(\pi | \rho \otimes \sigma)}, \quad (P'_\varepsilon)$$

where $\sigma = \sum_{i=1}^N \delta_{y_i}$, with the relation:

$$(P_{2\varepsilon}) = M_2(\rho) + M_2(\mu) - 2\varepsilon \mathcal{H}(\mu) - 2 \times (P'_\varepsilon).$$

Convergence Bounds for Entropic SDOT

Entropic Semi-discrete Optimal Transport

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- ▶ (P'_ε) admits a **unique solution** π^ε
 - ▶ by ε -strong concavity of (P'_ε) if $\varepsilon > 0$.
 - ▶ by Brenier (1991) theorem (ρ is a.c.) if $\varepsilon = 0$.

Convergence Bounds for Entropic SDOT

Entropic Semi-discrete Optimal Transport

- ▶ **(Semi-)Dual formulation** with strong duality (Genevay et al. (2016); Bercu and Bigot (2020)):

$$\min_{\psi \in \mathbb{R}^N} \int_{\mathcal{X}} \psi^{c,\varepsilon} d\rho + \langle \psi | \mu \rangle + \varepsilon, \quad (\text{D}_\varepsilon)$$

where $\psi^{c,\varepsilon}$ is the (c, ε) /Legendre transform of ψ :

$$\psi^{c,\varepsilon}(x) = \begin{cases} \varepsilon \log \left(\sum_{i=1}^N e^{\frac{\langle x | y_i \rangle - \psi_i}{\varepsilon}} \right) & \text{if } \varepsilon > 0, \\ \max_{i=1, \dots, N} \langle x | y_i \rangle - \psi_i = \psi^*(x) & \text{if } \varepsilon = 0. \end{cases}$$

Convergence Bounds for Entropic SDOT

Entropic Semi-discrete Optimal Transport

- ▶ (Semi-)Dual formulation:

$$\min_{\psi \in \mathbb{R}^N} \int_{\mathcal{X}} \psi^{c, \varepsilon} d\rho + \langle \psi | \mu \rangle + \varepsilon. \quad (D_\varepsilon)$$

- ▶ Notice that ψ and $\psi + c\mathbb{1}_N$ yield the same value:

$$\min_{\psi \in \mathbb{R}^N, \langle \psi | \mathbb{1}_N \rangle = 0} \int_{\mathcal{X}} \psi^{c, \varepsilon} d\rho + \langle \psi | \mu \rangle + \varepsilon. \quad (D_\varepsilon)$$

- ▶ By strict convexity, (D_ε) admits a **unique solution** $\psi^\varepsilon \in (\mathbb{1}_N)^\perp$.

Convergence Bounds for Entropic SDOT

Entropic Semi-discrete Optimal Transport

$$\min_{\psi \in \mathbb{R}^N, \langle \psi | \mathbb{1}_N \rangle = 0} \int_{\mathcal{X}} \psi^{c, \varepsilon} d\rho + \langle \psi | \mu \rangle + \varepsilon. \quad (D_\varepsilon)$$

► **First order condition:**

$$\mu(\{y_i\}) = \begin{cases} \int_{x \in \mathcal{X}} e^{\frac{\langle x | y_i \rangle - \psi_i^\varepsilon - (\psi^\varepsilon)^{c, \varepsilon}(x)}{\varepsilon}} d\rho(x) & \text{if } \varepsilon > 0, \\ \int_{x \in \mathcal{X}} \mathbb{1}_{\text{Lag}_i(\psi^0)}(x) d\rho(x) = \rho(\text{Lag}_i(\psi^0)) & \text{if } \varepsilon = 0, \end{cases}$$

where $\text{Lag}_i(\psi) = \{x \in \mathcal{X} \mid \forall j, \langle x | y_i \rangle - \psi_i \geq \langle x | y_j \rangle - \psi_j\}$.

► **Primal-dual relationship:** $\forall A \subset \mathcal{X}, i \in \{1, \dots, N\}$,

$$\pi^\varepsilon(A, \{y_i\}) = \begin{cases} \int_{x \in A} e^{\frac{\langle x | y_i \rangle - \psi_i^\varepsilon - (\psi^\varepsilon)^{c, \varepsilon}(x)}{\varepsilon}} d\rho(x) & \text{if } \varepsilon > 0, \\ \int_{x \in A} \mathbb{1}_{\text{Lag}_i(\psi^0)}(x) d\rho(x) = \rho(\text{Lag}_i(\psi^0) \cap A) & \text{if } \varepsilon = 0. \end{cases}$$

Convergence Bounds for Entropic SDOT

Entropic Semi-discrete Optimal Transport

- ▶ Laguerre cells: a 2-dimensional example



$$\rho = \mathbb{1}_{[a,b] \times [c,d]} \text{ and } \mu = \sum_{i=1}^N \mu_i \delta_{y_i}.$$

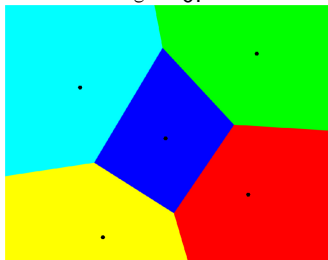
Convergence Bounds for Entropic SDOT

Entropic Semi-discrete Optimal Transport

$$\text{Lag}_i(\psi^0) = \{x \in \mathcal{X} \mid \forall j, \langle x \mid y_i \rangle - \psi_i^0 \geq \langle x \mid y_j \rangle - \psi_j^0\}.$$

(Figures inspired from Peyré and Cuturi (2019))

$\varepsilon = 0$:



Each color corresponds to one of $(\text{Lag}_i(\psi^0))_{i=1, \dots, N}$.

