

Quantitative Stability in Quadratic Optimal Transport

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EPFL

*CIRM Workshop PDE & Probability in interaction:
functional inequalities, optimal transport and particle systems*

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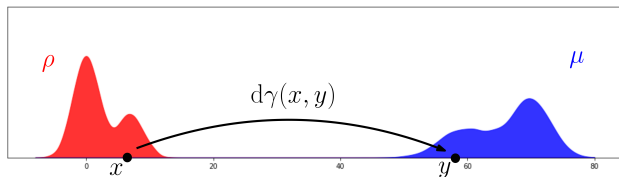
Introduction

Quadratic Optimal Transport problem (Monge, 1781; Kantorovich, 1942):

► Given $\rho, \mu \in \mathcal{P}_2(\mathbb{R}^d)$, solve

$$\inf_{\gamma \in \Gamma(\rho, \mu)} \int_{\mathbb{R}^d \times \mathbb{R}^d} \|x - y\|^2 d\gamma(x, y), \quad (\text{KP})$$

where $\Gamma(\rho, \mu) = \{\gamma \in \mathcal{P}_2(\mathbb{R}^d \times \mathbb{R}^d) \mid \forall A \subset \Omega, \gamma(A \times \mathbb{R}^d) = \rho(A), \gamma(\mathbb{R}^d \times A) = \mu(A)\}$.



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- ▶ 2-**Wasserstein distance** between ρ and μ :

$$W_2(\rho, \mu) := \left(\inf_{\gamma \in \Gamma(\rho, \mu)} \int_{\mathbb{R}^d \times \mathbb{R}^d} \|x - y\|^2 d\gamma(x, y) \right)^{1/2}.$$

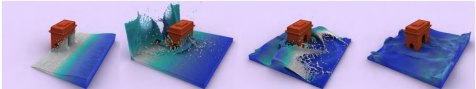
- ▶ 2-**Wasserstein space**: $(\mathcal{P}_2(\mathbb{R}^d), W_2)$.

→ Geodesic distance, interpolations, barycenters...

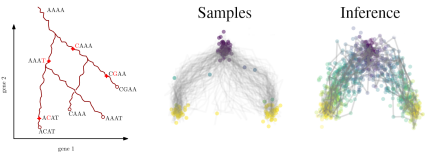
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► Strong physical modeling power:

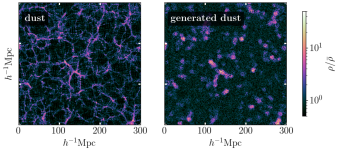
Euler equations: (de Goes et al., 2015)



Trajectory inference for single cell RNA-sequencing data: (Forrow et al., 2021; Chizat et al., 2022)



Cosmology: (Nikakhtar et al., 2023)



Quantum chemistry, meteorology, economics, image processing, machine learning...

Introduction

Is the quadratic optimal transport problem $\inf_{\gamma \in \Gamma(\rho, \mu)} \langle d^2 | \gamma \rangle$ **well-posed?**

1. Existence of optimal γ ? Verified.

(Kantorovich, 1942; Kellerer, 1984)

2. Uniqueness of optimal γ ? Not verified in general.

But well-studied and verified in many *particular* cases.

Theorem (Brenier, 1987): If ρ is **absolutely continuous**, then the optimal transport solution is **unique**. It is induced by a map $T : \mathbb{R}^d \rightarrow \mathbb{R}^d$ satisfying $T_{\#}\rho = \mu$ characterized by $T = \nabla\phi$ with ϕ convex.

For μ a.c. and under additional assumptions, optimal ϕ solution of the Monge-Ampère equation:

$$\forall x \in \Omega, \quad \det(D^2\phi(x))\mu(\nabla\phi(x)) = \rho(x).$$

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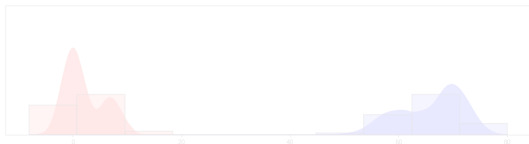
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Theorem (Villani, 2008): If $\rho_n \rightarrow \rho$, $\mu_n \rightarrow \mu$, then for $\gamma_n \in \Gamma(\rho_n, \mu_n)$ **optimal**, up to a subsequence, $\gamma_n \rightarrow \gamma \in \Gamma(\rho, \mu)$ **optimal**.

Example:



What is the *rate* of the convergence $\gamma_n \rightarrow \gamma$ in terms of the *rates* of convergence of $\rho_n \rightarrow \rho$ and $\mu_n \rightarrow \mu$?

→ Quantitative stability of optimal transport solutions?

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► **Quantitative stability** of optimal transport solutions w.r.t. problem data?

1. Beyond the case $\Omega = \mathbb{R}$, no general quantitative stability result.

2. Convex optimization viewpoint: $\min_{\gamma \in \Gamma(\rho, \mu)} \langle d^2 | \gamma \rangle$.

→ Strong/Uniform convexity? *Linear program.*

3. Elliptic PDE viewpoint: $\det(D^2\phi)\mu(\nabla\phi) = \rho$.

→ Uniform ellipticity? *Degenerate elliptic equation.*

Using the unconstrained dual problem, quantitative stability guarantees can be obtained.

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Part I.

Strong convexity of the dual quadratic optimal transport problem.

Part II.

Consequences: quantitative stability estimates for optimal transport maps, Wasserstein barycenters and entropic optimal transport.

