

# The Multi-Marginal Optimal Transport Problem and its Applications

Luca Nenna

(LMO) Université Paris-Saclay

Lecture 7 OT M2-OPT



- 1 Introduction: Classical vs Multi-Marginal Optimal Transport
  - The three universes of Numerical Optimal Transportation
  - The discretized problem
- 2 Entropic Optimal Transport
  - The numerical method
  - How the regularization works
- 3 Application I: MMOT for computing geodesics in the Wasserstein space
- 4 Application II: MMOT and the electron-electron repulsion

## 1 Introduction: Classical vs Multi-Marginal Optimal Transport

- The three universes of Numerical Optimal Transportation
- The discretized problem

## 2 Entropic Optimal Transport

- The numerical method
- How the regularization works

## 3 Application I: MMOT for computing geodesics in the Wasserstein space

## 4 Application II: MMOT and the electron-electron repulsion

- 1 Introduction: Classical vs Multi-Marginal Optimal Transport
  - The three universes of Numerical Optimal Transportation
  - The discretized problem
- 2 Entropic Optimal Transport
  - The numerical method
  - How the regularization works
- 3 Application I: MMOT for computing geodesics in the Wasserstein space
- 4 Application II: MMOT and the electron-electron repulsion

- 1 Introduction: Classical vs Multi-Marginal Optimal Transport
  - The three universes of Numerical Optimal Transportation
  - The discretized problem
- 2 Entropic Optimal Transport
  - The numerical method
  - How the regularization works
- 3 Application I: MMOT for computing geodesics in the Wasserstein space
- 4 Application II: MMOT and the electron-electron repulsion

# Introduction: Classical vs Multi-Marginal Optimal Transport

# Classical Optimal Transportation Theory

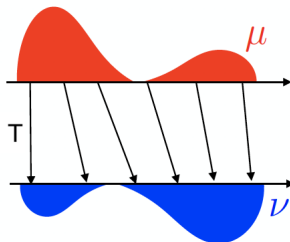
Let  $\mu \in \mathcal{P}(X)$  and  $\nu \in \mathcal{P}(Y)$  ( $X \subseteq \mathbb{R}^n$  and  $Y \subseteq \mathbb{R}^n$ ), the Optimal Transport (OT) problem is defined as follows

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

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

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

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



# The Multi-Marginal Optimal Transportation

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

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

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

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

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

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



# The Multi-Marginal Optimal Transportation

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

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

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

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

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

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

# The Multi-Marginal Optimal Transportation

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

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

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

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

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

**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**

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

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

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

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  $\phi, \psi$  such that  $\phi(x) + \psi(y) \leq c(x, y)$ .

## Remark

Notice that the constraint on a couple  $(\phi, \psi)$  may be rewritten as

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

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

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

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

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

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  $\phi, \psi$  such that  $\phi(x) + \psi(y) \leq c(x, y)$ .

## Remark

Notice that the constraint on a couple  $(\phi, \psi)$  may be rewritten as

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

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

# 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  $\gamma$  matches individuals from each team  $\mu_i$  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  $\gamma(x_1, \dots, x_N)$  returns the probability of finding electrons at position  $x_1, \dots, x_N$ ;
- Incompressible Euler Equations **(Yann Brenier 1989)** :  $\gamma(\omega)$  gives "the mass of fluid" which follows a path  $\omega$ . See also **(Jean-David Benamou, Guillaume Carlier, and Luca Nenna 2018)**.
- Variational Mean Field Games **(J.-D. Benamou, G. Carlier, S. Di Marino, and L. Nenna 2018)**;
- etc...

# 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  $\gamma$  matches individuals from each team  $\mu_i$  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  $\gamma(x_1, \dots, x_N)$  returns the probability of finding electrons at position  $x_1, \dots, x_N$ ;
- Incompressible Euler Equations **(Yann Brenier 1989)** :  $\gamma(\omega)$  gives “the mass of fluid” which follows a path  $\omega$ . See also **(Jean-David Benamou, Guillaume Carlier, and Luca Nenna 2018)**.
- Variational Mean Field Games **(J.-D. Benamou, G. Carlier, S. Di Marino, and L. Nenna 2018)**;
- etc...

# 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  $\gamma$  matches individuals from each team  $\mu_i$  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  $\gamma(x_1, \dots, x_N)$  returns the probability of finding electrons at position  $x_1, \dots, x_N$ ;
- Incompressible Euler Equations **(Yann Brenier 1989)** :  $\gamma(\omega)$  gives “the mass of fluid” which follows a path  $\omega$ . See also **(Jean-David Benamou, Guillaume Carlier, and Luca Nenna 2018)**.
- Variational Mean Field Games **(J.-D. Benamou, G. Carlier, S. Di Marino, and L. Nenna 2018)**;
- etc...

# 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  $\gamma$  matches individuals from each team  $\mu_i$  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  $\gamma(x_1, \dots, x_N)$  returns the probability of finding electrons at position  $x_1, \dots, x_N$ ;
- Incompressible Euler Equations **(Yann Brenier 1989)** :  $\gamma(\omega)$  gives “the mass of fluid” which follows a path  $\omega$ . See also **(Jean-David Benamou, Guillaume Carlier, and Luca Nenna 2018)**.
- Variational Mean Field Games (J.-D. Benamou, G. Carlier, S. Di Marino, and L. Nenna 2018);
- etc...



# 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  $\gamma$  matches individuals from each team  $\mu_i$  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  $\gamma(x_1, \dots, x_N)$  returns the probability of finding electrons at position  $x_1, \dots, x_N$ ;
- Incompressible Euler Equations **(Yann Brenier 1989)** :  $\gamma(\omega)$  gives “the mass of fluid” which follows a path  $\omega$ . See also **(Jean-David Benamou, Guillaume Carlier, and Luca Nenna 2018)**.
- Variational Mean Field Games **(J.-D. Benamou, G. Carlier, S. Di Marino, and L. Nenna 2018)**;
- etc...

# 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  $\gamma$  matches individuals from each team  $\mu_i$  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  $\gamma(x_1, \dots, x_N)$  returns the probability of finding electrons at position  $x_1, \dots, x_N$ ;
- Incompressible Euler Equations **(Yann Brenier 1989)** :  $\gamma(\omega)$  gives “the mass of fluid” which follows a path  $\omega$ . See also **(Jean-David Benamou, Guillaume Carlier, and Luca Nenna 2018)**.
- Variational Mean Field Games **(J.-D. Benamou, G. Carlier, S. Di Marino, and L. Nenna 2018)**;
- etc...

# 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  $\mu$  have an atomic form, i.e.  $\mu(x) = \sum_i \mu_i \delta_{x_i}$  (and  $\nu$  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.
- Continuous-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).
- Continuous-2-Continuous:  $\mu = \bar{\mu} dx$  and  $\nu = \bar{\nu} dy$ . Remarks:
  - The Brenier's Speed Limitation for Optimal Transport (Lafforgue, Mirebeau and V. Bonic 2020).

# 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  $\mu$  have an atomic form, i.e.  $\mu(x) = \sum_i \mu_i \delta_{x_i}$  (and  $\nu$  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.
- Continuous-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).
- Continuous-2-Continuous  $\mu = \bar{\mu}dx$  (and  $\nu$  too). **Remarks**
  - The Benamou-Brenier formulation for Optimal Transport! (J.-D. Benamou and Y. Brenier 2000)

# 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  $\mu$  have an atomic form, i.e.  $\mu(x) = \sum_i \mu_i \delta_{x_i}$  (and  $\nu$  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.
- Continuous-2-Discrete:  $\mu = \bar{\mu}dx$  and  $\nu(y) = \sum_i \nu_i \delta_{y_i}$ . **Remarks:**
  - The semi-discrete approach (**Méridot 2011**).
  - Used for generalized euler equations (kind of mmot problem) à la Brenier (**Méridot and Mirebeau 2016**).
- Continuous-2-Continuous  $\mu = \bar{\mu}dx$  (and  $\nu$  too). **Remarks**
  - The Benamou-Brenier formulation for Optimal Transport! (**J.-D. Benamou and Y. Brenier 2000**)

# 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  $\mu$  have an atomic form, i.e.  $\mu(x) = \sum_i \mu_i \delta_{x_i}$  (and  $\nu$  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.
- **Continuous-2-Discrete:**  $\mu = \bar{\mu}dx$  and  $\nu(y) = \sum_i \nu_i \delta_{y_i}$ . **Remarks:**
  - The semi-discrete approach (**Mérogot 2011**).
  - Used for generalized euler equations (kind of mmot problem) à la Brenier (**Mérogot and Mirebeau 2016**).
- **Continuous-2-Continuous**  $\mu = \bar{\mu}dx$  (and  $\nu$  too). **Remarks**
  - The Benamou-Brenier formulation for Optimal Transport! (**J.-D. Benamou and Y. Brenier 2000**)

# 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

$$\min \left\{ \sum_{i,j=1}^M c_{ij} \gamma_{ij} \mid \sum_{j=1}^M \gamma_{ij} = \mu_i \ \forall i, \sum_{i=1}^M \gamma_{ij} = \nu_j \ \forall j \right\} \quad (4)$$

and the dual problem

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

## Remarks

- The primal has  $M^2$  unknowns and  $M \times 2$  linear constraints.
- The dual has  $M \times 2$  unknowns, but  $M^2$  constraints.

