The Multi-Marginal Optimal Transport Problem and its Applications

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Lecture 3

Overview

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Introduction: Classical vs Multi-Marginal Optimal Transport

Classical Optimal Transportation Theory

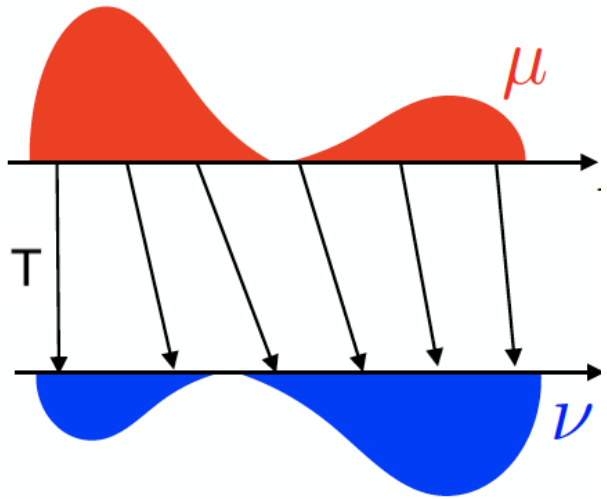
Let $\mu \in \mathcal{P}(X)$ and $\nu \in \mathcal{P}(Y)$ ($X \subseteq \mathbb{R}^n$ and $Y \subseteq \mathbb{R}^n$), the Optimal Transport (OT) problem is defined as follows

$$(\mathcal{MK}) \quad E_c(\mu,\nu) = \inf\{\mathcal{E}_c(\gamma) \mid \gamma \in \Pi(\mu,\nu)\} \tag{1}$$

where $\Pi(\mu,\nu) := \{\gamma \in \mathcal{P}(X \times Y) | \quad \pi_{1,\sharp}\gamma = \mu,\ \pi_{2,\sharp}\gamma = \nu\}$ and

$$\mathcal{E}_c(\gamma) := \int c(x_1,x_2)d\gamma(x_1,x_2).$$

Solution à la Monge : the transport plan γ is deterministic (or à la Monge) if $\gamma = (Id, T)_\sharp\mu$ where $T_\sharp\mu = \nu$.



The Multi-Marginal Optimal Transportation

Let us take N probability measures $\mu_i \in \mathcal{P}(X)$ with $i = 1, \cdots, N$ and $c : X^N \to [0, +\infty]$ a continuous cost function. Then the multi-marginal OT problem reads as:

$$(\mathcal{MK}_N) \quad E_c(\mu_1, \cdots, \mu_N) = \inf \{\mathcal{E}_c(\gamma) \mid \gamma \in \Pi_N(\mu_1, \cdots, \mu_N)\} \tag{2}$$

where $\Pi_N(\mu_1, \cdots, \mu_N)$ denotes the set of couplings $\gamma(x_1, \cdots, x_N)$ having μ_i as marginals and

$$\mathcal{E}_c(\gamma) := \int c(x_1, \cdots, x_N) d\gamma(x_1, \cdots, x_N)$$

Solution à la Monge : $\gamma = (Id, T_2, \ldots, T_N)_\sharp \mu_1$ where $T_{i\sharp}\mu_1 = \mu_i$.

Why is it a difficult problem to treat?

Example : $N = 3$, $d = 1$, $\mu_i = \mathcal{L}_{[0,1]}$ $\forall i$ and $c(x_1, x_2, x_3) = |x_1 + x_2 + x_3|^2$.

- Uniqueness fails (**Simone Di Marino, Augusto Gerolin, and Luca Nenna 2017**);
- $\exists$ T_i optimal, are not differentiable at any point and they are fractal maps **ibid., Thm 4.6**

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The dual formulation of $(\mathcal{MK})$

We consider the 2 marginals case for simplicity. The $(\mathcal{MK})$ problem admits a dual formulation:

$$\sup \{\mathcal{J}(\phi, \psi) \mid (\phi, \psi) \in \mathcal{K}\}. \tag{3}$$

where

$$\mathcal{J}(\phi, \psi) := \int_X \phi d\mu(x) + \int_Y \psi d\nu(y)$$

and $\mathcal{K}$ is the set of bounded and continuous functions ϕ, ψ such that $\phi(x) + \psi(y) \leq c(x, y)$.

Remark

Notice that the constraint on a couple (ϕ, ψ) may be rewritten as

$$\psi(y) \leq \inf_x c(x, y) - \phi(x) := \phi^c(y).$$

So for an admissible couple (ϕ, ψ) one has $\mathcal{J}(\phi, \phi^c) \geq \mathcal{J}(\phi, \psi)$

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Some applications

- The Wasserstein barycenter problem can be rewritten as a MMOT problem (see **(Agueh and G. Carlier 2011)**): statistics, machine learning, image processing;
- Matching for teams problem (see **(Guillaume Carlier and Ekeland 2010)**): economics. The transport plan γ matches individuals from each team μ_i minimizing a given cost;
- In Density Functional Theory: the electron-electron repulsion (see **(Buttazzo, De Pascale, and Paola Gori-Giorgi 2012; C. Cotar, G. Friesecke, and C. Klüppelberg 2013)**). The plan $\gamma(x_1, \cdots, x_N)$ returns the probability of finding electrons at position $x_1, \cdots, x_N$;
- Incompressible Euler Equations **(Yann Brenier 1989)** : $\gamma(\omega)$ gives "the mass of fluid" which follows a path ω. See also **(Jean-David Benamou, Guillaume Carlier, and Luca Nenna 2018)**.
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The three universes of Numerical Optimal Transportation

Let's consider the two marginal case then we can have the three following numerical approach to Optimal Transport

- Discrete-2-Discrete: the marginals μ have an atomic form, i.e. $\mu(x) = \sum_i \mu_i \delta_{x_i}$ (and ν as well). **Remarks:**
  - The problem becomes a standard linear programming problem.
  - Works for any kind of cost function.
  - Can be easily generalized to the multi-marginal case.
- Continous-2-Discrete: $\mu = \bar{\mu} dx$ and $\nu(y) = \sum_i \nu_i \delta_{y_i}$. **Remarks:**
  - The semi-discrete approach (**Mérigot 2011**).
  - Used for generalized euler equations (kind of mmot problem) à la Brenier (**Mérigot and Mirebeau 2016**).
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The discretized Monge-Kantorovich problem

Let's take $c_{ij} = c(x_i, y_j) \in \mathbb{R}^{M\times M}$ (M are the gridpoints used to discretize X) then the discretized $(\mathcal{MK})$, reads as

$$\min\{\sum_{i,j=1}^{M} c_{ij}\gamma_{ij} \mid \sum_{j=1}^{M} \gamma_{ij} = \mu_i \ \forall i, \ \sum_{i=1}^{M} \gamma_{ij} = \nu_j \ \forall j\} \tag{4}$$

and the dual problem

$$\max\{\sum_{i=1}^{M} \phi_i\mu_i + \sum_{j=1}^{M} \psi_j\nu_j \mid \phi_i + \psi_j \leq c_{ij} \ \forall (i,j) \in \{1, \cdots, M\}^2\}. \tag{5}$$

Remarks

- The primal has M^2 unknowns and $M \times 2$ linear constraints.
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The importance of being sparse

A multi-scale approach to reduce M **(J.-D. Benamou, G. Carlier, and L. Nenna 2016)**

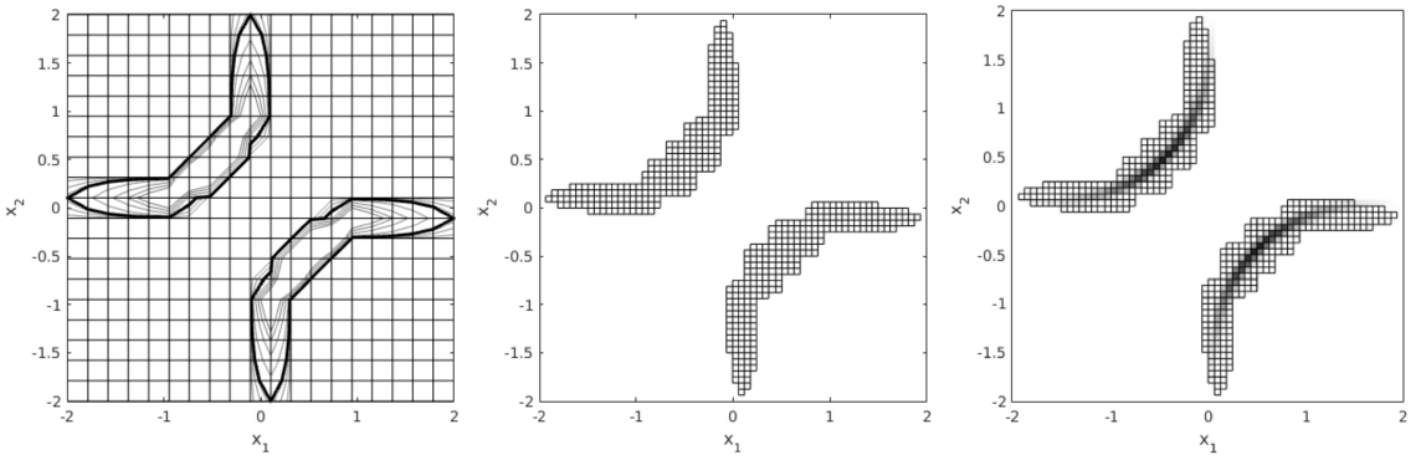

Figure: Support of the optimal γ for 2 marginals and the Coulomb cost

Some references:

Schmitzer, Bernhard (2019). "Stabilized sparse scaling algorithms for entropy regularized transport problems". In: *SIAM J. Sci. Comput.* 41.3, A1443–A1481. ISSN: 1064-8275. DOI: 10.1137/16M1106018. URL: https://mathscinet.ams.org/mathscinet-getitem?mr=3947294.

Mérigot, Quentin (2011). "A multiscale approach to optimal transport". In: *Computer Graphics Forum*. Vol. 30. 5. Wiley Online Library, pp. 1583–1592.

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$$\min\{ \sum_{(j_1,\cdots,j_N)=1}^{M} c_{j_1,\cdots,j_N}\gamma_{j_1,\cdots,j_N} \quad | \quad \sum_{j_k,k\neq i} \gamma_{j_1,\cdots,j_{i-1},j_{i+1},\cdots,j_N} = \mu^i_{j_i}\} \tag{6}$$

and the dual problem

$$\max\{\sum_{i=1}^{N}\sum_{j_i=1}^{M} u^i_{j_i}\mu^i_{j_i} \quad | \quad \sum_{k=1}^{N} u^k_{j_k} \leq c_{j_1,\dots,j_N} \quad \forall (j_1,\cdots,j_N) \in \{1,\cdots,M\}^N\}. \tag{7}$$

Drawbacks

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Entropic Optimal Transport (Repetita iuvant!)

The entropic OT problem

We present a numerical method to solve the regularized ((**Jean-David Benamou, Guillaume Carlier, Marco Cuturi, Luca Nenna, and Gabriel Peyré 2015; M. Cuturi 2013; Galichon and Salanié 2009**)) optimal transport problem (let us consider, for simplicity, 2 marginals)

$$\min_{\gamma \in \mathcal{C}} \sum_{i,j} c_{ij}\gamma_{ij} + \begin{cases} \epsilon \sum_{ij} \gamma_{ij} \log\left(\frac{\gamma_{ij}}{\mu_i \nu_j}\right) & \gamma \geq 0 \\ +\infty & \textit{otherwise} \end{cases} . \tag{8}$$

where C is the matrix associated to the cost, γ is the discrete transport plan and $\mathcal{C}$ is the intersection between $\mathcal{C}_1 = \{\gamma \mid \sum_j \gamma_{ij} = \mu_i\}$ and $\mathcal{C}_2 = \{\gamma \mid \sum_i \gamma_{ij} = \nu_j\}$.

Remark: Think at ϵ as the temperature, then entropic OT is just OT at positive temperature.

The problem (8) can be re-written as

$$\min_{\gamma \in \mathcal{C}} \mathcal{H}(\gamma|\bar{\gamma}) \tag{9}$$

where $\mathcal{H}(\gamma|\bar{\gamma}) = \sum_{ij} \gamma_{ij} \left(\log \frac{\gamma_{ij}}{\bar{\gamma}_{ij}} \right)$ ($= \mathrm{KL}(\gamma|\bar{\gamma})$ aka the Kullback-Leibler divergence) and $\bar{\gamma}_{ij} = e^{-\frac{c_{ij}}{\epsilon}} \mu_i \nu_j$.

Remarks:

- Unique and semi-explicit solution
- Problem (9) dates back to Schrödinger, (see Christian Léonard's web page).
- $\mathcal{H} \to \mathcal{MK}$ as $\epsilon \to 0$. (see (Guillaume Carlier, Duval, Gabriel Peyré, and Bernhard Schmitzer 2017; Léonard 2012)).
- The dual problem is an unconstrained optimization problem.

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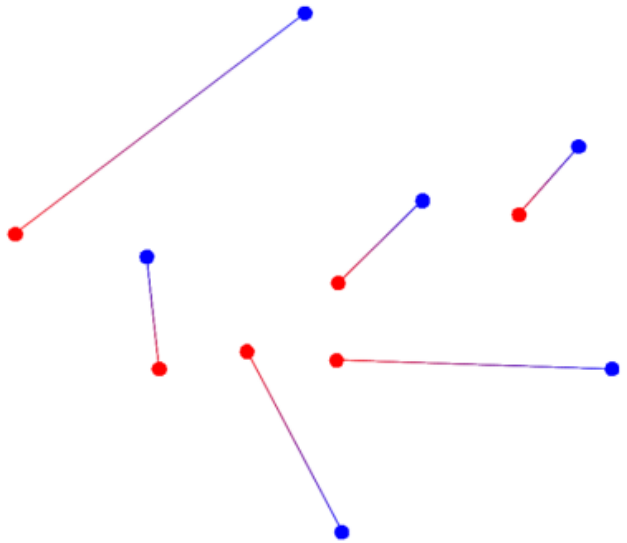
The "bridge" between quadratic Monge-Kantorovich and Schrödinger

From deterministic to stochastic matching **(Léonard 2012)**

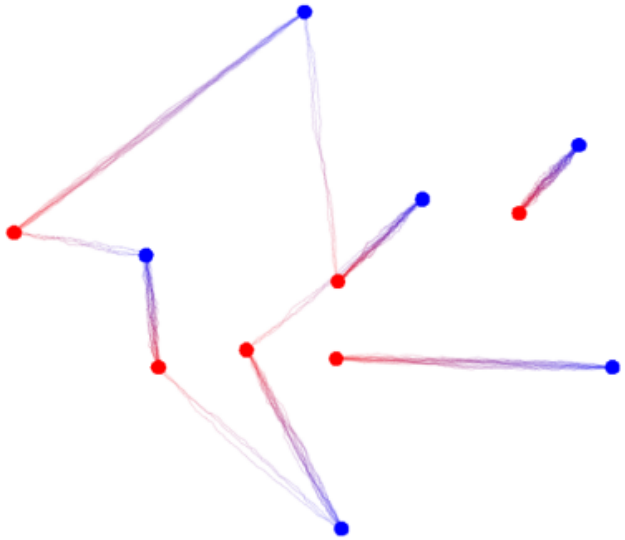


$$\varepsilon = 0$$

Figure: G. Peyre's twitter account

The "bridge" between quadratic Monge-Kantorovich and Schrödinger

From deterministic to stochastic matching **(Léonard 2012)**

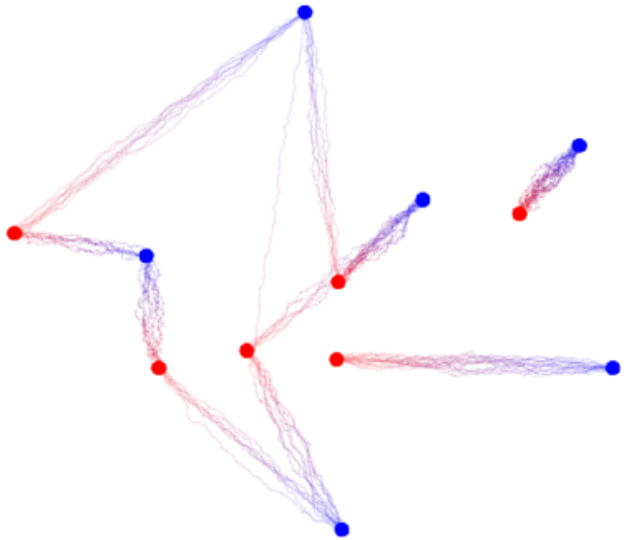


$$\varepsilon = .05$$

Figure: G. Peyre's twitter account

The "bridge" between quadratic Monge-Kantorovich and Schrödinger

From deterministic to stochastic matching **(Léonard 2012)**

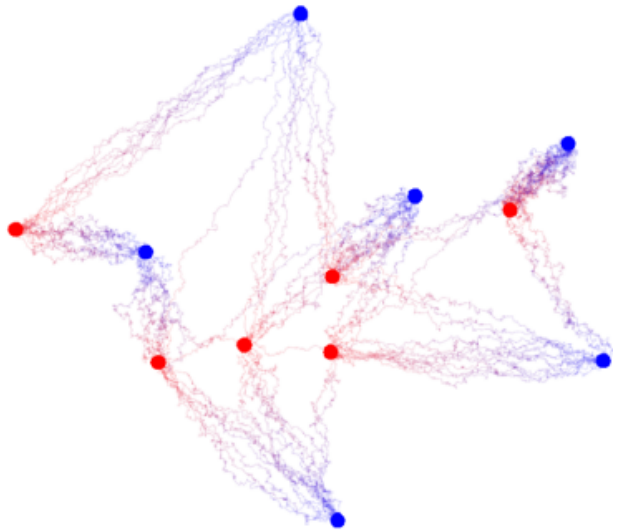


$$\varepsilon = 0.2$$

Figure: G. Peyre's twitter account

The "bridge" between quadratic Monge-Kantorovich and Schrödinger

From deterministic to stochastic matching **(Léonard 2012)**



$$\varepsilon = 1$$

Figure: G. Peyre's twitter account

How the regularization works: from spread to deterministic plan (quadratic cost)

Take the quadratic cost and solve the regularized problem. Then as $\epsilon \to 0$ ($N = 512$), we have

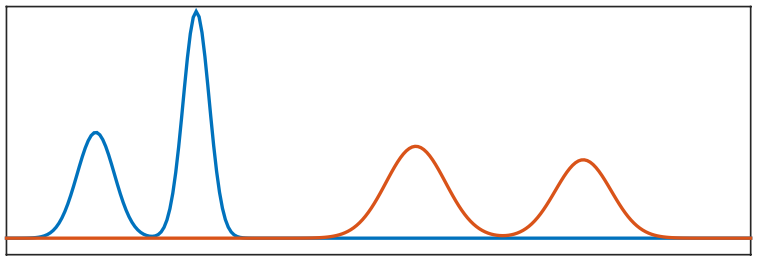


Figure: Marginals μ and ν

Figure: $\epsilon = 60/N$

How the regularization works: from spread to deterministic plan (quadratic cost)

Take the quadratic cost and solve the regularized problem. Then as $\epsilon \to 0$ ($N = 512$), we have

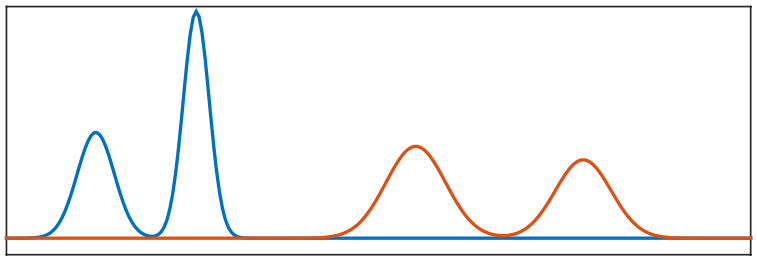


Figure: Marginals μ and ν

Figure: $\epsilon = 40/N$

How the regularization works: from spread to deterministic plan (quadratic cost)