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Dual problem

$$\min_{\gamma \in \Gamma(\rho, \mu)} \int \|x - y\|^2 d\gamma(x, y) = \int \|x\|^2 d\rho(x) + \int \|y\|^2 d\mu(y) - 2 \underbrace{\max_{\gamma \in \Gamma(\rho, \mu)} \int \langle x|y \rangle d\gamma(x, y)}_{:= \mathcal{T}(\rho, \mu)}.$$

- ▶ Get rid of constraint:

$$\mathcal{T}(\rho, \mu) = \max_{\gamma \geq 0} \int \langle \cdot | \cdot \rangle d\gamma + \min_{\phi, \psi} \int \phi d(\rho - \gamma_1) + \int \psi d(\mu - \gamma_2)$$

- ▶ Swap max and min:

$$\begin{aligned} \mathcal{T}(\rho, \mu) &= \min_{\phi, \psi} \int \phi d\rho + \int \psi d\mu + \max_{\gamma \geq 0} \int (\langle \cdot | \cdot \rangle - \phi \oplus \psi) d\gamma \\ &= \min_{\phi, \psi | \langle \cdot | \cdot \rangle \leq \phi \oplus \psi} \int \phi d\rho + \int \psi d\mu \\ &= \min_{\psi} \int \psi^* d\rho + \int \psi d\mu, \quad \text{where } \psi^*(x) = \sup_y \langle x|y \rangle - \psi(y). \end{aligned}$$

Remark: When ρ is a.c., $T = \nabla \psi^*$ where ψ is a minimizer.

Definition: $\mathcal{K}_\rho : \psi \mapsto \int \psi^* d\rho.$

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$$\boxed{\min_{\psi: \mathbb{R}^d \rightarrow \bar{\mathbb{R}}} \mathcal{K}_\rho(\psi) + \int \psi d\mu.} \quad (\text{DP})$$

► \mathcal{K}_ρ is convex. First order condition in (DP):

$$\psi_\mu \text{ minimizer in (DP)} \iff 0 \in \partial \mathcal{K}_\rho(\psi_\mu) + \mu \iff \psi_\mu \in (\partial \mathcal{K}_\rho)^{-1}(-\mu).$$

Stability estimate for $\mu \mapsto \psi_\mu$.

\iff

Strong/Uniform convexity estimate for $\psi \mapsto \mathcal{K}_\rho(\psi)$.

$F \in \mathcal{C}^2(\mathbb{R}^d)$ is strongly convex if there exists $\alpha > 0$ such that:

$$\forall x, y \in \mathbb{R}^d, t \in [0, 1], \quad \alpha \frac{t(1-t)}{2} \|x - y\|^2 \leq (1-t)F(x) + tF(y) - F((1-t)x + ty),$$

$$\iff \forall x, y \in \mathbb{R}^d, \quad \frac{\alpha}{2} \|x - y\|^2 \leq F(y) - F(x) - \langle \nabla F(x), y - x \rangle,$$

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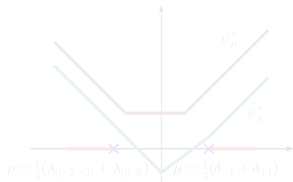
Strong convexity of the dual problem

► Strong convexity of $\mathcal{K}_\rho : \psi \mapsto \int \psi^* d\rho$?

1. Strong convexity should work "up to additive constants":

$$\forall c \in \mathbb{R}, \quad \mathcal{K}_\rho(\psi + c) = \mathcal{K}_\rho(\psi) - c.$$

2. Support of ρ should be connected:



$$\nabla \psi_\mu^* \# \rho = \nabla \tilde{\psi}_\mu^* \# \rho = \mu.$$

$$\implies \psi_\mu, \tilde{\psi}_\mu \in \arg \min_\psi \mathcal{K}_\rho(\psi) + \langle \psi | \mu \rangle.$$

$$\implies \forall t \in [0, 1],$$

$$\mathcal{K}_\rho((1-t)\psi_\mu + t\tilde{\psi}_\mu) = (1-t)\mathcal{K}_\rho(\psi_\mu) + t\mathcal{K}_\rho(\tilde{\psi}_\mu).$$

Assumption: Source ρ is absolutely continuous and satisfies a Poincaré-Wirtinger inequality: $\exists p \geq 1, C_{PW} \in (0, +\infty)$ s.t.

$$\forall f \in \mathcal{C}^1(\mathbb{R}^d), \quad \|f - \mathbb{E}_\rho f\|_{L^p(\rho)} \leq C_{PW} \|\nabla f\|_{L^p(\rho, \mathbb{R}^d)}.$$

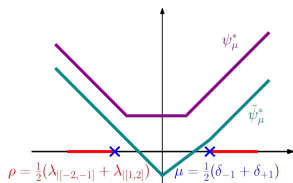
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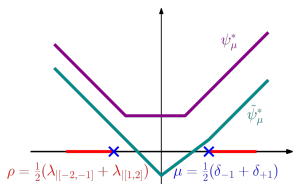
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$$\forall c \in \mathbb{R}, \quad \mathcal{K}_\rho(\psi + c) = \mathcal{K}_\rho(\psi) - c.$$

2. Support of ρ should be connected:



$$\nabla \psi_\mu^* \# \rho = \nabla \tilde{\psi}_\mu^* \# \rho = \mu.$$

$$\implies \psi_\mu, \tilde{\psi}_\mu \in \arg \min_\psi \mathcal{K}_\rho(\psi) + \langle \psi | \mu \rangle.$$

$$\implies \forall t \in [0, 1],$$

$$\mathcal{K}_\rho((1-t)\psi_\mu + t\tilde{\psi}_\mu) = (1-t)\mathcal{K}_\rho(\psi_\mu) + t\mathcal{K}_\rho(\tilde{\psi}_\mu).$$

Assumption: Source ρ is **absolutely continuous** and satisfies a **Poincaré-Wirtinger inequality**: $\exists \rho \geq 1, C_{PW} \in (0, +\infty)$ s.t.

$$\forall f \in \mathcal{C}^1(\mathbb{R}^d), \quad \|f - \mathbb{E}_\rho f\|_{L^p(\rho)} \leq C_{PW} \|\nabla f\|_{L^p(\rho, \mathbb{R}^d)}.$$

Strong convexity of the dual problem

- ▶ **"Subdifferential"** of \mathcal{K}_ρ ? (Fenchel-Young) $\forall \psi, \tilde{\psi} : \mathbb{R}^d \rightarrow \bar{\mathbb{R}},$

$$\langle \tilde{\psi} - \psi | -(\nabla \psi^*)_{\#} \rho \rangle \leq \mathcal{K}_\rho(\tilde{\psi}) - \mathcal{K}_\rho(\psi).$$

→ Gap in this inequality?