- ▶ First-order condition: $\mu(\{y_i\}) = \rho(\text{Lag}_i(\psi^0))$.
- ▶ Primal-dual relation: $\forall A \subset \mathcal{X}, \pi^0(A, \{y_i\}) = \rho(\text{Lag}_i(\psi^0) \cap A)$

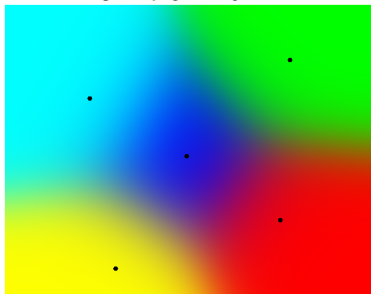
$$\implies \boxed{\text{Lag}_i(\psi^0) = (T_{\rho \rightarrow \mu})^{-1}(\{y_i\}).}$$

Convergence Bounds for Entropic SDOT

Entropic Semi-discrete Optimal Transport

$$\pi_{x,i}^\varepsilon := \frac{e^{(\langle x|y_i \rangle - \psi_i^\varepsilon)/\varepsilon}}{\sum_j e^{(\langle x|y_j \rangle - \psi_j^\varepsilon)/\varepsilon}}.$$

$$\varepsilon = 7.5 \times 10^{-2}:$$



Each color represents one of $(x \mapsto \pi_{x,i}^\varepsilon)_{i=1,\dots,N'}$, level of transparency = value.

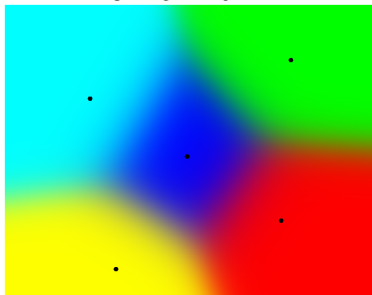
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Convergence Bounds for Entropic SDOT

Entropic Semi-discrete Optimal Transport

$$\pi_{x,i}^\varepsilon := \frac{e^{(\langle x|y_i \rangle - \psi_i^\varepsilon)/\varepsilon}}{\sum_j e^{(\langle x|y_j \rangle - \psi_j^\varepsilon)/\varepsilon}}.$$

$$\varepsilon = 5 \times 10^{-2}:$$



Each color represents one of $(x \mapsto \pi_{x,i}^\varepsilon)_{i=1,\dots,N}$, level of transparency = value.

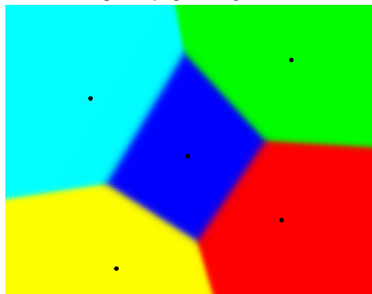
- ▶ First-order condition: $\mu(\{y_i\}) = \int_{x \in \mathcal{X}} \pi_{x,i}^\varepsilon d\rho(x)$.
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Convergence Bounds for Entropic SDOT

Entropic Semi-discrete Optimal Transport

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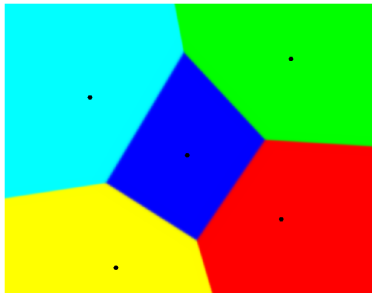
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Convergence Bounds for Entropic SDOT

Entropic Semi-discrete Optimal Transport

$$\pi_{x,i}^\varepsilon := \frac{e^{(\langle x|y_i \rangle - \psi_i^\varepsilon)/\varepsilon}}{\sum_j e^{(\langle x|y_j \rangle - \psi_j^\varepsilon)/\varepsilon}}.$$

$$\varepsilon = 2.5 \times 10^{-3}:$$



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Convergence Bounds for Entropic SDOT

Non-asymptotic Behavior of Potentials

- ▶ Recent result from Altschuler, Niles-Weed and Stromme (2021) (Theorem 1.1): *under regularity assumptions on ρ ,*

$$W_{2,\varepsilon}^2(\rho, \mu) = W_2^2(\rho, \mu) + \varepsilon^2 \frac{\pi^2}{12} \sum_{i < j} \frac{w_{ij}}{\|y_i - y_j\|} + o(\varepsilon^2),$$

where $w_{ij} = \int_{\text{Lag}_i(\psi^0) \cap \text{Lag}_j(\psi^0)} \rho(x) d\mathcal{H}^{d-1}(x)$.

Convergence Bounds for Entropic SDOT

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where $w_{ij} = \int_{\text{Lag}_i(\psi^0) \cap \text{Lag}_j(\psi^0)} \rho(x) d\mathcal{H}^{d-1}(x)$.

- ▶ Showed using (Theorem 1.3 in Altschuler et al. (2021)):

$$\lim_{\varepsilon \rightarrow 0} \frac{1}{\varepsilon} (\psi^\varepsilon - \psi^0) = \dot{\psi}^\varepsilon \Big|_{\varepsilon=0} = 0,$$

where $\dot{\psi}^\varepsilon = \frac{\partial}{\partial \varepsilon} \psi^\varepsilon$.

Convergence Bounds for Entropic SDOT

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$$\lim_{\varepsilon \rightarrow 0} \frac{1}{\varepsilon} (\psi^\varepsilon - \psi^0) = \dot{\psi}^\varepsilon \Big|_{\varepsilon=0} = 0.$$

This result can be extended and quantified with a non-asymptotic analysis.