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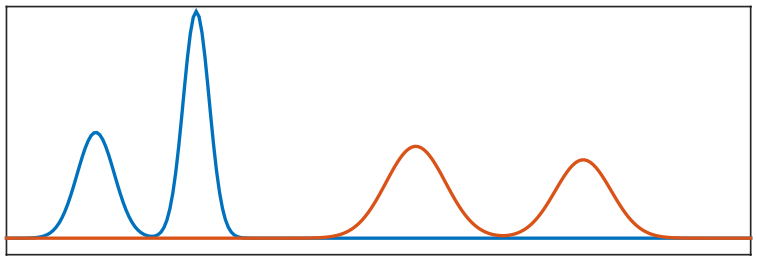

Figure: Marginals μ and ν

Figure: $\epsilon = 20/N$

How the regularization works: from spread to deterministic plan (quadratic cost)

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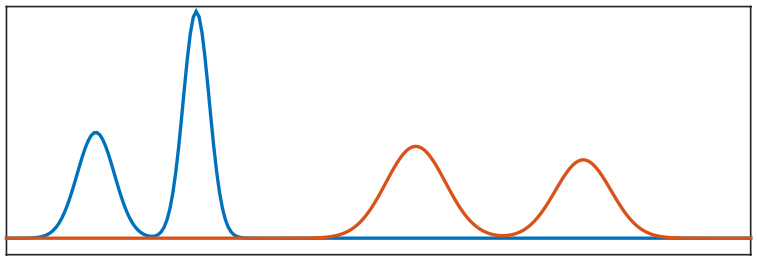

Figure: Marginals μ and ν

Figure: $\epsilon = 10/N$

How the regularization works: from spread to deterministic plan (quadratic cost)

Take the quadratic cost and solve the regularized problem. Then as $\epsilon \to 0$ ($N = 512$), we have

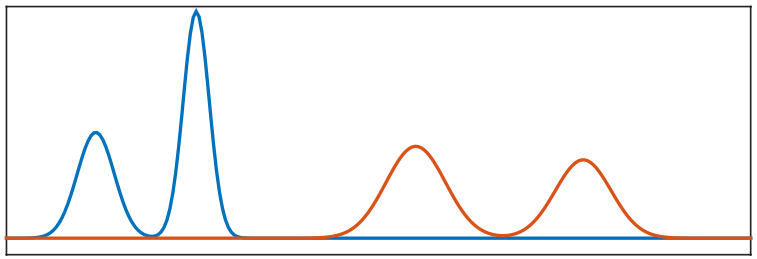

Figure: Marginals μ and ν

Figure: $\epsilon = 6/N$

How the regularization works: from spread to deterministic plan (quadratic cost)

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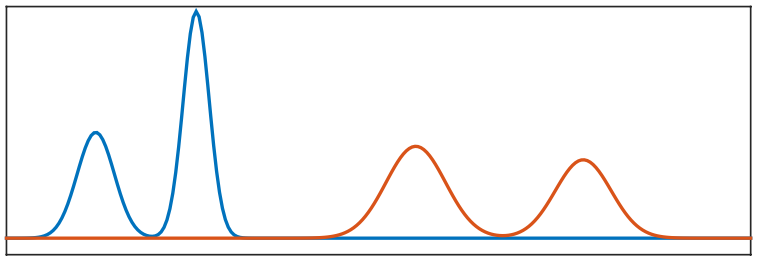

Figure: Marginals μ and ν

Figure: $\epsilon = 4/N$

The extension to the Multi-Marginal problem

The entropic multi-marginal problem becomes

$$\min_{\gamma \in \mathcal{C}} \mathcal{H}(\gamma|\bar{\gamma}) \tag{10}$$

where $\mathcal{H}(\gamma|\bar{\gamma}) = \sum_{i,j,k} \gamma_{ijk}(\log \frac{\gamma_{ijk}}{\bar{\gamma}_{ijk}} - 1)$ is the relative entropy, and $\mathcal{C} = \bigcap_{i=1}^{3} \mathcal{C}_i$ (i.e. $\mathcal{C}_1 = \{\gamma \quad | \quad \sum_{j,k} \gamma_{ijk} = \mu_i^1\}$).

The optimal plan $\gamma^\star$ becomes $\gamma^\star_{ijk} = a_i^\star b_j^\star c_k^\star \bar{\gamma}_{ijk}$ $a_i^\star$, $b_j^\star$ and $c_k^\star$ can be determined by the marginal constraints.

$$b_j^\star = \frac{\mu_j^2}{\sum_{ik} a_i^\star c_k^\star \bar{\gamma}_{ijk}}$$

$$c_k^\star = \frac{\mu_k^3}{\sum_{ij} a_i^\star b_j^\star \bar{\gamma}_{ijk}}$$

$$a_i^\star = \frac{\mu_i^1}{\sum_{jk} b_j^\star c_k^\star \bar{\gamma}_{ijk}}$$

$\Rightarrow$

$\Rightarrow$

$$b_j^{n+1} = \frac{\mu_j^2}{\sum_{ik} a_i^n c_k^n \bar{\gamma}_{ijk}}$$

$\Rightarrow$

$$c_k^{n+1} = \frac{\mu_k^3}{\sum_{ij} a_i^n b_j^{n+1} \bar{\gamma}_{ijk}}$$

$\Rightarrow$

$$a_i^{n+1} = \frac{\mu_i^1}{\sum_{jk} b_j^{n+1} c_k^{n+1} \bar{\gamma}_{ijk}}$$

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$$\begin{aligned}
b_j^\star &= \frac{\mu_j^2}{\sum_{ik} a_i^\star c_k^\star \bar{\gamma}_{ijk}} && \Rightarrow \\
c_k^\star &= \frac{\mu_k^3}{\sum_{ij} a_i^\star b_j^\star \bar{\gamma}_{ijk}} && \Rightarrow \\
a_i^\star &= \frac{\mu_i^1}{\sum_{jk} b_j^\star c_k^\star \bar{\gamma}_{ijk}} && \Rightarrow
\end{aligned}$$

$$\begin{aligned}
b_j^{n+1} &= \frac{\mu_j^2}{\sum_{ik} a_i^n c_k^n \bar{\gamma}_{ijk}} \\
c_k^{n+1} &= \frac{\mu_k^3}{\sum_{ij} a_i^n b_j^{n+1} \bar{\gamma}_{ijk}} \\
a_i^{n+1} &= \frac{\mu_i^1}{\sum_{jk} b_j^{n+1} c_k^{n+1} \bar{\gamma}_{ijk}}
\end{aligned}$$

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b_j^\star &= \frac{\mu_j^2}{\sum_{ik} a_i^\star c_k^\star \bar{\gamma}_{ijk}} & \Rightarrow \quad & b_j^{n+1} = \frac{\mu_j^2}{\sum_{ik} a_i^n c_k^n \bar{\gamma}_{ijk}} \\
c_k^\star &= \frac{\mu_k^3}{\sum_{ij} a_i^\star b_j^\star \bar{\gamma}_{ijk}} & \Rightarrow \quad & c_k^{n+1} = \frac{\mu_k^3}{\sum_{ij} a_i^n b_j^{n+1} \bar{\gamma}_{ijk}} \\
a_i^\star &= \frac{\mu_i^1}{\sum_{jk} b_j^\star c_k^\star \bar{\gamma}_{ijk}} & \Rightarrow \quad & a_i^{n+1} = \frac{\mu_i^1}{\sum_{jk} b_j^{n+1} c_k^{n+1} \bar{\gamma}_{ijk}}
\end{aligned}$$

Application I: MMOT for computing geodesics in the Wasserstein space

The three formulations of quadratic Optimal Transport

Three formulations of Optimal Transport problem) with the quadratic cost :

- The static

$$\inf\left\{\int_{X\times X}\frac{1}{2}|x-y|^2 d\gamma \mid \gamma\in\Pi(\mu,\nu)\right\}$$

- The dynamic (Lagrangian) ($C=H^1([0,1];X)$ and $e_t:[0,1]\to X$)

$$\inf\left\{\int_C\int_0^1\frac{1}{2}|\dot\omega|^2 dt dQ(\omega) \mid Q\in\mathcal{P}(C),\ (e_0)_\sharp Q=\mu,\ (e_1)_\sharp Q=\nu\right\}$$

- The dynamic (Eulerian), aka the Benamou-Brenier formulation

$$\inf\int_0^1\int_X\frac{1}{2}|v_t|^2\rho_t dx dt \quad s.t.\ \partial_t\rho_t+\nabla\cdot(\rho_t v_t)=0$$

$$\rho(0,\cdot)=\mu,\ \rho(1,\cdot)=\nu$$

Some remarks and a MMOT formulation

Remarks:

- Consider the optimal solutions for the three formulations $\gamma^\star, Q^\star, \rho_t^\star$ then

$$\pi_t(x,y)_\sharp \gamma = (e_t)_\sharp Q = \rho_t^\star,$$

  where $\pi_t(x,y) = (1-t)x + ty$.

- if we discretise in time (let take $T+1$ time steps) the Lagrangian formulation and imposing that $\omega(t_i) = x_i$ ($t_i = i\frac{1}{T}$ for $i = 0, \cdots, T$) we get the following discrete (in time) MMOT problem

$$\inf \int_{X^T} \frac{1}{2T} \sum_{i=0}^{T} |x_{i+1} - x_i|^2 d\gamma(x_0, \cdots, x_T) \text{ s.t}$$
$$\gamma \in \mathcal{P}(X^{T+1}),\ \pi_{0,\sharp}\gamma = \mu,\ \pi_{T,\sharp}\gamma = \nu$$

