Multi-Marginal Optimal Transportation: Numerics and Applications

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Overview

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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– Roman Andreev (Post Doc, U. Paris Diderot)
Applications

- 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 distribution $\mu$ and $\nu$ 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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NO MASS SPLITTING
$X \rightarrow T(X)$
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 \( \mu \) and \( \nu \):
  - \( \int \gamma(x, y)dy = \mu(x) \)
  - \( \int \gamma(x, y)dx = \nu(y) \)
- \( \gamma(x, y) \) minimizes the cost \( \int c(x, y)\gamma(x, y)dxdy \).
The Kantorovich (relaxed) problem

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  - $\int \gamma(x, y)dy = \mu(x)$
  - $\int \gamma(x, y)dx = \nu(y)$
- $\gamma(x, y)$ minimizes the cost $\int c(x, y)\gamma(x, y)dxdy$. 
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 \iff Monge pb?**

If the optimal plan has the form \( \gamma^*_T \) (which means that no splitting of mass occurs and \( \gamma^*_T \) 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 \( \mu \) to \( \nu \), this map is also the optimal transport between \( \mu \) to \( \nu \) for the quadratic cost (\( p = 2 \))

Thus, for \( p = 2 \) we have \( \gamma^*_T(x, y) = \mu(x)\delta(y - \nabla u(x)) \)
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 $\gamma^*_T$ (which means that no splitting of mass occurs and $\gamma^*_T$ 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 $\mu$ to $\nu$, this map is also the optimal transport between $\mu$ to $\nu$ for the quadratic cost ($p = 2$)

Thus, for $p = 2$ we have $\gamma^*_T(x, y) = \mu(x)\delta(y - \nabla u(x))$
Source, Target and Transport Plan

Source

Target
Transport Map between ellipses and McCann’s Interpolant

- $N$ distribution $\mu_i$ ($i = 1, \cdots, N$) 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

\[
\int c(T_1(x), T_2(x), \cdots, T_N(x)) \mu_1(x) \, dx \tag{1}
\]

- The standard cost function

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

**Example, $N = 3$**

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

- $N$ distribution $\mu_i$ ($i = 1, \cdots, N$) on $\mathbb{R}^d$ (for simplicity $d = 1$)
- Find the transport maps $T_i(x)$ such that:
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  - $T_i$ minimize the cost

$$\int c(T_1(x), T_2(x), \cdots, T_N(x)) \mu_1(x) dx$$  \hspace{1cm} (1)

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**Example, $N = 3$**

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\]
\[ \frac{1}{2} |T_2 - T_3|^2 \]
The Multi-Marginals (Kantorovich) Problem
[Gangbo-Święch,’98]

Find a joint distribution \( \gamma(x_1, \cdots, x_N) \) such that

- \( \gamma(x_1, \cdots, x_N) \) has marginals equals to \( \mu_i \ i = 1, \cdots, N \):

\[
\int \gamma(x_1, \cdots, x_i, \cdots, x_N) dx_1 \cdots dx_{i-1} dx_{i+1} \cdots dx_N = \mu_i(x_i)
\]  

(3)

- \( \gamma(x_1, \cdots, x_N) \) minimizes the cost \( \int c(x_1, \cdots, x_N) \gamma(x_1, \cdots, x_N) dx_1 \cdots dx_N \).

Example, \( N = 3 \)

(KP) \( c(x, y, z) = \frac{|x - y|^2}{2} + \frac{|y - z|^2}{2} + \frac{|x - z|^2}{2} \).
Find a joint distribution $\gamma(x_1, \cdots, x_N)$ such that

- $\gamma(x_1, \cdots, x_N)$ has marginals equals to $\mu_i$ $i = 1, \cdots, N$:
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  \int \gamma(x_1, \cdots, x_i, \cdots, x_N) dx_1 \cdots dx_{i-1} dx_{i+1} \cdots dx_N = \mu_i(x_i) \tag{3}
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- $\gamma(x_1, \cdots, x_N)$ minimizes the cost $\int c(x_1, \cdots, x_N) \gamma(x_1, \cdots, x_N) dx_1 \cdots dx_N$.

**Example, $N = 3$**

(KP) $c(x, y, z) = \frac{|x - y|^2}{2} + \frac{|y - z|^2}{2} + \frac{|x - z|^2}{2}$. 
Numerical Results-1D- \( N = 3 \)

\[ \mu_1 \]

\[ \mu_2 \]

\[ \mu_3 \]
Numerical Results-1D-Projection of $\gamma^*-N = 3$

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

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

The marginals $\rho$ 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 $x$. 
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Numerical results for $N = 2$ in 1D

$\mu = \nu = \rho$

$\mu = \nu = \rho$
\[ c(x, y, z) = \frac{1}{|x - y|} + \frac{1}{|y - z|} + \frac{1}{|z - x|} \]

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

Figure: \( \gamma_{\rho_1 \rightarrow \rho_3} \)
References


μν

μ

ν