Convergence Bounds for Entropic SDOT

Non-asymptotic Behavior of Potentials

- ▶ **Assumption:** *The compact set \mathcal{X} is convex. The source density ρ is α -Hölder continuous for some $\alpha \in (0, 1]$ and verifies on \mathcal{X} :*

$$0 < m_\rho \leq \rho \leq M_\rho < +\infty.$$

Convergence Bounds for Entropic SDOT

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$$0 < m_\rho \leq \rho \leq M_\rho < +\infty.$$

Theorem (D., 2021): *The mapping $\varepsilon \mapsto \psi^\varepsilon$ from \mathbb{R}_+^* to $(\mathbb{1}_N)^\perp$ is \mathcal{C}^1 . For any $\varepsilon > 0, \alpha' \in (0, \alpha)$,*

$$\|\dot{\psi}^\varepsilon\|_2 \lesssim \min(\varepsilon^{\alpha'}, 1),$$

where $\dot{\psi}^\varepsilon = \frac{\partial}{\partial \varepsilon} \psi^\varepsilon$ and \lesssim hides multiplicative constants that depend on $\mathcal{X}, \rho, \mathcal{Y}, \mu$.

Convergence Bounds for Entropic SDOT

Non-asymptotic Behavior of Potentials

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► **Remark:** A rough upperbound on the constant is

$$c^{(d)} \times \frac{N}{\underline{\mu}} \frac{M_\rho}{m_\rho} e^{R_{\mathcal{Y}} \text{diam}(\mathcal{X})} \left(N R_{\mathcal{X}} \text{diam}(\mathcal{Y}) + \log \frac{1}{\underline{\mu}} \right. \\ \left. + N^2 M_\rho \text{diam}(\mathcal{X})^{d-1} \left(1 + \frac{C_\rho}{\delta^\alpha} + R_{\mathcal{X}} \text{diam}(\mathcal{Y}) + \log \frac{1}{\underline{\mu}} \right) \right. \\ \left. + N^3 M_\rho \frac{\text{diam}(\mathcal{X})^{d-2} \text{diam}(\mathcal{Y})^4}{\cos(\theta/2)\delta^4} \left(1 + R_{\mathcal{X}} \text{diam}(\mathcal{Y}) + \log \frac{1}{\underline{\mu}} \right) \right),$$

where $\mathcal{X} \subset B(0, R_{\mathcal{X}})$, $\mathcal{Y} \subset B(0, R_{\mathcal{Y}})$, $\underline{\mu} = \min_i \mu_i > 0$, $\delta = \min_{i \neq j} \|y_i - y_j\| > 0$,

$$\theta = \max_{i,j,k} \{\angle y_i y_j y_k \mid \angle y_i y_j y_k < \pi\}, \quad \forall x, x' \in \mathcal{X}, \quad \left| \rho(x) - \rho(x') \right| \leq C_\rho \left\| x - x' \right\|^\alpha.$$

Convergence Bounds for Entropic SDOT

Non-asymptotic Behavior of Potentials

Corollary (D., 2021): *Let $0 < \varepsilon' \leq \varepsilon$. For any $\alpha' \in (0, \alpha)$,*

$$\left\| \psi^\varepsilon - \psi^{\varepsilon'} \right\|_\infty \lesssim \varepsilon^{\alpha'} (\varepsilon - \varepsilon').$$

Convergence Bounds for Entropic SDOT

Non-asymptotic Behavior of Potentials

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- ▶ **Remark:** May "justify" ε -scaling heuristic, where ε is decreased over the iterations of an algorithm that estimates ψ^0 .

Convergence Bounds for Entropic SDOT

Non-asymptotic Behavior of Potentials

Corollary (D., 2021): Let $0 < \varepsilon' \leq \varepsilon$. For any $\alpha' \in (0, \alpha)$,

$$\left\| \psi^\varepsilon - \psi^{\varepsilon'} \right\|_\infty \lesssim \varepsilon^{\alpha'} (\varepsilon - \varepsilon').$$

In particular, letting ε' go to 0 yields

$$\left\| \psi^\varepsilon - \psi^0 \right\|_\infty \lesssim \varepsilon^{1+\alpha'}.$$

Additionally, for ρ -a.e. $x \in \mathcal{X}$,

$$\left| \pi^\varepsilon(x, \cdot) - \pi^0(x, \cdot) \right| \lesssim e^{-c_x/\varepsilon},$$

where $c_x = \min_{i \in \{1, \dots, N\}} \{(\psi^0)^*(x) - \langle x | y_i \rangle + \psi_i^0 \mid \langle x | y_i \rangle - \psi_i^0 \neq (\psi^0)^*(x)\} > 0$.

Convergence Bounds for Entropic SDOT

Non-asymptotic Expansion of the Difference of Costs

Theorem (D., 2021): For any $\alpha' \in (0, \alpha)$ and $\varepsilon > 0$,

$$\left| W_{2,\varepsilon}^2(\rho, \mu) - W_2^2(\rho, \mu) - \varepsilon^2 \frac{\pi^2}{12} \sum_{i < j} \frac{w_{ij}}{\|y_i - y_j\|} \right| \lesssim \varepsilon^{2+\alpha'}.$$

This inequality is tight.

► **Remark:** No third-order expansion.

Sketch of proof for $\|\psi^\varepsilon\|_2 \lesssim \min(\varepsilon^{\alpha'}, 1)$

A governing O.D.E.

- ▶ Dual formulation:

$$\min_{\psi \in \mathbb{R}^N, \langle \psi | \mathbb{1}_N \rangle = 0} \int_{\mathcal{X}} \psi^{c, \varepsilon} d\rho + \langle \psi | \mu \rangle + \varepsilon. \quad (\text{D}_\varepsilon)$$

- ▶ Regularized Kantorovich's functional: $\forall \psi \in \mathbb{R}^N$,

$$\begin{aligned} \mathcal{K}^\varepsilon(\psi) &= \int_{\mathcal{X}} \psi^{c, \varepsilon} d\rho + \varepsilon \\ &= \int_{\mathcal{X}} \varepsilon \log \left(\sum_{i=1}^N \exp \left(\frac{\langle x | y_i \rangle - \psi_i}{\varepsilon} \right) \right) d\rho(x) + \varepsilon. \end{aligned}$$

- ▶ \mathcal{K}^ε strictly convex on $(\mathbb{1}_N)^\perp$. First-order condition for (D_ε) :
$$\nabla \mathcal{K}^\varepsilon(\psi^\varepsilon) = -\mu.$$

Sketch of proof for $\|\dot{\psi}^\varepsilon\|_2 \lesssim \min(\varepsilon^{\alpha'}, 1)$

A governing O.D.E.