The geodesic in 2D

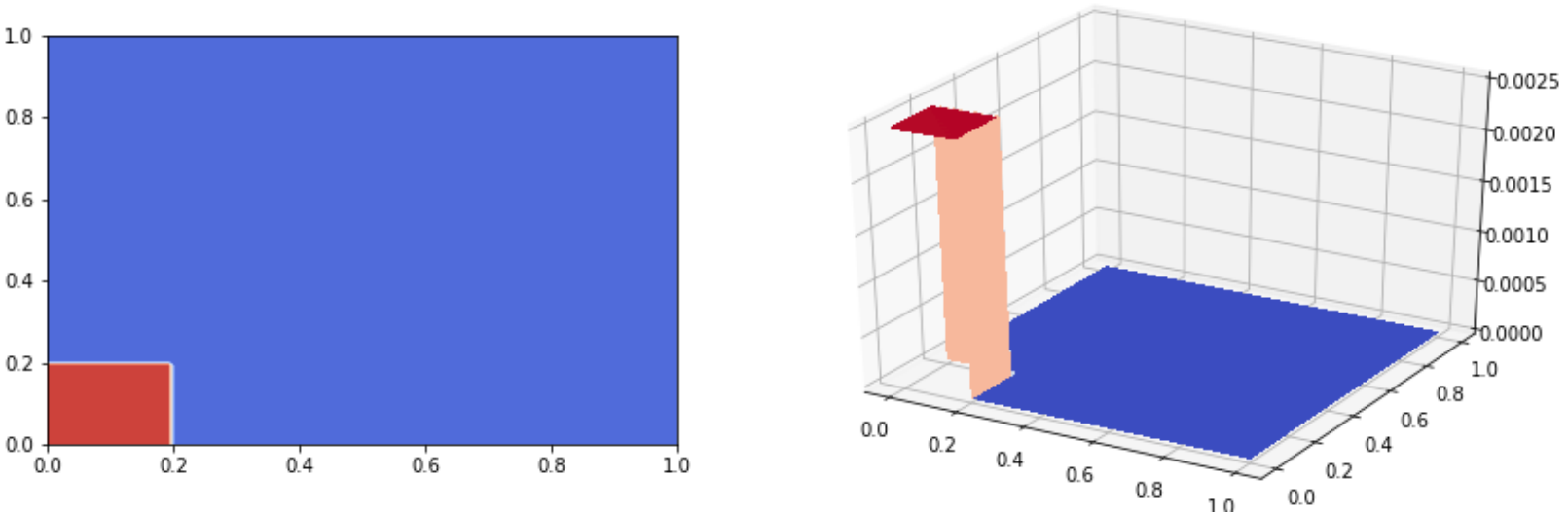

Figure: $t = 0$

The geodesic in 2D

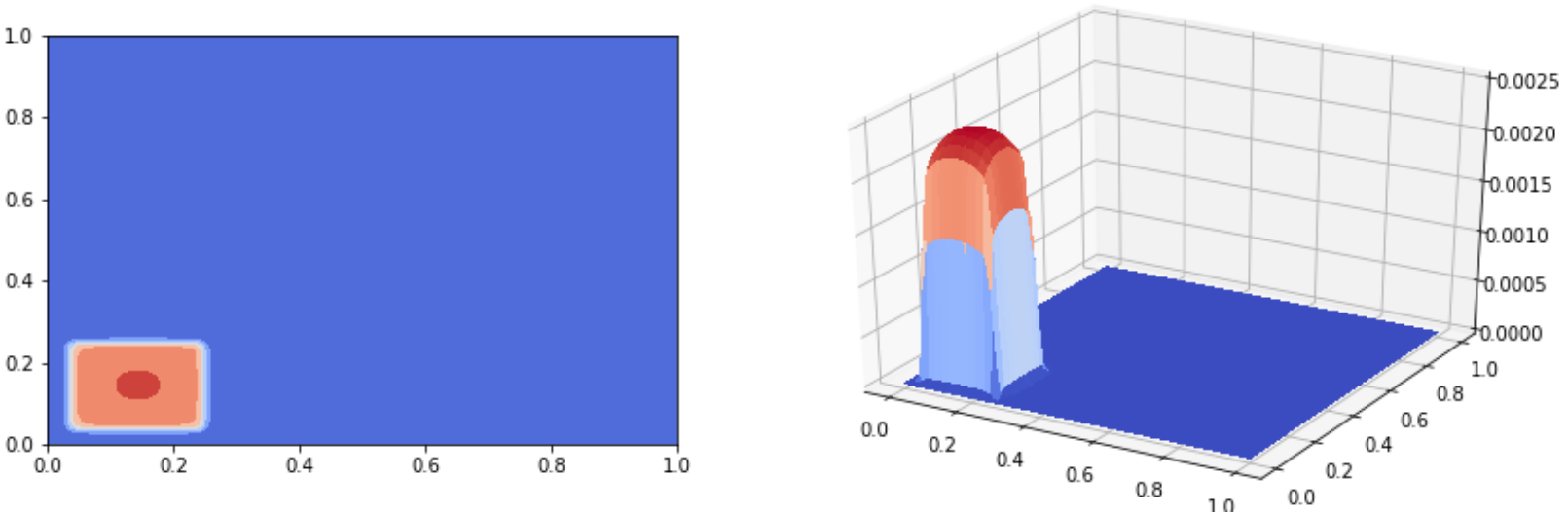

Figure: $t = \frac{1}{14}$

The geodesic in 2D

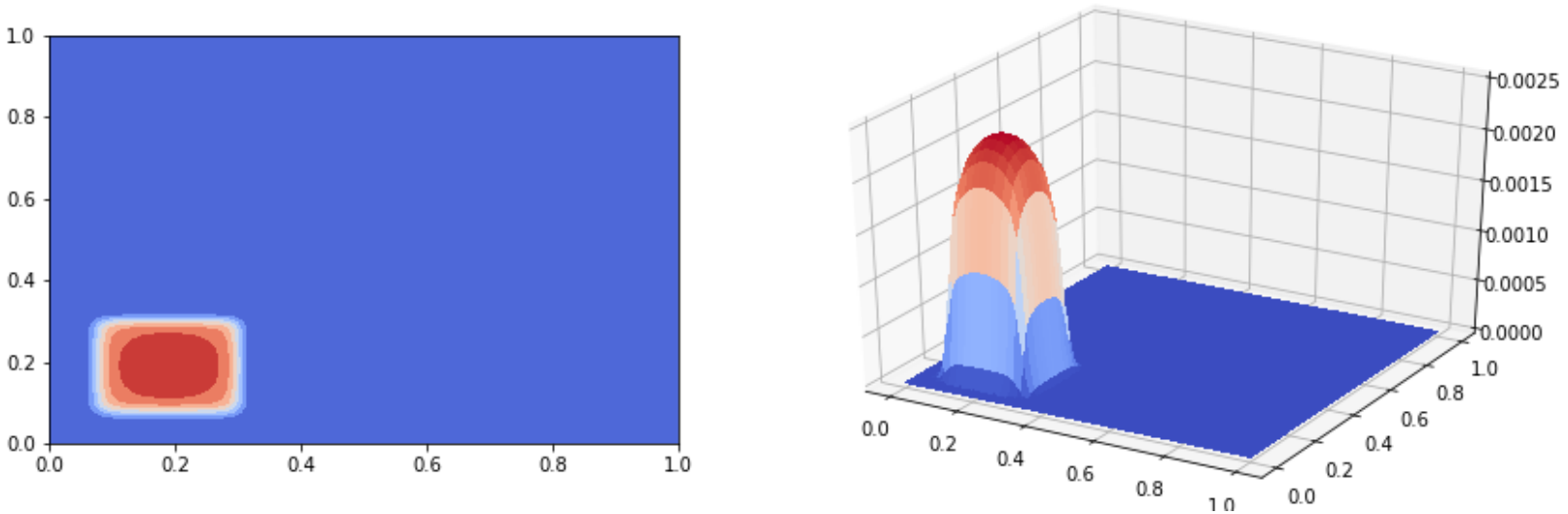

Figure: $t = \frac{2}{14}$

The geodesic in 2D

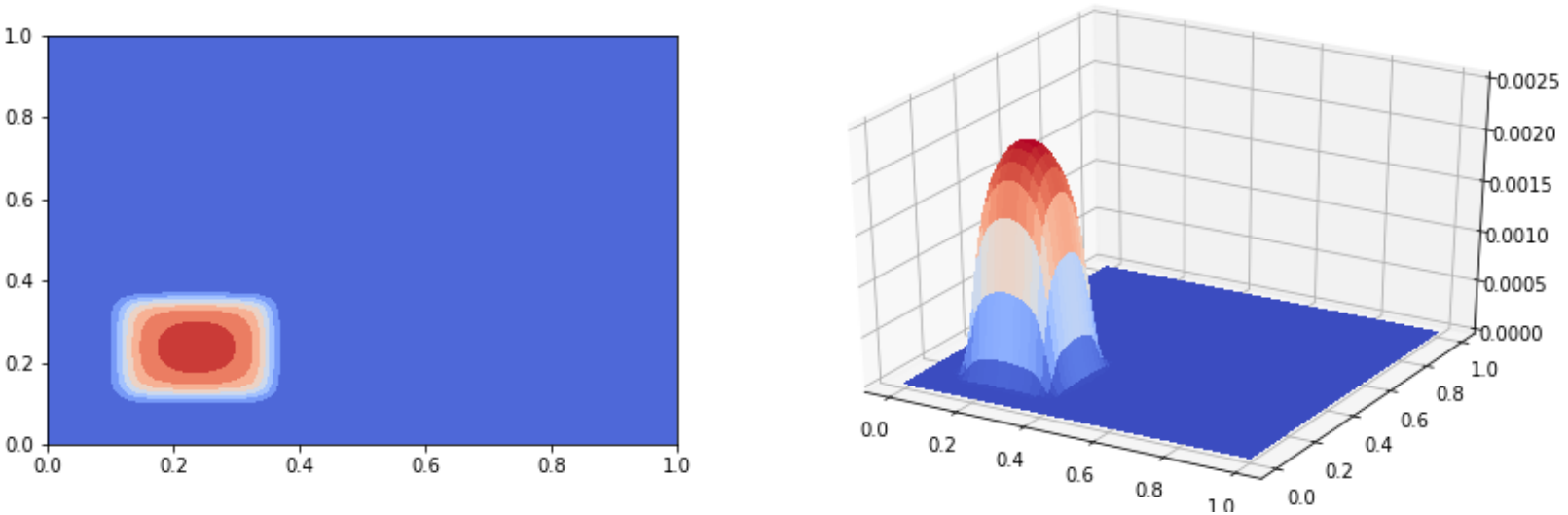

Figure: $t = \frac{3}{14}$

The geodesic in 2D

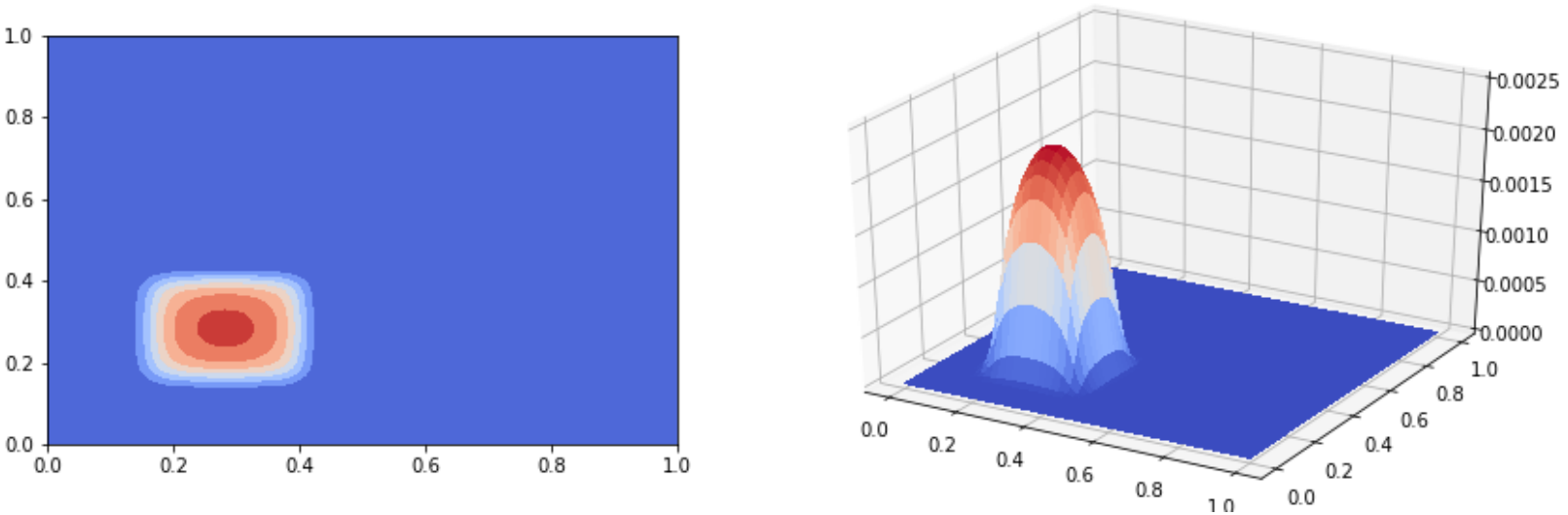

Figure: $t = \frac{4}{14}$

The geodesic in 2D

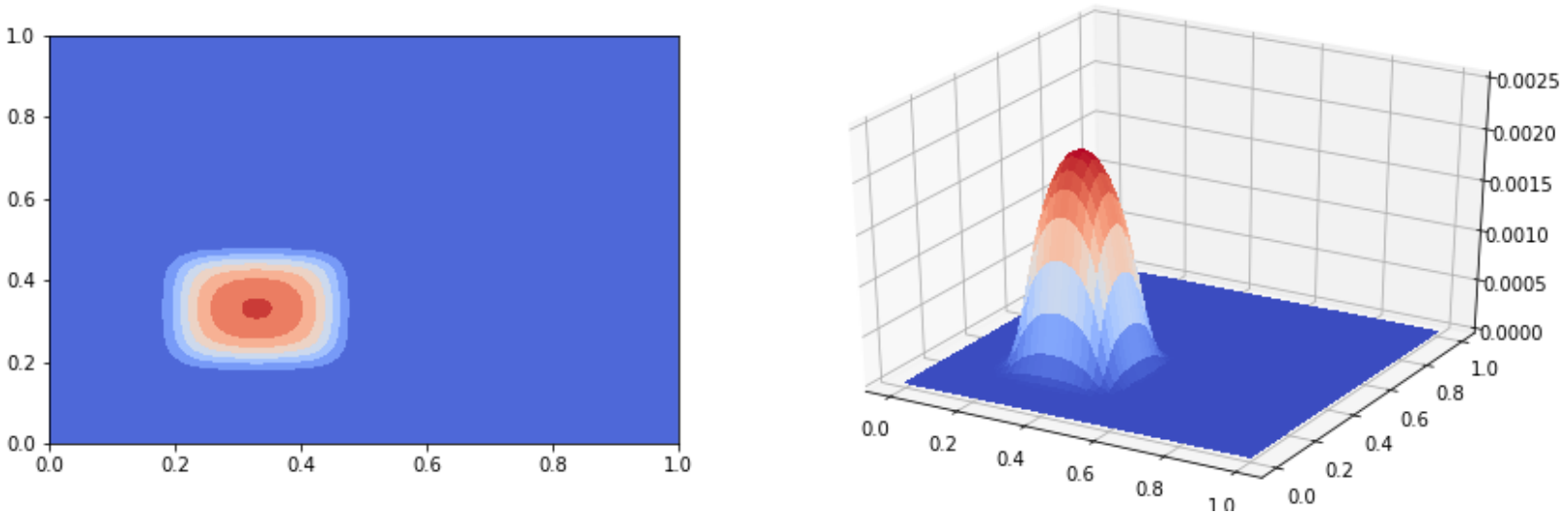

Figure: $t = \frac{5}{14}$

The geodesic in 2D

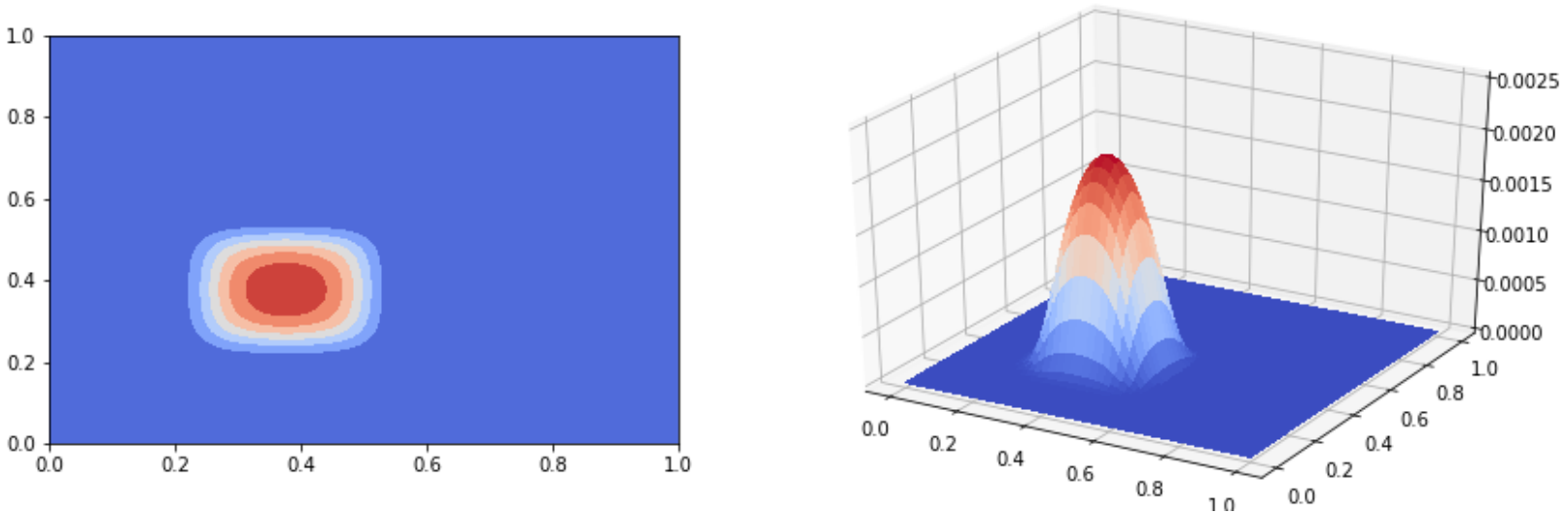

Figure: $t = \frac{6}{14}$

The geodesic in 2D

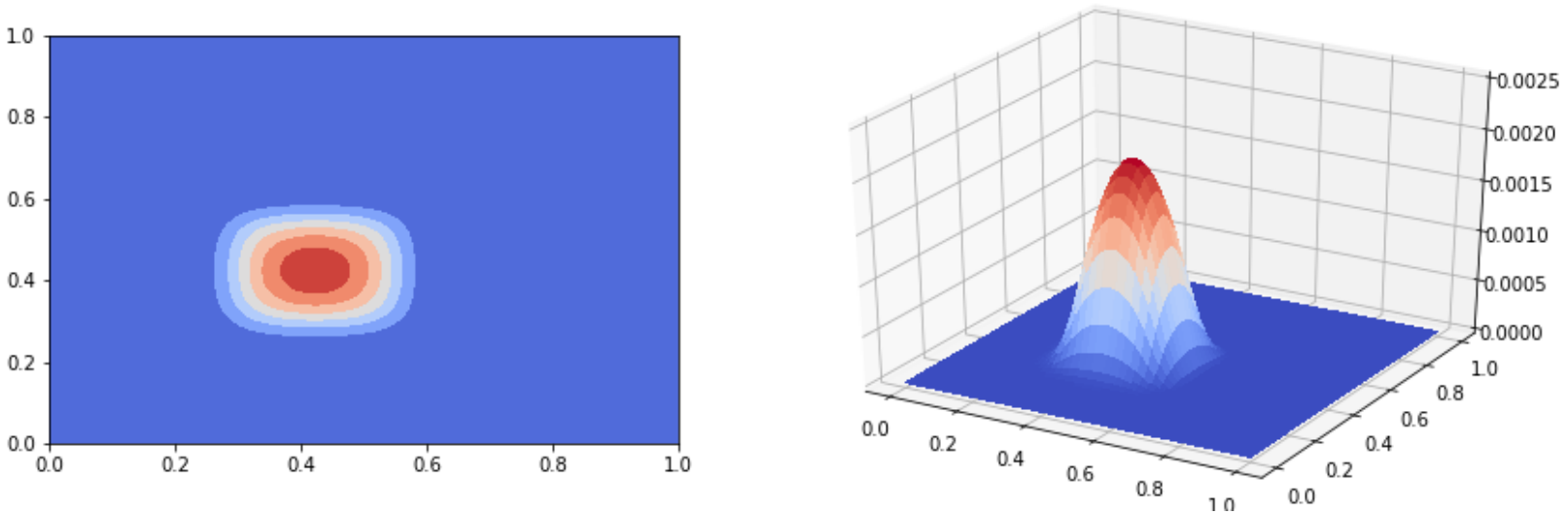

Figure: $t = \frac{7}{14}$

The geodesic in 2D

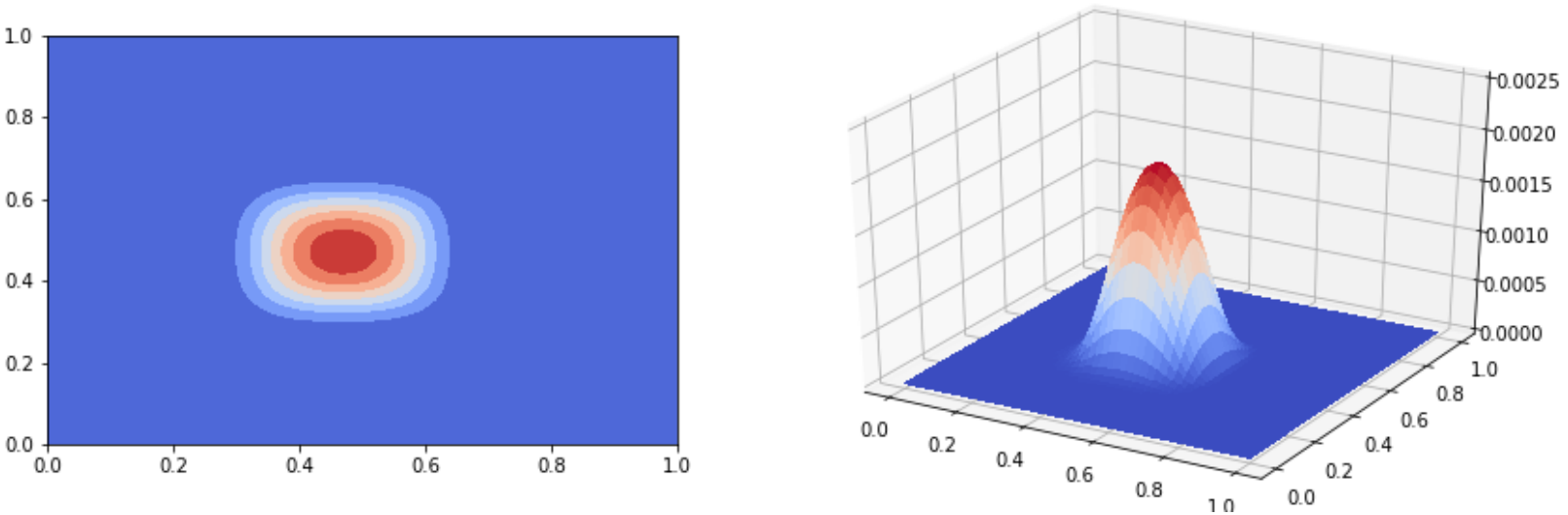

Figure: $t = \frac{8}{14}$

The geodesic in 2D

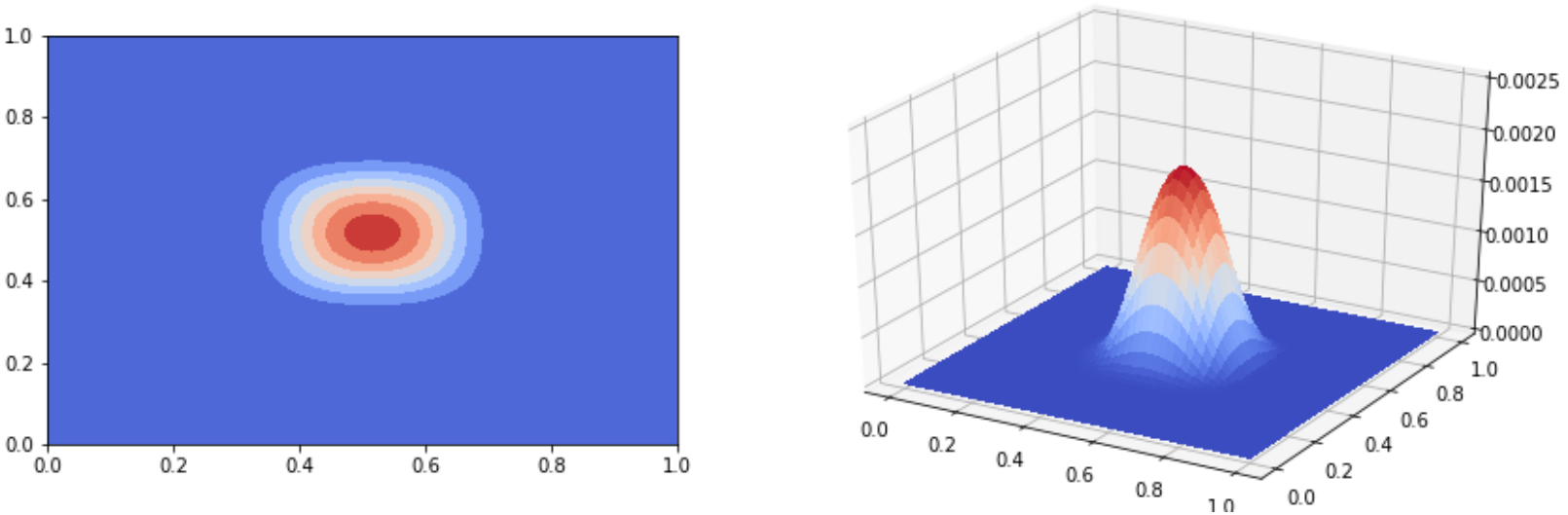

Figure: $t = \frac{9}{14}$

The geodesic in 2D

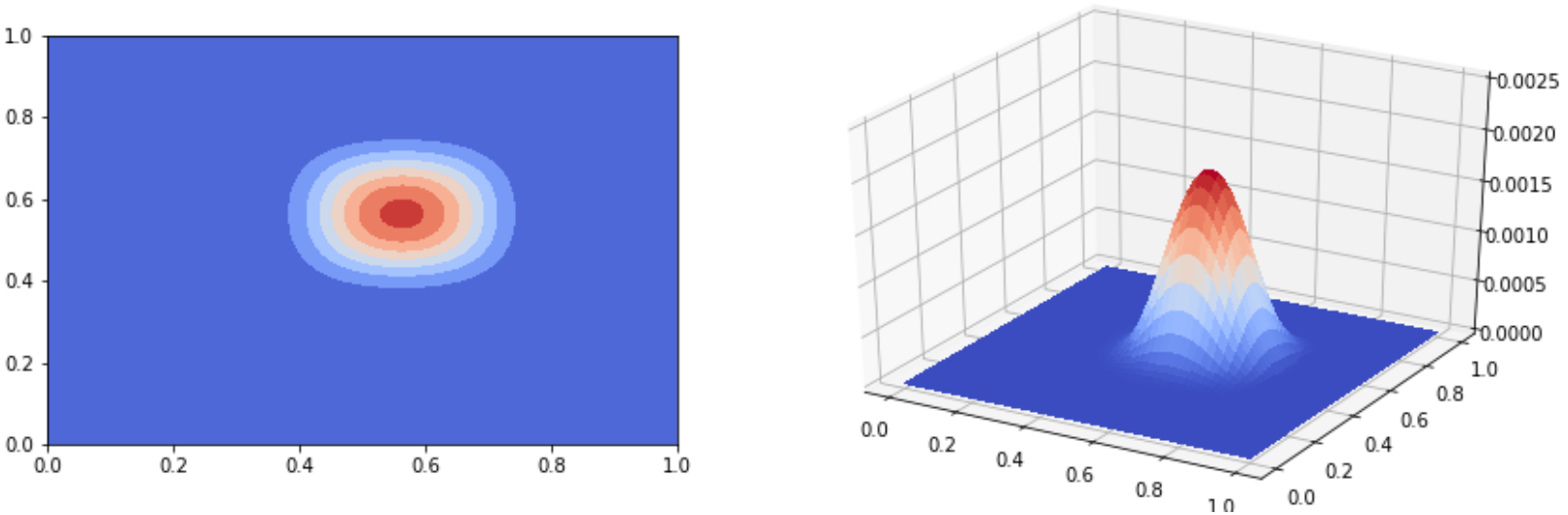

Figure: $t = \frac{10}{14}$

The geodesic in 2D

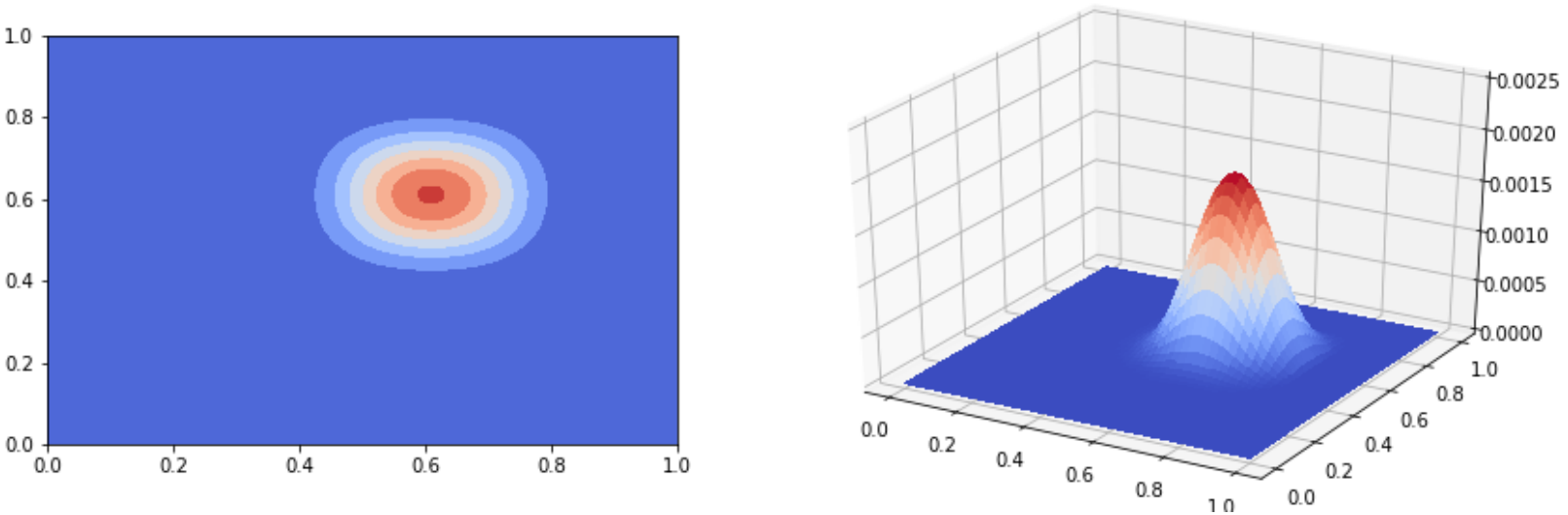

Figure: $t = \frac{11}{14}$

The geodesic in 2D

