

Disentangling entropy and suboptimality in Entropic optimal transport

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Optimal transport

Transport map

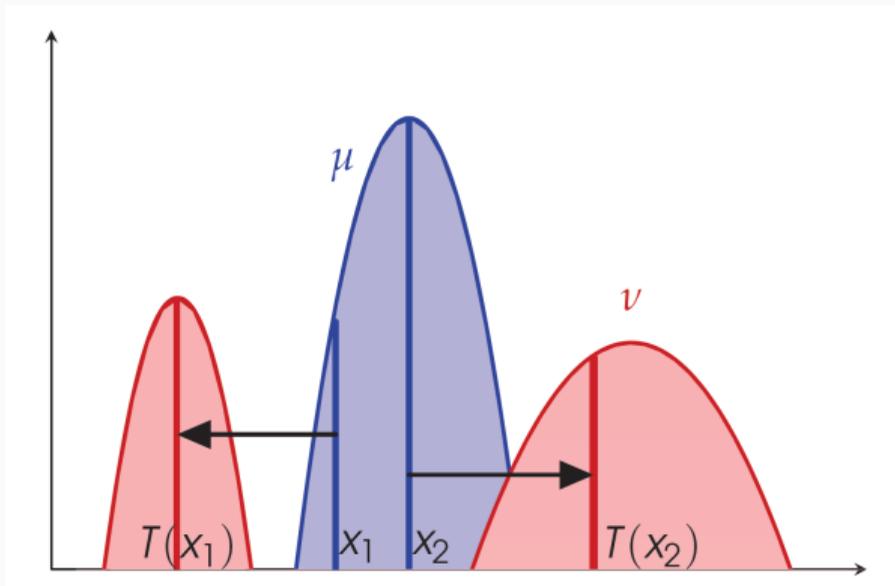


Figure 1: the map T transports μ onto ν : $T_{\#}\mu = \nu$

Transport plan

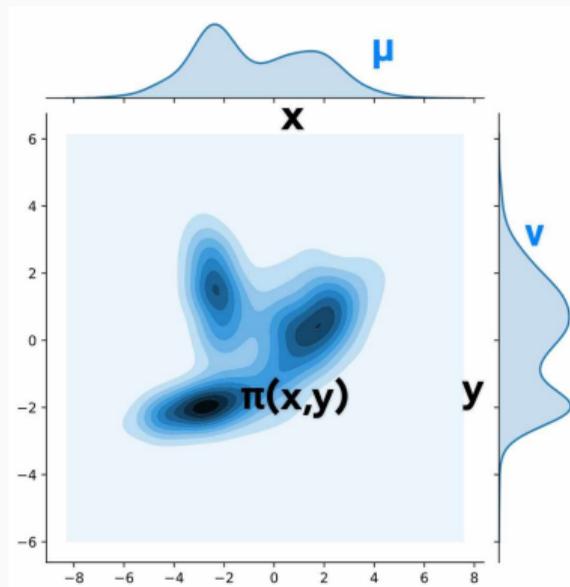


Figure 2: The plan π transports μ onto ν : $\pi \in \Pi(\mu, \nu)$ (image from Wikipedia)

Optimal transport

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- Monge problem (1781) is

$$\inf_{T \# \mu_0 = \mu_1} \int c(x, T(x)) d\mu_0(x) \quad (1)$$

- Kantorovich formulation:

$$OT_0(\mu, \nu) := \inf_{\gamma \in \Pi(\mu_0, \mu_1)} \int c(x, y) d\gamma(x, y) \quad (P)$$

- Dual problem:

$$OT_0(\mu, \nu) := \sup_{\phi \oplus \psi \leq c} \int \phi d\mu_0 + \int \psi d\mu_1 \quad (D)$$

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In the following, the cost function is $c(x, y) = \frac{1}{2}|x - y|^2$. It defines the Wasserstein

distance $W_2^2(\mu, \nu) := \inf_{\gamma \in \Pi(\mu_0, \mu_1)} \int |x - y|^2 d\gamma(x, y)$

Legendre transform

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- f^* is always convex
- if f is convex and if both f and f^* are differentiable, then

$$(\nabla f)^{-1} = \nabla f^* \quad (3)$$

Legendre transform

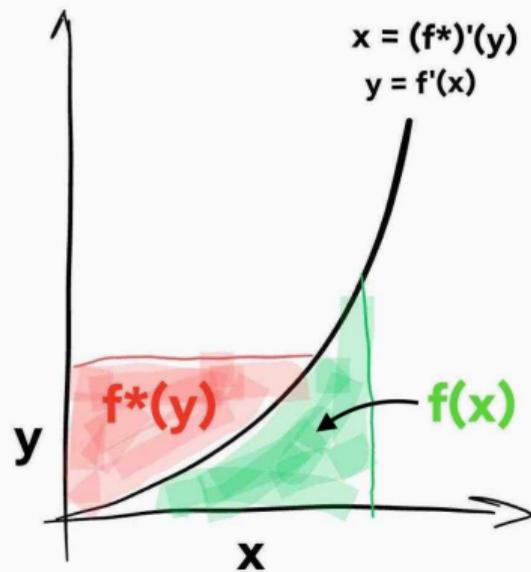


Figure 3: The Legendre transform in 1d

Structure of the optimizers

$$\inf_{T \# \mu_0 = \mu_1} \int c(x, T(x)) d\mu_0(x) \geq \min_{\gamma \in \Pi(\mu_0, \mu_1)} \int c(x, y) d\gamma(x, y) = \sup_{\phi \oplus \psi \leq c} \int \phi d\mu_0 + \int \psi d\mu_1 \quad (4)$$

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Theorem (Brenier)

For the quadratic cost $c(x, y) = \frac{1}{2}|x - y|^2$:

If $\mu_0 \in \mathcal{P}_{2,ac}(\mathbb{R}^d)$ then the solutions T, γ_0, ϕ, ψ can be expressed thanks to a unique convex function f :

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If $\mu_0 \in \mathcal{P}_{2,ac}(\mathbb{R}^d)$ then the solutions T, γ_0, ϕ, ψ can be expressed thanks to a unique convex function f :

- $T = \nabla f$,
- $\gamma_0 = (id, \nabla f) \# \mu_0$,
- $\phi(x) = \frac{1}{2}|x|^2 - f(x)$,
- $\psi(y) = \frac{1}{2}|y|^2 - f^*(y)$.