- ▶ Regularized Kantorovich's functional: $\forall \psi \in \mathbb{R}^N$,

$$\mathcal{K}^\varepsilon(\psi) = \int_{\mathcal{X}} \varepsilon \log \left(\sum_{i=1}^N \exp \left(\frac{\langle x | y_i \rangle - \psi_i}{\varepsilon} \right) \right) d\rho(x) + \varepsilon.$$

- ▶ \mathcal{K}^ε strictly convex on $(\mathbb{1}_N)^\perp$. First-order condition for (D_ε) :

$$\nabla \mathcal{K}^\varepsilon(\psi^\varepsilon) = -\mu.$$

- ▶ **Implicit function theorem:**

- ▶ $\psi \mapsto \mathcal{K}^\varepsilon(\psi)$ is a \mathcal{C}^2 strictly convex mapping from $(\mathbb{1}_N)^\perp$ to \mathbb{R} .
- ▶ $\varepsilon \mapsto \nabla \mathcal{K}^\varepsilon(\psi)$ is a \mathcal{C}^1 mapping from \mathbb{R}_+^* to \mathbb{R} .

$\implies \varepsilon \mapsto \psi^\varepsilon$ is a \mathcal{C}^1 mapping from \mathbb{R}_+^* to $(\mathbb{1}_N)^\perp$ and

$$\nabla^2 \mathcal{K}^\varepsilon(\psi^\varepsilon) \dot{\psi}^\varepsilon + \frac{\partial}{\partial \varepsilon} (\nabla \mathcal{K}^\varepsilon)(\psi^\varepsilon) = 0.$$

Sketch of proof for $\|\dot{\psi}^\varepsilon\|_2 \lesssim \min(\varepsilon^{\alpha'}, 1)$

A governing O.D.E.

- ▶ The potential ψ^ε satisfies

$$\nabla^2 \mathcal{K}^\varepsilon(\psi^\varepsilon) \dot{\psi}^\varepsilon + \frac{\partial}{\partial \varepsilon} (\nabla \mathcal{K}^\varepsilon)(\psi^\varepsilon) = 0.$$

- ▶ \implies An upper bound on $\|\dot{\psi}^\varepsilon\|$ may be obtained from:
 - ▶ A lower bound on $\nabla^2 \mathcal{K}^\varepsilon(\psi^\varepsilon) \rightarrow$ **Prékopa-Leindler inequality**.
 - ▶ An upper bound on $\frac{\partial}{\partial \varepsilon} (\nabla \mathcal{K}^\varepsilon)(\psi^\varepsilon) \rightarrow$ **"Laplace's method"**.

Sketch of proof for $\|\dot{\psi}^\varepsilon\|_2 \lesssim \min(\varepsilon^{\alpha'}, 1)$

Strong convexity estimate of \mathcal{K}^ε

Theorem (D., 2021): For any $\varepsilon > 0$ and $v \in \mathbb{R}^N$,

$$\text{Var}_\mu(v) \leq \left(e^{R_{\text{y diam}}(\mathcal{X})} \frac{M_\rho}{m_\rho} + \varepsilon \right) \langle v | \nabla^2 \mathcal{K}^\varepsilon(\psi^\varepsilon) v \rangle.$$

Sketch of proof for $\|\dot{\psi}^\varepsilon\|_2 \lesssim \min(\varepsilon^{\alpha'}, 1)$

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Theorem (D., 2021): For any $\varepsilon > 0$ and $v \in \mathbb{R}^N$,

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- **Remark:** this result is mainly deduced from the Prékopa-Leindler inequality:

Let $0 < \lambda < 1$ and $f, g, h : \mathbb{R}^N \rightarrow \mathbb{R}_+$. Assume that $\forall x, y \in \mathbb{R}^N$,

$$h((1 - \lambda)x + \lambda y) \geq f(x)^{1-\lambda} g(y)^\lambda.$$

Then

$$\|h\|_1 \geq \|f\|_1^{1-\lambda} \|g\|_1^\lambda.$$

Sketch of proof for $\|\dot{\psi}^\varepsilon\|_2 \lesssim \min(\varepsilon^{\alpha'}, 1)$

Strong convexity estimate of \mathcal{K}^ε

Theorem (D., 2021): For any $\varepsilon > 0$ and $v \in \mathbb{R}^N$,

$$\text{Var}_\mu(v) \leq \left(e^{R_{\mathcal{Y}} \text{diam}(\mathcal{X})} \frac{M_\rho}{m_\rho} + \varepsilon \right) \langle v | \nabla^2 \mathcal{K}^\varepsilon(\psi^\varepsilon) v \rangle.$$

- ▶ **Remark:** this result is deduced mainly from the Prékopa-Leindler inequality.
- ▶ **Remark:** as $\varepsilon \rightarrow 0$, recover a similar estimate in the unregularized case that was proved using the Brascamp-Lieb inequality (D. and Mériçot, 2021):

$$\text{Var}_\mu(v) \leq \left(e^{R_{\mathcal{Y}} \text{diam}(\mathcal{X})} \frac{M_\rho}{m_\rho} \right) \langle v | \nabla^2 \mathcal{K}^0(\psi^0) v \rangle.$$

Sketch of proof for $\|\dot{\psi}^\varepsilon\|_2 \lesssim \min(\varepsilon^{\alpha'}, 1)$

Bound on the second term $\frac{\partial}{\partial \varepsilon}(\nabla \mathcal{K}^\varepsilon)(\psi^\varepsilon)$

