Mappings valued in the Wasserstein space

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May 14th, 2020

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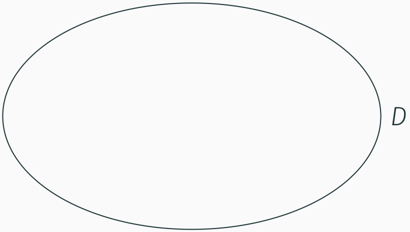
The Wasserstein[1] space

D convex and compact domain of $\mathbb{R}^d$.



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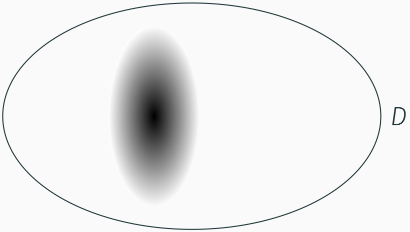

$\mathcal{P}(D)$ space of probability measures on D.

The **Wasserstein space** is the space $\mathcal{P}(D)$ endowed with the Wasserstein distance.

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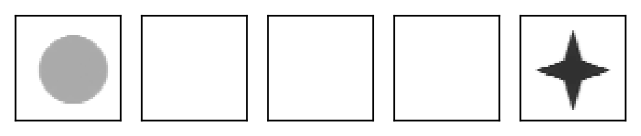

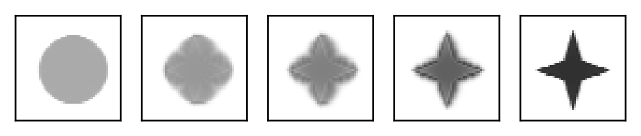

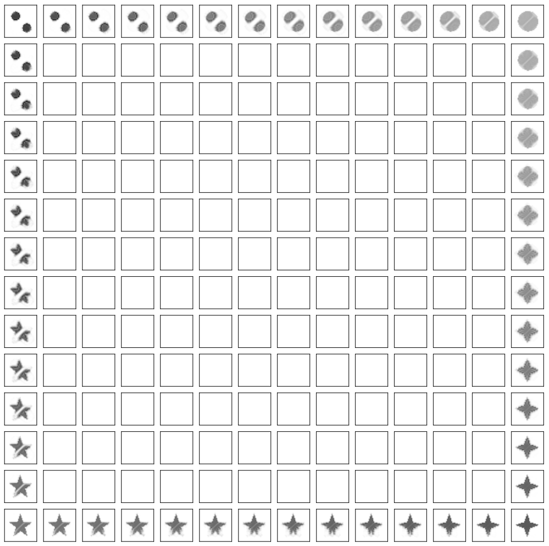

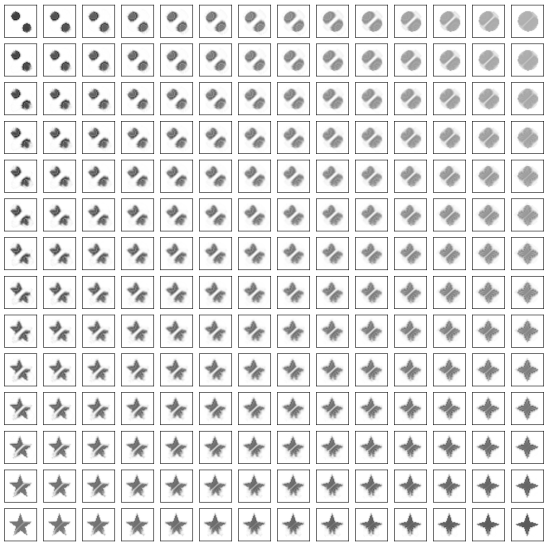

In this presentation

1. A quick introduction to the Wasserstein space
2. Harmonic mappings valued in the Wasserstein space
3. An application in nonlinear elasticity

1. A quick introduction to the Wasserstein space

The metric tensor in the Wasserstein space

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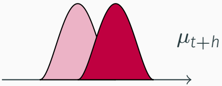

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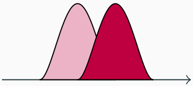
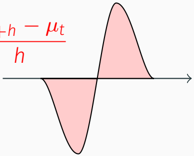


Vertical derivative

$$\frac{\mu_{t+h} - \mu_t}{h}$$



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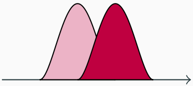

