

Multi-Marginal Optimal Transportation: Numerics and Applications

Luca Nenna

I.N.R.I.A. (MoKaPlan)

Junior Seminar, 17 March 2015

- 1 The Dream Team
- 2 Applications
- 3 Optimal Transportation (the standard case)
 - The Godfather(s) of Optimal Transportation
- 4 Numerical Results
 - 1D case
 - 2D case
- 5 The Multi-Marginals OT problem
- 6 Numerical Results
 - 1D case- $N = 3$
 - 2D case- $N = 3$
- 7 The DFT and the Optimal Transportation
- 8 Numerical results for $N = 2$ in 1D
- 9 Numerical results for $N = 3$ in 1D

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Ceremade (Paris-Dauphine):

- **Guillaume Carlier (PR)**
- **Gabriel Peyré (DR CNRS)**
- Francois-Xavier Vialard (MCF)
- Bernhard Schmitzer (Post Doc)
- Jingwei Liang (PhD)
- Lénaïc Chizat (PhD)
- Quentin Denoyelle (PhD)
- Maxime Laborde (PhD)
- Roméo Hatchi (PhD)
- Dario Prandi (Post Doc)

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- Yann Brenier (DR CNRS, CMLS X)
- Quentin Merigot (CR CNRS, Ceremade)
- Jean-Marie Mirebeau (CR CNRS, Ceremade)
- Roman Andreev (Post Doc, U. Paris Diderot)

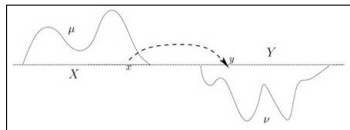
INRIA :

- **Jean-David Benamou (DR INRIA)**
- Vincent Duval (Ingenieur Corps des Mines, Détache)
- Simon Legrand (Research engineer ADT Mokabajour)
- Luca Nenna (PhD)

- Economy
- Finance
- Astrophysics
- Image Processing
- Machine Learning
- Optics (the reflector problem)
- Meteorology and Fluid models (semi-geostrophic equations)
- **Density Functional Theory**
- and so on ...

The Monge Problem

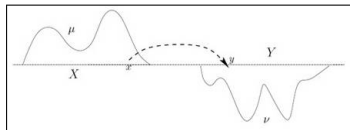
Once upon a time (namely 1781), Gaspard Monge...



- Two distributions μ and ν on \mathbb{R}^d (for simplicity $d = 1$) with **same total mass** ($\int \mu(x)dx = \int \nu(y)dy$)
- Find the transport map $T(x)$ such that:
 - T preserves mass ($\nu(T(x))T'(x)dx = \mu(x)dx$)
 - T minimizes the cost $\int c(x, T(x))\mu(x)dx$
- The standard cost function $c(x, y) = \frac{|x - y|^p}{p}$
 - $p = 1$ $c(x, y) = \frac{|x - y|}{2}$ (the problem introduced by Monge)
 - $p = 2 \Rightarrow$ Brenier's Theorem
- **NO MASS SPLITTING**

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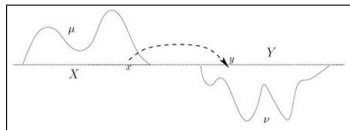
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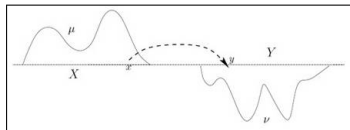


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x



$T(x)$



The Kantorovich (relaxed) problem

In 1942, Kantorovich (Nobel prize in 1975) proposed a relaxed formulation of the Monge problem which allows mass splitting. Find a joint distribution $\gamma(x, y)$ such that

- $\gamma(x, y)$ has marginals equals to μ and ν :
 - $\int \gamma(x, y) dy = \mu(x)$
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The Brenier's theorem

If $T(x)$ is a transport map then it induces a transport plan
 $\gamma_T(x, y) = \mu(x)\delta(y - T(x))$.

Kant pb \Leftrightarrow Monge pb ?

If the optimal plan has the form γ_T^* (which means that no splitting of mass occurs and γ_T^* is **concentrated**) then T is an optimal transport map.