Theorem (D., 2021): For any $\varepsilon > 0$,

$$\left\| \frac{\partial}{\partial \varepsilon}(\nabla \mathcal{K}^\varepsilon)(\psi^\varepsilon) \right\|_\infty \lesssim \min\left(\varepsilon^{\alpha'}, \frac{1}{\varepsilon}\right).$$

Sketch of proof for $\|\dot{\psi}^\varepsilon\|_2 \lesssim \min(\varepsilon^{\alpha'}, 1)$

Bound on the second term $\frac{\partial}{\partial \varepsilon}(\nabla \mathcal{K}^\varepsilon)(\psi^\varepsilon)$

Theorem (D., 2021): For any $\varepsilon > 0$,

$$\left\| \frac{\partial}{\partial \varepsilon}(\nabla \mathcal{K}^\varepsilon)(\psi^\varepsilon) \right\|_\infty \lesssim \min\left(\varepsilon^{\alpha'}, \frac{1}{\varepsilon}\right).$$

► **Proof idea:** We have

$$\left[\frac{\partial}{\partial \varepsilon}(\nabla \mathcal{K}^\varepsilon)(\psi^\varepsilon) \right]_i = \int_{\mathcal{X}} \sum_{j \neq i} \left(\frac{f_i^\varepsilon(x) - f_j^\varepsilon(x)}{\varepsilon^2} \right) \pi_{x,j}^\varepsilon \pi_{x,i}^\varepsilon d\rho(x),$$

where $\forall j, f_j^\varepsilon(x) = \langle x | y_j \rangle - \psi_j^\varepsilon$ and $\pi_{x,j}^\varepsilon = \frac{\exp(\frac{f_j^\varepsilon(x)}{\varepsilon})}{\sum_k \exp(\frac{f_k^\varepsilon(x)}{\varepsilon})}$.

⇒ Control $|f_i^\varepsilon(x) - f_j^\varepsilon(x)|$, $\pi_{x,i}^\varepsilon$, $\pi_{x,j}^\varepsilon$ depending on the position of x in $\mathcal{X} = \bigcup_i \text{Lag}_i(\psi^\varepsilon)$.

Numerical illustrations

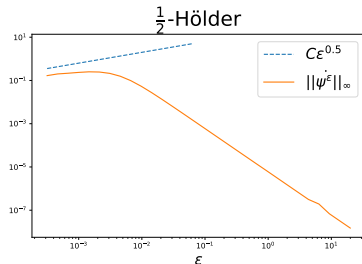
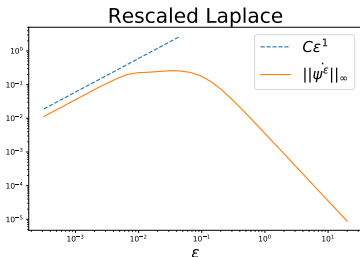
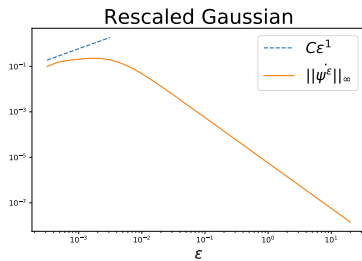
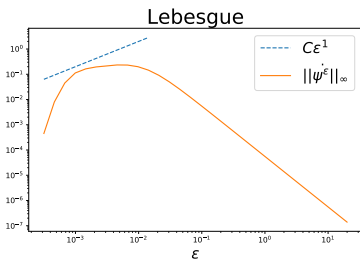
Behavior of $\varepsilon \mapsto \psi^\varepsilon$

- ▶ Let $\mathcal{X} = [-1, 1]$, ρ symmetric on \mathcal{X} and $\mu = \frac{1}{5} \sum_{i=1}^5 \delta_{y_i}$, where $\{y_1, \dots, y_5\} \subset \mathcal{X}$.
- ▶ Consider 4 different sources:
 - ▶ Lebesgue: $\rho(x) \propto \mathbb{1}_{[-1,1]}(x)$,
 - ▶ Rescaled Gaussian: $\rho(x) \propto e^{-x^2/2\sigma^2} \mathbb{1}_{[-1,1]}(x)$,
 - ▶ Rescaled Laplace: $\rho(x) \propto e^{-|x|} \mathbb{1}_{[-1,1]}(x)$,
 - ▶ $\frac{1}{2}$ -Hölder density: $\rho(x) \propto (1 - |x|^{1/2}) \mathbb{1}_{[-1,1]}(x)$.

Numerical illustrations

Behavior of $\varepsilon \mapsto \psi^\varepsilon$

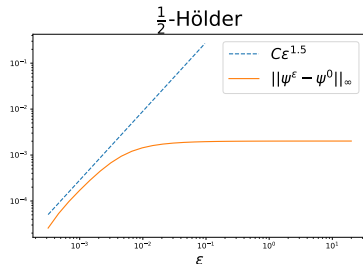
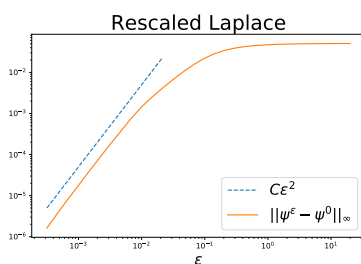
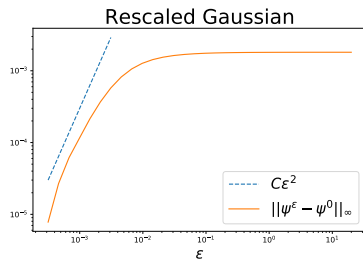
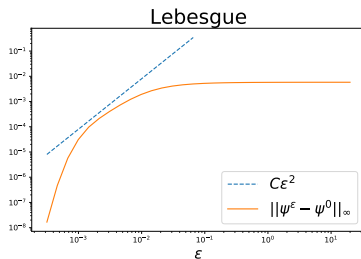
- ▶ Observe $\|\dot{\psi}^\varepsilon\|_2 \lesssim \min(\varepsilon^{\alpha'}, 1)$:



