A numerical method to solve Generalized Euler Equations

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Overview

1. A brief Introduction to Optimal Transportation
   - Classical Optimal Transportation
   - The Multi-Marginal Optimal Transportation
2. Numerical Method
   - The Regularised OT problem
   - The IPFP procedure (aka Sinkhorn algorithm)
3. The Generalized solutions for Euler Equations
   - Euler equations and the Arnold's principle
   - The Brenier's variational principle
   - From Brenier's problem to Multi-Marginal Optimal Transport
   - Numerical results

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Overview

Classical Optimal Transportation (Monge 1781-Kantorovich 1942-Brenier 1989)

Let us consider two probability measures $\mu, \nu \in \mathcal{P}(\mathbb{R}^d)$ and a continuous function $c : \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{R}$ then the Monge problem $(\mathcal{M})$ is defined as follows

$$\inf\{\int_{\mathbb{R}^d} c(x, T(x))d\mu(x) | \quad T : \mathbb{R}^d \to \mathbb{R}^d \quad T_\sharp \mu = \nu\}$$

Notice that no mass splitting occurs: all the mass on x must be sent onto $T(x)$. The high non-linearity of the constraint makes this problem quite difficult to treat. Thus, in 1942 Kantorovich introduced a relax formulation $(\mathcal{MK})$ which allows mass splitting

$$\inf\{\int_{\mathbb{R}^d \times \mathbb{R}^d} c(x, y)d\gamma(x, y) | \quad \gamma \in \Pi(\mathbb{R}^{2d}, \mu, \nu)\}$$

where $\Pi(\mathbb{R}^{2d}, \mu, \nu) := \{\gamma \in \mathcal{P}(\mathbb{R}^{2d}) | \quad \pi_{1,\sharp}\gamma = \mu \quad \pi_{2,\sharp}\gamma = \nu\}$.

Remark

If the optimal γ has the form $\gamma_T = (Id, T)_\sharp \mu$ (it's a **deterministic** plan) then T is an optimal map for $(\mathcal{M})$.

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The Multi-Marginal Optimal Transportation

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

$$\inf\{\int_{\mathbb{R}^d} c(x, T_2(x), \cdots, T_N(x)) d\mu_1(x) | \quad T_i : \mathbb{R}^d \to \mathbb{R}^d \quad T_{i,\sharp}\mu_1 = \mu_i\}$$

And its relaxed formulation of $(\mathcal{MK}_N)$

$$\inf\{\int_{\mathbb{R}^{dN}} c(x_1, \cdots, x_N) d\gamma(x_1, \cdots, x_N) | \quad \gamma \in \Pi(\mathbb{R}^{dN}, \mu_1, \cdots, \mu_N)\}$$

where $\Pi(\mathbb{R}^{dN}, \mu_1, \cdots, \mu_N)$ denotes the set of couplings $\gamma(x_1, \cdots, x_N)$ having μ_i as marginals. One can also looks at the dual formulation of $(\mathcal{MK}_N)$

$$\sup\{\sum_{i=1}^N \int_{\mathbb{R}^d} \phi_i d\mu_i(x_i) | \quad \boldsymbol{\phi} \in \mathcal{K}_N\}.$$

where $\mathcal{K}_N$ is the set of all $N-$tuples $\boldsymbol{\phi} = (\phi_1, \cdots, \phi_N)$ such that $\phi_i \in L^1(\mathbb{R}^d, \mu_i)$ and $\sum_{i=1}^N \phi_i(x_i) \le c(x_1, \cdots, x_N) \quad \forall \{x\}_{i=1}^N$.

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If the optimal γ has the form $\gamma_T = (Id, T_2, \cdots, T_N)_\sharp \mu_1$ (it's a **deterministic** plan) then T_i are optimal maps for $(\mathcal{M}_N)$.

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The discretized Monge-Kantorovich problem

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

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

and the dual problem

$$\max\{\sum_{i=1}^{N}\sum_{j_i=1}^{M} u^i_{j_i}\mu^i_{j_i} \quad | \quad \sum_{k=1}^{N} u^k_{j_k} \leq c_{j_1,\ldots,j_N} \quad \forall (j_1,\cdots,j_N) \in \{1,\cdots,M\}^N\}. \tag{2}$$