Theorem [Brenier '91] for $p = 2$

There exists a unique map of the form $T = \nabla u$ with u convex that transports μ to ν , this map is also the optimal transport between μ to ν for the quadratic cost ($p = 2$)

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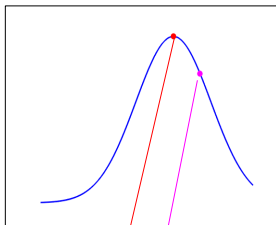
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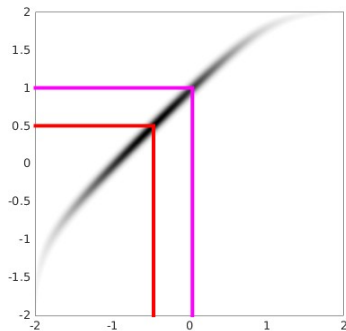
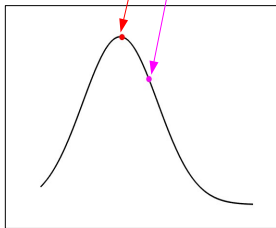
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Source, Target and Transport Plan

Source



Target



Transport Map between ellipses and McCann's Interpolant

The Multi-Marginals (Monge) Problem [Gangbo-Świąch, '98]

- N distribution μ_i ($i = 1, \dots, N$) on \mathbb{R}^d (for simplicity $d = 1$)
- Find the transport maps $T_i(x)$ such that:
 - T_i preserve mass ($\mu_i(T_i(x))T_i(x)' dx = \mu_1(x)dx$ and $T_1(x) = x$)
 - T_i minimize the cost

$$\int c(T_1(x), T_2(x), \dots, T_N(x)) \mu_1(x) dx \quad (1)$$

- The standard cost function

$$c(T_1(x), T_2(x), \dots, T_N(x)) = \int \sum_{i=1}^N \sum_{j=i+1}^N \frac{|T_i(x) - T_j(x)|^2}{2} \mu_1(x) dx. \quad (2)$$

Example, $N = 3$

$$(\text{MP}) \quad c(x, T_2(x), T_3(x)) = \frac{|x - T_2(x)|^2}{2} + \frac{|T_2(x) - T_3(x)|^2}{2} + \frac{|x - T_3(x)|^2}{2}.$$

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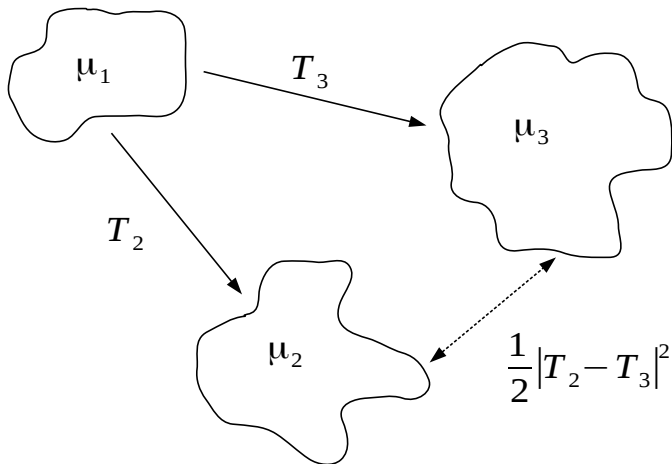
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$$(KP) \quad c(x, y, z) = \frac{|x - y|^2}{2} + \frac{|y - z|^2}{2} + \frac{|x - z|^2}{2}.$$

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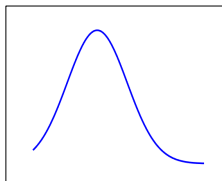
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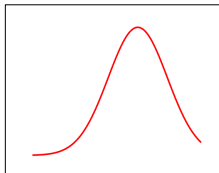
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Numerical Results-1D- $N = 3$