- ▶ A known result:

Theorem (Ambrosio, Gigli, 2011):

Assume $\psi, \tilde{\psi} \in C^1(\mathbb{R}^d)$, ψ is convex and $\tilde{\psi}$ is α -strongly convex for some $\alpha > 0$. Then,

$$\frac{\alpha}{2C_{PW}} \text{Var}_\rho(\tilde{\psi}^* - \psi^*) \leq \frac{\alpha}{2} \left\| \nabla \tilde{\psi}^* - \nabla \psi^* \right\|_{L^2(\rho, \mathbb{R}^d)}^2 \leq \mathcal{K}_\rho(\tilde{\psi}) - \mathcal{K}_\rho(\psi) + \langle \tilde{\psi} - \psi | (\nabla \psi^*)_{\#} \rho \rangle.$$

Strong assumption: $\tilde{\psi}$ is α -strongly convex $\iff \nabla \tilde{\psi}^*$ is $\frac{1}{\alpha}$ -Lipschitz continuous!

→ Not satisfied in general.

→ Implies that $\nabla \tilde{\psi}^*_{\#} \rho$ has a connected support.

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Strong convexity of the dual problem

Strong convexity estimate for the Kantorovich functional:

Theorem (D., Mérigot, 2021):

- ▶ Let $\mathcal{X} \subset \mathbb{R}^d$ compact convex, $\rho \in \mathcal{P}_{a.c.}(\mathcal{X})$ with $0 < m_\rho \leq \rho \leq M_\rho$.
- ▶ Let $\mathcal{Y} = B(0, R_Y) \subset \mathbb{R}^d$ compact and let $\mu, \nu \in \mathcal{P}(\mathcal{Y})$.

Then for ψ_μ, ψ_ν Kantorovich potentials between ρ and μ, ν ,

$$C_{d,\mathcal{X},\rho,\mathcal{Y}} \text{Var}_{\frac{1}{2}(\mu+\nu)}(\psi_\nu - \psi_\mu) \leq \mathcal{K}_\rho(\psi_\nu) - \mathcal{K}_\rho(\psi_\mu) + \langle \psi_\nu - \psi_\mu | \mu \rangle,$$

where $C_{d,\mathcal{X},\rho,\mathcal{Y}} = \left(e(d+1)2^{d-1}R_Y \text{diam}(\mathcal{X}) \frac{M_\rho^2}{m_\rho^2} \right)^{-1}$.

Strong convexity of the dual problem

$$\mathbb{V}\text{ar}_{\frac{1}{2}(\mu+\nu)}(\psi_\nu - \psi_\mu) \lesssim \mathcal{K}_\rho(\psi_\nu) - \mathcal{K}_\rho(\psi_\mu) + \langle \psi_\nu - \psi_\mu | \mu \rangle.$$

► Remarks:

1. Reference $\frac{1}{2}(\mu + \nu)$? Fenchel-Young (in)equality:

Proposition (D., Mériqot, 2021): $\frac{1}{2} \mathbb{V}\text{ar}_\rho(\psi_\mu^* - \psi_\nu^*) \leq \mathbb{V}\text{ar}_{\frac{1}{2}(\mu+\nu)}(\psi_\nu - \psi_\mu)$.

2. Optimal exponents.
3. Similar result with **non-compact targets**: main assumption is boundedness of ψ_μ^*, ψ_ν^* on \mathcal{X} . Satisfied if μ, ν have bounded moment of order $p > d$ (Morrey's inequality).
4. $\text{spt}(\rho) = \mathcal{X}$ **convex**? Can be relaxed.

Corollary (Carlier, D., Mériqot, 2022): If \mathcal{X} is a **connected finite union of convex sets** s.t. ρ satisfies a L^1 **Poincaré-Wirtinger inequality**, a similar estimate holds.

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$$\text{Var}_{\frac{1}{2}(\mu^0 + \mu^1)}(\psi^1 - \psi^0) \lesssim \mathcal{K}_\rho(\psi^1) - \mathcal{K}_\rho(\psi^0) + \langle \psi^1 - \psi^0 | \mu^0 \rangle.$$

► Elements of proof:

1. Let $v := \psi^1 - \psi^0$. For $t \in [0, 1]$, $\psi^t := \psi^0 + tv$, $\phi^t := (\psi^t)^*$ and $\tilde{v}^t = v(\nabla\phi^t)$. Then *under regularity assumptions*:

$$\frac{d}{dt}\mathcal{K}_\rho(\psi^t) = -\mathbb{E}_\rho \tilde{v}^t \quad \text{and} \quad \frac{d^2}{dt^2}\mathcal{K}_\rho(\psi^t) = \mathbb{E}_\rho \langle \nabla \tilde{v}^t | (D^2\phi^t)^{-1} \cdot \nabla \tilde{v}^t \rangle.$$

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4. With $\mu^t = (\nabla\phi^t)_{\#}\rho$, $\text{Var}_{\mu^t}(v) \leq \frac{M_\rho}{m_\rho} \exp(M_\phi - m_\phi) \frac{d^2}{dt^2}\mathcal{K}_\rho(\psi^t).$

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Outline

Part I.

Strong convexity of the dual quadratic optimal transport problem.

Part II.

Consequences: quantitative stability estimates for optimal transport maps, Wasserstein barycenters and entropic optimal transport.

Quantitative stability of optimal transport maps

► Motivation: (Approximated) Wasserstein geometry.

Theorem (Brenier, 1987): If $\rho \in \mathcal{P}_{2,a.c.}(\mathbb{R}^d)$, $\exists!$ ρ -a.e. $T_\mu : \mathbb{R}^d \rightarrow \mathbb{R}^d$ s.t. $(T_\mu)_\# \rho = \mu$, and $T_\mu = \nabla \phi_\mu$ with ϕ_μ **convex**.