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 Regularised OT problem

Numerics for the multi-marginal problem have not been extensively developed. Here, we present a numerical method to solve the regularised **(Benamou,Carlier, Cuturi, N., Peyré-'15)** optimal transport problem (let us consider, for simplicity, 2 marginals)

$$\min_{\gamma\in\mathcal{C}}\langle C,\gamma\rangle + \begin{cases} \epsilon\sum_{ij}\gamma_{ij}(\log(\gamma_{ij})-1) & \gamma>0 \\ +\infty & otherwise \end{cases} . \quad (3)$$

where C is the matrix associated to the cost, γ is the discrete transport plan and $\mathcal{C}$ is the intersection between $\mathcal{C}_1 = \{\gamma \quad | \quad \sum_j \gamma_{ij} = \mu_i\}$ and $\mathcal{C}_2 = \{\gamma \quad | \quad \sum_i \gamma_{ij} = \nu_j\}$. The problem (3) can be re-written as

$$\min_{\gamma\in\mathcal{C}} KL(\gamma|\bar{\gamma})$$

where $KL(\gamma|\bar{\gamma}) = \sum_{i,j}\gamma_{ij}(\log\frac{\gamma_{ij}}{\bar{\gamma}_{ij}} - 1)$ is the Kullback-Leibler distance and $\bar{\gamma}_{ij} = e^{-\frac{c_{ij}}{\epsilon}}$.

Theorem

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

$$b^\star_j = \frac{\nu_j}{\sum_i a^\star_i \bar{\gamma}_{ij}}, \; a^\star_i = \frac{\mu_i}{\sum_j b^\star_j \bar{\gamma}_{ij}}.$$

The IPFP procedure

$$b^{n+1}_j = \frac{\nu_j}{\sum_i a^n_i \bar{\gamma}_{ij}}, \; a^{n+1}_i = \frac{\mu_i}{\sum_j b^{n+1}_j \bar{\gamma}_{ij}}.$$

Theorem

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

Remark (1)

$u_i = \epsilon log(a_i)$ and $v_j = \epsilon log(b_j)$ are the (regularised) Kantorovich potentials.

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The extension to the Multi-Marginal problem

The problem (3), in the multi-marginal framework, becomes

$$\min_{\gamma \in \mathcal{C}} KL(\gamma|\bar{\gamma}) \tag{4}$$

where $KL(\gamma|\bar{\gamma}) = \sum_{i,j,k} \gamma_{ijk}(\log \frac{\gamma_{ijk}}{\bar{\gamma}_{ijk}} - 1)$ is the Kullback-Leibler distance, $\bar{\gamma}_{ijk} = e^{-\frac{c_{ijk}}{\epsilon}}$ 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. And the IPFP becomes

$$b_j^{n+1} = \frac{\mu_j^2}{\sum_{ik} a_i^n c_k^n \bar{\gamma}_{ijk}}, \quad c_k^{n+1} = \frac{\mu_k^3}{\sum_{ij} a_i^n b_j^{n+1} \bar{\gamma}_{ijk}}, \quad a_i^{n+1} = \frac{\mu_i^1}{\sum_{jk} b_j^{n+1} c_k^{n+1} \bar{\gamma}_{ijk}}.$$

Euler Equations

In 1755 Euler introduced the equations governing the motion of an incompressible fluid flows. Take a domain $D \subseteq \mathbb{R}^d$ and an interval $I = [0, T]$ of time then we have

$$\partial_t \mathbf{u} + (\mathbf{u} \cdot \nabla)\mathbf{u} = -\nabla p, \tag{5}$$

$$div(\mathbf{u}) = 0, \tag{6}$$

$$\mathbf{u} \cdot \mathbf{n} = 0 \qquad on \quad \partial D \tag{7}$$

where $\mathbf{u} : I \times D \to \mathbb{R}^d$ is the velocity field and $p : I \times D \to \mathbb{R}$ is the pressure. Consider now the flow $g : I \times D \to D$ of the velocity field (we want to describe the motion of fluid particles in Lagrangian coordinates), then it is defined $\forall t \geq 0$ by the following ODE:

$$g(0, x) = x, \qquad \partial_t g(t, x) = u(t, g(t, x)). \tag{8}$$

Arnold's principle

Remark

The incompressibility constraint $div\mathbf{u} = 0$ implies

$$det(\nabla g(t,x)) = 1 \quad \forall t \in [0,T],$$

so $g(t) := g(t,\cdot)$ belongs to the space $\mathbb{S}Diff(D)$ of orientation and measure-preserving diffeomorphisms of D.

In 1966 Arnold interpreted the Euler equations in Lagrangian coordinates as the geodesic equation on $\mathbb{S}Diff(D)$ equipped with the L^2 metric. Take an initial $g_\star = Id$ and a final position $g^\star = h(x)$, then the geodesic equation $(\mathcal{A})$ is define as follows:

$$\inf\{\int_0^T \|\dot{g}\|^2 dt \quad | \quad g(t,x) \in H^1([0,T],\mathbb{S}Diff), g(0,x) = Id, g(T,x) = h(x)\}. \tag{9}$$