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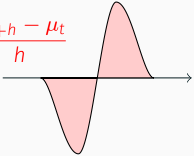

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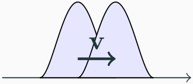

A particle located at x moves to $x + h\mathbf{v}(x)$

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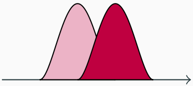

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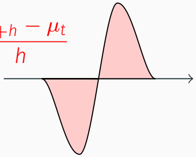
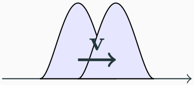


$$\boxed{\partial_t \mu = -\nabla \cdot (\mu \mathbf{v})}$$



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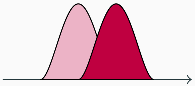

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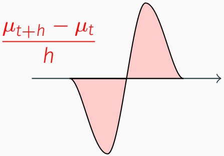

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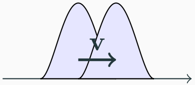

A particle located at x moves to $x + h\mathbf{v}(x)$

- Quadratic Optimal Transport: the square of the norm of the speed is

$$\min_{\mathbf{v}: D \to \mathbb{R}^d} \left\{ \int_D |\mathbf{v}(y)|^2 \, \mu(\mathrm{d}y) \ : \ -\nabla \cdot (\mu \mathbf{v}) = \partial_t \mu \right\}.$$

Action and geodesics

If $\mu : [0,1] \to \mathcal{P}(D)$ is given, its **action** is

$$\mathcal{A}(\mu) := \min_{\mathbf{v}} \left\{ \frac{1}{2} \int_0^1 \int_D |\mathbf{v}_t|^2 \, \mathrm{d}\mu_t \, \mathrm{d}t \ : \ \partial_t \mu_t + \nabla \cdot (\mu_t \mathbf{v}_t) = 0 \right\}.$$

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The Wasserstein distance W_2 is

$$\frac{1}{2} W_2^2(\rho, \nu) = \min_{\mu} \left\{ \mathcal{A}(\mu) \ : \ \mu_0 = \rho, \ \mu_1 = \nu \right\},$$

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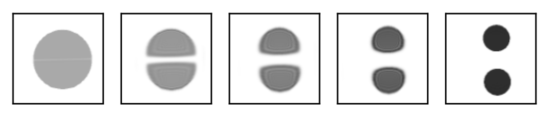

and the minimizers are the constant-speed geodesics.

Wasserstein spaces on manifolds

The definition can be extended for D Riemannian manifold, and similar numerical methods can be used[2].

[2] H. Lavenant, S. Claici, E. Chien and J. Solomon. *Dynamical Optimal Transport on Discrete Surfaces*. 2018.

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Why use Wasserstein distances?

Finding matching between distributions of mass is an ubiquitous task.

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- **Data fitting** in machine learning[6].

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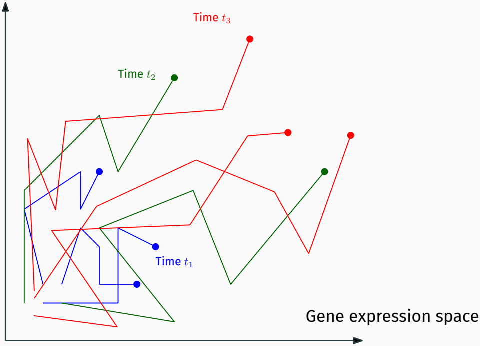
Regularizer in machine learning[7]



- Stochastic process (X_t), access to *independent samples* at different times.

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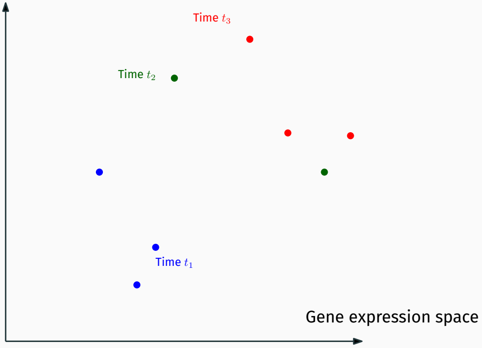