# 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

$$\min \left\{ \sum_{i,j=1}^M c_{ij} \gamma_{ij} \mid \sum_{j=1}^M \gamma_{ij} = \mu_i \ \forall i, \sum_{i=1}^M \gamma_{ij} = \nu_j \ \forall j \right\} \quad (4)$$

and the dual problem

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

## Remarks

- The primal has  $M^2$  unknowns and  $M \times 2$  linear constraints.
- The dual has  $M \times 2$  unknowns, but  $M^2$  constraints.



# The importance of being sparse

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

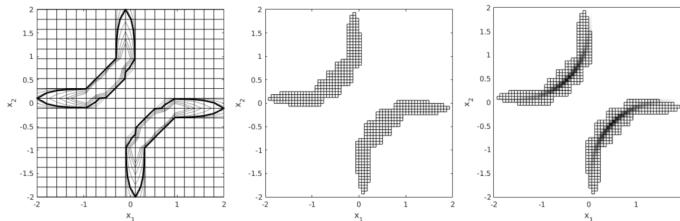


Figure: Support of the optimal  $\gamma$  for 2 marginals and the Coulomb cost

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.

# The discretized Monge-Kantorovich problem

Let's take  $c_{j_1, \dots, j_N} = c(x_{j_1}, \dots, x_{j_N}) \in \otimes_1^N \mathbb{R}^M$  ( $M$  are the gridpoints used to discretize  $\mathbb{R}^d$ ) then the discretized  $(\mathcal{MK}_N)$ , reads as

$$\min \left\{ \sum_{(j_1, \dots, j_N)=1}^M c_{j_1, \dots, j_N} \gamma_{j_1, \dots, j_N} \mid \sum_{j_k, k \neq i} \gamma_{j_1, \dots, j_{i-1}, j_{i+1}, \dots, j_N} = \mu_{j_i}^i \right\} \quad (6)$$

and the dual problem

$$\max \left\{ \sum_{i=1}^N \sum_{j_i=1}^M u_{j_i}^i \mu_{j_i}^i \mid \sum_{k=1}^N u_{j_k}^k \leq c_{j_1, \dots, j_N} \quad \forall (j_1, \dots, j_N) \in \{1, \dots, M\}^N \right\}. \quad (7)$$

## Drawbacks

- The primal has  $M^N$  unknowns and  $M \times N$  linear constraints.
- The dual has  $M \times N$  unknowns, but  $M^N$  constraints.

# The discretized Monge-Kantorovich problem

Let's take  $c_{j_1, \dots, j_N} = c(x_{j_1}, \dots, x_{j_N}) \in \otimes_1^N \mathbb{R}^M$  ( $M$  are the gridpoints used to discretize  $\mathbb{R}^d$ ) then the discretized  $(\mathcal{MK}_N)$ , reads as

$$\min \left\{ \sum_{(j_1, \dots, j_N)=1}^M c_{j_1, \dots, j_N} \gamma_{j_1, \dots, j_N} \mid \sum_{j_k, k \neq i} \gamma_{j_1, \dots, j_{i-1}, j_{i+1}, \dots, j_N} = \mu_{j_i}^i \right\} \quad (6)$$

and the dual problem

$$\max \left\{ \sum_{i=1}^N \sum_{j_i=1}^M u_{j_i}^i \mu_{j_i}^i \mid \sum_{k=1}^N u_{j_k}^k \leq c_{j_1, \dots, j_N} \quad \forall (j_1, \dots, j_N) \in \{1, \dots, M\}^N \right\}. \quad (7)$$

## Drawbacks

- The primal has  $M^N$  unknowns and  $M \times N$  linear constraints.
- The dual has  $M \times N$  unknowns, but  $M^N$  constraints.

# Entropic Optimal Transport

# 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)

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

where  $C$  is the matrix associated to the cost,  $\gamma$  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  $\epsilon$  as the temperature, then entropic OT is just OT at positive temperature.

The problem (8) can be re-written as

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

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

Remarks:

- Unique and semi-explicit solution (we will see it in 2/3 minutes!)
- Problem (9) dates back to Schrödinger, (see Christian Léonard's web page).
- $\mathcal{H}_\epsilon \rightarrow \text{MK}$  as  $\epsilon \rightarrow 0$ . (see (Guillaume Carlier, Duval, Gabriel Peyré, and Bernhard Schmitzer 2017; Léonard 2012)).
- The dual problem is an unconstrained optimization problem.

The problem (8) can be re-written as

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

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

**Remarks:**

- **Unique and semi-explicit solution** (we will see it in 2/3 minutes!)
- **Problem (9) dates back to Schrödinger**, (see [Christian Léonard's web page](#)).
- $\mathcal{H} \rightarrow \mathcal{MK}$  as  $\epsilon \rightarrow 0$ . (see (Guillaume Carlier, Duval, Gabriel Peyré, and Bernhard Schmitzer 2017; Léonard 2012)).
- The dual problem is an unconstrained optimization problem.

The problem (8) can be re-written as

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

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

**Remarks:**

- **Unique and semi-explicit solution** (we will see it in 2/3 minutes!)
- **Problem (9) dates back to Schrödinger**, (see [Christian Léonard's web page](#)).
- $\mathcal{H} \rightarrow \mathcal{MK}$  as  $\epsilon \rightarrow 0$ . (see **(Guillaume Carlier, Duval, Gabriel Peyré, and Bernhard Schmitzer 2017; Léonard 2012)**).
- The dual problem is an unconstrained optimization problem.



The problem (8) can be re-written as

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

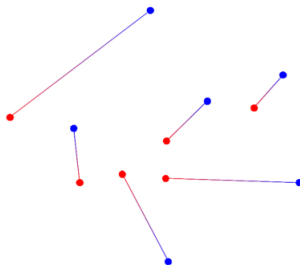
where  $\mathcal{H}(\gamma | \bar{\gamma}) = \sum_{ij} \gamma_{ij} \left( \log \frac{\gamma_{ij}}{\bar{\gamma}_{ij}} \right)$  ( $= \text{KL}(\gamma | \bar{\gamma})$  aka the Kullback-Leibler divergence ) and  $\bar{\gamma}_{ij} = e^{-\frac{c_{ij}}{\epsilon}} \mu_i \nu_j$ .

**Remarks:**

- **Unique and semi-explicit solution** (we will see it in 2/3 minutes!)
- **Problem (9) dates back to Schrödinger**, (see [Christian Léonard's web page](#)).
- $\mathcal{H} \rightarrow \mathcal{MK}$  as  $\epsilon \rightarrow 0$ . (see **(Guillaume Carlier, Duval, Gabriel Peyré, and Bernhard Schmitzer 2017; Léonard 2012)**).
- The dual problem is an unconstrained optimization problem.