Energy gap

Let define the Energy gap function

$$E(x, y) := c(x, y) - \phi(x) - \psi(y) \quad (5)$$

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- $\forall (x, y) \in \mathbb{R}^{2d} \quad E(x, y) \geq 0,$
- $(x, y) \in \text{Supp}(\gamma_0) \Rightarrow E(x, y) = 0,$
- If $\gamma \in \Pi(\mu_0, \mu_1)$ then

$$\int c d\gamma - \int c d\gamma_0 = \int E d\pi,$$

- For the quadratic cost,

$$E(x, y) = f(x) + f^*(y) - x \cdot y,$$

Legendre transform

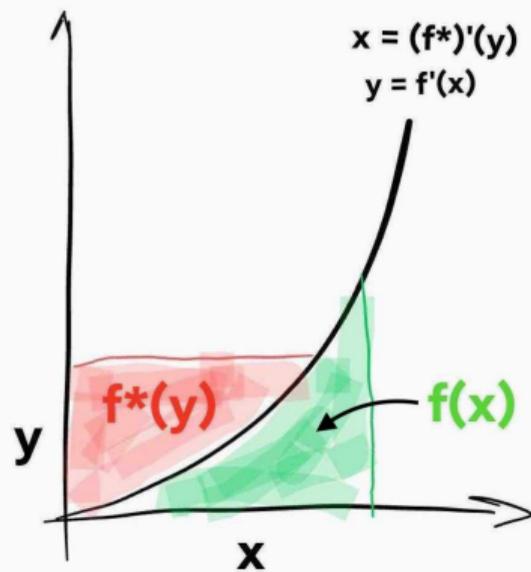


Figure 4: We can identify $E(x, y) = f(x) + f^*(y) - x \cdot y$ on this drawing

Energy gap

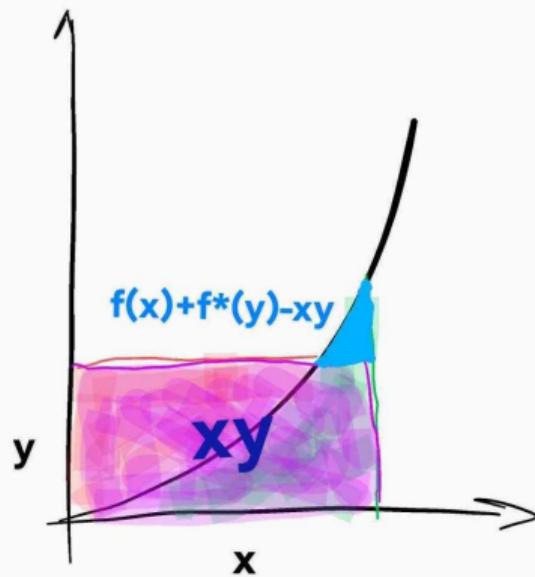


Figure 5: The energy gap in 1d

Benamou-Brenier formulation

Let $\mu_0, \mu_1 \in \mathcal{P}_2(\mathbb{R}^d)$, for the quadratic cost, the Benamou-Brenier formulation is:

$$OT_0(\mu_0, \mu_1) = \inf_{\substack{\partial_t \rho + \nabla \cdot (\rho v) = 0 \\ \rho_0 = \mu_0, \rho_1 = \mu_1}} \iint \frac{1}{2} |v_t|^2 \rho_t dt \quad (\text{BB})$$

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(The advection equation $\partial_t \rho + \nabla \cdot (\rho v) = 0$ means that the density ρ is transported by the velocity field v)

Entropic optimal transport

Let $\rho \in \mathcal{P}_{2,ac}(\mathbb{R}^k)$ be a continuous measure with finite variance, define

$$\underbrace{H(\rho) := \int_{\mathbb{R}^k} \rho(x) \ln \rho(x) dx}_{\text{differential entropy}} \quad \text{and} \quad \underbrace{I(\rho) := \int_{\mathbb{R}^k} \rho(x) |\nabla \ln \rho(x)|^2 dx}_{\text{Fisher information}} \quad (6)$$

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$I(\rho) < +\infty$ implies $H(\rho) < +\infty$ Let c be a C^2 cost function.

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Let $\mu_0, \mu_1 \in \mathcal{P}_{ac}(\mathbb{R}^d)$ be such that $H(\mu_i) < +\infty$.