1.

$$\implies W_2(\rho, \mu) = \|T_\mu - \text{id}\|_{L^2(\rho, \mathbb{R}^d)}.$$

2. Riemannian interpretation of $(\mathcal{P}_2(\mathbb{R}^d), W_2)$ (Otto, 2001; Ambrosio, Gigli, Savaré, 2004):

	Riemannian geometry	Optimal transport
Point	$x \in M$	$\mu \in \mathcal{P}_2(\mathbb{R}^d)$
Geodesic distance	$d_g(x, y)$	$W_2(\mu, \nu)$
Tangent space	$\mathcal{T}_\rho M$	$\mathcal{T}_\rho \mathcal{P}_2(\mathbb{R}^d) \subseteq L^2(\rho, \mathbb{R}^d)$
Inverse exponential map	$\exp^{-1}(x) \in \mathcal{T}_\rho M$	$T_\mu - \text{id} \in \mathcal{T}_\rho \mathcal{P}_2(\mathbb{R}^d)$
Distance in tangent space	$\ \exp^{-1}(x) - \exp^{-1}(y)\ _{g(\rho)}$	$\ T_\mu - T_\nu\ _{L^2(\rho, \mathbb{R}^d)}$

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Hilbertian distance used in image analysis (Wang et al., 2013) and other ML applications.

How much does $W_{2,\rho}$ distort W_2 ?

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How much does $\|T_\mu - T_\nu\|_{L^2(\rho, \mathbb{R}^d)}$ distort $W_2(\mu, \nu)$?

- ▶ Elementary results: $\mu \mapsto T_\mu$ is **continuous** and **reverse-Lipschitz**.

$$W_2(\mu, \nu) \leq \|T_\mu - T_\nu\|_{L^2(\rho, \mathbb{R}^d)}.$$

- ▶ Negative results: $\mu \mapsto T_\mu$ is **not better than $\frac{1}{2}$ -Hölder**.

Theorem (Andoni, Naor, Neiman, 2018):
 $(\mathcal{P}_2(\mathbb{R}^3), W_2)$ does not admit a bi-Hölder embedding into any L^p space.

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Theorem (Ambrosio, Gigli, 2011): Let $\Omega \subset \mathbb{R}^d$ compact, $\rho \in \mathcal{P}_{a.c.}(\Omega)$ and $\mu, \nu \in \mathcal{P}(\Omega)$. Assume that T_μ is L -Lipschitz. Then,

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$$\|T_\mu - T_\nu\|_{L^2(\rho, \mathbb{R}^d)} \leq C_{d, \rho, \mathcal{X}, \mathcal{Y}} W_1(\mu, \nu)^{\frac{1}{2(d-1)(d+2)}}.$$

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$$\|T_\mu - T_\nu\|_{L^2(\rho, \mathbb{R}^d)} \leq C_{d, \rho, \mathcal{X}, \mathcal{Y}}W_1(\mu, \nu)^{\frac{1}{2^{(d-1)(d+2)}}}.$$

Quantitative stability of optimal transport maps

Global & dimension-independent stability result (compact case):

Theorem (D., Mérigot, 2021):

- ▶ Let $\mathcal{X} \subset \mathbb{R}^d$ compact convex, $\rho \in \mathcal{P}_{a.c.}(\mathcal{X})$ with $0 < m_\rho \leq \rho \leq M_\rho$.
- ▶ Let $\mathcal{Y} = B(0, R_\mathcal{Y}) \subset \mathbb{R}^d$ bounded and $\mu, \nu \in \mathcal{P}(\mathcal{Y})$.

Then the OT maps T_μ, T_ν between ρ and μ, ν satisfy

$$\|T_\mu - T_\nu\|_{L^2(\rho, \mathbb{R}^d)} \leq C_{d, \rho, \mathcal{X}, \mathcal{Y}} W_1(\mu, \nu)^{1/6}.$$

▶ Remarks:

1. Optimal Hölder exponent? $\frac{1}{6} < \frac{1}{2}$.
2. The constant is explicit: $C_{d, \rho, \mathcal{X}, \mathcal{Y}} \approx C_d \left(\frac{M_\rho}{m_\rho}\right)^3 \text{diam}(\mathcal{X})^{d+1} R_\mathcal{Y}^2$.
3. **Proof idea:** strong convexity of \mathcal{K}_ρ and new Galgaliardo-Nirenberg type inequality:

Proposition (D., Mérigot, 2021):

For $K \subset \mathbb{R}^d$ compact and $u, v : K \rightarrow \mathbb{R}$ Lipschitz convex,

$$\|\nabla u - \nabla v\|_{L^2(K, \mathbb{R}^d)}^2 \leq C_d \mathcal{H}^{d-1}(\partial K)^{\frac{2}{3}} (\text{Lip}(u) + \text{Lip}(v))^{\frac{4}{3}} \|u - v\|_{L^2(K)}^{\frac{2}{3}}.$$

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Quantitative stability of optimal transport maps

Global stability result (non-compact case):

Theorem (Chazal, D., Mérigot, 2020/2021):

- ▶ Let $\mathcal{X} \subset \mathbb{R}^d$ compact convex, $\rho \in \mathcal{P}_{a.c.}(\mathcal{X})$ with $0 < m_\rho \leq \rho \leq M_\rho$.
- ▶ Let $p > d$ and $p \geq 4$ and let $\mu, \nu \in \mathcal{P}(\mathbb{R}^d)$ with p -th moment upper bounded by $M_p < +\infty$.

Then the OT maps T_μ, T_ν between ρ and μ, ν satisfy

$$\|T_\mu - T_\nu\|_{L^2(\rho, \mathbb{R}^d)} \leq C_{d, \rho, \mathcal{X}, p, M_p} W_1(\mu, \nu)^{\frac{p}{6p+16d}}.$$

▶ Remarks:

1. Concerns all sub-Gaussian and sub-exponential probability measures.
2. $\mu \mapsto T_\mu$ is a bi-Hölder embedding of $B_{W_p}(\delta_0, M_p) \subset (\mathcal{P}_2(\mathbb{R}^d), W_2)$ into $L^2(\rho, \mathbb{R}^d)$.

Outline

Part I.

Strong convexity of the dual quadratic optimal transport problem.

Part II.