# The “bridge” between quadratic Monge-Kantorovich and Schrödinger

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

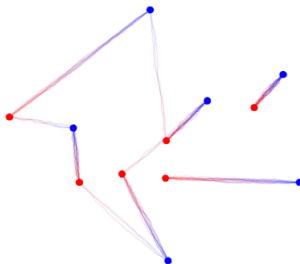


$$\varepsilon = 0$$

Figure: G. Peyre's twitter account

# The “bridge” between quadratic Monge-Kantorovich and Schrödinger

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

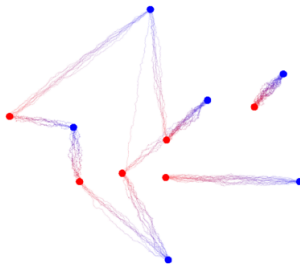


$$\varepsilon = .05$$

Figure: G. Peyre's twitter account

# The “bridge” between quadratic Monge-Kantorovich and Schrödinger

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

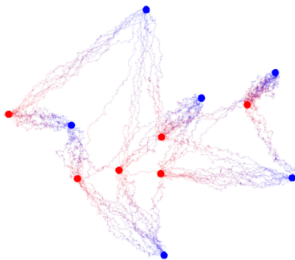


$$\varepsilon = 0.2$$

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

# The Sinkhorn algorithm

## Theorem ((Franklin and Lorenz 1989))

The optimal plan  $\gamma^*$  has the form  $\gamma_{ij}^* = a_i^* b_j^* \bar{\gamma}_{ij}$ . Moreover  $a_i^*$  and  $b_j^*$  can be uniquely determined (up to a multiplicative constant) as follows

$$b_j^* = \frac{\nu_j}{\sum_i a_i^* \bar{\gamma}_{ij}}, \quad a_i^* = \frac{\mu_i}{\sum_j b_j^* \bar{\gamma}_{ij}}$$

## The Sinkhorn algorithm (aka IPFP)

$$b_j^{n+1} = \frac{\nu_j}{\sum_i a_i^n \bar{\gamma}_{ij}}, \quad a_i^{n+1} = \frac{\mu_i}{\sum_j b_j^{n+1} \bar{\gamma}_{ij}}$$

## Theorem ((ibid.))

$a^n$  and  $b^n$  converge to  $a^*$  and  $b^*$

**Remark:**  $\phi_i = \epsilon \log(a_i)$  and  $\psi_j = \epsilon \log(b_j)$  are the (regularized) Kantorovich potentials.

# The Sinkhorn algorithm

## Theorem ((Franklin and Lorenz 1989))

*The optimal plan  $\gamma^*$  has the form  $\gamma_{ij}^* = a_i^* b_j^* \bar{\gamma}_{ij}$ . Moreover  $a_i^*$  and  $b_j^*$  can be uniquely determined (up to a multiplicative constant) as follows*

$$b_j^* = \frac{\nu_j}{\sum_i a_i^* \bar{\gamma}_{ij}}, \quad a_i^* = \frac{\mu_i}{\sum_j b_j^* \bar{\gamma}_{ij}}$$

## The Sinkhorn algorithm (aka IPFP)

$$b_j^{n+1} = \frac{\nu_j}{\sum_i a_i^n \bar{\gamma}_{ij}}, \quad a_i^{n+1} = \frac{\mu_i}{\sum_j b_j^{n+1} \bar{\gamma}_{ij}}$$

## Theorem ((ibid.))

$a^n$  and  $b^n$  converge to  $a^*$  and  $b^*$

**Remark:**  $\phi_i = \epsilon \log(a_i)$  and  $\psi_j = \epsilon \log(b_j)$  are the (regularized) Kantorovich potentials.

# The Sinkhorn algorithm

## Theorem ((Franklin and Lorenz 1989))

The optimal plan  $\gamma^*$  has the form  $\gamma_{ij}^* = a_i^* b_j^* \bar{\gamma}_{ij}$ . Moreover  $a_i^*$  and  $b_j^*$  can be uniquely determined (up to a multiplicative constant) as follows

$$b_j^* = \frac{\nu_j}{\sum_i a_i^* \bar{\gamma}_{ij}}, \quad a_i^* = \frac{\mu_i}{\sum_j b_j^* \bar{\gamma}_{ij}}$$

## The Sinkhorn algorithm (aka IPFP)

$$b_j^{n+1} = \frac{\nu_j}{\sum_i a_i^n \bar{\gamma}_{ij}}, \quad a_i^{n+1} = \frac{\mu_i}{\sum_j b_j^{n+1} \bar{\gamma}_{ij}}$$

## Theorem ((ibid.))

$a^n$  and  $b^n$  converge to  $a^*$  and  $b^*$

Remark:  $\phi_i = \epsilon \log(a_i)$  and  $\psi_j = \epsilon \log(b_j)$  are the (regularized) Kantorovich potentials.



# The Sinkhorn algorithm

## Theorem ((Franklin and Lorenz 1989))

The optimal plan  $\gamma^*$  has the form  $\gamma_{ij}^* = a_i^* b_j^* \bar{\gamma}_{ij}$ . Moreover  $a_i^*$  and  $b_j^*$  can be uniquely determined (up to a multiplicative constant) as follows

$$b_j^* = \frac{\nu_j}{\sum_i a_i^* \bar{\gamma}_{ij}}, \quad a_i^* = \frac{\mu_i}{\sum_j b_j^* \bar{\gamma}_{ij}}$$

## The Sinkhorn algorithm (aka IPFP)

$$b_j^{n+1} = \frac{\nu_j}{\sum_i a_i^n \bar{\gamma}_{ij}}, \quad a_i^{n+1} = \frac{\mu_i}{\sum_j b_j^{n+1} \bar{\gamma}_{ij}}$$

## Theorem ((ibid.))

$a^n$  and  $b^n$  converge to  $a^*$  and  $b^*$

**Remark:**  $\phi_i = \epsilon \log(a_i)$  and  $\psi_j = \epsilon \log(b_j)$  are the (regularized) Kantorovich potentials.

- In **(Franklin and Lorenz 1989)** proved the convergence of Sinkhorn by using the Hilbert metric.
- The entropic regularization spreads the support and this helps to stabilize: it defines a strongly convex program with a unique solution.
- The solution can be obtained through elementary operations (trivially parallelizable).
- The regularized solution  $\gamma^\epsilon$  converges to the solution  $\gamma^{ot}$  of  $\mathcal{MK}$  pb. with minimal entropy as  $\epsilon \rightarrow 0$  (in **(Cominetti and San Martin 1994)** the authors proved that the convergence is exponential).
- The complexity depends on the cost function: with Euler's cost  $O((N-1)M^{2.37})$ ...still exponential in  $N$  for the Coulomb cost : ( .

- In **(Franklin and Lorenz 1989)** proved the convergence of Sinkhorn by using the Hilbert metric.
- The entropic regularization spreads the support and this helps to stabilize: it defines a strongly convex program with a unique solution.
- The solution can be obtained through elementary operations (trivially parallelizable).
- The regularized solution  $\gamma^\epsilon$  converges to the solution  $\gamma^{ot}$  of  $\mathcal{MK}$  pb. with minimal entropy as  $\epsilon \rightarrow 0$  (in **(Cominetti and San Martin 1994)** the authors proved that the convergence is exponential).
- The complexity depends on the cost function: with Euler's cost  $O((N-1)M^{2.37})$ ...still exponential in  $N$  for the Coulomb cost : ( .

- In **(Franklin and Lorenz 1989)** proved the convergence of Sinkhorn by using the Hilbert metric.
- The entropic regularization spreads the support and this helps to stabilize: it defines a strongly convex program with a unique solution.
- The solution can be obtained through elementary operations (trivially parallelizable).
- The regularized solution  $\gamma^\epsilon$  converges to the solution  $\gamma^{ot}$  of  $\mathcal{MK}$  pb. with minimal entropy as  $\epsilon \rightarrow 0$  (in **(Cominetti and San Martin 1994)** the authors proved that the convergence is exponential).
- The complexity depends on the cost function: with Euler's cost  $\mathcal{O}((N-1)M^{2.37})$ ...still exponential in  $N$  for the Coulomb cost : ( .

- In **(Franklin and Lorenz 1989)** proved the convergence of Sinkhorn by using the Hilbert metric.
- The entropic regularization spreads the support and this helps to stabilize: it defines a strongly convex program with a unique solution.
- The solution can be obtained through elementary operations (trivially parallelizable).
- The regularized solution  $\gamma^\epsilon$  converges to the solution  $\gamma^{ot}$  of  $\mathcal{MK}$  pb. with minimal entropy as  $\epsilon \rightarrow 0$  (in **(Cominetti and San Martin 1994)** the authors proved that the convergence is exponential).
- The complexity depends on the cost function: with Euler's cost  $O((N-1)M^{2.37})$ ...still exponential in  $N$  for the Coulomb cost : ( .

- In **(Franklin and Lorenz 1989)** proved the convergence of Sinkhorn by using the Hilbert metric.
- The entropic regularization spreads the support and this helps to stabilize: it defines a strongly convex program with a unique solution.
- The solution can be obtained through elementary operations (trivially parallelizable).
- The regularized solution  $\gamma^\epsilon$  converges to the solution  $\gamma^{ot}$  of  $\mathcal{MK}$  pb. with minimal entropy as  $\epsilon \rightarrow 0$  (in **(Cominetti and San Martin 1994)** the authors proved that the convergence is exponential).
- The complexity depends on the cost function: with Euler's cost  $\mathcal{O}((N-1)M^{2.37})$ ...still exponential in  $N$  for the Coulomb cost : ( .