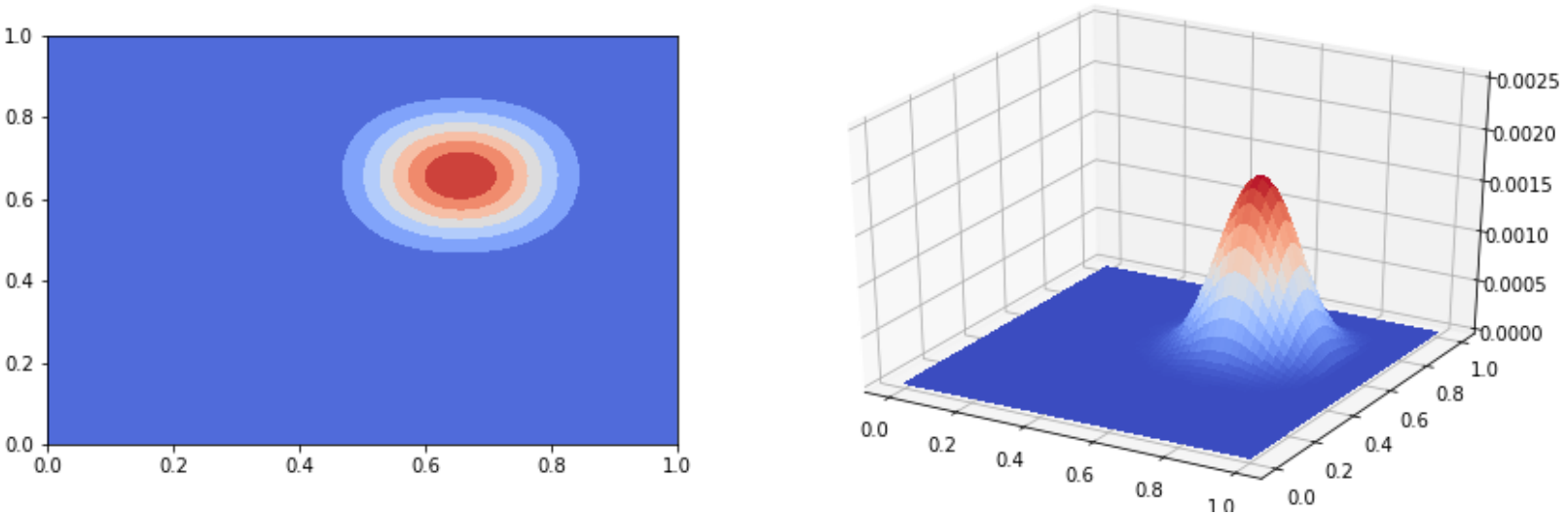

Figure: $t = \frac{12}{14}$

The geodesic in 2D

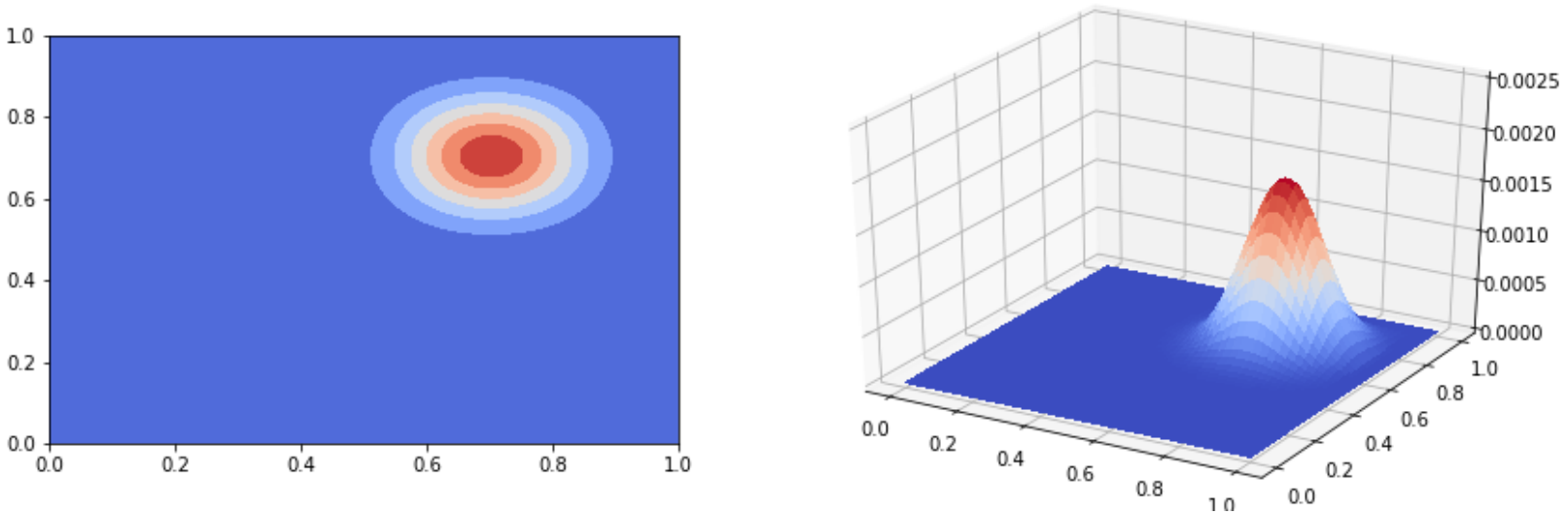

Figure: $t = \frac{13}{14}$

The geodesic in 2D

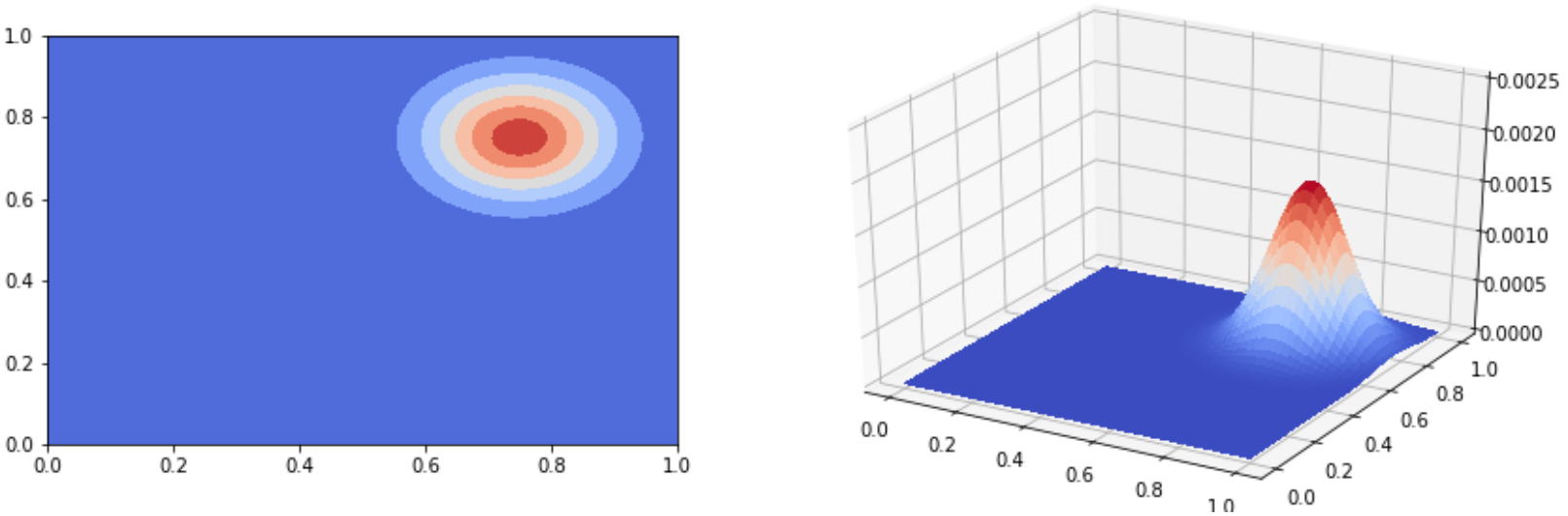

Figure: $t = 1$

The geodesic between images

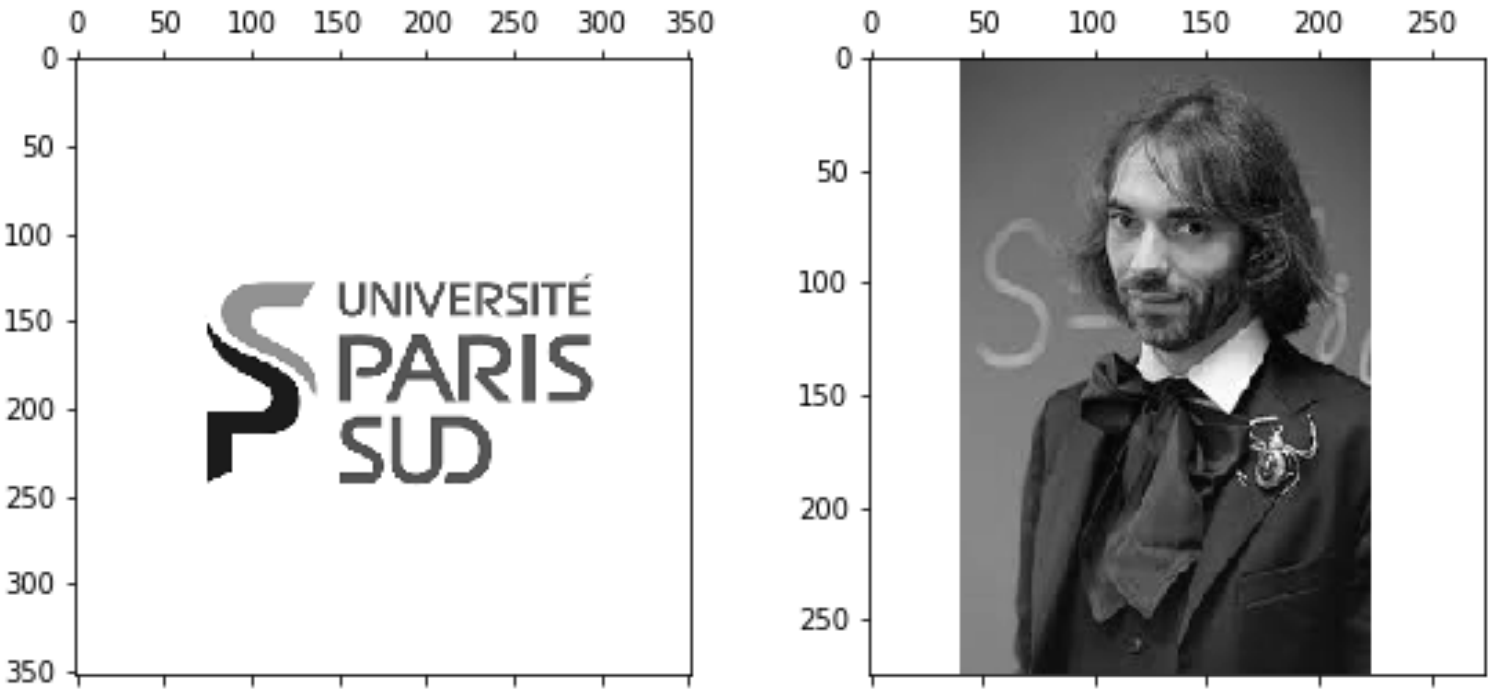

Figure: $t = 0$

The geodesic between images

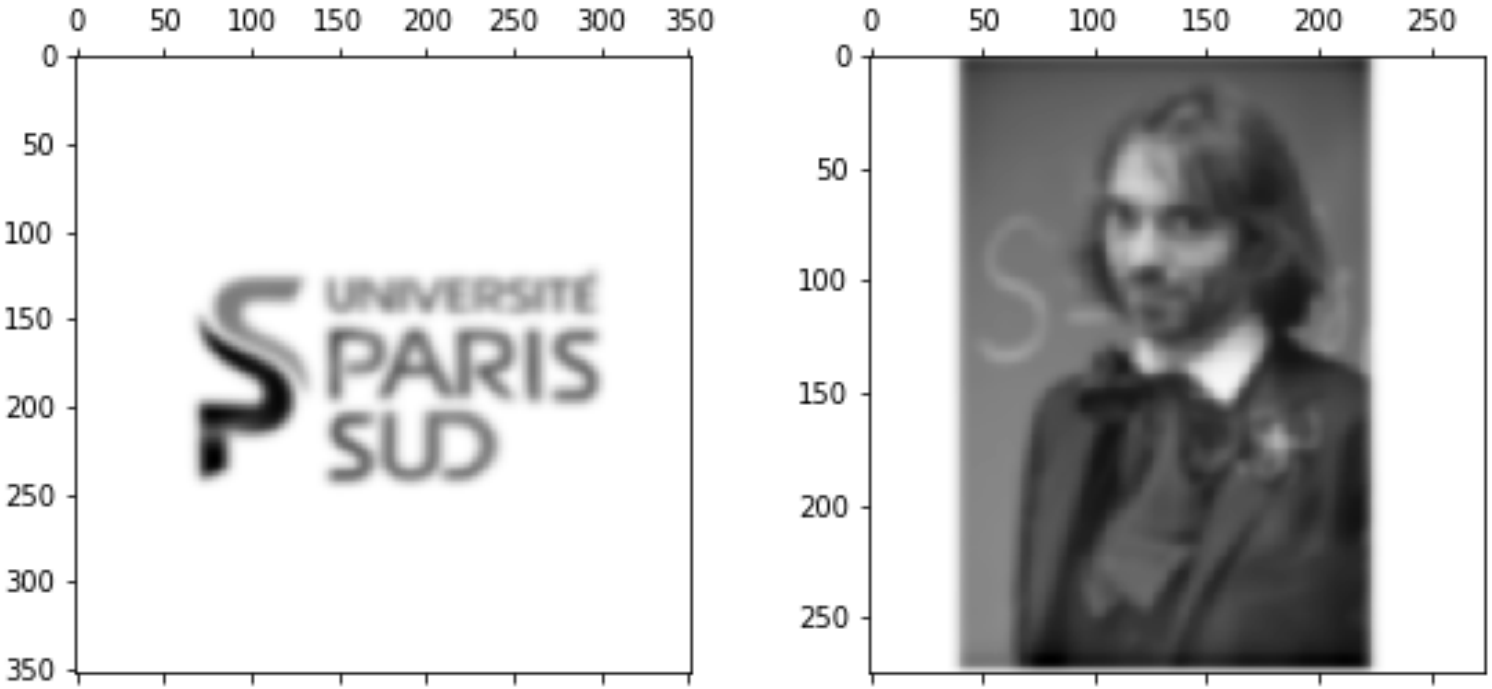

Figure: $t = \frac{1}{14}$

The geodesic between images

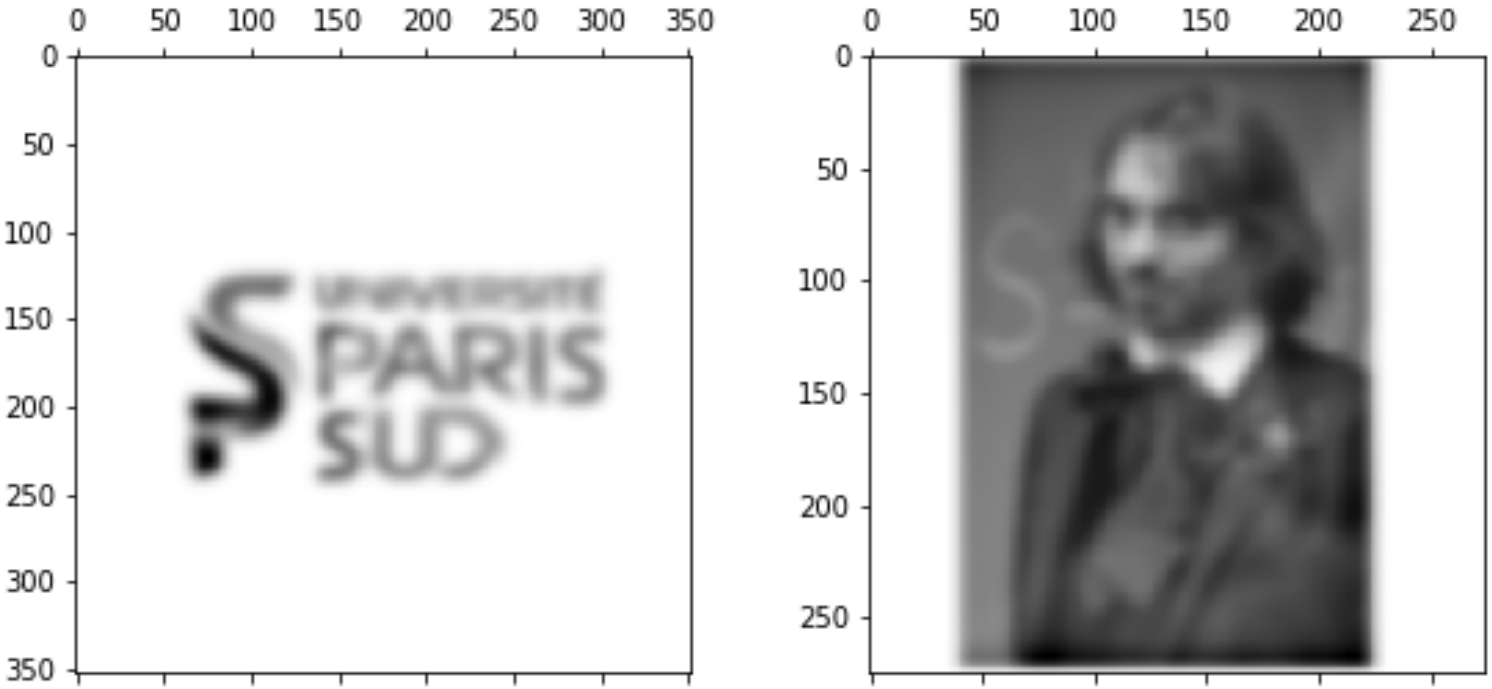

Figure: $t = \frac{2}{14}$

The geodesic between images

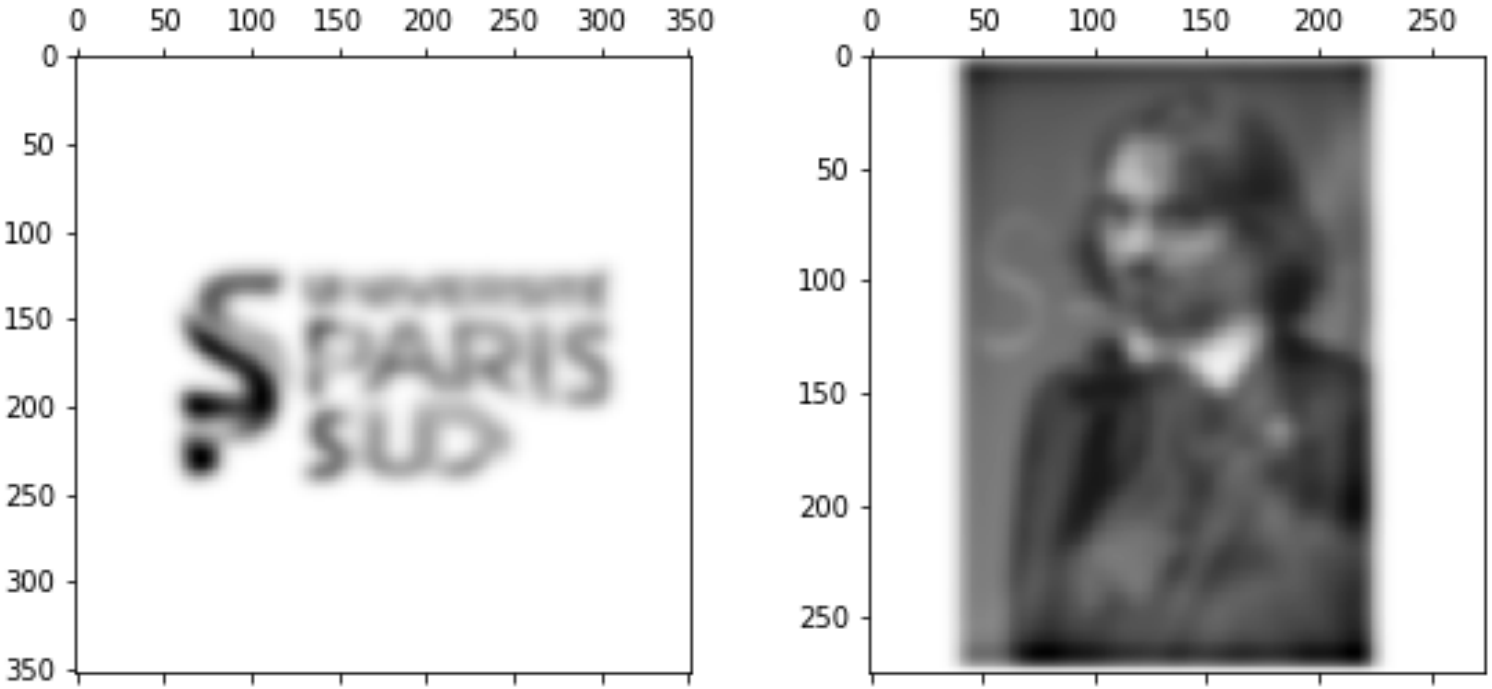

Figure: $t = \frac{3}{14}$

The geodesic between images

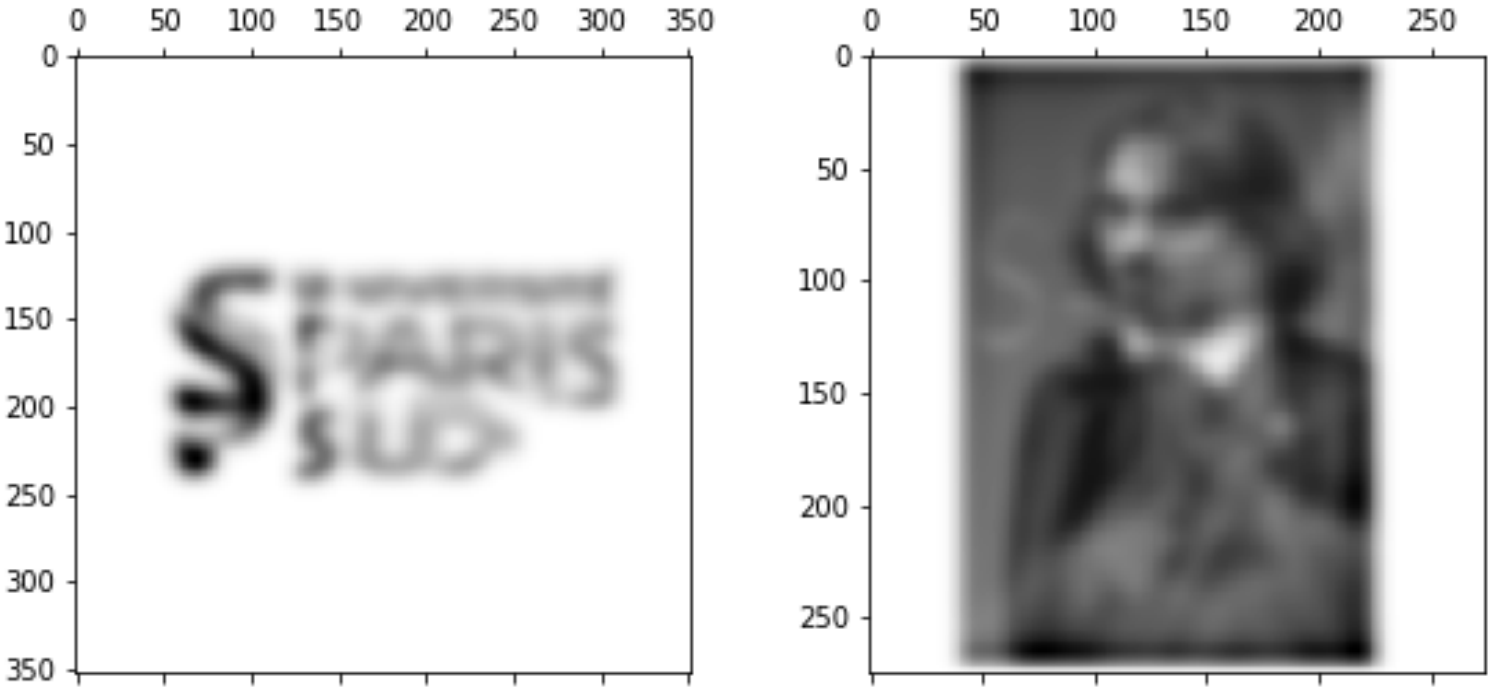

Figure: $t = \frac{4}{14}$

The geodesic between images

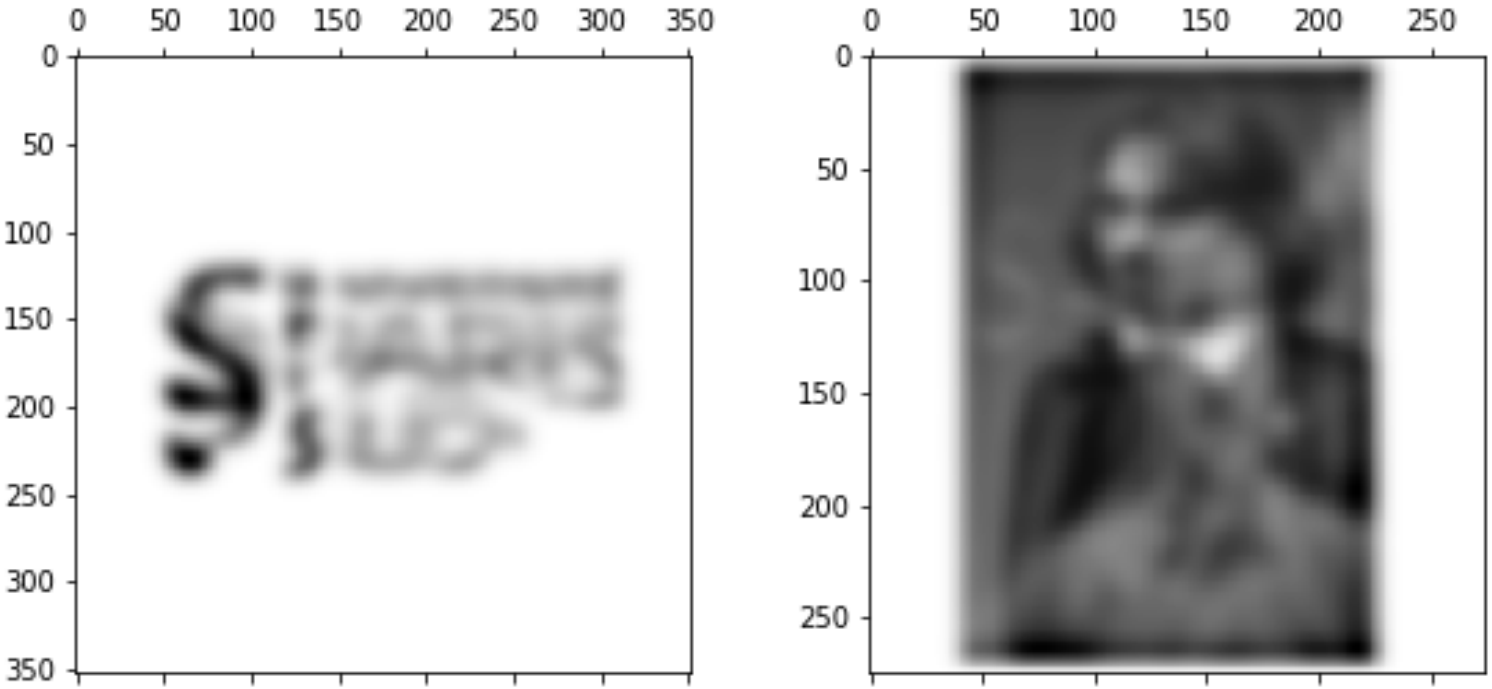

Figure: $t = \frac{5}{14}$

The geodesic between images

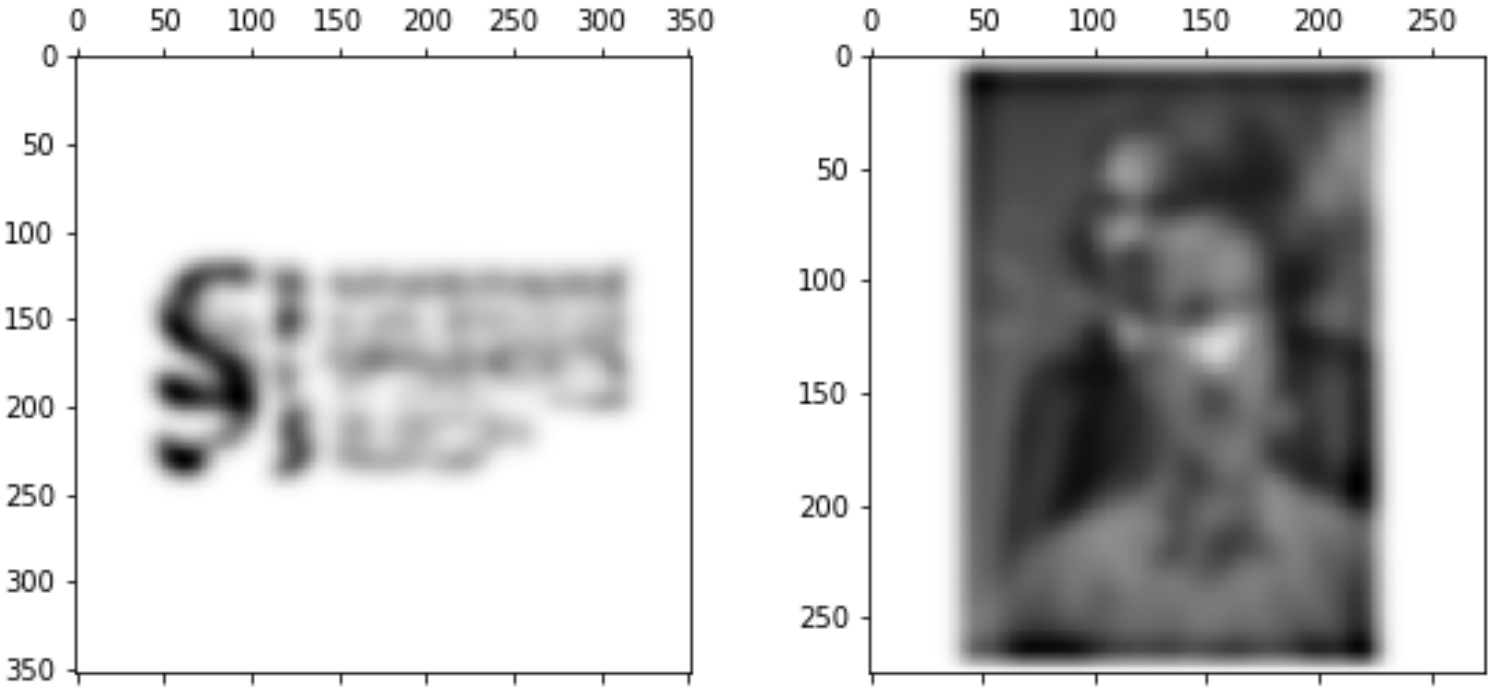

Figure: $t = \frac{6}{14}$

The geodesic between images

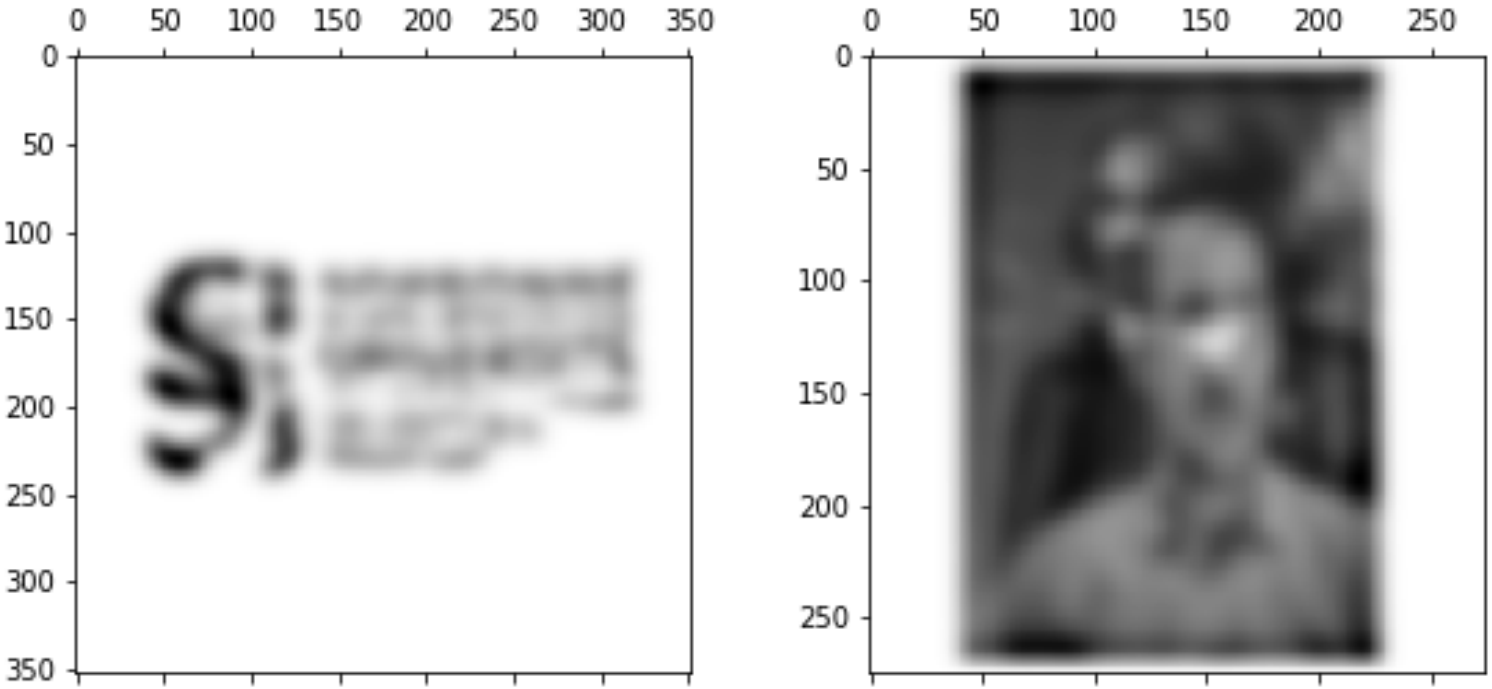

Figure: $t = \frac{7}{14}$

The geodesic between images

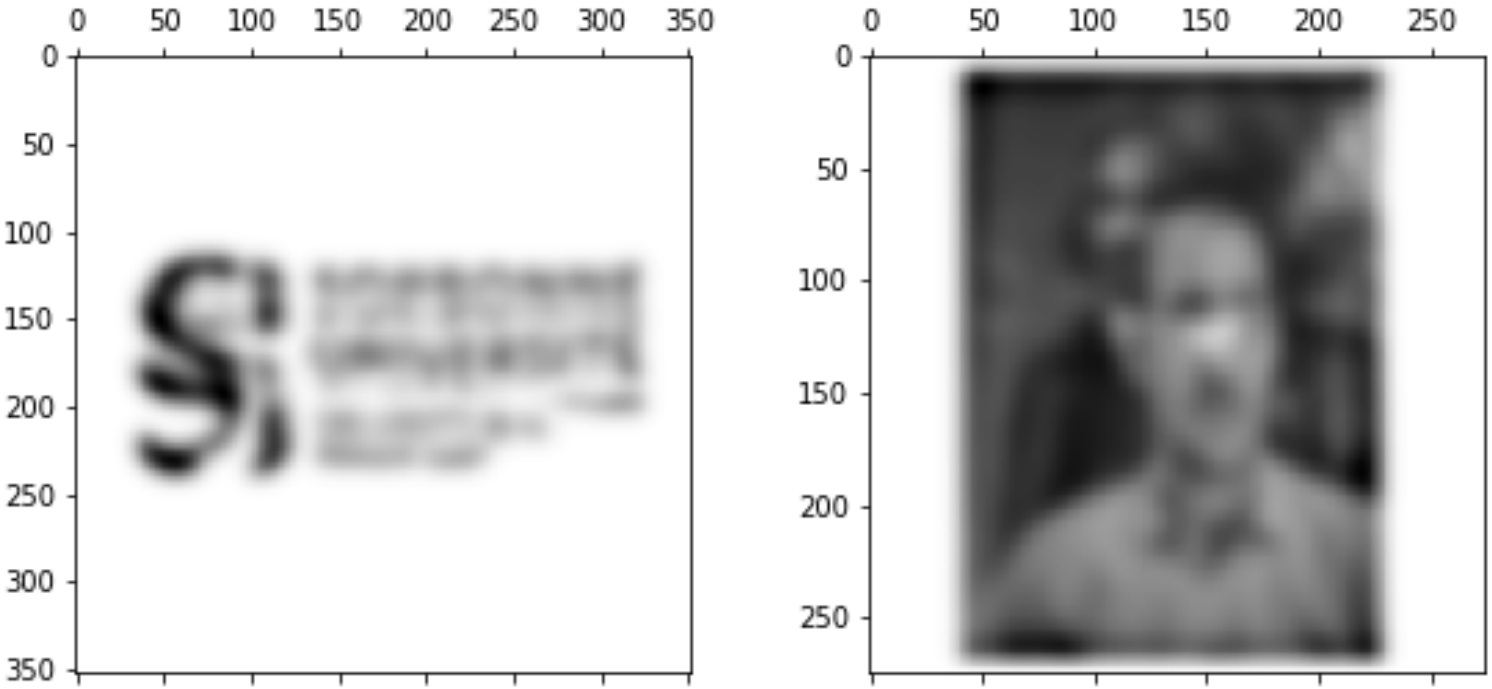

Figure: $t = \frac{8}{14}$