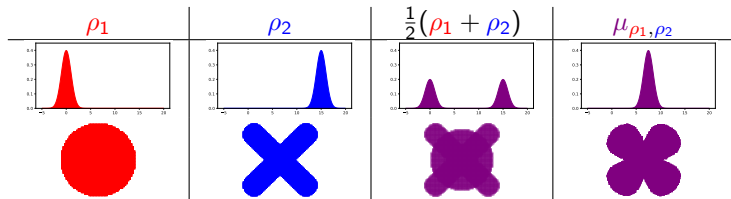
Consequences: quantitative stability estimates for optimal transport maps, Wasserstein barycenters and entropic optimal transport.

Quantitative stability of Wasserstein barycenters

Definition: Let $\Omega \subset \mathbb{R}^d$ compact. Wasserstein barycenter of $\rho_1, \dots, \rho_N \in \mathcal{P}(\Omega)$:

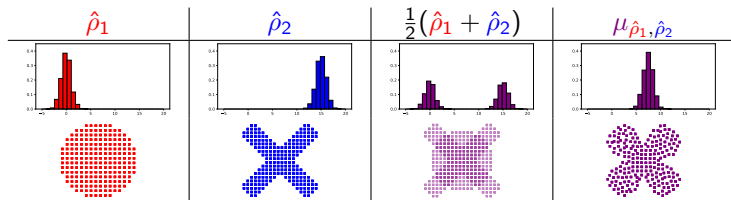
$$\mu_{\rho_1, \dots, \rho_N} \in \arg \min_{\mu \in \mathcal{P}(\Omega)} \frac{1}{2N} \sum_{i=1}^N W_2^2(\rho_i, \mu).$$

- ▶ Geometrically faithful "average" of probability measures:



Quantitative stability of Wasserstein barycenters

- ▶ Many applications, e.g. in
 1. Image processing (Rabin et al., 2011).
 2. Geometry processing (Solomon et al., 2015).
 3. Language processing (Colombo et al., 2021).
- ▶ ρ_1, ρ_2 often **not directly accessible**, but $\hat{\rho}_1, \hat{\rho}_2$ instead:



Can we bound $W_2(\mu_{\hat{\rho}_1, \hat{\rho}_2}, \mu_{\rho_1, \rho_2})$ in terms of $W_2(\hat{\rho}_1, \rho_1)$ and $W_2(\hat{\rho}_2, \rho_2)$?

Quantitative stability of Wasserstein barycenters

► Known positive results:

Theorem (Le Gouic, Loubes, 2017): If $\forall i, W_2(\rho_i^n, \rho_i) \xrightarrow{n \rightarrow \infty} 0$, then $(\mu_{\rho_1^n, \dots, \rho_N^n})_n$ is pre-compact and any limit is a barycenter of ρ_1, \dots, ρ_N .

Proposition: In dimension $d = 1$, $W_2(\alpha, \beta) = \|F_\alpha^{-1} - F_\beta^{-1}\|_{L^2([0,1])}$ so that:

$$W_2(\mu_{\rho_1, \dots, \rho_N}, \mu_{\tilde{\rho}_1, \dots, \tilde{\rho}_N}) \leq \frac{1}{N} \sum_{i=1}^N W_2(\rho_i, \tilde{\rho}_i).$$

Quantitative stability result in dimension $d \geq 2$?

Quantitative stability of Wasserstein barycenters

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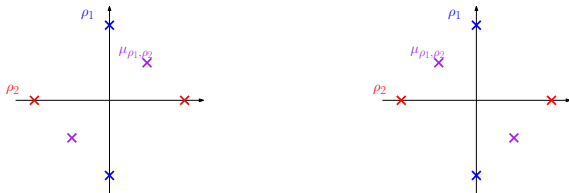
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Quantitative stability result in dimension $d \geq 2$?

Quantitative stability of Wasserstein barycenters

► Negative results:

When $d \geq 2$, barycenter may not be unique:



Proposition (Aguéh, Carlier, 2011): If one of the ρ_i 's is absolutely continuous, the barycenter is unique.

Even with an a.c. marginal, α -Hölder behaviour for any $\alpha \in (0, 1)$ is possible:

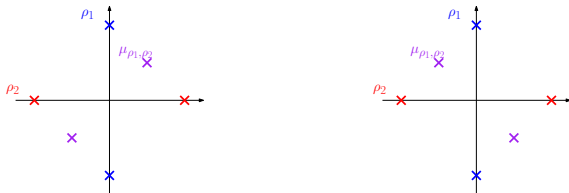


$$W_2(\rho_2^0, \rho_2^\varepsilon) = \varepsilon \text{ while } W_2(\mu_{\rho_1, \rho_2^0}, \mu_{\rho_1, \rho_2^\varepsilon}) \sim \varepsilon^\alpha.$$

Quantitative stability of Wasserstein barycenters

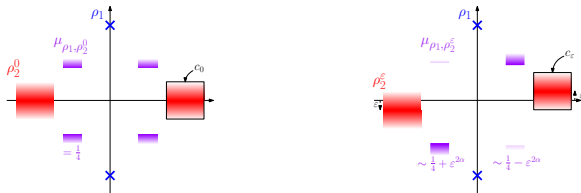
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Quantitative stability of Wasserstein barycenters

Hölder stability estimate for Wasserstein barycenters:

Theorem (Carlier, D., Mérigot, 2022):

- ▶ Let $\Omega = B(0, R_\Omega) \subset \mathbb{R}^d$ and $\rho_1, \dots, \rho_N, \tilde{\rho}_1, \dots, \tilde{\rho}_N \in \mathcal{P}(\Omega)$.
- ▶ Assume ρ_1 is a.c. with $0 < m_{\rho_1} \leq \rho_1 \leq M_{\rho_1}$ on $\mathcal{X}_1 = \text{spt}(\rho_1)$ convex.