For $\varepsilon \geq 0$

$$OT_\varepsilon(\mu_0, \mu_1) := \inf_{\gamma \in \Pi(\mu_0, \mu_1)} \int c\gamma + \varepsilon H(\gamma) \quad (\varepsilon\text{EOT})$$

Entropic optimal transport

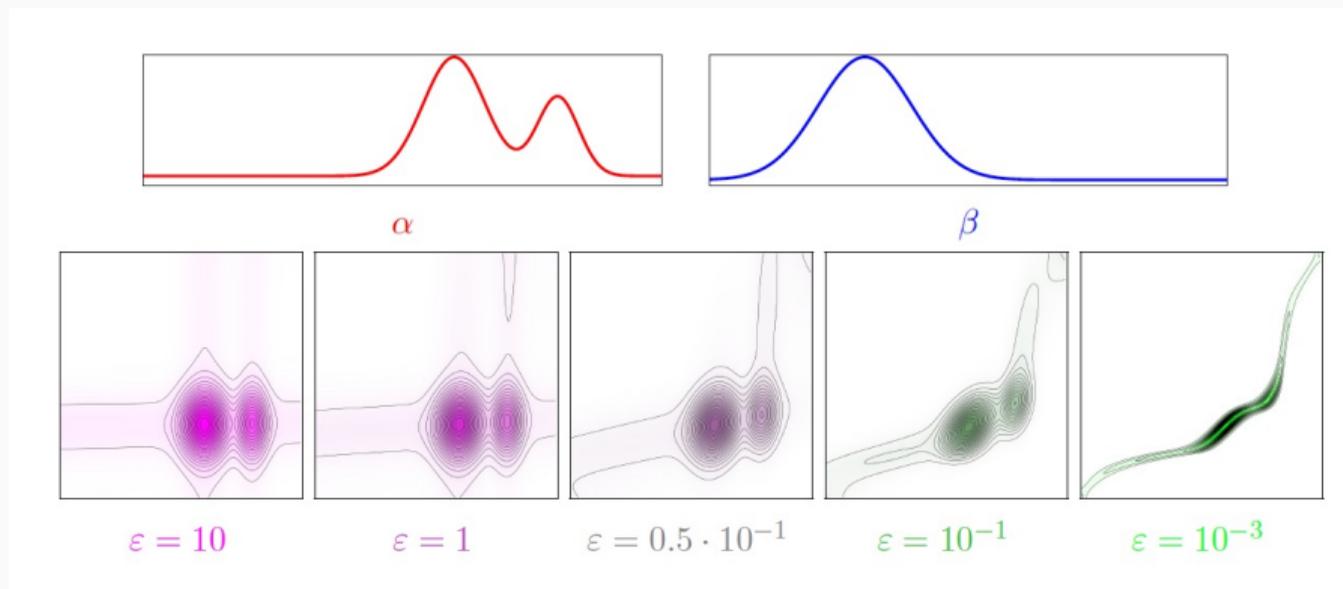


Figure 6: Entropic optimal transport in 1d (image from [PC18])

Sinkhorn algorithm

The dual problem of (ε EOT) is

$$OT_{\varepsilon}(\mu_0, \mu_1) = \sup_{\phi, \psi} \int \phi d\mu_0 + \int \psi d\mu_1 - \varepsilon \int e^{\frac{\phi \oplus \psi - c}{\varepsilon}} d\mu_0 d\mu_1 + \varepsilon \quad (7)$$

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The optimality conditions are

$$\phi(x) = -\varepsilon \ln \int e^{\frac{\psi(y) - c(x,y)}{\varepsilon}} d\mu_1(y), \quad \psi(y) = -\varepsilon \ln \int e^{\frac{\phi(x) - c(x,y)}{\varepsilon}} d\mu_0(x). \quad (8)$$

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$$\phi_{n+1}(x) = -\varepsilon \ln \int e^{\frac{\psi_n(y) - c(x,y)}{\varepsilon}} d\mu_1(y), \quad \psi_{n+1}(y) = -\varepsilon \ln \int e^{\frac{\phi_{n+1}(x) - c(x,y)}{\varepsilon}} d\mu_0(x). \quad (9)$$

Entropic optimal transport

For $\varepsilon \geq 0$

$$OT_\varepsilon(\mu_0, \mu_1) := \inf_{\gamma \in \Pi(\mu_0, \mu_1)} \int c\gamma + \varepsilon H(\gamma) \quad (\varepsilon\text{EOT})$$

Question: What happens when $\varepsilon \rightarrow 0$?

Qualitative convergence results.

- Γ -convergence : [Mik04],[MT08],[Lé13],[CDPS15]

Quantitative convergence results.

- Discrete optimal transport: [CM94]
- Semi-discrete optimal transport: [ANWS21],[Del21]
- Finite Fisher information: [ADPZ11],[EMR15],[Con19]
- Finite entropy: [Pal19],[EN22],[CPT22]
- Multimarginal: [NP23]
- Sinkhorn divergence: [FSV⁺18, CRL⁺20]

Proposition [ADPZ11][EMR15]

Assume $c(x, y) = \frac{1}{2}\|x - y\|^2$, and that $Supp(\mu_i)$ are compact with $I(\mu_i) < +\infty$ then

$$OT_\varepsilon - OT_0 = -\frac{d}{2}\varepsilon \ln(2\pi\varepsilon) + \varepsilon \frac{H(\mu_0) + H(\mu_1)}{2} + o(\varepsilon) \quad (TE-OT_\varepsilon)$$

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Proposition [EN22, CPT22]

Assume c is infinitesimally twisted and $Supp(\mu_i)$ compact then

$$\left(-\frac{d}{2}\varepsilon \ln(\varepsilon) + C'\varepsilon \leq\right) OT_\varepsilon - OT_0 \leq -\frac{d}{2}\varepsilon \ln(\varepsilon) + C\varepsilon \quad (10)$$

Questions

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$$OT_{\epsilon} - OT_0 = \underbrace{\int c\gamma_{\epsilon} - \int c\gamma_0}_{\text{suboptimality}} + \epsilon \underbrace{H(\gamma_{\epsilon})}_{\text{entropy}}$$

Can we disentangle ?