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

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

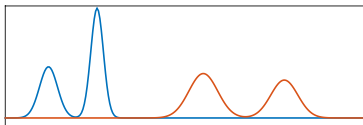


Figure: Marginals  $\mu$  and  $\nu$



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  $\epsilon \rightarrow 0$  ( $N = 512$ ), we have

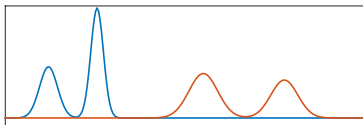


Figure: Marginals  $\mu$  and  $\nu$



Figure:  $\epsilon = 40/N$



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

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

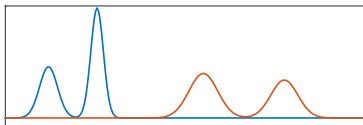


Figure: Marginals  $\mu$  and  $\nu$



Figure:  $\epsilon = 20/N$

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

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

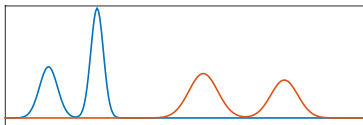


Figure: Marginals  $\mu$  and  $\nu$



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  $\epsilon \rightarrow 0$  ( $N = 512$ ), we have

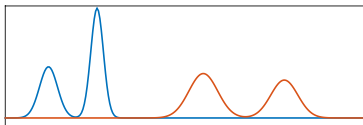


Figure: Marginals  $\mu$  and  $\nu$



Figure:  $\epsilon = 6/N$

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

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

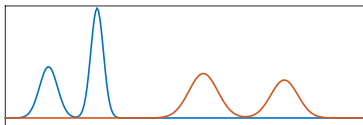


Figure: Marginals  $\mu$  and  $\nu$



Figure:  $\epsilon = 4/N$

# The extension to the Multi-Marginal problem

The entropic multi-marginal problem becomes

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

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.  $\mathcal{C}_1 = \{\gamma \mid \sum_{j,k} \gamma_{ijk} = \mu_i^1\}$ ).

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

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

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

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

$\Rightarrow$   
 $\Rightarrow$   
 $\Rightarrow$   
 $\Rightarrow$   
 $\Rightarrow$   
 $\Rightarrow$

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

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

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

# The extension to the Multi-Marginal problem

The entropic multi-marginal problem becomes

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

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.  $\mathcal{C}_1 = \{\gamma \mid \sum_{j,k} \gamma_{ijk} = \mu_i^1\}$ ).

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

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

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

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

$\Rightarrow$   
 $\Rightarrow$   
 $\Rightarrow$   
 $\Rightarrow$   
 $\Rightarrow$   
 $\Rightarrow$

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

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

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

# The extension to the Multi-Marginal problem

The entropic multi-marginal problem becomes

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

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.  $\mathcal{C}_1 = \{\gamma \mid \sum_{j,k} \gamma_{ijk} = \mu_i^1\}$ ).

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

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

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

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

$\Rightarrow$   
 $\Rightarrow$   
 $\Rightarrow$   
 $\Rightarrow$   
 $\Rightarrow$   
 $\Rightarrow$

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

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

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

# 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  $e_t : [0, 1] \rightarrow X$ )

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

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

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

# Some remarks and a MMOT formulation

## Remarks:

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

$$\pi_t(x, y)_{\#} \gamma = (e_t)_{\#} Q = \rho_t^*,$$

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  $i = 0, \dots, T$ ) we get the following discrete (in time) MMOT problem

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

# The geodesic in 2D

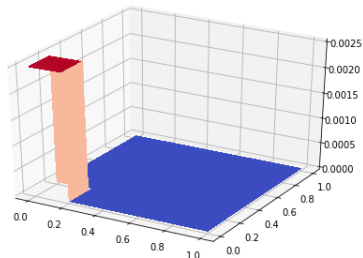
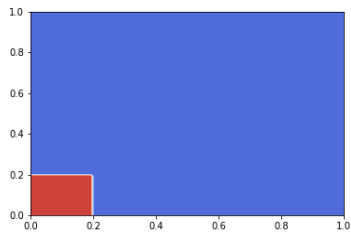


Figure:  $t = 0$

# The geodesic in 2D

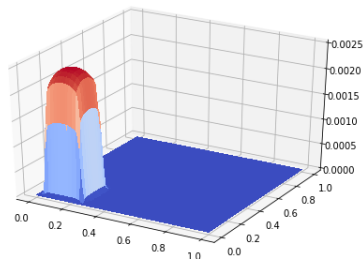
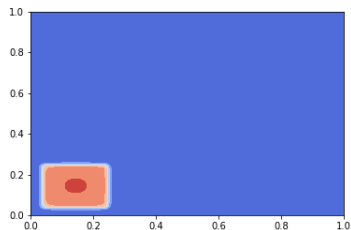


Figure:  $t = \frac{1}{14}$

# The geodesic in 2D

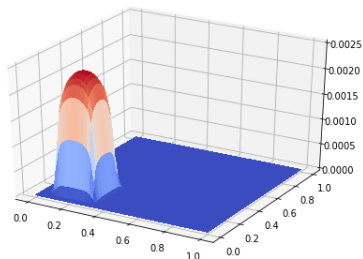
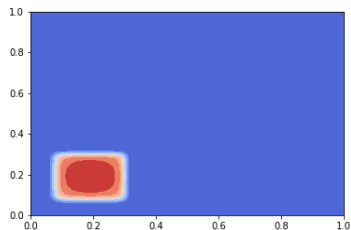


Figure:  $t = \frac{2}{14}$

# The geodesic in 2D

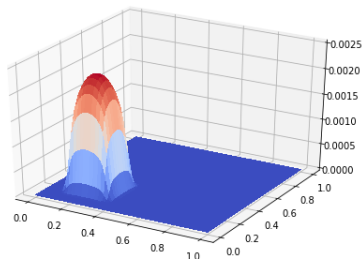
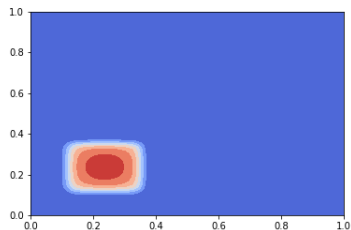


Figure:  $t = \frac{3}{14}$

# The geodesic in 2D

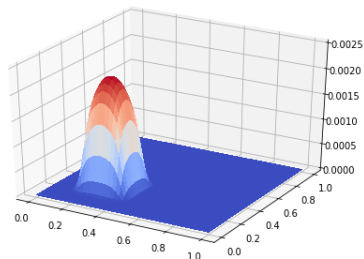
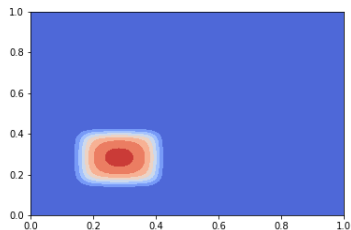


Figure:  $t = \frac{4}{14}$

# The geodesic in 2D

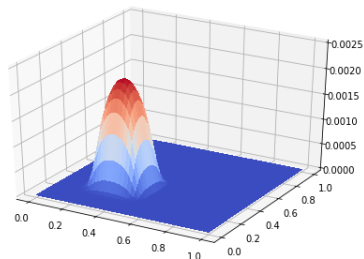
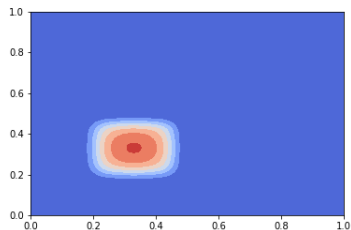


Figure:  $t = \frac{5}{14}$



# The geodesic in 2D

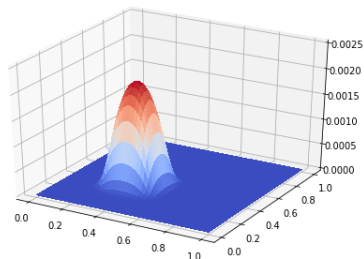
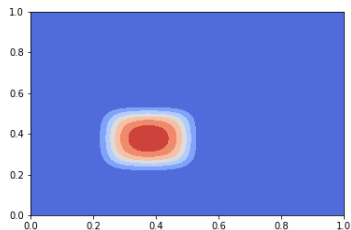