Then,
$$W_2(\mu_{\rho_1, \dots, \rho_N}, \mu_{\tilde{\rho}_1, \dots, \tilde{\rho}_N}) \leq C_{d, \Omega, \rho_1} \left(\sum_{i=1}^N W_2(\rho_i, \tilde{\rho}_i) \right)^{1/6}.$$

▶ Remarks:

1. Optimal Hölder exponent?
2. The constant is explicit: $C_{d, \Omega, \rho_1} \approx C_d (R_\Omega \text{diam}(\mathcal{X}_1))^{d+1} \left(\frac{M_{\rho_1}}{m_{\rho_1}} \right)^{1/6}$.
3. Main assumption on ρ_1 : \mathcal{K}_{ρ_1} should satisfy a strong convexity estimate.
4. **Proof idea:** strong convexity of $\mathcal{K}_{\rho_1} \Rightarrow$ "strong convexity" of $\frac{1}{2} W_2^2(\rho_1, \cdot)$:

Proposition (Carlier, D., Mérigot, 2022): Under the assumptions on ρ_1 ,

$$\forall \mu, \nu \in \mathcal{P}(\Omega), \quad W_2^6(\mu, \nu) \lesssim \frac{1}{2} W_2^2(\rho_1, \nu) - \frac{1}{2} W_2^2(\rho_1, \mu) - \left\langle \frac{1}{2} \|\cdot\|^2 - \psi_{\rho_1 \rightarrow \mu} \mid \nu - \mu \right\rangle.$$

Quantitative stability of Wasserstein barycenters

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Quantitative stability of Wasserstein barycenters

► Statistical consequence:

Theorem (Fournier, Guillin, 2015):

- Let $\rho \in \mathcal{P}(\Omega)$ and $\hat{\rho}^n = \frac{1}{n} \sum_{j=1}^n \delta_{x_j}$ where $(x_j)_{1 \leq j \leq n} \sim \rho^{\otimes n}$. Then:

$$\mathbb{E}W_2^2(\hat{\rho}^n, \rho) \leq C_d R^2 \begin{cases} n^{-1/2} & \text{if } d < 4, \\ n^{-1/2} \log(n) & \text{if } d = 4, \\ n^{-2/d} & \text{else.} \end{cases}$$

Corollary (Carlier, D., Mérigot, 2022):

- Under the assumptions of the theorem, if $\forall i, \tilde{\rho}_i = \frac{1}{n} \sum_{j=1}^n \delta_{x_{i,j}}$ where $(x_{i,j})_{1 \leq j \leq n} \sim \rho_i^{\otimes n}$, then

$$\mathbb{E}W_2^2(\mu_{\rho_1, \dots, \rho_N}, \mu_{\hat{\rho}_1^n, \dots, \hat{\rho}_N^n}) \lesssim N^{1/3} \begin{cases} n^{-1/12} & \text{if } d < 4, \\ n^{-1/12} \log(n)^{1/6} & \text{if } d = 4, \\ n^{-1/(3d)} & \text{else.} \end{cases}$$

Outline

Part I.

Strong convexity of the dual quadratic optimal transport problem.

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Consequences: quantitative stability estimates for optimal transport maps, Wasserstein barycenters and entropic optimal transport.

Quantitative stability of entropic regularization

Entropic optimal transport: (Schrödinger, 1931; Léonard, 2014; Peyré and Cuturi, 2019)

► Primal and dual problems: for $\varepsilon > 0$,

$$\max_{\gamma \in \Gamma(\rho, \mu)} \int \langle x|y \rangle d\gamma(x, y) - \varepsilon \text{KL}(\gamma | \rho \otimes \mu) = \min_{\psi: \mathbb{R}^d \rightarrow \bar{\mathbb{R}}} \int \psi^{c, \varepsilon, \mu} d\rho + \int \psi d\mu + \varepsilon,$$

where $\psi^{c, \varepsilon, \mu}(\cdot) = \varepsilon \log \int e^{\frac{\langle \cdot | y \rangle - \psi(y)}{\varepsilon}} d\mu(y)$.

$$\mathcal{K}_\rho^{c, \varepsilon, \mu} : \psi \mapsto \int \psi^{c, \varepsilon, \mu} d\rho.$$

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Strong convexity of the dual entropic problem

Strong convexity estimate for the entropic Kantorovich functional:

Theorem (D., 2022):

- ▶ Let \mathcal{X} compact convex, $\rho \in \mathcal{P}_{a.c.}(\mathcal{X})$ with $0 < m_\rho \leq \rho \leq M_\rho$.
- ▶ Let $\mathcal{Y} = B(0, R_\mathcal{Y})$ compact and let $\mu \in \mathcal{P}(\mathcal{Y})$.

Then for ψ_μ an entropic potential between ρ and μ and any $v : \mathbb{R}^d \rightarrow \mathbb{R}$,

$$C_{\mathcal{X}, \rho, \mathcal{Y}, \varepsilon} \operatorname{Var}_\mu(v) \leq \left. \frac{d^2}{dt^2} \mathcal{K}_\rho^{\varepsilon, \mu}(\psi_\mu + tv) \right|_{t=0},$$

where $C_{\mathcal{X}, \rho, \mathcal{Y}, \varepsilon} = \left(e^{R_\mathcal{Y} \operatorname{diam}(\mathcal{X})} \frac{M_\rho}{m_\rho} + \varepsilon \right)^{-1}$.

Remarks:

1. Allows to recover the *non-entropic* estimate when $\varepsilon \rightarrow 0$.
2. Constant improves when $\varepsilon \rightarrow 0$.

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$$C_{\mathcal{X},\rho,\mathcal{Y},\varepsilon} \text{Var}_{\mu}(v) \leq \frac{d^2}{dt^2} \mathcal{K}_{\rho}^{\varepsilon,\mu}(\psi_{\mu} + tv),$$

► Elements of proof:

1. Define $I : \psi \mapsto \log(\int_{\mathcal{X}} e^{-\psi^{c,\varepsilon,\mu}})$, and using the Prékopa-Leindler inequality, show

$$\forall \varphi, \psi : \mathbb{R}^d \rightarrow \mathbb{R}, t \in [0, 1], \quad I((1-t)\varphi + t\psi) \geq (1-t)I(\varphi) + tI(\psi).$$

2. Noticing that I is \mathcal{C}^2 , conclude with

$$\frac{d^2}{dt^2} I(\psi_{\mu} + tv) = -\frac{d^2}{dt^2} \mathcal{K}_{\rho}^{\varepsilon,\mu}(\psi_{\mu} + tv) + \text{Var}_{\bar{\mu}}(v) \leq 0.$$

- Remark: with $I : \psi \mapsto \log \int e^{-\psi^*}$, this argument recovers Brascamp-Lieb from Prékopa-Leindler.