The geodesic between images

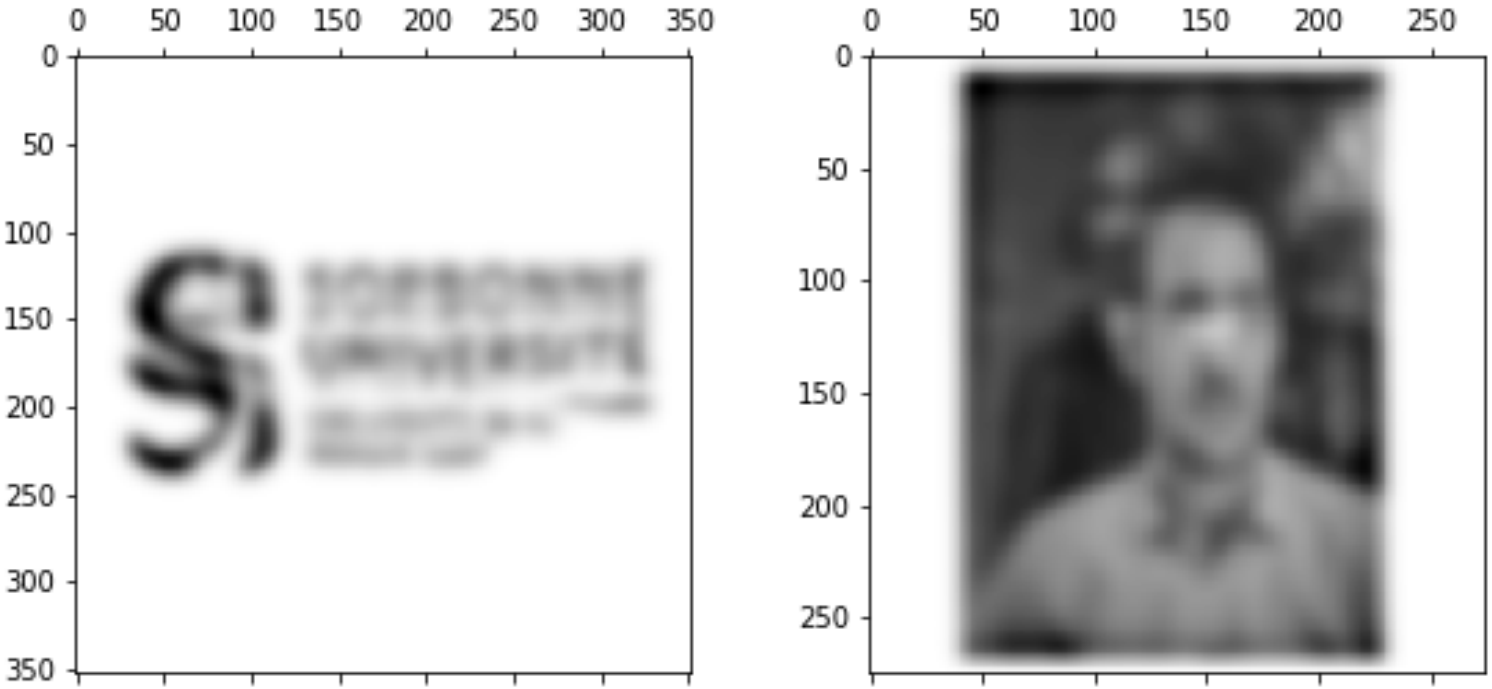

Figure: $t = \frac{9}{14}$

The geodesic between images

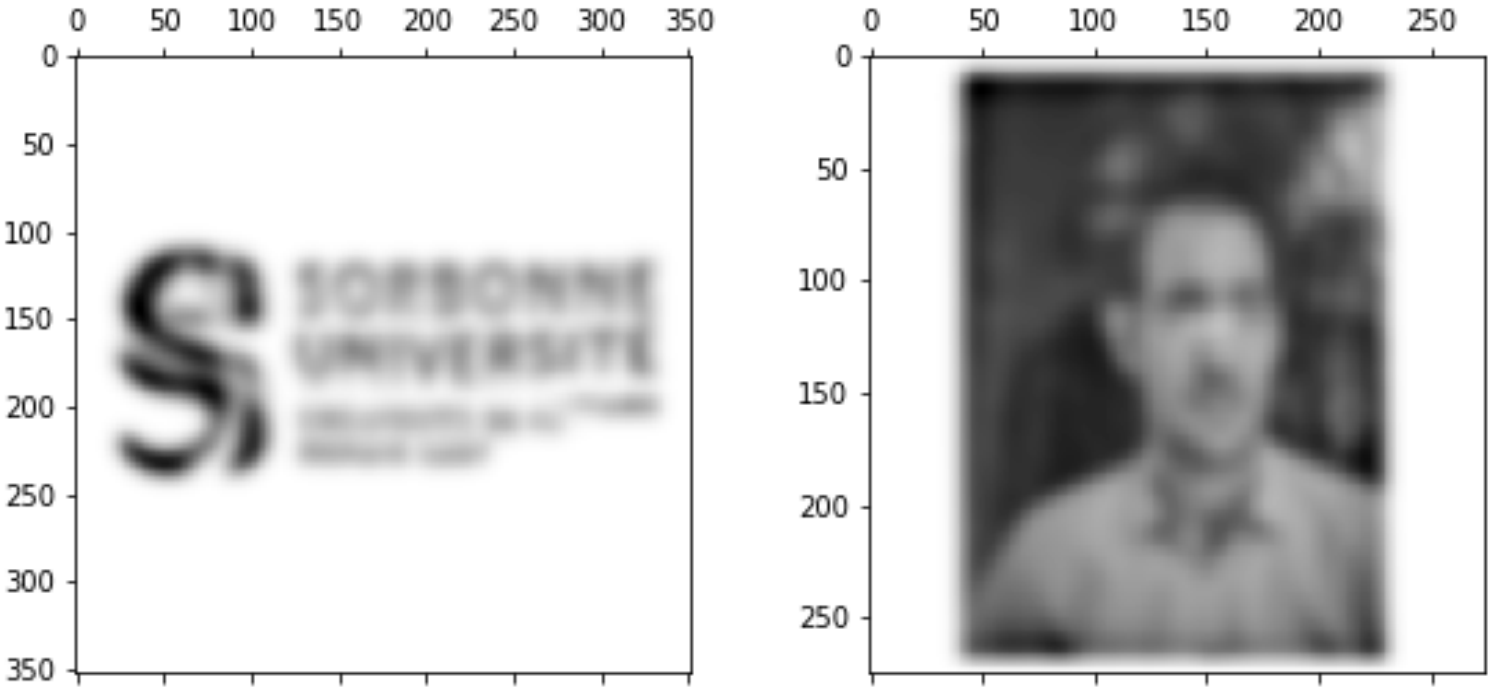

Figure: $t = \frac{10}{14}$

The geodesic between images

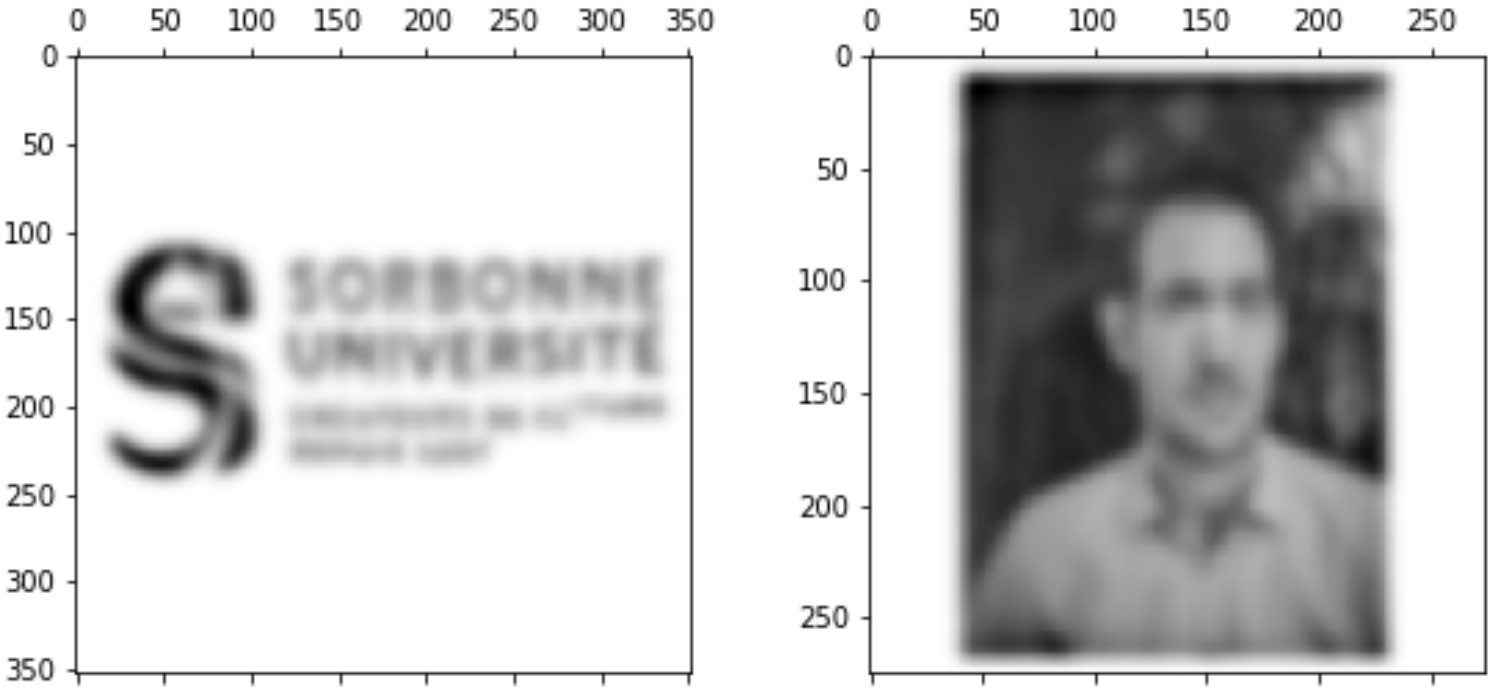

Figure: $t = \frac{11}{14}$

The geodesic between images

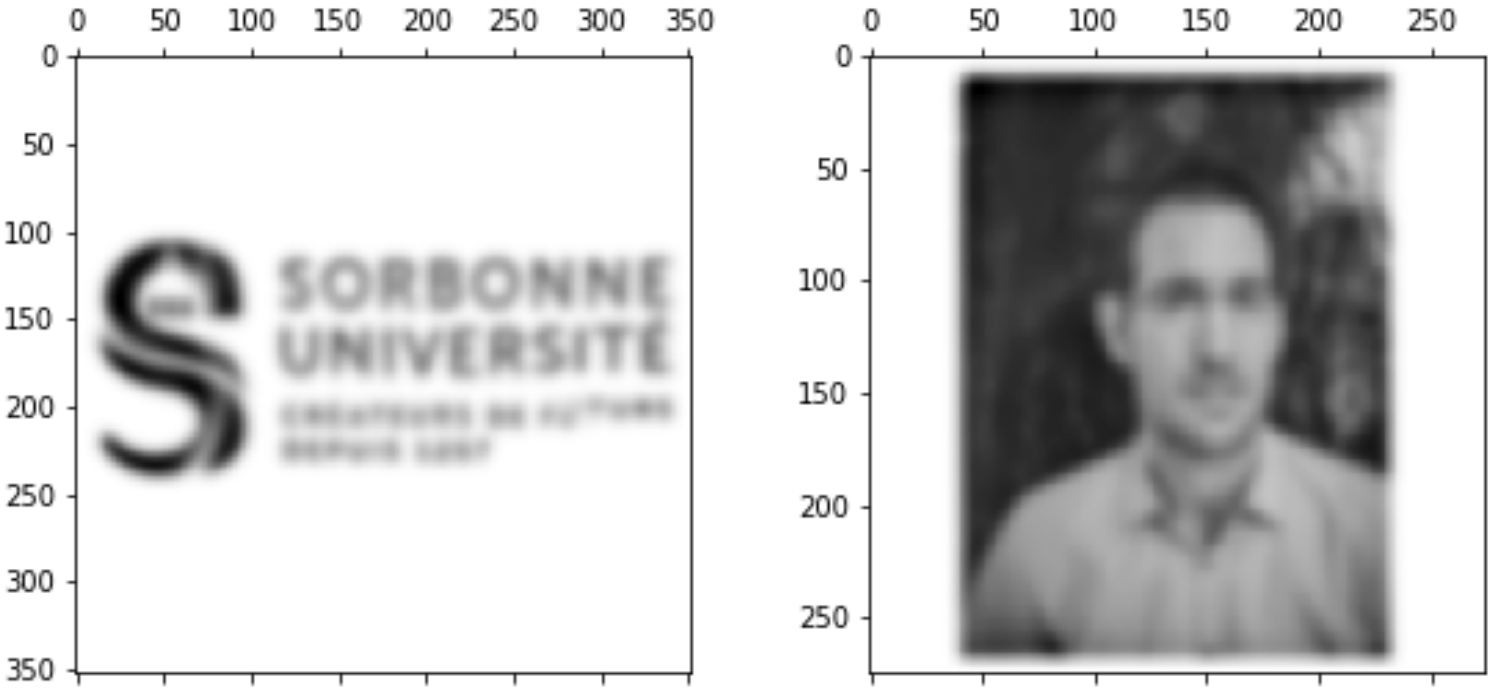

Figure: $t = \frac{12}{14}$

The geodesic between images

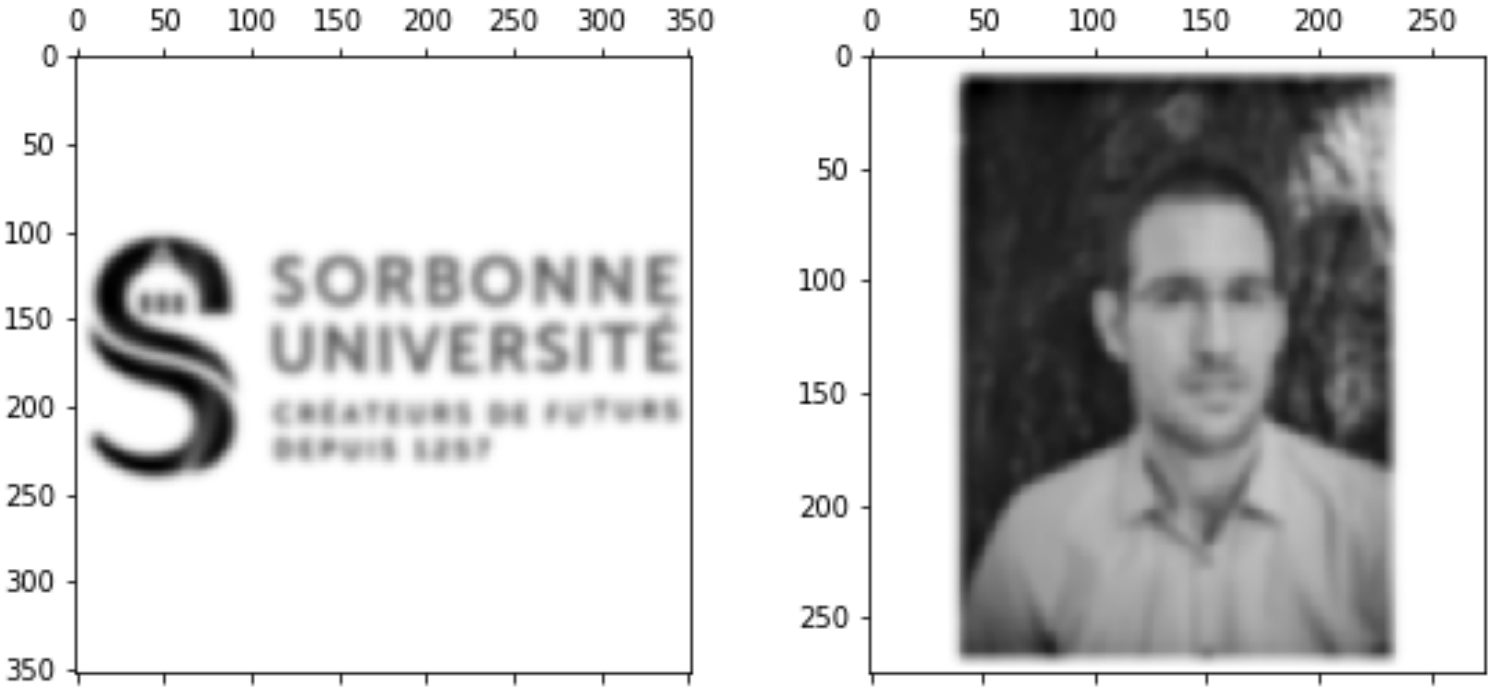

Figure: $t = \frac{13}{14}$

The geodesic between images

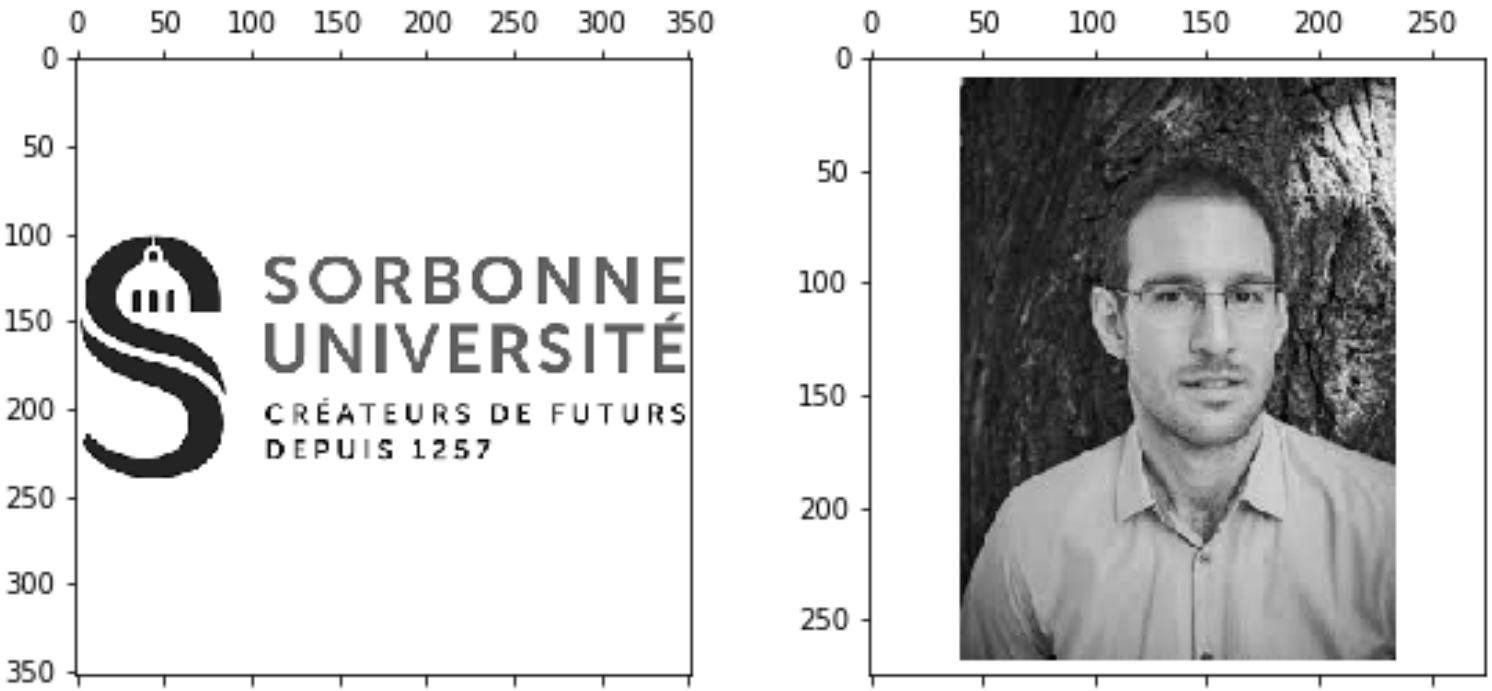

Figure: $t = 1$

Application II: MMOT and the electron-electron repulsion

Why Repulsive OT? The Density Functional Theory

Let denote by $\Psi(x_1, s_1, \dots, x_N, s_N)$ the wavefunction for N electrons and $\gamma = N \sum_{s_1, \cdots, s_N \in \mathbb{Z}_2} |\Psi(x_1, s_1, \dots, x_N, s_N)|^2 \overset{def}{=}$ joint probability density of electrons at positions $x_1, \dots, x_N \in \mathbb{R}^d$.
Then the **Density Functional Theory** consists in studying the following variational principle

Rayleigh-Ritz variational principle