Figure:  $t = \frac{6}{14}$

# The geodesic in 2D

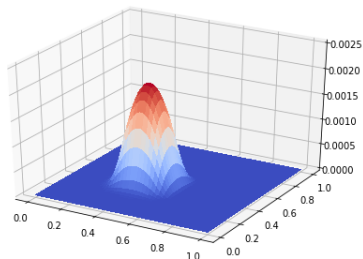
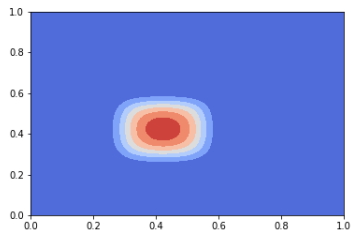


Figure:  $t = \frac{7}{14}$

# The geodesic in 2D

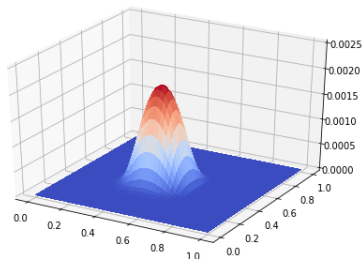
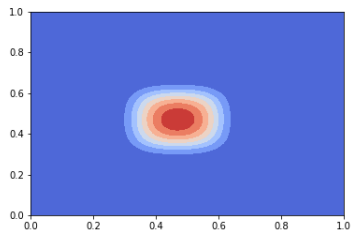


Figure:  $t = \frac{8}{14}$

# The geodesic in 2D

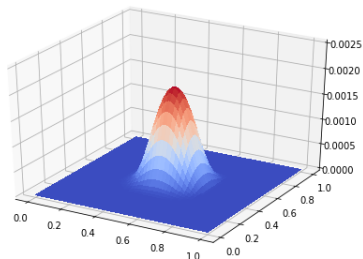
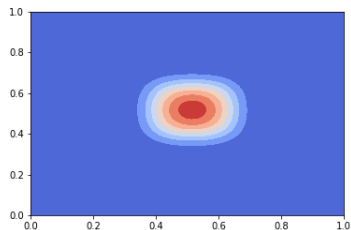


Figure:  $t = \frac{9}{14}$

# The geodesic in 2D

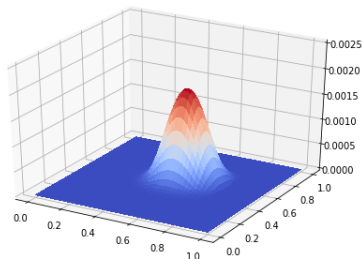
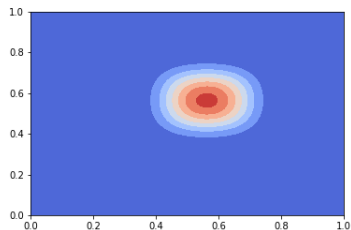


Figure:  $t = \frac{10}{14}$

# The geodesic in 2D

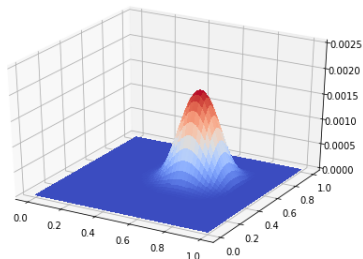
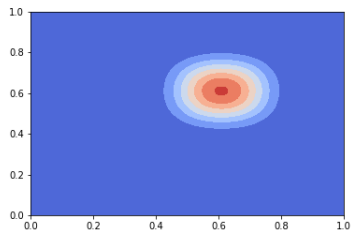


Figure:  $t = \frac{11}{14}$

# The geodesic in 2D

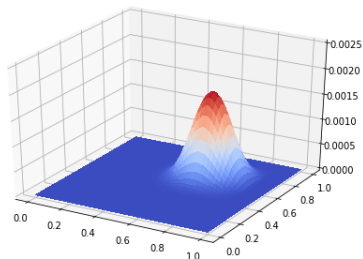
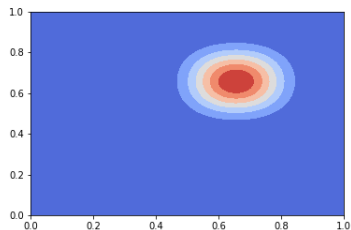


Figure:  $t = \frac{12}{14}$

# The geodesic in 2D

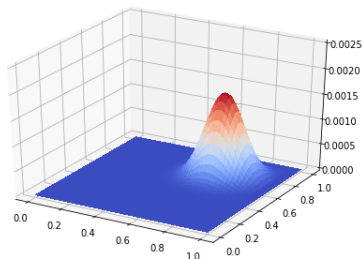
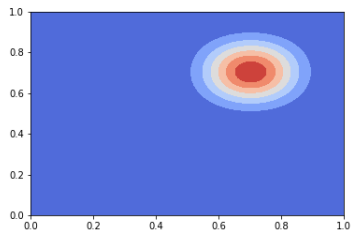


Figure:  $t = \frac{13}{14}$



# The geodesic in 2D

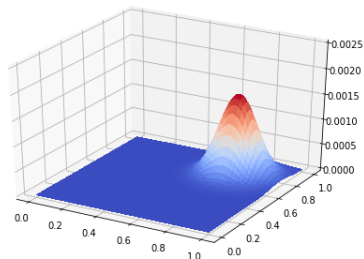
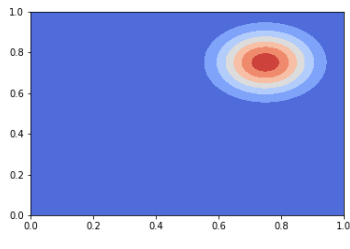