Numerical illustrations

Behavior of $\varepsilon \mapsto \psi^\varepsilon$

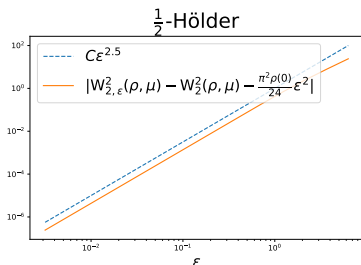
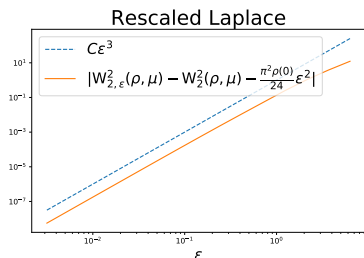
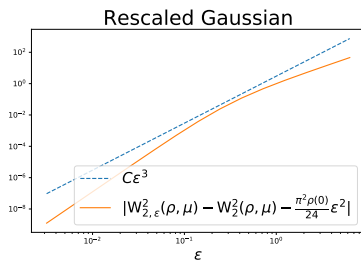
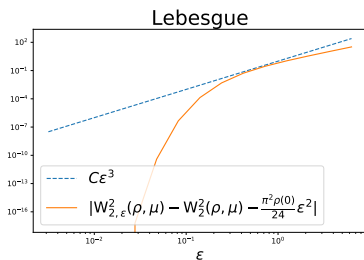
- ▶ Observe $\|\psi^\varepsilon - \psi^0\|_2 \lesssim \varepsilon^{1+\alpha'}$:



Numerical illustrations

Difference of Costs

- Observe $\left| W_{2,\varepsilon}^2(\rho, \mu) - W_2^2(\rho, \mu) - \varepsilon^2 \frac{\pi^2}{12} \sum_{i < j} \frac{w_{ij}}{\|y_i - y_j\|} \right| \lesssim \varepsilon^{2+\alpha'}$:



Thank you for your attention!

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ε -scaling

Corollary (D., 2021): Let $0 < \varepsilon' \leq \varepsilon$. For any $\alpha' \in (0, \alpha)$,

$$\left\| \psi^\varepsilon - \psi^{\varepsilon'} \right\|_\infty \lesssim \varepsilon^{\alpha'} (\varepsilon - \varepsilon').$$

- ▶ **Remark:** (ε -scaling) Assume we know an algorithm `approx_psi` such that

$$\widetilde{\psi}^\varepsilon := \text{approx_psi}(\rho, \mu, \varepsilon, \psi^{init}) \approx \psi^\varepsilon.$$

Fast if ε big or $\left\| \psi^\varepsilon - \psi^{init} \right\|$ small.

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Fast if ε big or $\|\psi^\varepsilon - \psi^{init}\|$ small.

ε -scaling approximates ψ^0 with $\widetilde{\psi}^{\varepsilon_K}$ for some $K \in \mathbb{N}^*$, where:

- ▶ $\varepsilon_0 > 0$ (**big**), $\widetilde{\psi}^{\varepsilon_0} := \text{approx_psi}(\rho, \mu, \varepsilon_0, \psi^{init})$,
- ▶ $\varepsilon_{k+1} = \varepsilon_k/2$,
- ▶ $\widetilde{\psi}^{\varepsilon_{k+1}} := \text{approx_psi}(\rho, \mu, \varepsilon_{k+1}, \widetilde{\psi}^{\varepsilon_k})$.

ε -scaling

Corollary (D., 2021): Let $0 < \varepsilon' \leq \varepsilon$. For any $\alpha' \in (0, \alpha)$,

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- $\varepsilon_{k+1} = \varepsilon_k/2$,
- $\widetilde{\psi}^{\varepsilon_{k+1}} := \text{approx_psi}(\rho, \mu, \varepsilon_{k+1}, \widetilde{\psi}^{\varepsilon_k})$.

Hope that $\left\| \widetilde{\psi}^{\varepsilon_k} - \psi^{\varepsilon_{k+1}} \right\|$ gets small as $\varepsilon_k \rightarrow 0$. See for instance Kosowsky and Yuille (1994); Schmitzer (2019); Feydy (2020).

Corollary (D., 2021): Let $0 < \varepsilon' \leq \varepsilon$. For any $\alpha' \in (0, \alpha)$,

$$\left\| \psi^\varepsilon - \psi^{\varepsilon'} \right\|_\infty \lesssim \varepsilon^{\alpha'} (\varepsilon - \varepsilon').$$

- ▶ **Remark:** (ε -scaling) Originally introduced for Bertsekas' auction algorithm (Bertsekas and Eckstein (1988)) for the N -assignment problem. Reduced worst case complexity:

$$O\left(\frac{N^2}{\varepsilon}\right) \rightarrow O\left(N^3 \log\left(\frac{1}{\varepsilon}\right)\right)$$

in order to get an ε -approximate solution.