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Question 3:

Is there a rate of convergence for $W_2(\gamma_{\epsilon}, \gamma_0)$?

Definition

Let $\mu, \nu \in \mathcal{P}_{2,ac}(\mathbb{R}^d)$ and $\gamma \in \Pi(\mu, \nu)$.

Let $\delta > 0$ and $(Q_i^\delta)_i$ be a partition of \mathbb{R}^d into cubes of side length δ .

The block approximation of γ is defined by

$$\forall x, y \in Q_j^\delta \times Q_k^\delta, \quad \gamma^\delta(x, y) = \gamma(Q_j^\delta \times Q_k^\delta) \frac{\mu(x)\nu(y)}{\mu(Q_j^\delta)\nu(Q_k^\delta)} \quad (11)$$

Block approximation

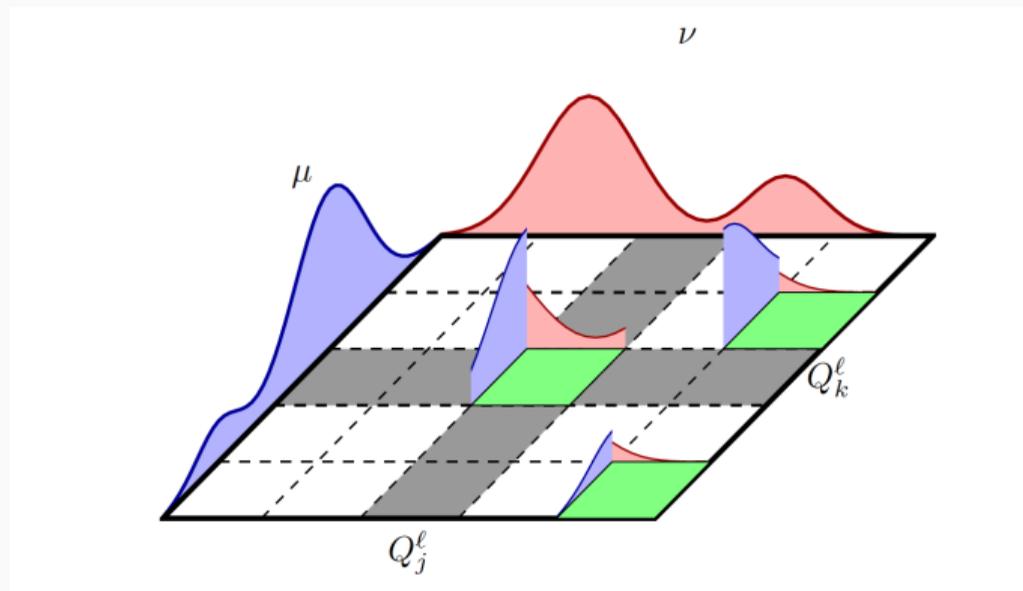


Figure 7: The block approximation in 1d (image from [CDPS17])

Block approximation

[[CPT22]] Let $\mu, \nu \in \mathcal{P}_{2,ac}(\mathbb{R}^d)$ and $\gamma \in \Pi(\mu, \nu)$ be the optimal transport plan. Let $\delta > 0$ and γ^δ be the block approximation of γ .

Then

$$\int c\gamma^\delta - \int c\gamma = \int E\gamma^\delta \leq C\delta^2 \quad \text{and} \quad H(\gamma^\delta) \leq -d \ln(\delta) + C \quad (12)$$

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So for $\delta = \sqrt{\varepsilon}$, we have

$$OT_\varepsilon(\mu, \nu) \leq \int c\gamma^\delta + \varepsilon H(\gamma^\delta) \leq -\frac{d}{2} \ln(\varepsilon) + C\varepsilon \quad (13)$$

Proposition [ADPZ11][EMR15]

Assume $c(x, y) = \frac{1}{2}\|x - y\|^2$, and that $Supp(\mu_i)$ are compact with $I(\mu_i) < +\infty$ then

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Fisher information and quadratic cost

Theorem [MS23]

Suppose that the cost is quadratic, that is $c(x, y) = \frac{1}{2}|x - y|^2$. Further assume that $I(\mu_i) < \infty$ and $Supp(\mu_i)$ compact. Then

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where $H_m = \frac{H(\mu_0) + H(\mu_1)}{2}$.

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where $H_m = \frac{H(\mu_0) + H(\mu_1)}{2}$. Moreover

$$\int c\gamma_\varepsilon - \int c\gamma_0 = \frac{d}{2}\varepsilon + o(\varepsilon) \quad (16)$$

Sketch of proof

Recall $H_m = \frac{H(\mu_0) + H(\mu_1)}{2}$. The dynamic formulation [Lé13] is

$$OT_\varepsilon = \varepsilon H_m - \frac{d}{2} \varepsilon \ln(2\pi\varepsilon) + \min_{\substack{\partial\rho + \nabla \cdot (\rho v) = 0 \\ \rho_0 = \mu_0, \rho_1 = \mu_1}} \iint \frac{1}{2} |v_t|^2 \rho_t t + \frac{\varepsilon^2}{8} \int_0^1 I(\rho_t) t \quad (\varepsilon\text{BB})$$

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Known asymptotics (TE- OT_ε) is

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Thus thanks to (εBB)

$$\frac{1}{\varepsilon} \underbrace{\left(\iint \frac{1}{2} |v_t^\varepsilon|^2 \rho_t^\varepsilon t - OT_0 \right)}_{\text{suboptimality}} + \frac{\varepsilon}{8} \underbrace{\int_0^1 I(\rho_t^\varepsilon) t}_{\text{regularity term}} = o(1) \quad (18)$$

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Since both terms are positive they both tend to 0.