$$E_0 = \inf_{\Psi \in H^1_a, ||\Psi||_2 = 1} \epsilon T[\Psi] + V_{ee}[\Psi] + \int \sum_{s_1, \cdots, s_N \in \mathbb{Z}_2} \sum_{i=1}^{N} v_{ext}(x_i) |\Psi|^2 dx \qquad (11)$$

$T[\Psi]$ is the kinetic energy, v_{ext} is an external attractive potential and $V_{ee}[\Psi]$ is the electron-electron repulsion

$$V_{ee}[\Psi] = \int_{\mathbb{R}^{dN}} \sum_{s_1, \cdots, s_N \in \mathbb{Z}_2} \sum_{i<j} \frac{1}{|x_i - x_j|} |\Psi|^2 dx_1 \cdots dx_N.$$

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The Levy-Lieb functional

The minimizing problem can be partitioned into a double minimization. First minimize over Ψ subject to a fixed ρ, then minimize over ρ:

$$E_0 = \inf_{\rho \in \mathcal{R}} F_{LL}[\rho] + \int v_{ext}(x)\rho(x)dx \tag{12}$$

where $\mathcal{R} := \{\rho | \rho \geq 0, \sqrt{\rho} \in H^1, \int \rho(x) = N\}$ and $F_{LL}[\rho]$ is the Levy-Lieb functional

$$F_{LL}[\rho] = \min_{\Psi \to \rho} \epsilon T[\Psi] + V_{ee}[\Psi] \tag{13}$$

Then we have **(Bindini and De Pascale 2017; Codina Cotar, Gero Friesecke, and Claudia Klüppelberg 2018; Lewin 2018)**...