Strong convexity estimate of \mathcal{K}^ε

Theorem (D., 2021): For any $\varepsilon > 0$ and $v \in \mathbb{R}^N$,

$$\text{Var}_\mu(v) \leq \left(e^{R_Y \text{diam}(\mathcal{X})} \frac{M_\rho}{m_\rho} + \varepsilon \right) \langle v | \nabla^2 \mathcal{K}^\varepsilon(\psi^\varepsilon) v \rangle.$$

► Notice that

$$\nabla^2 \mathcal{K}^\varepsilon(\psi) = \frac{1}{\varepsilon} \mathbb{E}_{x \sim \rho} \left(\text{diag}(\pi_x^\varepsilon(\psi)) - \pi_x^\varepsilon(\psi) \pi_x^\varepsilon(\psi)^\top \right),$$

where $\pi_x^\varepsilon(\psi) \in \mathbb{R}^N$ and $\forall i \in \{1, \dots, N\}$,

$$\pi_x^\varepsilon(\psi)_i = \frac{\exp\left(\frac{\langle x | y_i \rangle - \psi_i}{\varepsilon}\right)}{\sum_{j=1}^N \exp\left(\frac{\langle x | y_j \rangle - \psi_j}{\varepsilon}\right)}.$$

Strong convexity estimate of \mathcal{K}^ε

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► Introduce $I : \mathbb{R}^N \rightarrow \mathbb{R}, \psi \mapsto \log(\int_{\mathcal{X}} e^{-\psi^{c,\varepsilon}})$. Notice that I is \mathcal{C}^2 :

$$\begin{aligned} \nabla^2 I(\psi^\varepsilon) &= -\frac{1}{\varepsilon} \mathbb{E}_{x \sim \tilde{\rho}^\varepsilon} \left(\text{diag}(\pi_x^\varepsilon(\psi^\varepsilon)) - \pi_x^\varepsilon(\psi^\varepsilon) \pi_x^\varepsilon(\psi^\varepsilon)^\top \right) \\ &\quad + \mathbb{E}_{x \sim \tilde{\rho}^\varepsilon} \pi_x^\varepsilon(\psi^\varepsilon) \pi_x^\varepsilon(\psi^\varepsilon)^\top - \mathbb{E}_{x \sim \tilde{\rho}^\varepsilon} \pi_x^\varepsilon(\psi^\varepsilon) \mathbb{E}_{x \sim \tilde{\rho}^\varepsilon} \pi_x^\varepsilon(\psi^\varepsilon)^\top, \end{aligned}$$

where $\tilde{\rho}^\varepsilon := \frac{e^{-(\psi^\varepsilon)^{c,\varepsilon}}}{\int_{\mathcal{X}} e^{-(\psi^\varepsilon)^{c,\varepsilon}}}$.

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Theorem (D., 2021): For any $\varepsilon > 0$ and $v \in \mathbb{R}^N$,

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- $I : \psi \mapsto \log(\int_{\mathcal{X}} e^{-\psi^{c,\varepsilon}})$ is concave: Let $\psi, \varphi \in \mathbb{R}^N, 0 < \lambda < 1$. For any $u, v \in \mathcal{X}$, we have:

$$\begin{aligned} & (\lambda\psi + (1-\lambda)\varphi)^{c,\varepsilon}(\lambda u + (1-\lambda)v) \\ &= \varepsilon \log \left(\sum_{i=1}^N e^{\frac{\langle \lambda u + (1-\lambda)v | y_i \rangle - (\lambda\psi + (1-\lambda)\varphi)(y_i)}{\varepsilon}} \right) \\ &= \varepsilon \log \left(\sum_{i=1}^N \left(e^{\frac{\langle u | y_i \rangle - \psi(y_i)}{\varepsilon}} \right)^\lambda \left(e^{\frac{\langle v | y_i \rangle - \varphi(y_i)}{\varepsilon}} \right)^{1-\lambda} \right) \\ &\leq \varepsilon \log \left[\left(\sum_{i=1}^N e^{\frac{\langle u | y_i \rangle - \psi(y_i)}{\varepsilon}} \right)^\lambda \left(\sum_{i=1}^N e^{\frac{\langle v | y_i \rangle - \varphi(y_i)}{\varepsilon}} \right)^{1-\lambda} \right] \\ &= \lambda\psi^{c,\varepsilon}(u) + (1-\lambda)\varphi^{c,\varepsilon}(v). \end{aligned}$$

Strong convexity estimate of \mathcal{K}^ε

Theorem (D., 2021): For any $\varepsilon > 0$ and $v \in \mathbb{R}^N$,

$$\text{Var}_\mu(v) \leq \left(e^{R \text{diam}(\mathcal{X})} \frac{M_\rho}{m_\rho} + \varepsilon \right) \langle v | \nabla^2 \mathcal{K}^\varepsilon(\psi^\varepsilon) v \rangle.$$

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$$(\lambda\psi + (1-\lambda)\varphi)^{c,\varepsilon}(\lambda u + (1-\lambda)v) \leq \lambda\psi^{c,\varepsilon}(u) + (1-\lambda)\varphi^{c,\varepsilon}(v).$$

Denoting

$$h(u) = e^{-(\lambda\psi + (1-\lambda)\varphi)^{c,\varepsilon}(u)},$$
$$f(u) = e^{-\psi^{c,\varepsilon}(u)}, \quad g(u) = e^{-\varphi^{c,\varepsilon}(u)},$$

we thus have shown that

$$h(\lambda u + (1-\lambda)v) \geq f(u)^\lambda g(v)^{1-\lambda}.$$

⇒ Prékopa–Leindler inequality:

$$\int_{\mathcal{X}} h \geq \left(\int_{\mathcal{X}} f \right)^\lambda \left(\int_{\mathcal{X}} g \right)^{1-\lambda}.$$

Strong convexity estimate of \mathcal{K}^ε

Theorem (D., 2021): For any $\varepsilon > 0$ and $v \in \mathbb{R}^N$,

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► $I : \psi \mapsto \log\left(\int_{\mathcal{X}} e^{-\psi^c, \varepsilon}\right)$ is concave: Prékopa–Leindler inequality:

$$\int_{\mathcal{X}} h \geq \left(\int_{\mathcal{X}} f \right)^\lambda \left(\int_{\mathcal{X}} g \right)^{1-\lambda}.$$

$\implies I$ is concave:

$$\begin{aligned} I(\lambda\psi + (1-\lambda)\varphi) &= \log\left(\int_{\mathcal{X}} h\right) \\ &\geq \lambda \log\left(\int_{\mathcal{X}} f\right) + (1-\lambda) \log\left(\int_{\mathcal{X}} g\right) \\ &= \lambda I(\psi) + (1-\lambda)I(\varphi). \end{aligned}$$