Theorem

Let X be a set and $f : \mathbb{R} \times X \rightarrow \mathbb{R}$ be a function.

Let $F : \mathbb{R} \rightarrow \mathbb{R}$ be defined by

$$F(\varepsilon) = \inf_{x \in X} f(\varepsilon, x) \quad (19)$$

Let x_ε be a minimizer of $f(\varepsilon, \cdot)$. If F and $f(\cdot, x_\varepsilon)$ are differentiable at ε then their derivatives are the same:

$$F'(\varepsilon) = \frac{\partial f}{\partial \varepsilon}(\varepsilon, x_\varepsilon) \quad (20)$$

From dynamic to static and back

$$\underbrace{\int c\gamma_\varepsilon + \varepsilon H(\gamma_\varepsilon)}_{(a) \text{ static}} = \underbrace{\varepsilon H_m - \frac{d}{2}\varepsilon \ln(2\pi\varepsilon)}_{(b)} + \underbrace{\iint \frac{1}{2}|\mathbf{v}_t^\varepsilon|^2 \rho_t^\varepsilon t + \frac{\varepsilon^2}{8} \int_0^1 I(\rho_t^\varepsilon) t}_{(c) \text{ dynamic}} \quad (\varepsilon\text{BB})$$

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Envelop theorem

$$\frac{d}{d\varepsilon}(a) = \frac{d}{d\varepsilon}(b) + \frac{d}{d\varepsilon}(c)$$

$$H(\gamma_\varepsilon) = H_m - \frac{d}{2} \ln(2\pi\varepsilon) - \frac{d}{2} + \frac{\varepsilon}{4} \int l(\rho_t^\varepsilon) t$$

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$$H(\gamma_\varepsilon) = H_m - \frac{d}{2} \ln(2\pi\varepsilon) - \frac{d}{2} + \frac{\varepsilon}{4} \int I(\rho_t^\varepsilon) t$$

$$\begin{cases} \int c\gamma_\varepsilon - OT_0 = \iint \frac{1}{2} |v_t^\varepsilon|^2 \rho_t^\varepsilon t - OT_0 - \frac{\varepsilon^2}{8} \int I(\rho_t^\varepsilon) t + \frac{d}{2}\varepsilon \\ H(\gamma_\varepsilon) = \frac{\varepsilon}{4} \int_0^1 I(\rho_t^\varepsilon) t - \frac{d}{2} \ln(2\pi\varepsilon) + H_m - \frac{d}{2} \end{cases} \quad (21)$$

Quadratic cost without Fisher information

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Suppose that the cost is quadratic, that is $c(x, y) = \frac{1}{2}\|x - y\|^2$. Further assume that $\mu_i \in \mathcal{P}_{2+\delta, ac}(\mathbb{R}^d)$ for some $\delta > 0$.

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Suppose that the cost is quadratic, that is $c(x, y) = \frac{1}{2}\|x - y\|^2$. Further assume that $\mu_i \in \mathcal{P}_{2+\delta, ac}(\mathbb{R}^d)$ for some $\delta > 0$. Then

$$\int c\gamma_\varepsilon - \int c\gamma_0 = \Theta(\varepsilon), \quad H(\gamma_\varepsilon) = -\frac{d}{2} \ln(\varepsilon) + O(1), \quad (22)$$

$$W_2(\gamma_\varepsilon, \gamma_0) \geq C\sqrt{\varepsilon}. \quad (23)$$

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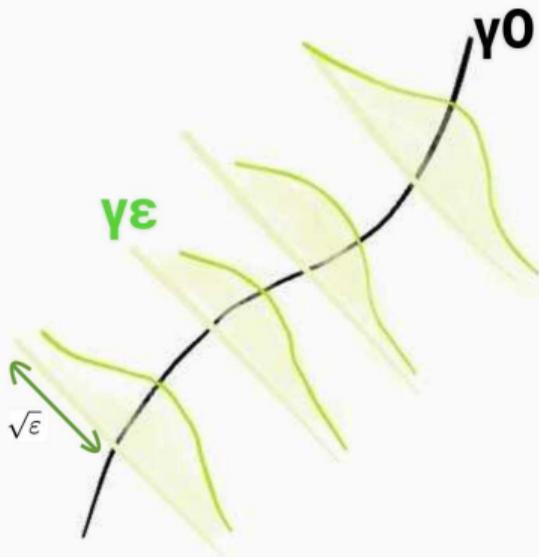


Figure 8: The best to do is to convolve γ_0 with a Gaussian in the transverse direction

Minty's coordinates

Minty's coordinates (u, v) are defined by

$$u = \frac{x + y}{\sqrt{2}}, \quad v = \frac{y - x}{\sqrt{2}} \quad (26)$$

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Then

$$T = \nabla f \text{ with } f \text{ convex} \Leftrightarrow S \text{ 1-Lipschitz}$$