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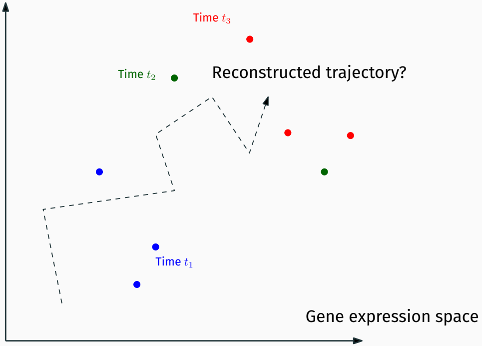

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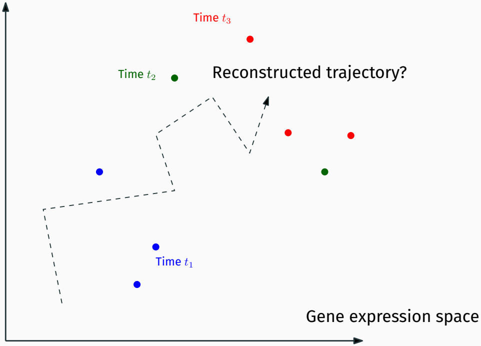

- Stochastic process (X_t), access to *independent samples* at different times.
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- Presence of noise? Handling birth and death of cells?

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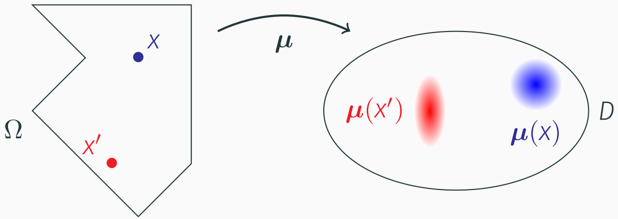
2. Harmonic mappings valued in the Wasserstein space

Measure-valued mappings[8]

Ω bounded set of $\mathbb{R}^n$ with Lipschitz boundary

We study $\boldsymbol{\mu} : \Omega \to \mathcal{P}(D)$.



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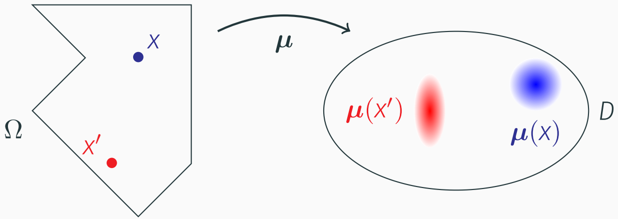

Definition of $\mathrm{Dir}(\boldsymbol{\mu}) = \dfrac{1}{2}\displaystyle\int_\Omega |\nabla \boldsymbol{\mu}|^2$ the **Dirichlet energy** generalizing $\mathcal{A}$.

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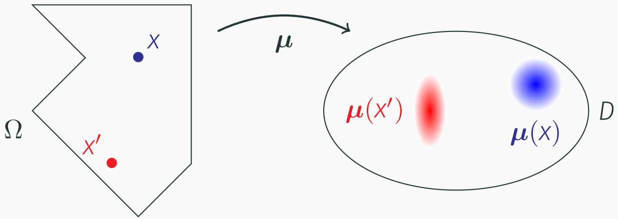

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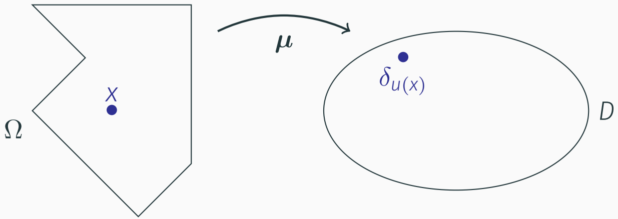

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If $u : \Omega \to D$ and $\boldsymbol{\mu}(x) := \delta_{u(x)}$ then $\mathrm{Dir}(\boldsymbol{\mu}) = \dfrac{1}{2}\displaystyle\int_\Omega |\nabla u|^2$.

[8] H. Lavenant. *Harmonic mappings valued in the Wasserstein space.* 2019.

The Dirichlet energy[9]

Definition

If $\boldsymbol{\mu} : \Omega \to \mathcal{P}(D)$ is given,

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where $\mathbf{v} : \Omega \times D \to \mathbb{R}^{nd}$ "density of Jacobian matrix".

If $\Omega = [0,1]$ it coincides with $\mathcal{A}$.