Figure:  $t = 1$

# The geodesic between images

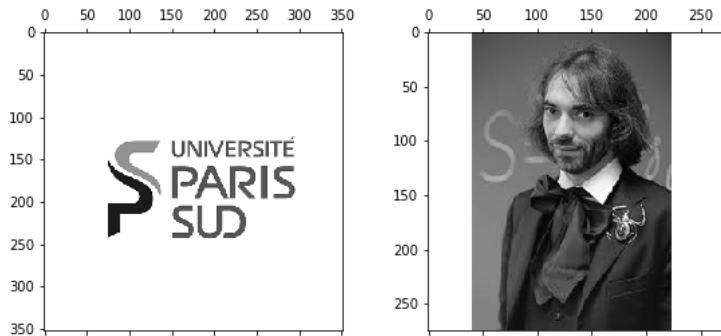


Figure:  $t = 0$

# The geodesic between images

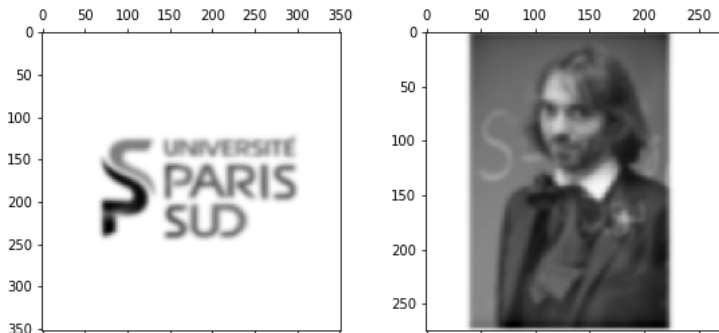


Figure:  $t = \frac{1}{14}$

# The geodesic between images

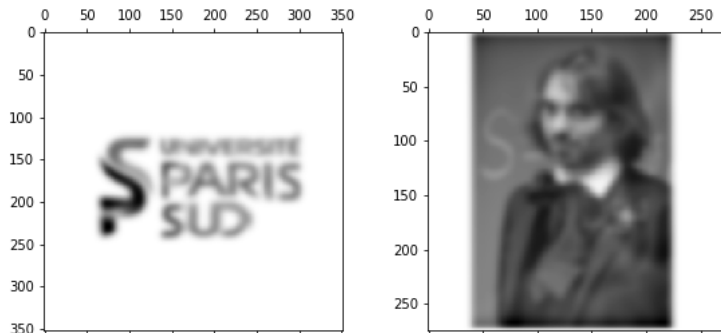


Figure:  $t = \frac{2}{14}$

# The geodesic between images

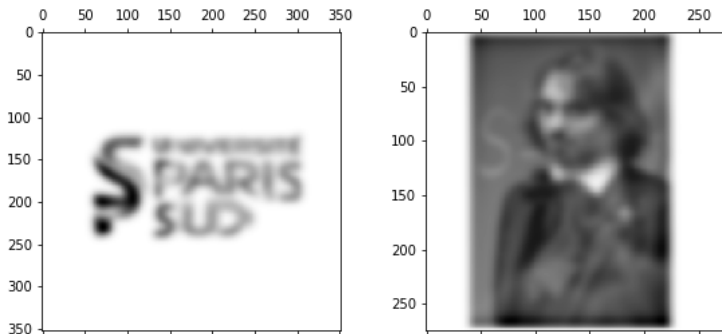


Figure:  $t = \frac{3}{14}$

# The geodesic between images

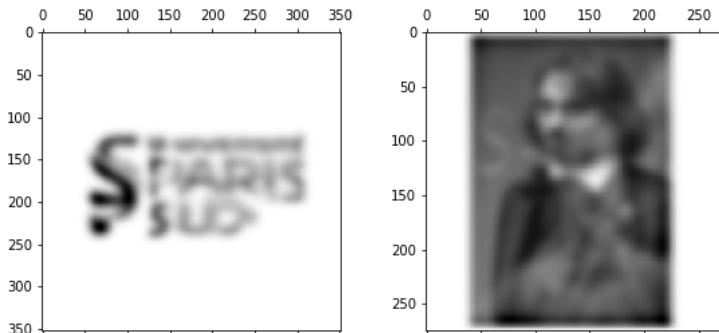


Figure:  $t = \frac{4}{14}$

# The geodesic between images

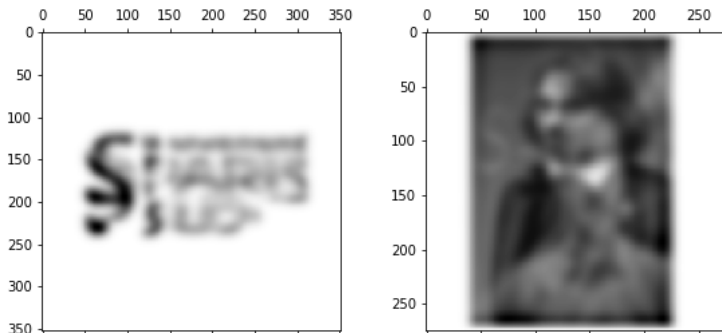


Figure:  $t = \frac{5}{14}$

# The geodesic between images

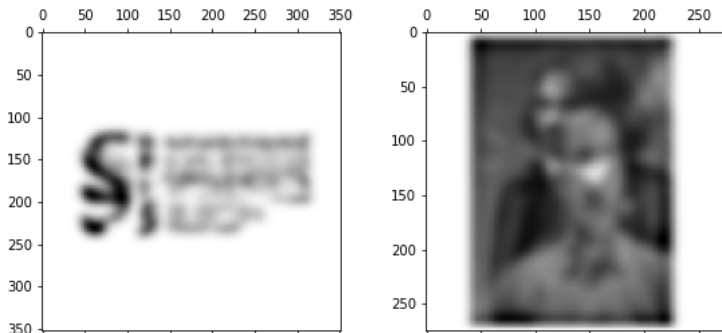


Figure:  $t = \frac{6}{14}$



# The geodesic between images

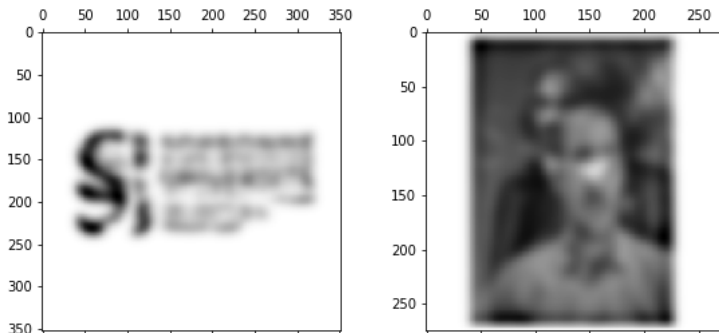


Figure:  $t = \frac{7}{14}$

# The geodesic between images

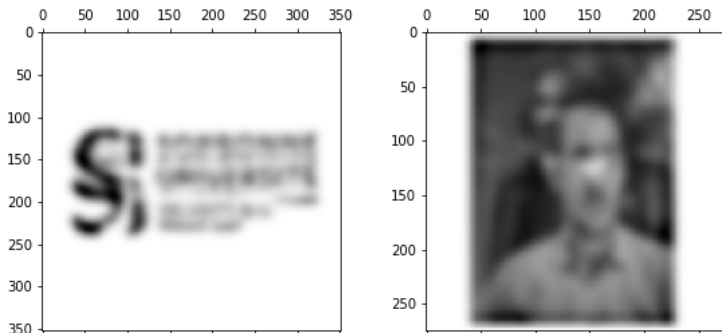


Figure:  $t = \frac{8}{14}$

# The geodesic between images

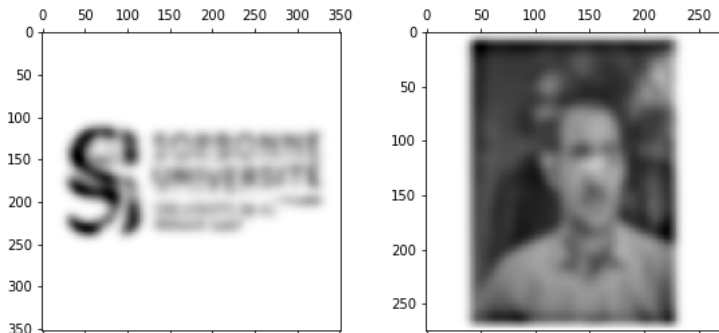


Figure:  $t = \frac{9}{14}$

# The geodesic between images

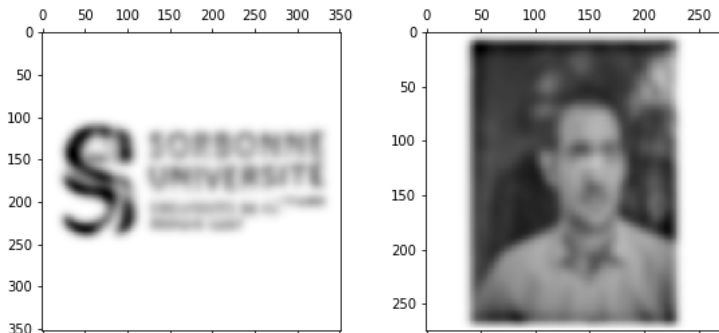


Figure:  $t = \frac{10}{14}$

# The geodesic between images

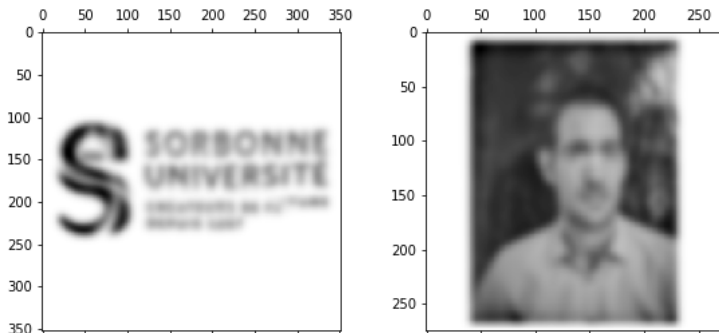


Figure:  $t = \frac{11}{14}$

# The geodesic between images

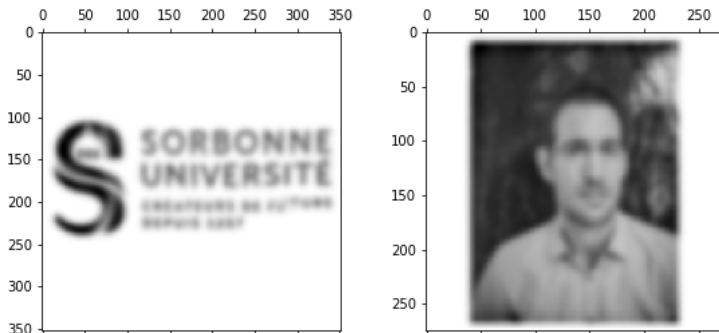


Figure:  $t = \frac{12}{14}$

# The geodesic between images

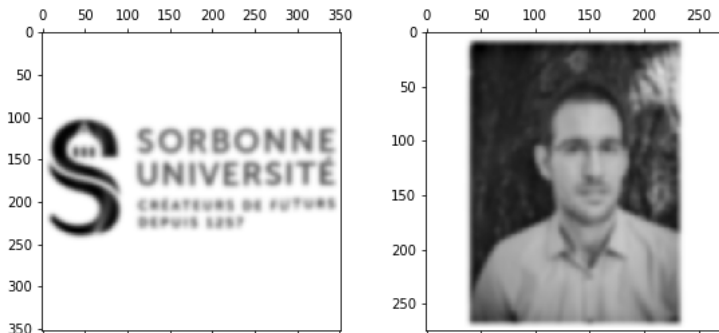


Figure:  $t = \frac{13}{14}$

# The geodesic between images

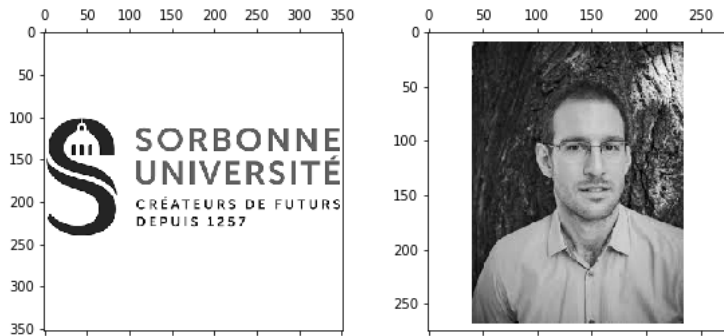


Figure:  $t = 1$



## 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  $\gamma = N \sum_{s_1, \dots, s_N \in \mathbb{Z}_2} |\Psi(x_1, s_1, \dots, x_N, s_N)|^2 \stackrel{\text{def}}{=} \text{joint probability density of electrons at positions } x_1, \dots, x_N \in \mathbb{R}^d$ .

Then the **Density Functional Theory** consists in studying the following variational principle

Rayleigh-Ritz variational principle

$$E_0 = \inf_{\Psi \in H^1_0, \|\Psi\|_2=1} \epsilon T[\Psi] + V_{ee}[\Psi] + \int \sum_{s_1, \dots, s_N \in \mathbb{Z}_2} \sum_{i=1}^N v_{\text{ext}}(x_i) |\Psi|^2 dx \quad (11)$$

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

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

# 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  $\gamma = N \sum_{s_1, \dots, s_N \in \mathbb{Z}_2} |\Psi(x_1, s_1, \dots, x_N, s_N)|^2 \stackrel{\text{def}}{=} \text{joint probability density of electrons at positions } x_1, \dots, x_N \in \mathbb{R}^d$ .

Then the **Density Functional Theory** consists in studying the following variational principle

## Rayleigh-Ritz variational principle

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

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

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

# The Levy-Lieb functional

The minimizing problem can be partitioned into a double minimization. First minimize over  $\Psi$  subject to a fixed  $\rho$ , then minimize over  $\rho$ :

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

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

$$F_{LL}[\rho] = \min_{\Psi \rightarrow \rho} T[\Psi] + V_{ee}[\Psi] \quad (13)$$

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