Minty's coordinates

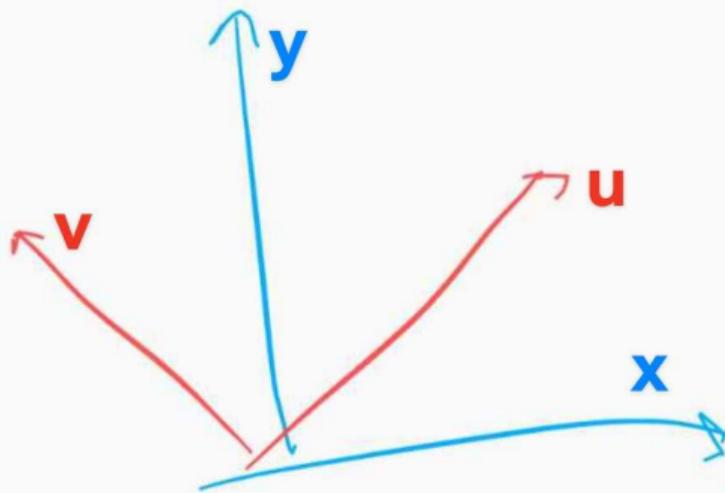


Figure 9: Minty's coordinates in 1d

Minty's coordinates

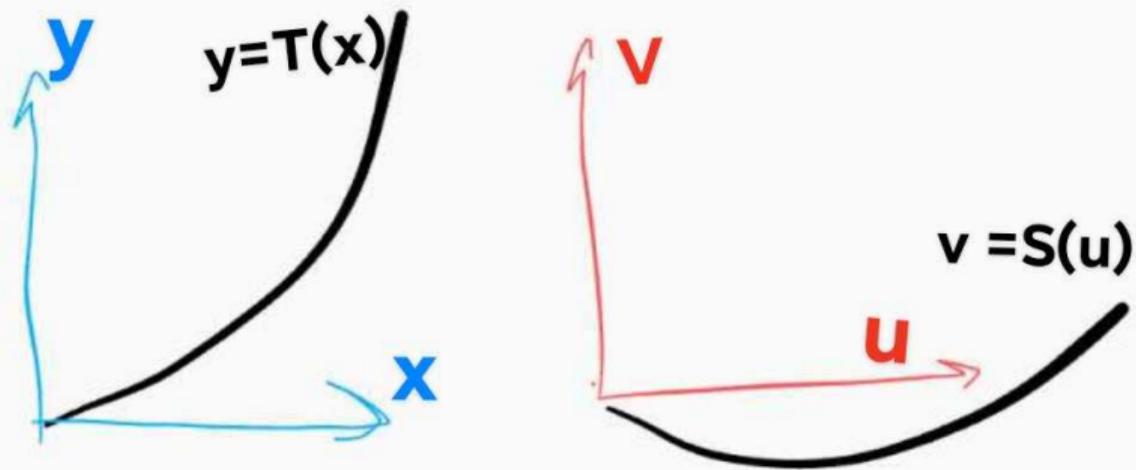


Figure 10: Minty's coordinates in 1d

Linearity of the entropy

Let $\gamma \in \mathcal{P}_{2,ac}(\mathbb{R}^{2d})$ be disintegrated in Minty's coordinates as

$$\gamma(u, v) = \gamma^u(v) \hat{\gamma}(u). \quad (27)$$

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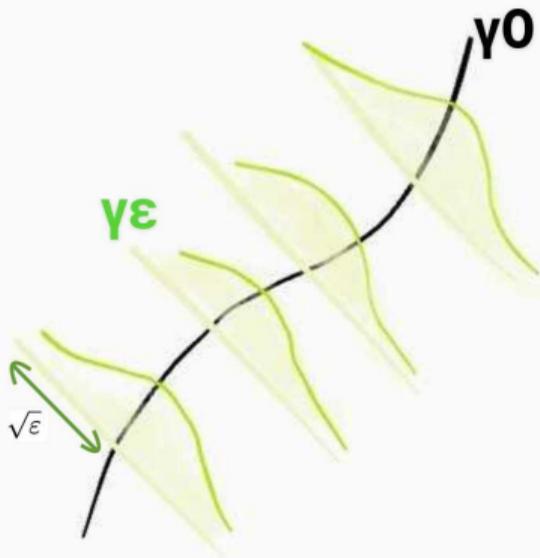


Figure 11: The best to do is to choose γ^u to be a Gaussian

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Proposition

Let $C_d = -d \ln(\frac{2\pi e}{d})$. Then

$$\int H(\gamma^u) d\hat{\gamma}(u) \geq -\frac{d}{2} \ln\left(\int |v - S(u)|^2 d\gamma(u, v)\right) + C_d \quad (30)$$

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Question: What do we do with this term $\int |v - S(u)|^2 d\gamma(u, v)$?

Wasserstein distance and Lipschitz function

Since γ_0 is supported by the graph of S , 1-Lipschitz, $\int |v - S(u)|^2 d\gamma(u, v)$ is bounded by the Wasserstein distance to γ_0 .

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Proposition

Let $\gamma, \gamma_0 \in \mathcal{P}_2(\mathbb{R}^{2d})$ be two plans.

If γ_0 is supported by the graph of a 1-Lipschitz function S , then

$$W_2^2(\gamma, \gamma_0) \geq \int \frac{|v - S(u)|^2}{2} d\gamma(u, v) \quad (31)$$