[9] Brenier. *Extended Monge-Kantorovich theory*. 2003.

Equivalence with a metric definition[10]

$$\frac{W_2^2(\boldsymbol{\mu}(x), \boldsymbol{\mu}(x'))}{\varepsilon^2}$$

[10] Korevaar and Schoen. *Sobolev spaces and harmonic maps for metric space targets.* 1993.

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$$\frac{1}{\varepsilon^n} \int_\Omega \frac{W_2^2(\boldsymbol{\mu}(x), \boldsymbol{\mu}(x'))}{\varepsilon^2} \mathbb{1}_{|x-x'|\leqslant \varepsilon} \, \mathrm{d}x'$$

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$$\mathrm{Dir}_\varepsilon(\boldsymbol{\mu}) := \frac{C_n}{2} \int_\Omega \frac{1}{\varepsilon^n} \int_\Omega \frac{W_2^2(\boldsymbol{\mu}(x), \boldsymbol{\mu}(x'))}{\varepsilon^2} \mathbb{1}_{|x-x'| \leqslant \varepsilon} \, \mathrm{d}x' \, \mathrm{d}x$$

Proposed by Korevaar, Schoen (and Jost) for mappings valued in metric spaces.

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Theorem

There holds

$$\lim_{\varepsilon \to 0} \mathrm{Dir}_\varepsilon = \mathrm{Dir},$$

and the convergence holds pointwisely and in the sense of Γ*-convergence along the sequence* $\varepsilon_m = 2^{-m}$.

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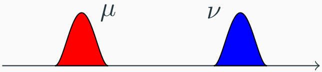
Curvature and convexity

If $\mu, \nu \in \mathcal{P}(D)$, two ways to interpolate.



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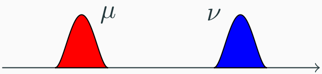

The **displacement** interpolation

- Midpoint of the geodesic in the Wasserstein space.
- The space $(\mathcal{P}(D), W_2)$ is a **positively curved space**: no convexity of W_2^2 nor Dir.

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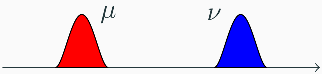

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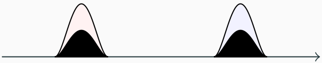
The **Linear** interpolation



- The Wasserstein distance square W_2^2 and the Dirichlet energy are convex.
- Tools from convex analysis.

The Dirichlet problem

The Dirichlet problem

We choose $\boldsymbol{\mu}_b : \partial\Omega \to \mathcal{P}(D)$ the boundary data.

Definition

The Dirichlet problem is

$$\min_{\boldsymbol{\mu}} \left\{ \mathrm{Dir}(\boldsymbol{\mu}) \ : \ \boldsymbol{\mu} = \boldsymbol{\mu}_b \text{ on } \partial\Omega \right\}.$$

The solutions of the Dirichlet problem are called harmonic mappings (valued in the Wasserstein space).

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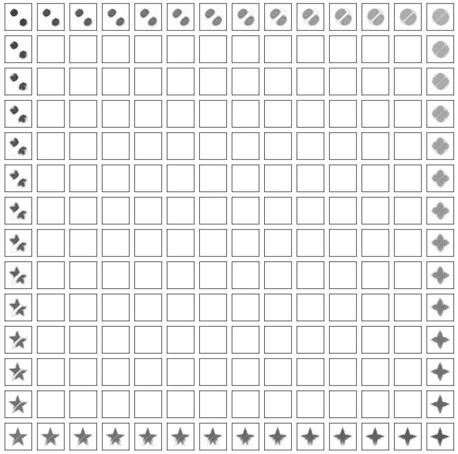
Theorem

Assume $\boldsymbol{\mu}_b : \partial\Omega \to (\mathcal{P}(D), W_2)$ is a Lipschitz mapping. Then there exists at least one solution to the Dirichlet problem.

Uniqueness is an open question.