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Quantitative stability of entropic regularization

► Denote $\psi^\varepsilon = \arg \min_{\psi} \mathcal{K}_\rho^{\varepsilon, \mu}(\psi) + \langle \psi | \mu \rangle + \varepsilon. \implies \boxed{\nabla \mathcal{K}_\rho^{\varepsilon, \mu}(\psi^\varepsilon) + \mu = 0.}$

► Implicit function theorem $\implies \boxed{\nabla^2 \mathcal{K}_\rho^{\varepsilon, \mu}(\psi^\varepsilon) \psi^\varepsilon + \frac{\partial}{\partial \varepsilon} (\nabla \mathcal{K}_\rho^{\varepsilon, \mu})(\psi^\varepsilon) = 0.}$

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- Let $\mathcal{X} \subset \mathbb{R}^d$ compact convex. Let $\rho \in \mathcal{P}_{a.c.}(\mathcal{X})$ with $0 < m_\rho \leq \rho \leq M_\rho$ and assume ρ is α -Hölder continuous.
- Let $\mu = \sum_{i=1}^N \mu_i \delta_{y_i}$.

Then $\varepsilon \mapsto \psi^\varepsilon$ is \mathcal{C}^1 . For any $\varepsilon > 0$ and $\alpha' \in (0, \alpha)$,

$$\|\dot{\psi}^\varepsilon\|_2 \leq C_{\mathcal{X}, \rho, \mathcal{Y}, \mu} \min(\varepsilon^{\alpha'}, 1)$$

► **Remark:** $\varepsilon \mapsto \psi^\varepsilon$ is Lipschitz continuous \rightarrow numerical optimal transport.

Corollary (D., 2022): Under the same assumptions, $\forall \varepsilon > 0, \forall \alpha' \in (0, \alpha)$,

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► Remark: $\varepsilon \mapsto \psi^\varepsilon$ is Lipschitz continuous \rightarrow numerical optimal transport.

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where $\mathbb{W}_{2,\varepsilon}^2(\rho, \mu) = \int \|x - y\|^2 d\gamma^\varepsilon(x, y)$. The last bound is tight.

Quantitative stability of entropic regularization

► Denote $\psi^\varepsilon = \arg \min_{\psi} \mathcal{K}_\rho^{\varepsilon, \mu}(\psi) + \langle \psi | \mu \rangle + \varepsilon. \implies \boxed{\nabla \mathcal{K}_\rho^{\varepsilon, \mu}(\psi^\varepsilon) + \mu = 0.}$

► Implicit function theorem $\implies \boxed{\nabla^2 \mathcal{K}_\rho^{\varepsilon, \mu}(\psi^\varepsilon) \psi^\varepsilon + \frac{\partial}{\partial \varepsilon} (\nabla \mathcal{K}_\rho^{\varepsilon, \mu})(\psi^\varepsilon) = 0.}$

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- Let $\mathcal{X} \subset \mathbb{R}^d$ compact convex. Let $\rho \in \mathcal{P}_{a.c.}(\mathcal{X})$ with $0 < m_\rho \leq \rho \leq M_\rho$ and assume ρ is α -Hölder continuous.
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Conclusion

▶ Main ideas:

1. **Dual quadratic OT problem** may enjoy form of **strong/uniform convexity**.
2. Strong convexity deduced from **Brascamp-Lieb/Prékopa-Leindler** inequalities → reinforces the link between OT and these functional inequalities.
3. Allows to prove **stability results in OT**:
 - ▶ Guarantees for statistical/numerical approximation of OT maps and Wasserstein barycenters.
 - ▶ Partial embedding of $(\mathcal{P}_2(\mathbb{R}^d), W_2)$ into $L^2(\rho, \mathbb{R}^d)$.
 - ▶ Quantitative control of entropic regularization.

▶ Open questions:

1. **Generalizations of strong convexity results**: source measure, ground cost?
2. **Numerical consequences of strong convexity result**: Newton methods, interior point methods, etc.

Thank you for your attention!

Appendix

Quantitative stability of optimal transport maps

$$\|T_\mu - T_\nu\|_{L^2(\rho, \mathbb{R}^d)} \leq C_{d, \rho, \mathcal{X}, \mathcal{Y}} W_1(\mu, \nu)^{1/6}.$$

- **Proof idea:** strong convexity of \mathcal{K}_ρ and new Galgaliardo-Nirenberg type inequality:

Proposition (D., Mérigot, 2021): For $K \subset \mathbb{R}^d$ compact and $u, v : K \rightarrow \mathbb{R}$ Lipschitz convex,

$$\|\nabla u - \nabla v\|_{L^2(K, \mathbb{R}^d)}^2 \leq C_d \mathcal{H}^{d-1}(\partial K)^{\frac{2}{3}} (\text{Lip}(u) + \text{Lip}(v))^{\frac{4}{3}} \|u - v\|_{L^2(K)}^{\frac{2}{3}}.$$

Let ϕ_μ, ϕ_ν be convex Brenier potentials between ρ and μ, ν :

$$\begin{aligned} \|T_\mu - T_\nu\|_{L^2(\rho, \mathbb{R}^d)} &= \|\nabla \phi_\mu - \nabla \phi_\nu\|_{L^2(\rho, \mathbb{R}^d)} \\ &\lesssim \text{Var}_\rho(\phi_\mu - \phi_\nu)^{1/6} \\ &\leq \text{Var}_{\frac{1}{2}(\mu+\nu)}(\phi_\mu^* - \phi_\nu^*)^{1/6} \\ &\lesssim (\mathcal{K}_\rho(\psi_\nu) - \mathcal{K}_\rho(\psi_\mu) + \langle \psi_\nu - \psi_\mu | \mu \rangle)^{1/6} \\ &\lesssim W_1(\mu, \nu)^{1/6}. \end{aligned}$$