Semiclassical limit

$\lim_{\epsilon \to 0} F_{LL}[\rho] = \mathcal{MK}[\rho]$

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Semiclassical limit

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Remarks

- We consider only wavefunctions Ψ real and spinless .
- $\gamma = |\Psi|^2$ is the **transport plan** and the electron-electron repulsion becomes

$$V_{ee}[\Psi] = \int_{\mathbb{R}^{dN}} \sum_{i<j} \frac{1}{|x_i - x_j|} \gamma(x_1, \cdots, x_N) dx_1 \cdots dx_N$$

- The marginal density $\rho = \int_{\mathbb{R}^{d(N-1)}} \gamma dx_2 \cdots dx_N$ is the electron density and $\int_{\mathbb{R}^d} \rho(x) dx = 1$.
- $|\nabla \Psi|^2 = |\nabla \sqrt{\gamma}|^2 = \frac{1}{4} \frac{|\nabla \gamma|^2}{\gamma}$ so the kinetic energy can be re-written as

$$T[\Psi] = \int_{\mathbb{R}^{dN}} \frac{1}{4} \frac{|\nabla \gamma|^2}{\gamma} dx_1 \cdots dx_N.$$

The entropic inequality

One can prove the following inequality

The Entropic Inequality (Seidl, Di Marino, A. Gerolin, L. Nenna, Giesbertz, and P. Gori-Giorgi 2017)

$$\min_{\gamma\to\rho}\int_{\mathbb{R}^{dN}}\epsilon\frac{1}{4}\frac{|\nabla\gamma|^2}{\gamma}+\sum_{i<j}\frac{1}{|x_i-x_j|}\gamma\geq\min_{\gamma\to\rho}\int_{\mathbb{R}^{dN}}\epsilon C\gamma\log(\gamma)+\sum_{i<j}\frac{1}{|x_i-x_j|}\gamma=\mathcal{H}(\gamma|\bar{\gamma}). \tag{14}$$

where $\int\frac{1}{4}\frac{|\nabla\gamma|^2}{\gamma}\geq C\int\gamma\log(\gamma)$ is the log-sobolev inequality (or Fisher information) and the entropic functional $\mathcal{H}(\gamma|\bar{\gamma})$ corresponds to minimize the Kullback-Leibler distance between γ and $\bar{\gamma}=e^{-\sum_{i<j}\frac{1}{|x_i-x_j|}\frac{1}{C\epsilon}}$.

Remarks on MMOT with Coulomb cost

Consider now the cost function

$$c(x_1, \cdots, x_N) = \sum_{i \neq j} \frac{1}{|x_i - x_j|},$$

and $\mu_1 = \cdots = \mu_N = \rho$ (we refer to ρ as the electronic density) then the MMOT gives the electronic configuration (namely the optimal transport plan γ) which minimises the electron-electron repulsion.

Remarks:

- Since the cost is symmetric in the marginals then the dual problem reduces to look for only one potential;
- The cost is also radially symmetric which means that when ρ is radially symmetric then the $d = 3$ pb. reduces to a one dimensional pb;
- Existence of Monge solutions is still an open problem for $d > 1$;

The limit as $\epsilon \to 0$

Take the Coulomb cost and solve the regularized problem. Then as $\epsilon \to 0$ ($N = 512$), we have

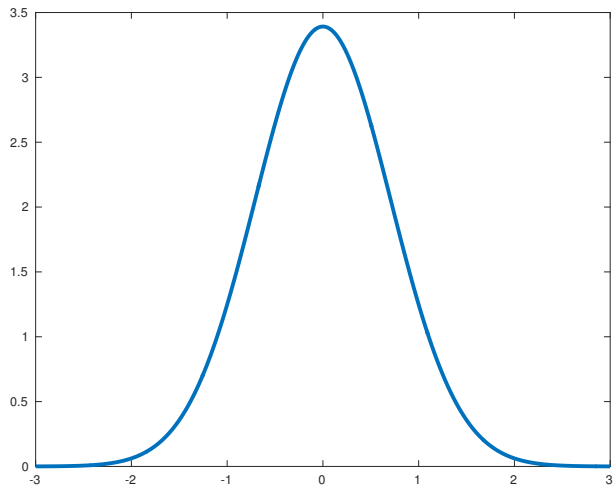


Figure: Marginals ρ (and ρ)

Figure: $\epsilon = 10$

The limit as $\epsilon \to 0$

Take the Coulomb cost and solve the regularized problem. Then as $\epsilon \to 0$ ($N = 512$), we have

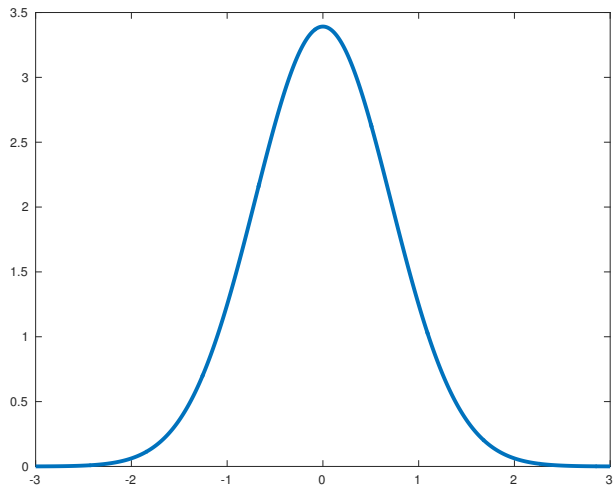


Figure: Marginals ρ (and ρ)

Figure: $\epsilon = 5$

The limit as $\epsilon \to 0$

Take the Coulomb cost and solve the regularized problem. Then as $\epsilon \to 0$ ($N = 512$), we have

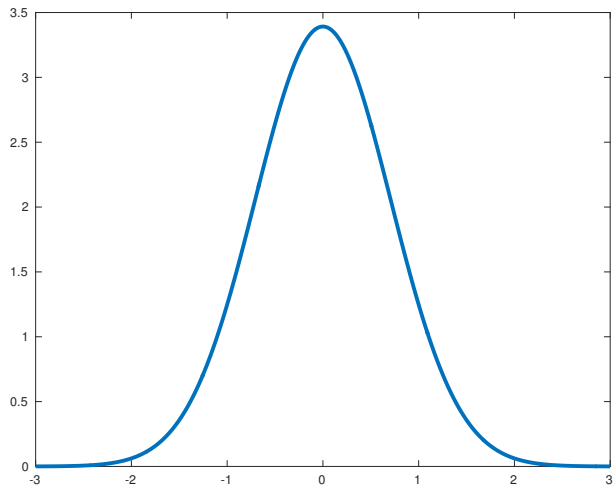


Figure: Marginals ρ (and ρ)

Figure: $\epsilon = 1$

The limit as $\epsilon \to 0$

Take the Coulomb cost and solve the regularized problem. Then as $\epsilon \to 0$ ($N = 512$), we have

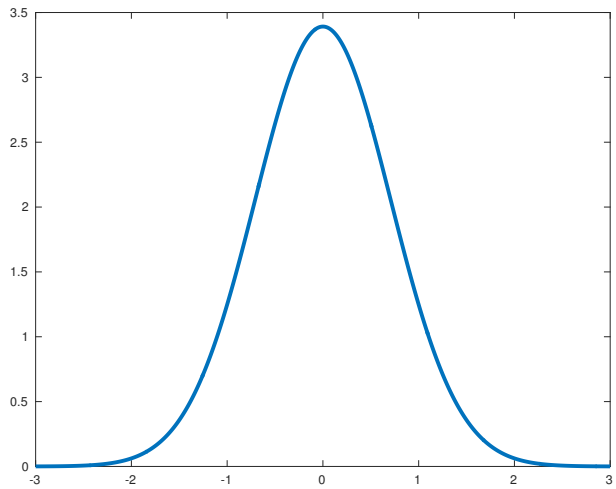


Figure: Marginals ρ (and ρ)

Figure: $\epsilon = 0.1$

The limit as $\epsilon \to 0$

Take the Coulomb cost and solve the regularized problem. Then as $\epsilon \to 0$ ($N = 512$), we have

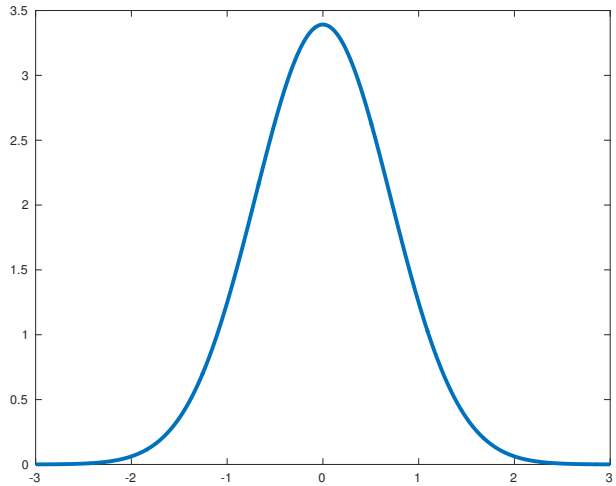


Figure: Marginals ρ (and ρ)

Figure: $\epsilon = 0.01$

The limit as $\epsilon \to 0$

Take the Coulomb cost and solve the regularized problem. Then as $\epsilon \to 0$ ($N = 512$), we have

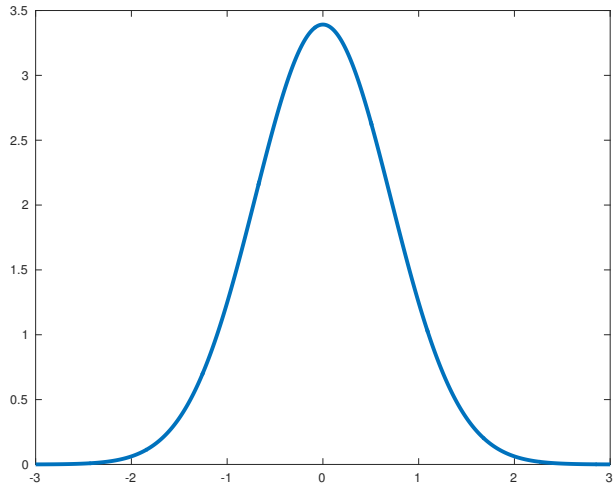
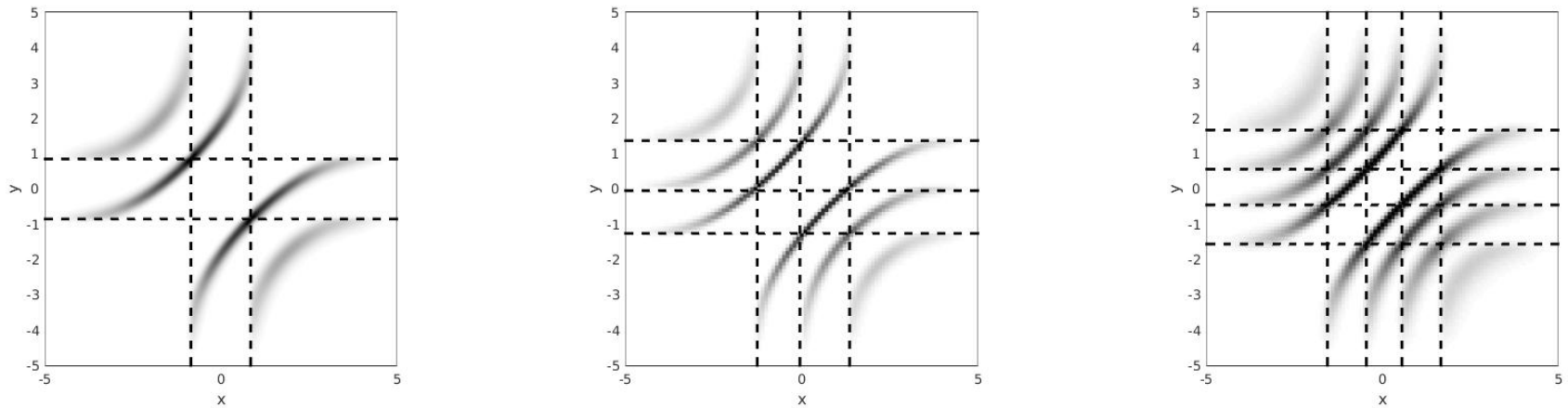


Figure: Marginals ρ (and ρ)

Figure: $\epsilon = 0.002$

Some simulations for $N = 3, 4, 5$ in 1D

We take the density $\rho(x) = \frac{N}{10}(1 + \cos(\frac{\pi}{5}x))$ and...



$N = 3$ $N = 4$ $N = 5$

Figure: *Support of the projected plan* $\pi_{12}(\gamma)$

The transition from spread to deterministic plans for $N = 3$ and $d = 3$

Take $\rho_\alpha(r) = \alpha\rho_{Li}(r) + (1-\alpha)\rho_{exp}(r)$ and $\alpha \in [0,1]$ then...

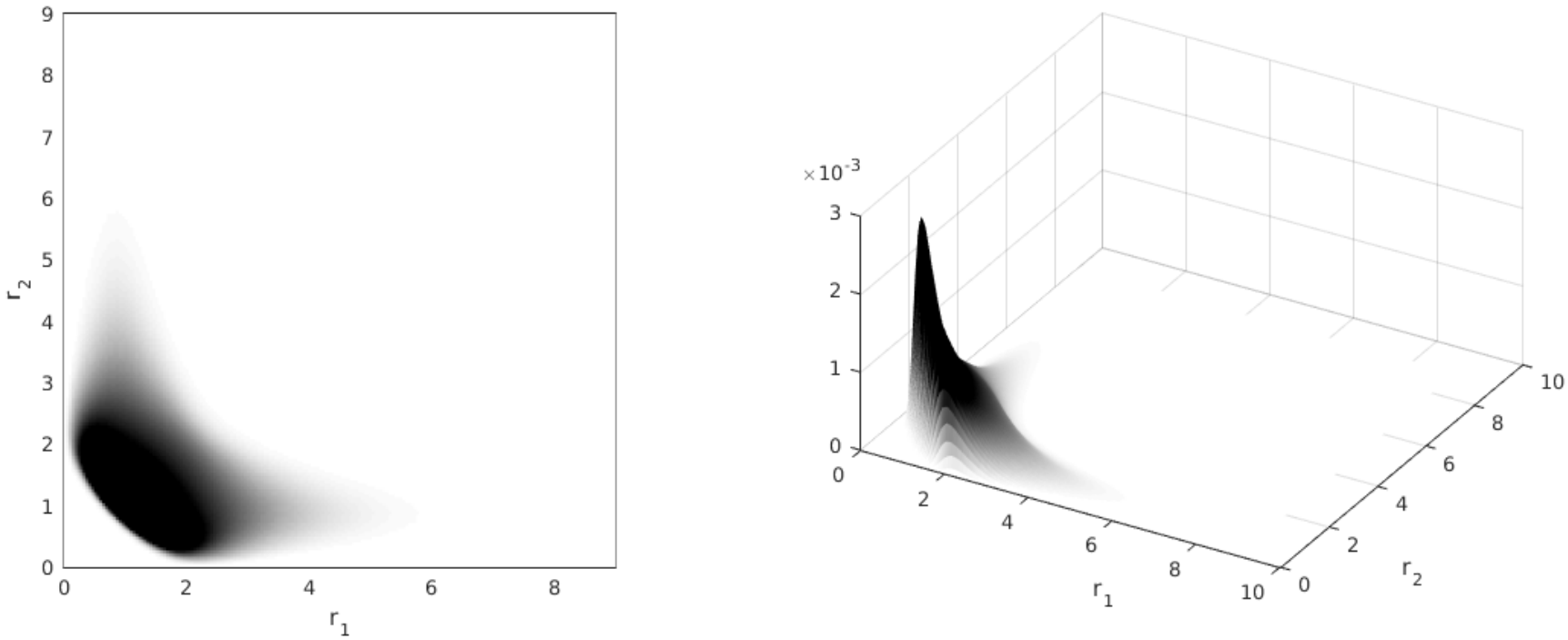


Figure: $\alpha = 0$

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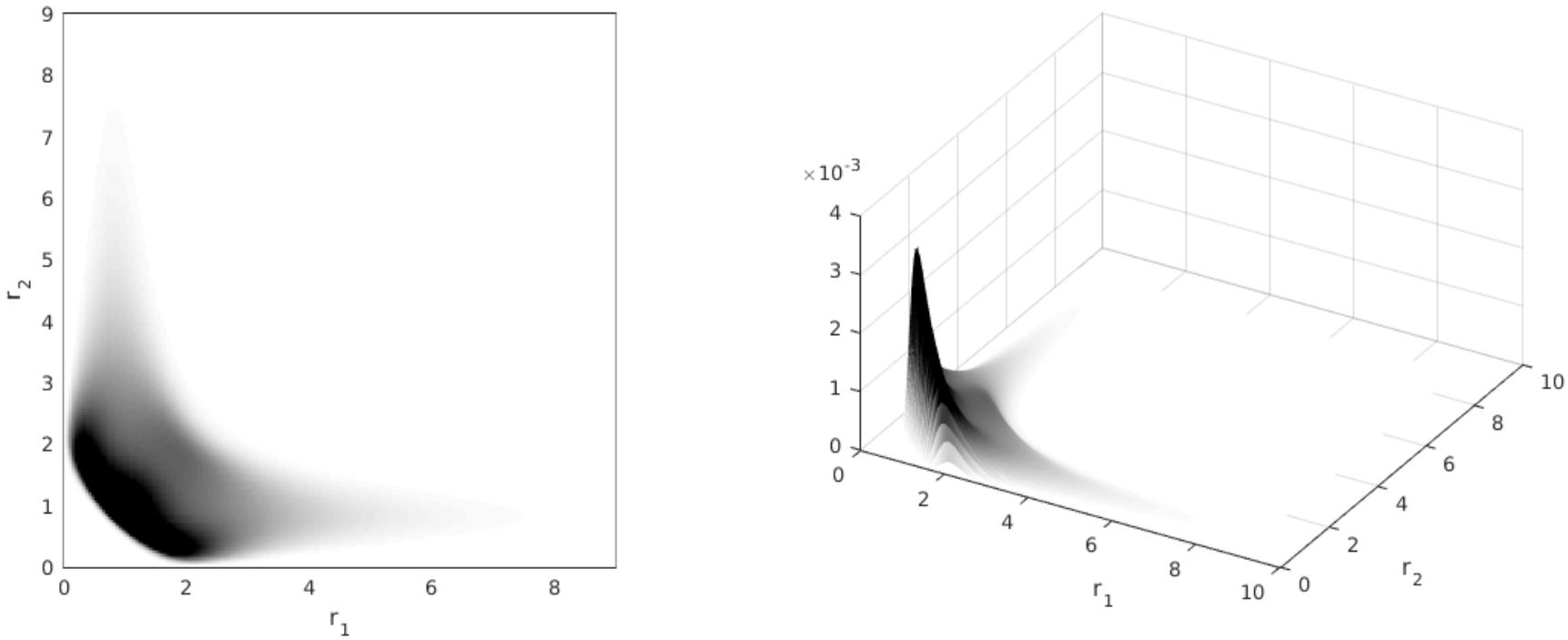

Figure: $\alpha = 0.1429$

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Take $\rho_\alpha(r) = \alpha\rho_{Li}(r) + (1-\alpha)\rho_{exp}(r)$ and $\alpha \in [0,1]$ then...