## Semiclassical limit

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

# The Levy-Lieb functional

The minimizing problem can be partitioned into a double minimization. First minimize over  $\Psi$  subject to a fixed  $\rho$ , then minimize over  $\rho$ :

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

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

$$F_{LL}[\rho] = \min_{\Psi \rightarrow \rho} T[\Psi] + V_{ee}[\Psi] \quad (13)$$

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

## Semiclassical limit

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

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

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

- 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)

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

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  $\gamma$  and  $\bar{\gamma} = e^{-\sum_{i < j} \frac{1}{|x_i - x_j|} \frac{1}{C\epsilon}}$ .

Consider now the cost function

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

and  $\mu_1 = \dots = \mu_N = \rho$  (we refer to  $\rho$  as the electronic density) then the MMOT gives the electronic configuration (namely the optimal transport plan  $\gamma$ ) 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  $\rho$  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 $\epsilon \rightarrow 0$

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

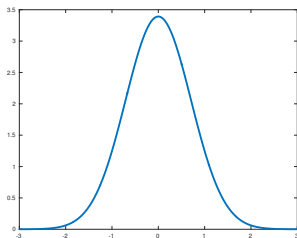


Figure: Marginals  $\rho$  (and  $\rho$ )



Figure:  $\epsilon = 10$

# The limit as $\epsilon \rightarrow 0$

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

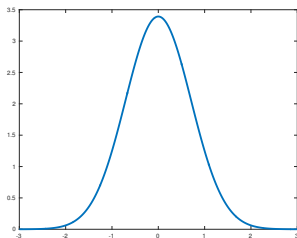


Figure: Marginals  $\rho$  (and  $\rho$ )



Figure:  $\epsilon = 5$

# The limit as $\epsilon \rightarrow 0$

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

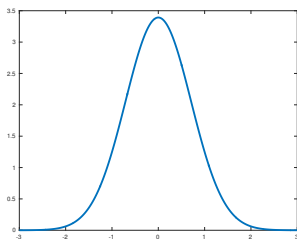


Figure: Marginals  $\rho$  (and  $\rho$ )



Figure:  $\epsilon = 1$

# The limit as $\epsilon \rightarrow 0$

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

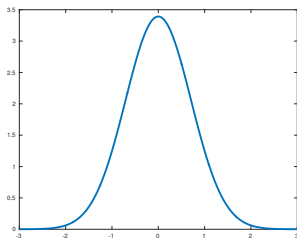


Figure: Marginals  $\rho$  (and  $\rho$ )



Figure:  $\epsilon = 0.1$

# The limit as $\epsilon \rightarrow 0$

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

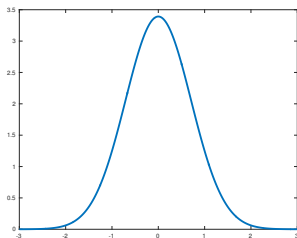


Figure: Marginals  $\rho$  (and  $\rho$ )



Figure:  $\epsilon = 0.01$

# The limit as $\epsilon \rightarrow 0$

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

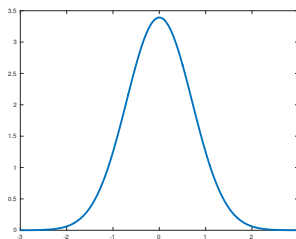


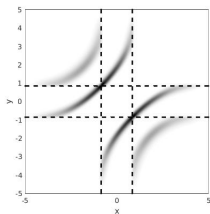
Figure: Marginals  $\rho$  (and  $\rho$ )



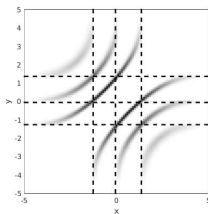
Figure:  $\epsilon = 0.002$

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

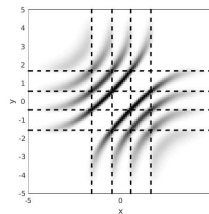
We take the density  $\rho(x) = \frac{N}{10}(1 + \cos(\frac{\pi}{5}x))$  and...



$N = 3$



$N = 4$



$N = 5$

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...

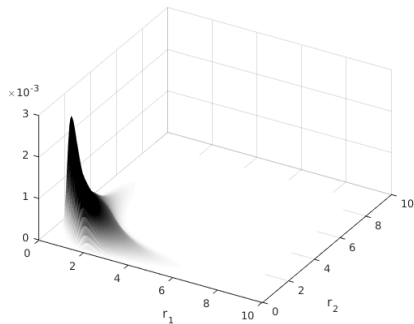
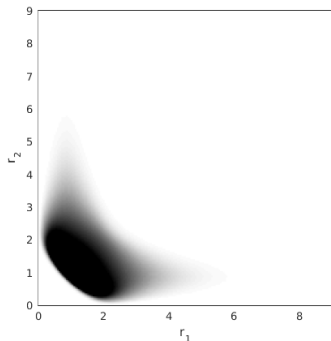


Figure:  $\alpha = 0$



# 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...

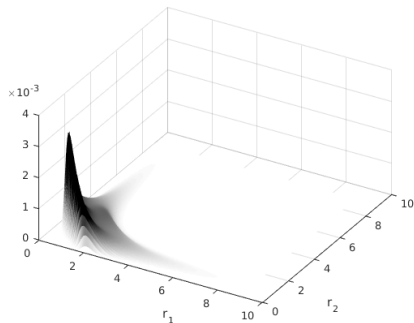
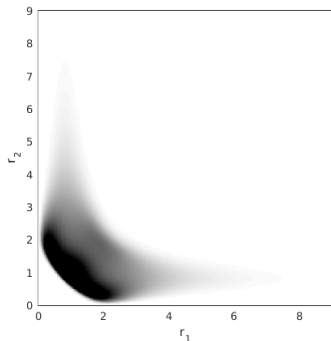