Strong convexity estimate of \mathcal{K}^ε

Theorem (D., 2021): For any $\varepsilon > 0$ and $v \in \mathbb{R}^N$,

$$\text{Var}_\mu(v) \leq \left(e^{R_{\text{y diam}}(\mathcal{X})} \frac{M_\rho}{m_\rho} + \varepsilon \right) \langle v | \nabla^2 \mathcal{K}^\varepsilon(\psi^\varepsilon) v \rangle.$$

► Notice that

$$\nabla^2 \mathcal{K}^\varepsilon(\psi) = \frac{1}{\varepsilon} \mathbb{E}_{x \sim \rho} (\text{diag}(\pi_x^\varepsilon(\psi)) - \pi_x^\varepsilon(\psi) \pi_x^\varepsilon(\psi)^\top).$$

► Introduce $I : \mathbb{R}^N \rightarrow \mathbb{R}, \psi \mapsto \log(\int_{\mathcal{X}} e^{-\psi^{c,\varepsilon}})$. Notice that I is \mathcal{C}^2 and **concave**:

$$\begin{aligned} \nabla^2 I(\psi^\varepsilon) &= -\frac{1}{\varepsilon} \mathbb{E}_{x \sim \tilde{\rho}^\varepsilon} (\text{diag}(\pi_x^\varepsilon(\psi^\varepsilon)) - \pi_x^\varepsilon(\psi^\varepsilon) \pi_x^\varepsilon(\psi^\varepsilon)^\top) \\ &\quad + \mathbb{E}_{x \sim \tilde{\rho}^\varepsilon} \pi_x^\varepsilon(\psi^\varepsilon) \pi_x^\varepsilon(\psi^\varepsilon)^\top - \mathbb{E}_{x \sim \tilde{\rho}^\varepsilon} \pi_x^\varepsilon(\psi^\varepsilon) \mathbb{E}_{x \sim \tilde{\rho}^\varepsilon} \pi_x^\varepsilon(\psi^\varepsilon)^\top \leq 0, \end{aligned}$$

where $\tilde{\rho}^\varepsilon := \frac{e^{-(\psi^\varepsilon)^{c,\varepsilon}}}{\int_{\mathcal{X}} e^{-(\psi^\varepsilon)^{c,\varepsilon}}}$.

Upper bound on $\left\| \frac{\partial}{\partial \varepsilon} (\nabla \mathcal{K}^\varepsilon)(\psi^\varepsilon) \right\|_\infty$

Theorem (D., 2021): For any $\varepsilon > 0$,

$$\left\| \frac{\partial}{\partial \varepsilon} (\nabla \mathcal{K}^\varepsilon)(\psi^\varepsilon) \right\|_\infty \lesssim \varepsilon^{\alpha'}.$$

► We have

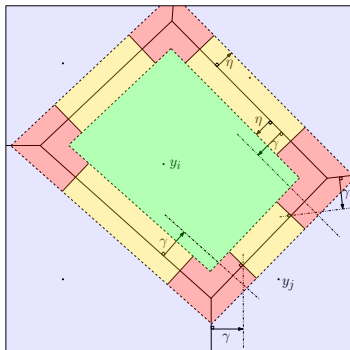
$$\left[\frac{\partial}{\partial \varepsilon} (\nabla \mathcal{K}^\varepsilon)(\psi^\varepsilon) \right]_i = \int_{\mathcal{X}} \sum_{j \neq i} \left(\frac{f_i^\varepsilon(x) - f_j^\varepsilon(x)}{\varepsilon^2} \right) \pi_{x,j}^\varepsilon \pi_{x,i}^\varepsilon d\rho(x),$$

where $\forall j, f_j^\varepsilon(x) = \langle x | y_j \rangle - \psi_j^\varepsilon$ and $\pi_{x,j}^\varepsilon = \frac{\exp(\frac{f_j^\varepsilon(x)}{\varepsilon})}{\sum_k \exp(\frac{f_k^\varepsilon(x)}{\varepsilon})}$.

Upper bound on $\left\| \frac{\partial}{\partial \varepsilon} (\nabla \mathcal{K}^\varepsilon)(\psi^\varepsilon) \right\|_\infty$

We have:

$$\left[\frac{\partial}{\partial \varepsilon} (\nabla \mathcal{K}^\varepsilon)(\psi^\varepsilon) \right]_i = \int_{\mathcal{X}} \sum_{j \neq i} \left(\frac{f_i^\varepsilon(x) - f_j^\varepsilon(x)}{\varepsilon^2} \right) \pi_{x,j}^\varepsilon \pi_{x,i}^\varepsilon d\rho(x).$$



Key technical result: for any $\eta, \gamma > 0$,

$$\begin{aligned} \left[\frac{\partial}{\partial \varepsilon} (\nabla \mathcal{K}^\varepsilon)(\psi) \right]_i &\lesssim \frac{1}{\varepsilon^2} e^{-\eta/\varepsilon} + \frac{\eta^{2+\alpha}}{\varepsilon^2} \\ &\quad + \frac{\gamma^2}{\varepsilon^2} (\eta + e^{-\eta/\varepsilon}) \\ &\quad + \frac{1}{\varepsilon^2} e^{-\tilde{\gamma}/\varepsilon} \left(\eta + \varepsilon \eta e^{\eta/\varepsilon} \right. \\ &\quad \quad \left. - \varepsilon^2 (e^{\eta/\varepsilon} - 1) \right), \end{aligned}$$

where $\tilde{\gamma} = \gamma\delta - \frac{\text{diam}(\mathcal{Y})^2}{\delta} \eta$ and
 $\delta = \min_{i \neq j} \|y_i - y_j\| > 0$.