Numerics: example



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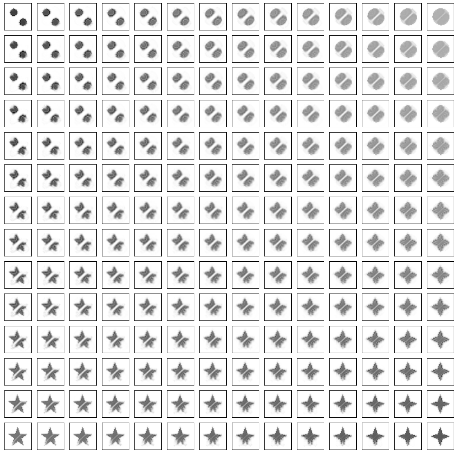

Numerics: adaptation of Benamou and Brenier[11]

The Dirichlet problem is a convex optimization problem.

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Unknowns ($\mathbf{m} = \boldsymbol{\mu}\mathbf{v}$ is the momentum):

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Objective:

$$\min_{\boldsymbol{\mu},\mathbf{m}} \left\{ \iint_{\Omega \times D} \frac{|\mathbf{m}|^2}{2\boldsymbol{\mu}} \right\}$$

under the constraints:

$$\begin{cases} \nabla_\Omega \boldsymbol{\mu} + \nabla_D \cdot \mathbf{m} = 0, \\ \boldsymbol{\mu} = \boldsymbol{\mu}_b \text{ on } \partial\Omega. \end{cases}$$

[11] J.-D. Benamou, and Y. Brenier. *A computational fluid mechanics solution to the Monge-Kantorovich mass transfer problem.* 2000.

Numerics: convergence? (for geodesics $\Omega = [0, 1]$)

In practice: finite-dimensional "approximation" with two convex optimization problems in duality, then **ADMM**.

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- Convergence of the solutions of the **discretized problem to the continuous one**[14].

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Maximum principle

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Some functionals $F : \mathcal{P}(D) \to \mathbb{R} \cup \{+\infty\}$ are convex along geodesics, e.g.

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Then there exists at least one solution $\boldsymbol{\mu}$ of the Dirichlet problem with boundary conditions $\boldsymbol{\mu}_b$ such that

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Already known for harmonic mappings valued in Riemannian manifolds (Ishihara) and Non Positively Curved spaces (Sturm).

3. An application in nonlinear elasticity

A variational problem inspired from elasticity theory

$\mathcal{L}_\Omega$ and $\mathcal{L}_D$ Lebesgue measures restricted to D and Ω respectively.

$$\min_{u:\Omega\to D}\left\{E(u) := \int_\Omega \left(\frac{1}{2}|\nabla u(x)|^2 - f(x)\cdot u(x)\right)\mathrm{d}x \ : \ u = g \text{ on } \partial\Omega \text{ and } u\#\mathcal{L}_\Omega = \mathcal{L}_D\right\}$$

- $f : \Omega \to \mathbb{R}^d$ exterior force.
- $g : \partial\Omega \to \partial D$ prescribed deformation on the boundary.
- $u\#\mathcal{L}_\Omega = \mathcal{L}_D \Leftrightarrow \forall B \subset D,\ \mathcal{L}_\Omega(u^{-1}(B)) = \mathcal{L}_D(B)$.
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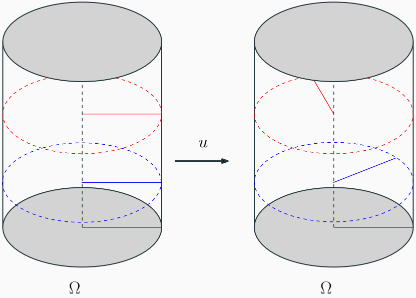
$$|\det \nabla u| = 1.$$

Critical points satisfy $\Delta u + f = (\nabla\omega)\circ u$ in the interior of Ω, where $\omega : D \to \mathbb{R}$ is a Lagrange multiplier.

An example: pure torsion of a cylinder



$\Omega = D = B(0,1) \times [0,1]$. For $a > 0$,

$$u_a \begin{pmatrix} x \\ y \\ z \end{pmatrix} = \begin{pmatrix} R_{az} \begin{pmatrix} x \\ y \end{pmatrix} \\ z \end{pmatrix}$$

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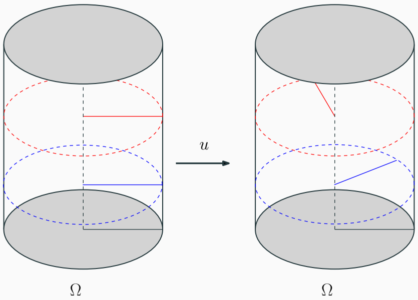

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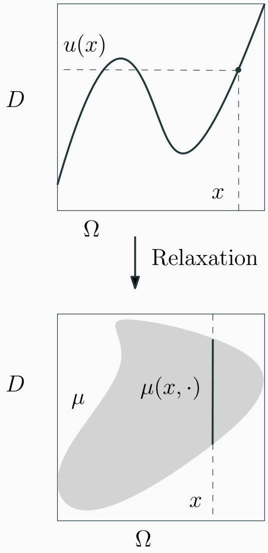
Result $(f \equiv 0)$

For all a, the function u_a is a critical point of the energy.