Figure:  $\alpha = 0.1429$

# 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...

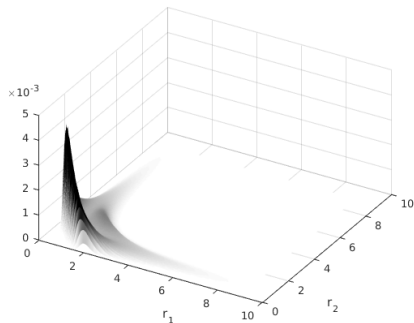
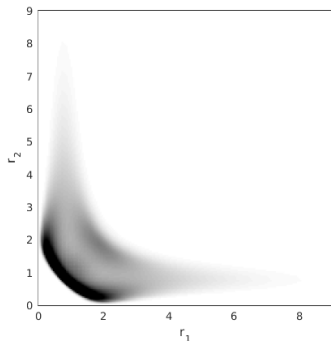


Figure:  $\alpha = 0.2857$

# 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...

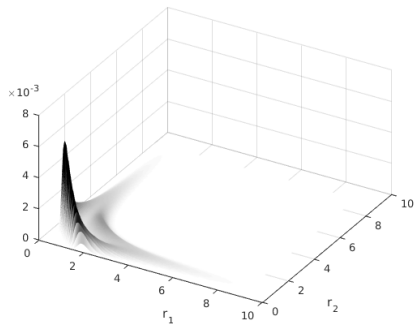
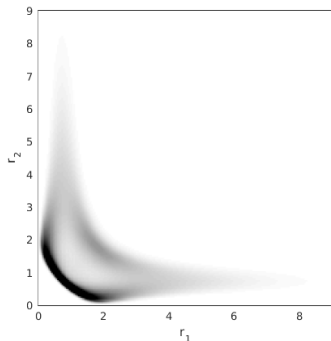


Figure:  $\alpha = 0.4286$

# 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...

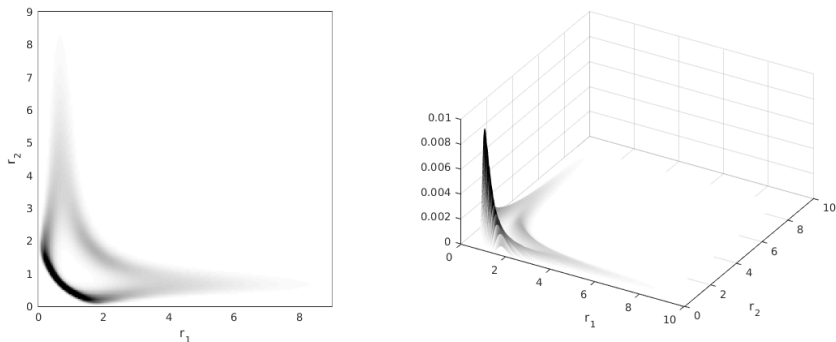


Figure:  $\alpha = 0.5714$

# 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...

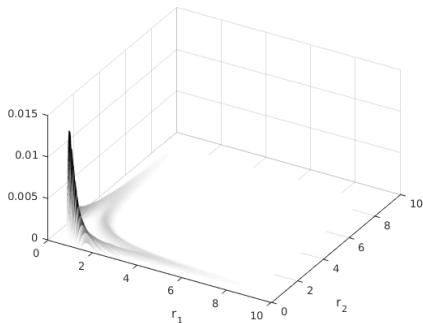
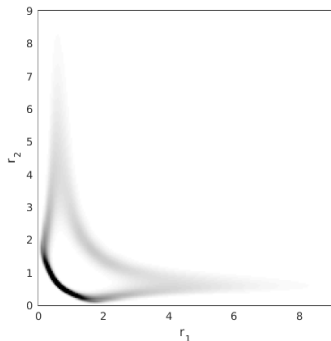


Figure:  $\alpha = 0.7143$

# 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...

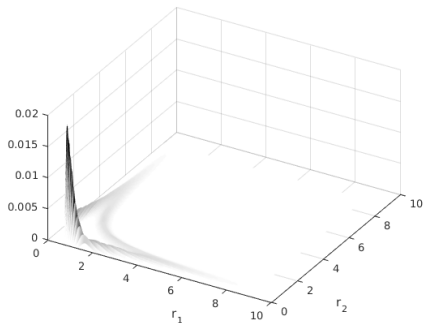
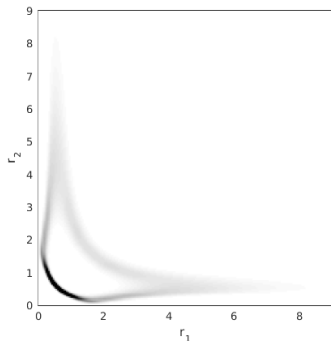


Figure:  $\alpha = 0.8571$

# 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...

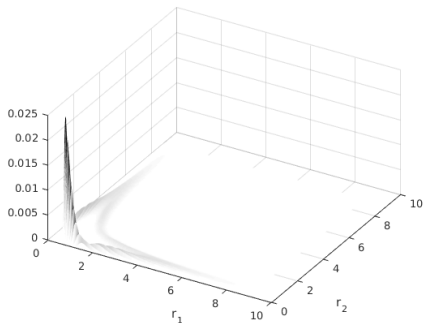
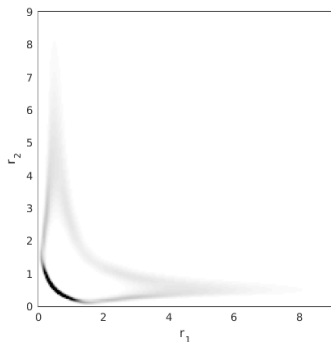


Figure:  $\alpha = 1$

# References

- Benamou, J.-D., G. Carlier, & L. Nenna (2016). "A Numerical Method to solve Multi-Marginal Optimal Transport Problems with Coulomb Cost". In: *Splitting Methods in Communication, Imaging, Science, and Engineering*. Springer International Publishing, pp. 577–601.
- Benamou, Jean-David, Guillaume Carlier, Marco Cuturi, Luca Nenna, & Gabriel Peyré (2015). "Iterative Bregman projections for regularized transportation problems". In: *SIAM J. Sci. Comput.* 37.2, A1111–A1138. ISSN: 1064-8275. DOI: 10.1137/141000439. URL: <http://dx.doi.org/10.1137/141000439>.
- Nenna, Luca (2016). "Numerical methods for multi-marginal optimal transportation". PhD thesis. PSL Research University.
- Peyré, Gabriel & Marco Cuturi (2017). *Computational optimal transport*. Tech. rep.
- Chizat, L., G. Peyré, B. Schmitzer, & F.-X. Vialard (2016). *Scaling Algorithms for Unbalanced Transport Problems*. Tech. rep. <http://arxiv.org/abs/1607.05816>.
- Léonard, C. (2012). "From the Schrödinger problem to the Monge-Kantorovich problem". In: *Journal of Functional Analysis* 262.4, pp. 1879–1920.
- Mérigot, Quentin (2011). "A multiscale approach to optimal transport". In: *Computer Graphics Forum*. Vol. 30. 5. Wiley Online Library, pp. 1583–1592.
- Cuturi, M. (2013). "Sinkhorn Distances: Lightspeed Computation of Optimal Transport.". In: *Advances in Neural Information Processing Systems (NIPS)* 26, pp. 2292–2300.
- Galichon, A. & B. Salanié (2009). *Matching with Trade-offs: Revealed Preferences over Competing Characteristics*. Tech. rep. Preprint SSRN-1487307.
- Buttazzo, Giuseppe, Luigi De Pascale, & Paola Gori-Giorgi (2012). "Optimal-transport formulation of electronic density-functional theory". In: *Physical Review A* 85.6, p. 062502.
- Cotar, C., G. Friesecke, & C. Klüppelberg (2013). "Density Functional Theory and Optimal Transportation with Coulomb Cost". In: *Communications on Pure and Applied Mathematics* 66.4, pp. 548–599. ISSN: 1097-0312. DOI: 10.1002/cpa.21437. URL: <http://dx.doi.org/10.1002/cpa.21437>.
- Di Marino, Simone, Augusto Gerolin, & Luca Nenna (2017). "Optimal transportation theory with repulsive costs". In: *Topological Optimization and Optimal Transport*. Radon Series on Computational and Applied Mathematics. <https://www.degruyter.com/view/books/9783110430417/9783110430417-010/9783110430417-010.xml>: De Gruyter. Chap. 9.