Wasserstein distance and Lipschitz function

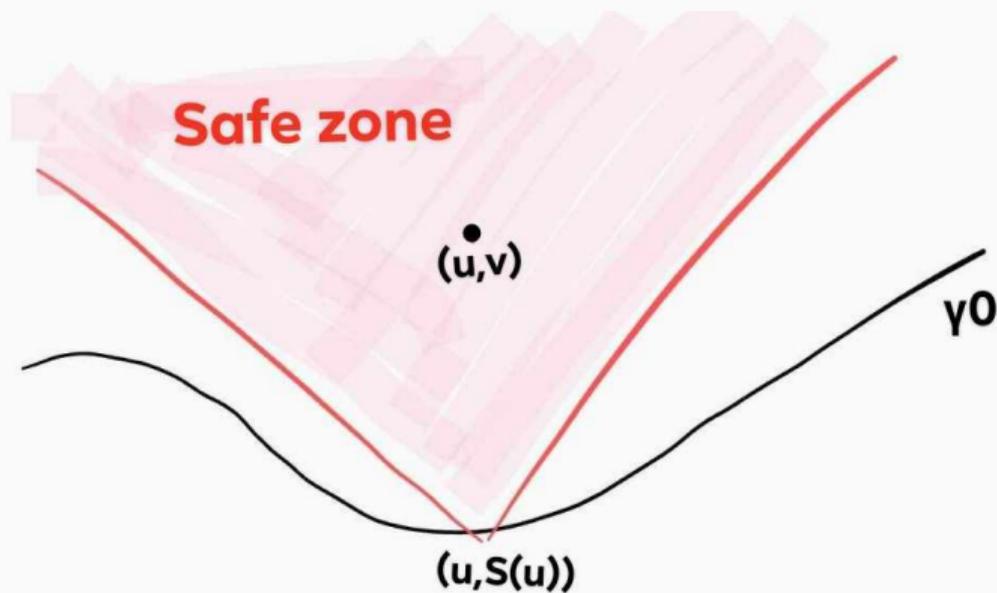


Figure 12: There is nothing much better to do than going down

Minty's trick

For the quadratic cost, the energy gap has a quadratic detachment in Minty's coordinates:

$$\forall u, v, \quad E(u, v) \geq \frac{|v - S(u)|^2}{2} \quad (32)$$

Consequence: if $\gamma \in \mathcal{P}_{2,ac}(\mathbb{R}^{2d})$, then

$$\int E\gamma \geq \int \frac{|v - S(u)|^2}{2} \gamma(u, v) du dv \quad (33)$$

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Quadratic detachment

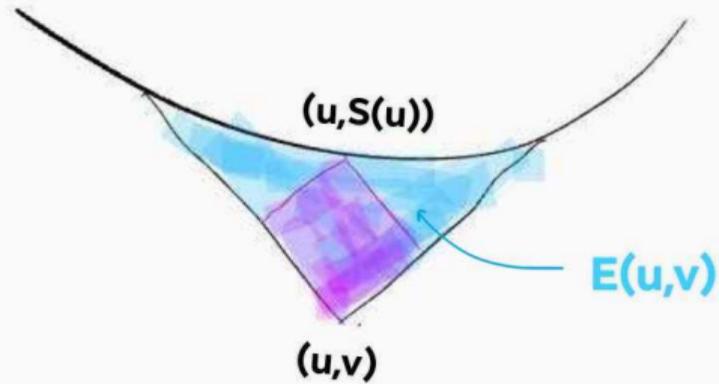


Figure 13: Quadratic detachment in 1d

Bound the transverse distance

Question: What do we do with this term $\int |v - S(u)|^2 d\gamma(u, v)$?

Answer: we can bound it with meaningful quantities

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Proposition

If $\gamma \in \mathcal{P}_2(\mathbb{R}^{2d})$, then

$$\int |v - S(u)|^2 d\gamma(u, v) \leq 2W_2^2(\gamma, \gamma_0)$$

$$\int |v - S(u)|^2 d\gamma(u, v) \leq 2 \int E\gamma$$

Remark that if $\gamma \in \Pi(\mu, \nu)$,

$$\int E\gamma = \int c\gamma - \int c\gamma_0.$$

We had

$$H(\gamma) \geq -\frac{d}{2} \ln \left(\int |v - S(u)|^2 d\gamma(u, v) \right) + C, \quad (34)$$

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$$H(\gamma_\epsilon) \gtrsim -\frac{d}{2} \ln W_2^2(\gamma_\epsilon, \gamma_0) \quad \text{and} \quad H(\gamma_\epsilon) \gtrsim -\frac{d}{2} \ln \left(\int c d\gamma_\epsilon - \int c d\gamma_0 \right)$$

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$$-\frac{d}{2} \varepsilon \ln(\varepsilon) \gtrsim OT_\varepsilon - OT_0$$

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Combining both,

$$W_2^2(\gamma_\varepsilon, \gamma_0) \gtrsim \varepsilon.$$

Suboptimality

Our result:

$$H(\gamma_\varepsilon) \gtrsim -\frac{d}{2} \ln\left(\int c\gamma_\varepsilon - \int c\gamma_0\right)$$

Existing literature:

$$-\frac{d}{2}\varepsilon \ln(\varepsilon) + C\varepsilon \geq \int c\gamma_\varepsilon - \int c\gamma_0 + \varepsilon H(\gamma_\varepsilon)$$

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Combining both,

$$C \geq \frac{\int c\gamma_\varepsilon - \int c\gamma_0}{\varepsilon} - \frac{d}{2} \ln\left(\frac{\int c\gamma_\varepsilon - \int c\gamma_0}{\varepsilon}\right) \quad (36)$$

the map $x \mapsto x - \frac{d}{2} \ln(x)$ is coercive, so

$$C_1\varepsilon \leq \int c\gamma_\varepsilon - \int c\gamma_0 \leq C_2\varepsilon$$

Theorem [MS23]

Suppose that the cost is quadratic, that is $c(x, y) = \frac{1}{2}\|x - y\|^2$. Further assume that $\mu_i \in \mathcal{P}_{2+\delta, ac}(\mathbb{R}^d)$ for some $\delta > 0$.