At least for small a, it is a global minimizer with boundary condition $g = u_a|_{\partial\Omega}$.

Transport plan



Method

$u : \Omega \to D$ is replaced by $\boldsymbol{\mu} : \Omega \to \mathcal{P}(D)$.

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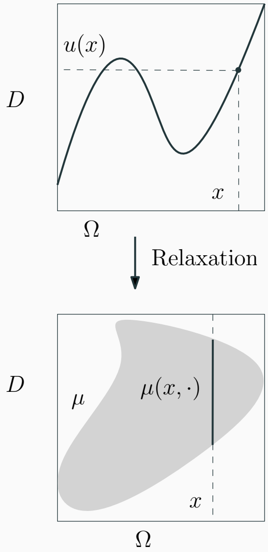

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- By disintegration/fubinization, one can see a mapping $\boldsymbol{\mu} : \Omega \to \mathcal{P}(D)$ as $\boldsymbol{\mu} \in \mathcal{P}(\Omega \times D)$ whose first marginal is $\mathcal{L}_\Omega$.
- The constraint $u\#\mathcal{L}_\Omega = \mathcal{L}_D$ is replaced by the second marginal of $\boldsymbol{\mu}$ being $\mathcal{L}_D$. We write $\boldsymbol{\mu} \in \Pi(\mathcal{L}_\Omega, \mathcal{L}_D)$.
- The marginal constraints are linear. For instance, for all $a \in C(\Omega)$:

$$\iint_{\Omega \times D} a(x)\, \boldsymbol{\mu}(\mathrm{d}x, \mathrm{d}y) = \int_\Omega a(x)\, \mathrm{d}x$$

A convex relaxation[15]

$$\min_{u:\Omega\to D}\left\{\int_\Omega\left(\frac{1}{2}|\nabla u(x)|^2 - f(x)\cdot u(x)\right)\mathrm{d}x \;:\; u = g \text{ on } \partial\Omega \text{ and } u\#\mathcal{L}_\Omega = \mathcal{L}_D\right\}$$

$$\downarrow$$

$$\min_{\boldsymbol{\mu}:\Omega\to\mathcal{P}(D)}\left\{\mathrm{Dir}(\boldsymbol{\mu}) - \iint_{D\times\Omega} f(x)\cdot y\,\boldsymbol{\mu}(\mathrm{d}x,\mathrm{d}y) \;:\; \boldsymbol{\mu}(x,\cdot) = \delta_{g(x)} \text{ for } x\in\partial\Omega \text{ and } \boldsymbol{\mu}\in\Pi(\mathcal{L}_\Omega,\mathcal{L}_D)\right\}$$

Without Dirichlet energy, it's exactly the relaxation used by Yann Brenier in 1987 to prove polar factorization!

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Remark

It's a convex problem!

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Tightness of the relaxation

Let $\lambda_1(\Omega)$ the first eigenvalue of the Dirichlet Laplacian on Ω.

Theorem

Let $u : \Omega \to D$ a smooth function satisfying $u = g$ on $\partial\Omega$ and $\omega \in C(D)$ such that

$$\Delta u + f = (\nabla\omega) \circ u.$$

If ω can be extended on $\mathbb{R}^d$ in a λ-**convex** function **with** $\lambda > -\lambda_1(\Omega)$ then u is the unique global minimizer global of the energy and and of the relaxed energy.

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Remark

There exists a simpler proof of this consequence which does not rely on the convex relaxation.

Conclusion

- Working on optimal transport by studying curves and mappings valued in the space of probability distributions.
- Some promising directions in Data Science using optimal transport as a regularizer.
- Definition of harmonic mappings valued in the Wasserstein space, with applications in nonlinear elasticity.

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Thank you for your attention