Quantitative stability of Wasserstein barycenters

► General result: infinite number of marginals

Definition: Let $\Omega \subset \mathbb{R}^d$ compact. Wasserstein barycenter of $\mathbb{P} \in \mathcal{P}(\mathcal{P}(\Omega))$:

$$\mu_{\mathbb{P}} \in \arg \min_{\mu \in \mathcal{P}(\Omega)} \frac{1}{2} \int_{\mathcal{P}(\Omega)} W_2^2(\rho, \mu) d\mathbb{P}(\rho).$$

Theorem (Carlier, D., Mérigot, 2022):

► Let $\mathbb{P}, \mathbb{Q} \in \mathcal{P}(\mathcal{P}(\Omega))$ and $\exists S_{\mathbb{P}} \subset \mathcal{P}(\Omega)$ s.t. $\mathbb{P}(S_{\mathbb{P}}) = \alpha_{\mathbb{P}} > 0$ and $\forall \rho \in S_{\mathbb{P}}$,

1. ρ is a.c.
2. $0 < m \leq \rho \leq M < +\infty$ on its support.
3. $\mathcal{H}^{d-1}(\partial \text{spt}(\rho)) \leq \text{per} < +\infty$.
4. $\forall \psi, \tilde{\psi} \in \mathcal{C}(\Omega)$,

$$c \text{Var}_{\rho}(\tilde{\psi}^* - \psi^*) \leq \mathcal{K}_{\rho}(\tilde{\psi}) - \mathcal{K}_{\rho}(\psi) - \langle \tilde{\psi} - \psi | \nabla \mathcal{K}_{\rho}(\psi) \rangle.$$

Then,

$$W_2(\mu_{\mathbb{P}}, \mu_{\mathbb{Q}}) \lesssim \frac{1}{\alpha_{\mathbb{P}}^{1/4}} W_1(\mathbb{P}, \mathbb{Q})^{1/6}.$$

$$\forall \mathbb{P}, \mathbb{Q} \in \mathcal{P}(\mathcal{P}(\Omega)), \quad W_1(\mathbb{P}, \mathbb{Q}) := \min_{\gamma \in \Pi(\mathbb{P}, \mathbb{Q})} \int_{\mathcal{P}(\Omega) \times \mathcal{P}(\Omega)} W_2(\rho, \tilde{\rho}) d\gamma(\rho, \tilde{\rho}).$$

Quantitative stability of entropic regularization

► Let $c(x, y) = \|x - y\|^2$.

	<i>Classical OT</i>	<i>Entropic OT</i>
Problem	$(P_0)_{\rho, \mu} : \min_{\gamma \in \Gamma(\rho, \mu)} \langle c \gamma \rangle$	$(P_\epsilon)_{\rho, \mu} : \min_{\gamma \in \Gamma(\rho, \mu)} \langle c \gamma \rangle + \epsilon \text{KL}(\gamma \rho \otimes \mu)$
Computational complexity (n support points)	$\tilde{O}(n^3)$	$\tilde{O}(n^2/\epsilon^2)$
Sample complexity $\mathbb{E} \left (P_\cdot)_{\hat{\rho}^n, \hat{\mu}^n} - (P_\cdot)_{\rho, \mu} \right $ $(\hat{\rho}^n = \frac{1}{n} \sum_i \delta_{x_i}, x_i \sim \rho,$ $\hat{\mu}^n = \frac{1}{n} \sum_j \delta_{y_j}, y_j \sim \mu)$	$O(n^{-1/d})$	$\lesssim \frac{e^{1/\epsilon}}{\epsilon^{d/2}} n^{-1/2}$
Minimizer	γ^0	γ^ϵ
Geometry?	$W_2(\rho, \mu) := \sqrt{\langle c \gamma^0 \rangle}$ is a distance	$W_{2, \epsilon}(\rho, \mu) := \sqrt{\langle c \gamma^\epsilon \rangle}$ is not a distance

Quantitative stability of entropic regularization

- ▶ **Semi-discrete setting:**

- ▶ Let $\mathcal{X} \subset \mathbb{R}^d$ compact and $\rho \in \mathcal{P}_{a.c.}(\mathcal{X})$ absolutely continuous.

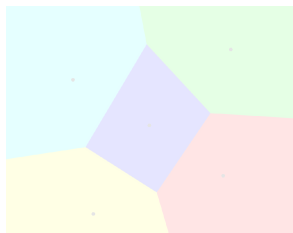
- ▶ Let $\mathcal{Y} = \{y_1, \dots, y_N\} \subset \mathbb{R}^d$ and $\mu = \sum_{i=1}^N \mu_i \delta_{y_i} \in \mathcal{P}(\mathcal{Y})$.

→ Natural framework in **statistics** and **numerical analysis**.

- ▶ A 2-dimensional example:



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



($\varepsilon = 0$)

$T_{\rho \rightarrow \mu}$ is piece-wise constant.

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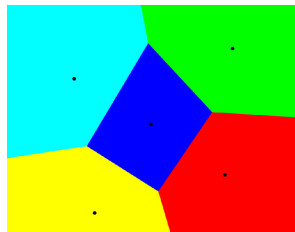
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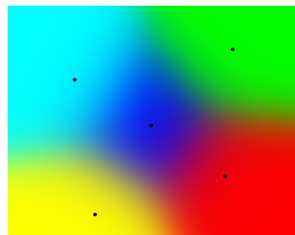
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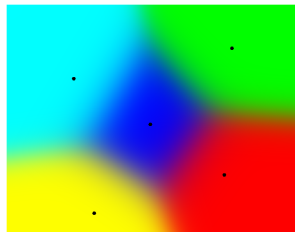
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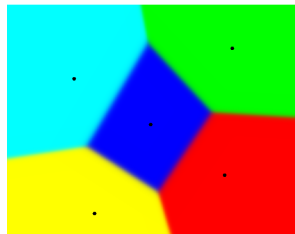
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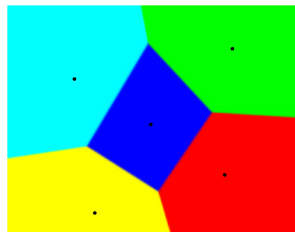
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