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Brenier's relaxation

Consider the space of continuous paths $\Omega := \mathcal{C}([0,T],D)$ and $e_t(\omega) := \omega(t)$ the evaluation map at time $t \in [0,T]$, then the geodesic equation admits a convex relaxation $(\mathcal{B})$ posed on probability measures on Ω

$$\inf\{\frac{T}{2}\int_\Omega\int_0^T |\dot\omega|^2 dtd\gamma(\omega) \quad \gamma \in \mathcal{P}(\Omega) \tag{10}$$

$$e_{t,\sharp}\gamma = \mathcal{L}_D, \quad \forall t \in [0,T] \tag{11}$$

$$(e_0,e_T)_\sharp\gamma = (Id,h)_\sharp\mathcal{L}_D\} \tag{12}$$

Let us fix the number of time steps (indeed we are discretizing the time interval $I=[0,T]$) then the time discretization of $(\mathcal{B})$ becomes

$$\inf \frac{T}{N}\int_D \sum_{i=1}^N |x_i - x_{i-1}|^2 d\gamma(x_1,\cdots,x_N) \quad s.t. \tag{13}$$

$$\pi_{i,\sharp}\gamma = \mathcal{L}_D \quad \forall i = 1,\cdots,N \tag{14}$$

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From Brenier's problem to Multi-Marginal Optimal Transport

Moreover the last constraint can be taken into account by defining the following cost function

$$c(x_1, \cdots, x_N) = \sum_{i=1}^{N} |x_i - x_{i-1}|^2 + |x_N - h(x_1)|^2, \tag{16}$$

then the problem can be re-written as a multi-marginal optimal transport problem

$$\inf\{\int_D c(x_1, \cdots, x_N) d\gamma(x_1, \cdots, x_N) | \quad \gamma \in \Pi(\mathbb{R}^{dN}, \mathcal{L}_D)\}, \tag{17}$$

where $\Pi(\mathbb{R}^{dN}, \mathcal{L}_D)$ is the set of all probability measures on $\mathbb{R}^{dN}$ whose N marginals are all equal to $\mathcal{L}_D$. **Remarks**:

- We can solve the multi-marginal problem by using the IPFP.
- If we add an entropy term, we cannot expect deterministic transport plans.
- In Brenier '89- Brenier, Roesch '98- Merigot, Mirebeau '15 the authors developed different numerical methods to solve $(\mathcal{B})$ in $d = 1$ and $d = 2$ based on permutations and semi-discret optimal transport, respectively.

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$1D$ Numerical experiments

We take $D = [0, 1]$ and we plot the coupling $\gamma_{0,t} = (e_0, e_t)_\sharp \gamma$ for $t = \frac{i}{N}$ $i = 1, \cdots, N$ and $N = 32$

Figure: Generalized solution $h = x + \frac{1}{2} mod 1$ and $T = 1$

Figure: Generalized solution $h = 1 - x$ and $T = 1$.

$2D$ Numerical experiments - Unit disk

Take $D = B_1(0) \subset \mathbb{R}^2$, then if $T = \pi$ we find that $h = -Id$. Then, if we consider the coupling $\gamma_{0,t}(x,y)$, we plot $\eta(y) = \gamma_{0,t}(\bar{x},y)$ where $\bar{x}$ is fixed.

$2D$ Numerical experiments - Beltrami Flow

Beltrami flow: $u(x_1, x_2) = (-cos(\pi x_1)sin(\pi x_2), sin(\pi x_1)cos(\pi x_2))$. $g_\star = Id_{[0,1]^2}$ and $g^\star$ is obtained by solving $\dot{g} = u$ in $[0, T]$. Then we consider the coupling $\gamma_{0,t}(x, y)$ and we plot $\eta(y) = \int_{D_k} \gamma_{0,t}(x, y)dx$ where $D_k = [k, \frac{k+1}{3}] \times [0, 1]$ $k = 0, 1, 2$.

Figure: ODE Solution for Beltrami flow $T = 0.9$.

Figure: Generalized solution for Beltrami flow $T = 0.9$.

$2D$ Numerical experiments - Beltrami Flow

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Figure: ODE Solution for Beltrami flow $T = \pi$.

Figure: Generalized solution for Beltrami flow $T = \pi$.

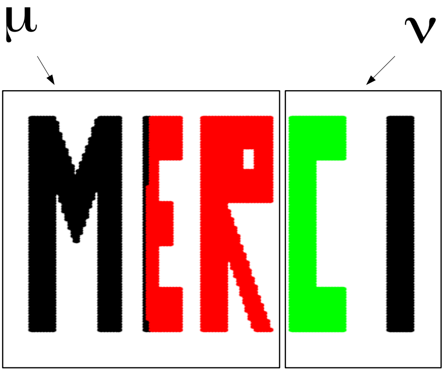
Conclusion

Conclusion:

- A numerical method to solve Multi-Marginal OT problems
- We can visualize the split of mass

On-going work:

- 3D numerical simulation
- Has the entropy a physical meaning? Of course (the next time)


μ
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