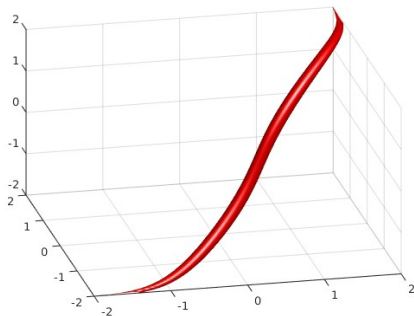
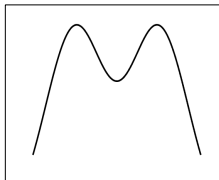
μ_1



μ_2



μ_3



Numerical Results-1D-Projection of γ^* - $N = 3$

$$\gamma_{\mu_i \rightarrow \mu_j} = \int \gamma^*(x_1, \dots, x_N) dx_1 \cdots dx_{i-1} dx_{i+1} \cdots dx_{j-1} dx_{j+1} \cdots dx_N$$



Figure : $\gamma_{\mu_1 \rightarrow \mu_2}$

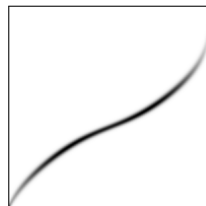


Figure : $\gamma_{\mu_1 \rightarrow \mu_3}$

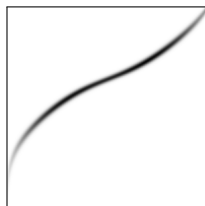


Figure : $\gamma_{\mu_2 \rightarrow \mu_3}$

Transport Maps

Transport Maps

The long (and hard) way from the DFT to Optimal Transportation

The Density Functional Theory describes the behaviour of an atom (or a molecule). After (a lot of) computations [Buttazzo, De Pascale, Gori-Giorgi '12; Cotar, Friesecke, Klüppelberg '13], we obtain the following problem: Find $\gamma(x, y)$ such that

- $\gamma(x, y)$ has marginals equals to ρ and ρ (electrons are indistinguishable so $\mu = \nu = \rho$)
- $\gamma(x, y)$ minimizes the cost $\int c(x, y) \gamma(x, y) dx dy$.

The marginals ρ are the electrons (in this case we have 2 electrons) and the cost function is the electron-electron repulsion (namely the Coulomb cost)

$$c(x, y) = \frac{1}{|x - y|}.$$

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- $T(x)$ is called co-motion function: it gives the position of the second electron when the first one is in x .

The Monge Problem

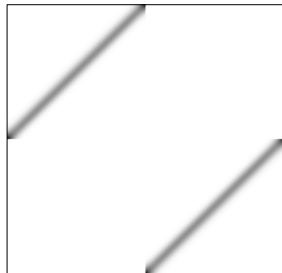
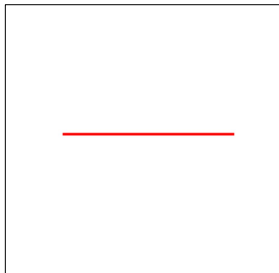
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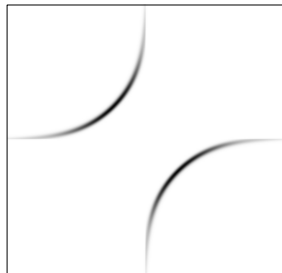
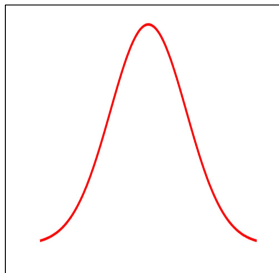
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Numerical results for $N = 2$ in 1D

$\mu=v=\rho$



$\mu=v=\rho$



$$c(x, y, z) = \frac{1}{|x - y|} + \frac{1}{|y - z|} + \frac{1}{|z - x|}$$

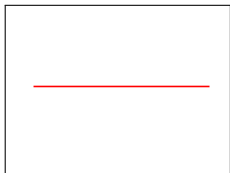


Figure : $\rho = \chi_{[0,1]}(x)$

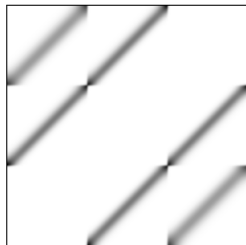








Figure : $\gamma_{\rho_1 \rightarrow \rho_3}$

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