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Maps

Theorem [MS23]

Suppose that the cost is quadratic, that is $c(x, y) = \frac{1}{2}\|x - y\|^2$. Further assume that $\mu_i \in \mathcal{P}_{2+\delta, ac}$ for some $\delta > 0$ and that the Monge map ∇f is Lipschitz. Then

$$C_1\sqrt{\varepsilon} \geq W_2(\gamma_\varepsilon, \gamma_0) \geq C_2\sqrt{\varepsilon}, \quad (39)$$

Theorem [MS23]

Suppose that the cost is quadratic, that is $c(x, y) = \frac{1}{2}\|x - y\|^2$. Further assume that $\mu_i \in \mathcal{P}_{2+\delta, ac}$ for some $\delta > 0$ and that the Monge map ∇f is Lipschitz. Then

$$C_1\sqrt{\varepsilon} \geq W_2(\gamma_\varepsilon, \gamma_0) \geq C_2\sqrt{\varepsilon}, \quad (39)$$

and

$$\|\nabla f_\varepsilon - \nabla f\|_{L^2(\mu_0)}^2 \leq C\varepsilon \quad (40)$$

Where f_ε is the Schrödinger potential and ∇f_ε is the barycentric map.

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Suppose that the cost is quadratic, that is $c(x, y) = \frac{1}{2}\|x - y\|^2$. Further assume that $\mu_i \in \mathcal{P}_{2+\delta, ac}$ for some $\delta > 0$ and that the Monge map ∇f is Lipschitz. Then

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Where f_ε is the Schrödinger potential and ∇f_ε is the barycentric map. ∇f_ε is the barycentric map means

$$\nabla f_\varepsilon(x) = \int y d\gamma_\varepsilon^x(y)$$

We got interested in $\int |v - S(u)|^2 d\gamma_\varepsilon(u, v)$, we can also be interested in $\int |y - T(x)|^2 d\gamma_\varepsilon(x, y)$. Two good reasons:

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- by Jensen inequality

$$\int \left| \int y d\gamma_\epsilon^x(y) - T(x) \right|^2 d\hat{\gamma}_\epsilon(x) \leq \int |y - T(x)|^2 d\gamma_\epsilon(x, y)$$

- $(x, y) \mapsto x, T(x)$ is a transport map between γ_ϵ and γ_0 , so

$$W_2^2(\gamma_\epsilon, \gamma_0) \leq \int |y - T(x)|^2 d\gamma_\epsilon(x, y)$$

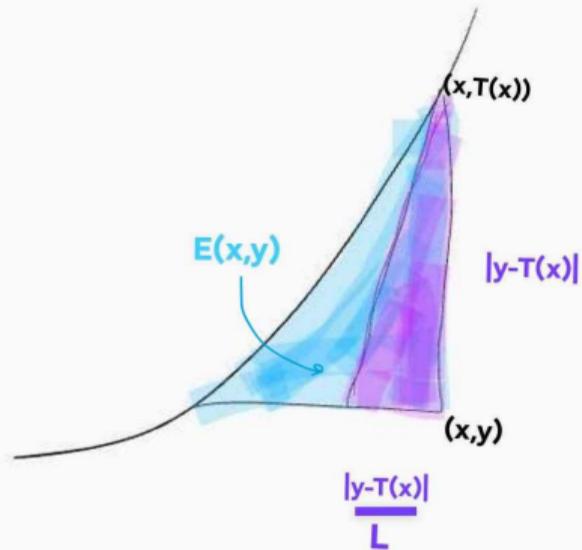


Figure 14: The energy gap $E(x, y)$ is bounded by $\frac{|y - T(x)|^2}{2L}$

$$E(x, y) \leq \frac{|y - T(x)|^2}{2L}$$

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Proposition

If ∇f is L -lipschitz, then

$$\int |y - T(x)|^2 d\gamma_\epsilon(x, y) \leq 2L \left(\int c\gamma_\epsilon - \int c\gamma_0 \right).$$

Theorem [MS23]

Suppose that the cost is quadratic, that is $c(x, y) = \frac{1}{2}\|x - y\|^2$. Further assume that $\mu_i \in \mathcal{P}_{2+\delta, ac}$ for some $\delta > 0$ and that the Monge map ∇f is Lipschitz. Then

$$C_1\sqrt{\varepsilon} \geq W_2(\gamma_\varepsilon, \gamma_0) \geq C_2\sqrt{\varepsilon}, \quad (41)$$

and

$$\|\nabla f_\varepsilon - \nabla f\|_{L^2(\mu_0)}^2 \leq C\varepsilon \quad (42)$$

Where f_ε is the Schrödinger potential and ∇f_ε is the barycentric map.

Infinitesimally twisted costs and compact supports

Definition

$c \in \mathcal{C}^2(\Omega^2)$ is said to be infinitesimally twisted if $\nabla_{xy}^2 c(x, y) = (\partial_{x_i y_j}^2 c(x, y))_{i,j} \in M_d(\mathbb{R})$ is invertible for every $(x, y) \in \Omega^2$.

Theorem

Suppose that the cost is \mathcal{C}^2 and infinitesimally twisted . Further assume that μ_i is compactly supported then

$$(c, \gamma_\varepsilon) = OT_0 + \Theta(\varepsilon), \quad H(\gamma_\varepsilon \mid \mathcal{H}^{2d}) = -\frac{d}{2} \ln(\varepsilon) + O(1), \quad \sqrt{\varepsilon} = O(W_2(\gamma_\varepsilon, \gamma_0)) \quad (43)$$

Note that here γ_0 is any optimal transport plan.

Thank you !

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