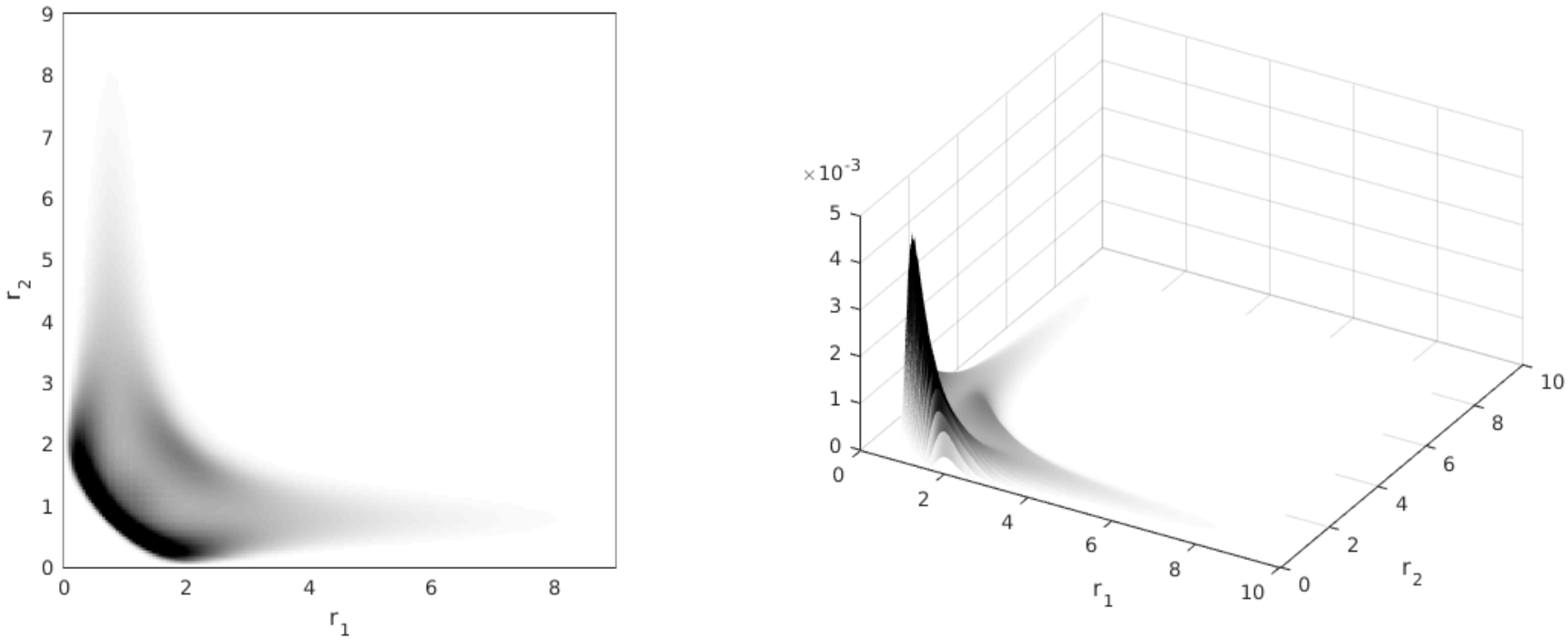

Figure: $\alpha = 0.2857$

The transition from spread to deterministic plans for $N = 3$ and $d = 3$

Take $\rho_\alpha(r) = \alpha\rho_{Li}(r) + (1-\alpha)\rho_{exp}(r)$ and $\alpha \in [0,1]$ then...

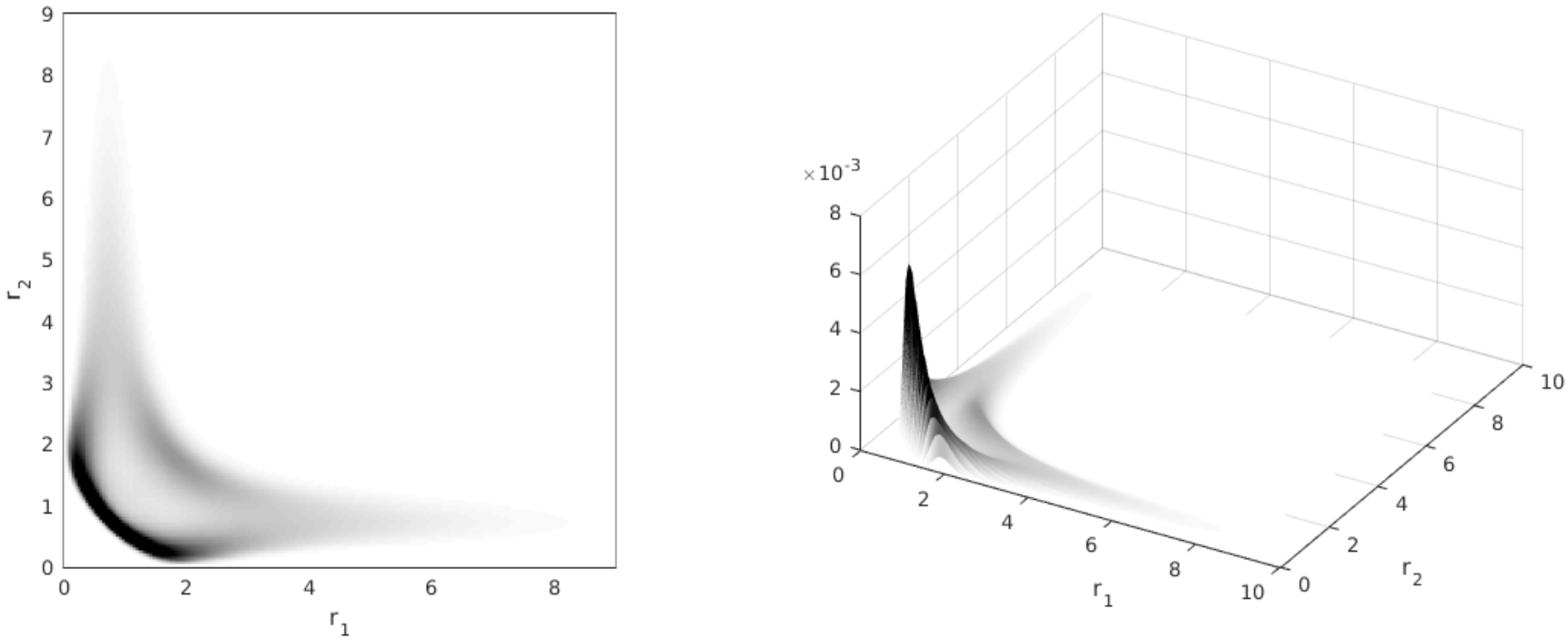

Figure: $\alpha = 0.4286$

The transition from spread to deterministic plans for $N = 3$ and $d = 3$

Take $\rho_\alpha(r) = \alpha\rho_{Li}(r) + (1-\alpha)\rho_{exp}(r)$ and $\alpha \in [0,1]$ then...

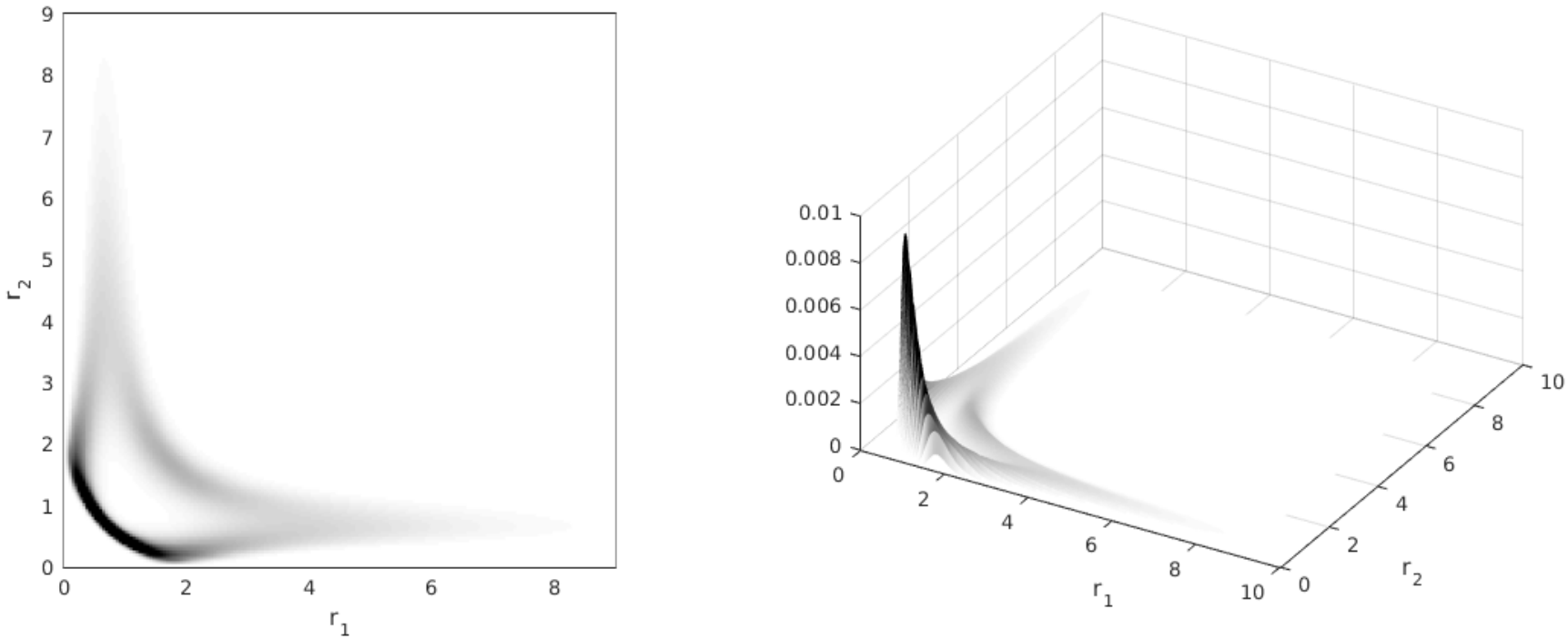

Figure: $\alpha = 0.5714$

The transition from spread to deterministic plans for $N = 3$ and $d = 3$

Take $\rho_\alpha(r) = \alpha\rho_{Li}(r) + (1-\alpha)\rho_{exp}(r)$ and $\alpha \in [0,1]$ then...

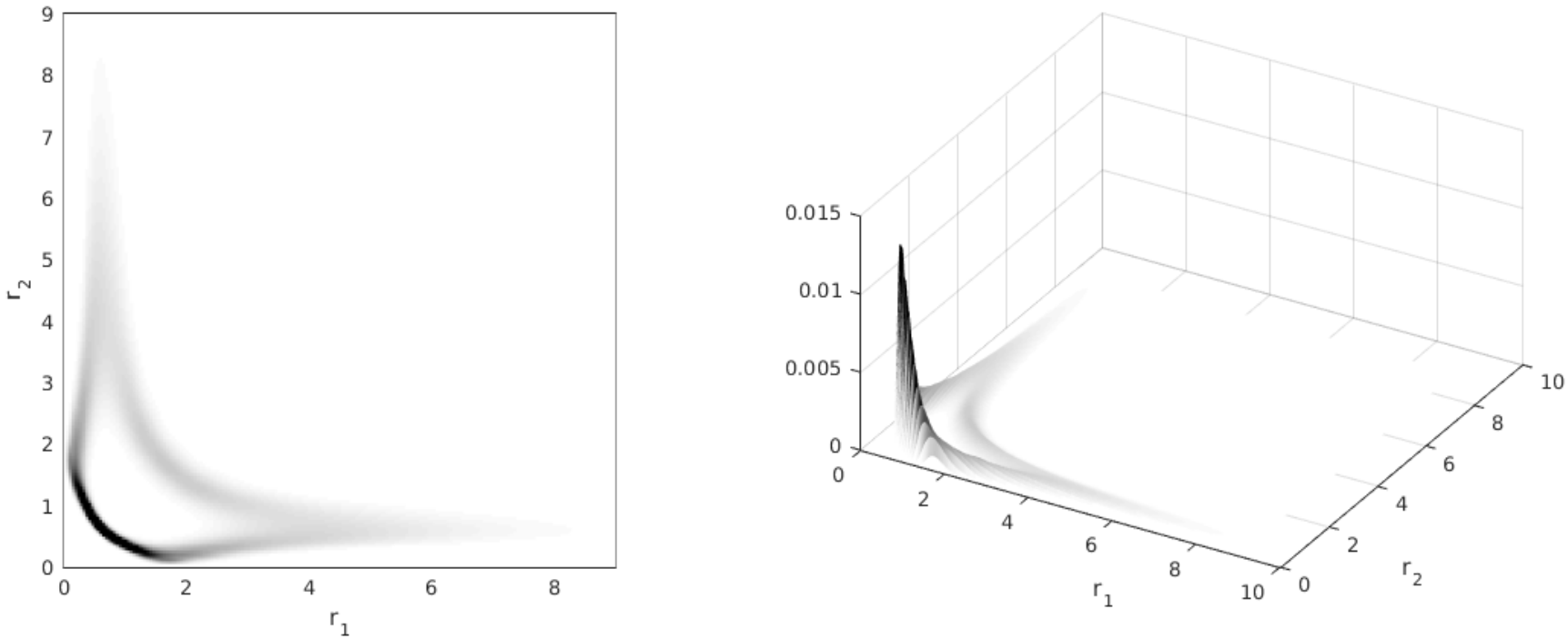

Figure: $\alpha = 0.7143$

The transition from spread to deterministic plans for $N = 3$ and $d = 3$

Take $\rho_\alpha(r) = \alpha\rho_{Li}(r) + (1-\alpha)\rho_{exp}(r)$ and $\alpha \in [0,1]$ then...

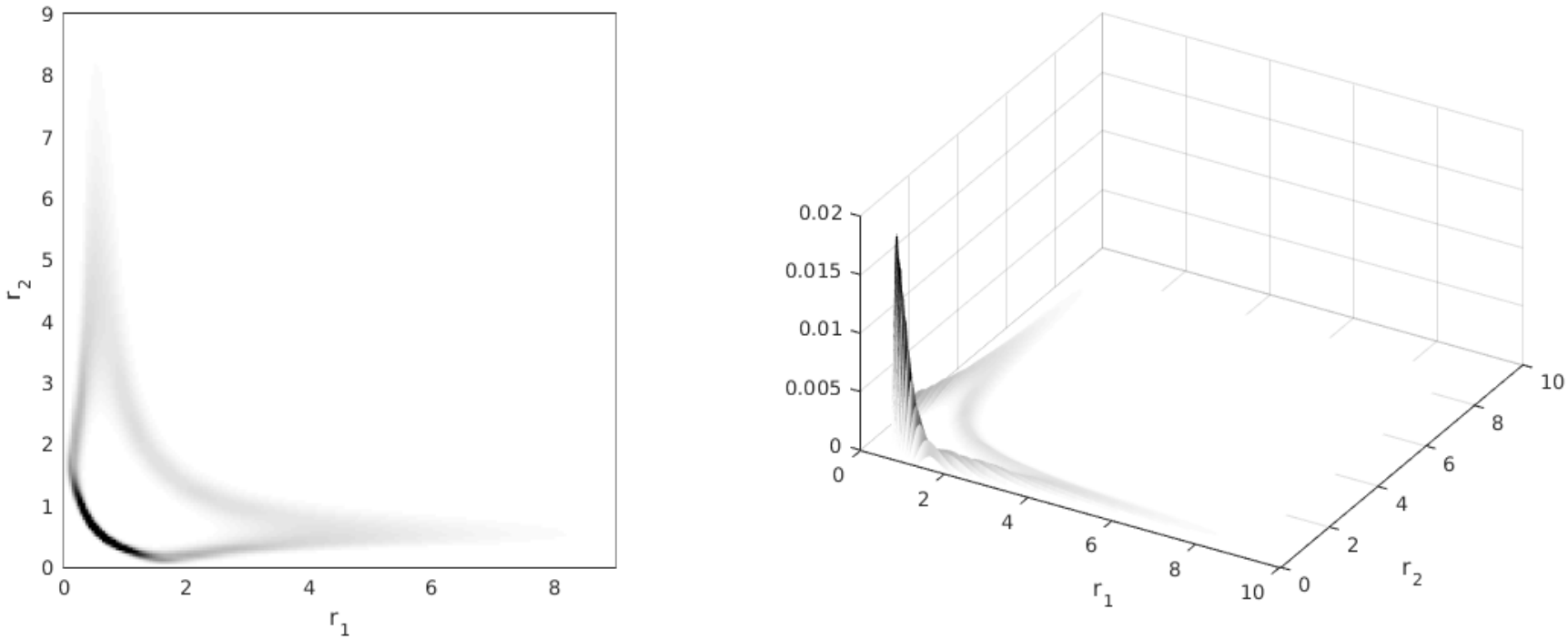

Figure: $\alpha = 0.8571$

The transition from spread to deterministic plans for $N = 3$ and $d = 3$

Take $\rho_\alpha(r) = \alpha\rho_{Li}(r) + (1-\alpha)\rho_{exp}(r)$ and $\alpha \in [0,1]$ then...

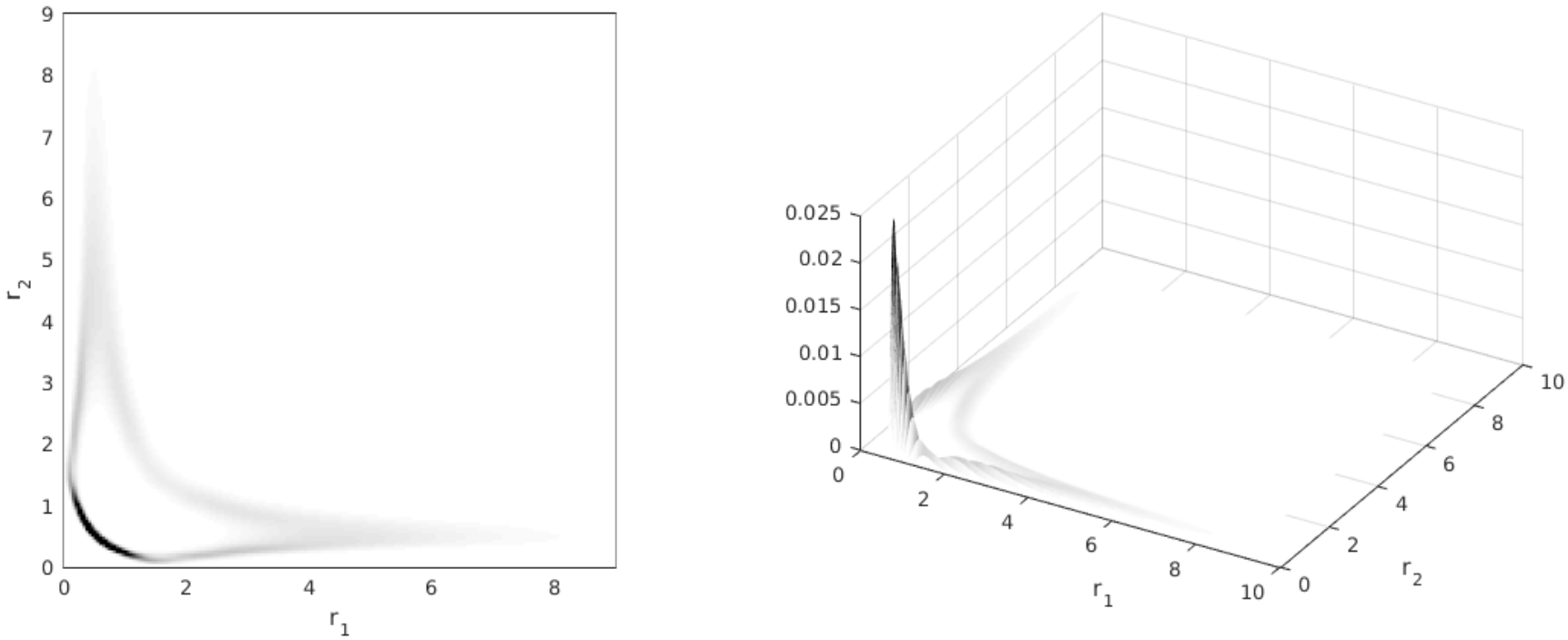

Figure: $\alpha = 1$

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