An ODE characterisation of entropic (multi-marginal) optimal transport

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joint work with B. Pass

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Overview

1. A crash introduction to (multi-marginal) Optimal Transport

   Classical Optimal transport

   Multi-marginal optimal transport

2. Connecting 2−marginal OT and MOT

   Characterisations of $\mathcal{W}^2_\nu(\mu_0, \mu_1)$

3. Entropic Multi-Marginal Optimal Transport

4. The algorithm and some numerical results

A crash introduction to (multi-marginal) Optimal Transport

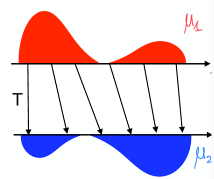
Classical Optimal Transportation Theory

Consider two probability measures μ_i on $X_i \subseteq \mathbb{R}^d$, and c a cost function (e.g. continuous or l.s.c.), the Optimal Transport (OT) problem is defined as follows

$$\mathrm{OT}_0 := \inf \left\{ \int_{\boldsymbol{X}} c(x_1, x_2) \mathrm{d}\gamma(x_1, x_2) \mid \gamma \in \Pi(\mu_1, \mu_2) \right\} \tag{1}$$

where $\Pi(\mu_1, \mu_2)$ denotes the set of couplings $\gamma(x_1, x_2) \in \mathcal{P}(\boldsymbol{X})$ having μ_1 and μ_2 as marginals.

• Solution à la Monge the transport plan γ is deterministic (or à la Monge) if $\gamma = (Id, T)_\sharp \mu$ where $T_\sharp \mu_1 = \mu_2$.



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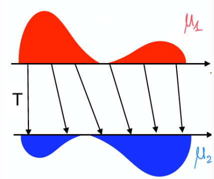

- Duality:

$$\sup\left\{ \mathcal{J}(\phi_1, \phi_2) \mid (\phi_1, \phi_2) \in \mathcal{K} \right\}. \tag{2}$$

where

$$\mathcal{J}(\phi_1, \phi_2) := \int_{X_1} \phi_1 \mathrm{d}\mu_1 + \int_{X_2} \phi_2 \mathrm{d}\mu_2$$

and $\mathcal{K}$ is the set of bounded and continuous functions (ϕ_1, ϕ_2) such that $\phi_1(x_1) + \phi(x_2) \leq c(x_1, x_2)$.

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Why is it a difficult problem to treat? (the discrete case)

Let $c_{j_1, \cdots, j_m} = c(x_{j_1}, \cdots, x_{j_m}) \in \otimes_1^N \mathbb{R}^M$ (M is the number of gridpoints to discretize $\mathbb{R}^{d_i}$)

$$\inf_{\gamma \in \Pi(\mu_1, \dots, \mu_m)} \sum_{(j_1, \cdots, j_m)=1}^{M} c_{j_1, \cdots, j_m} \gamma_{j_1, \cdots, j_m}$$

M^m **unknowns!**

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- Multi-period martingale transport, etc **[Hiew, N., Pass '24]**

Connecting $2-$marginal OT and MOT

The $\nu-$based Wasserstein distance

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$$\mathcal{W}_\nu^2(\mu_1, \mu_2) = \inf \left\{ \int |x_1 - x_2|^2 d\gamma(y, x_1, x_2); \gamma \in \mathcal{P}(X^2 \times Y),\ \gamma_{y,x_i} \in \Pi_O(\mu_i, \nu) \right\},$$

where $\Pi_O(\mu_i, \nu)$ is the set of optimal plans between μ_i and ν.

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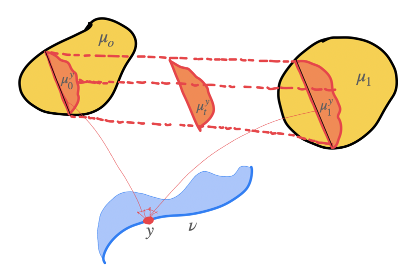

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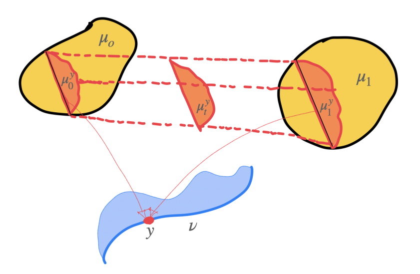

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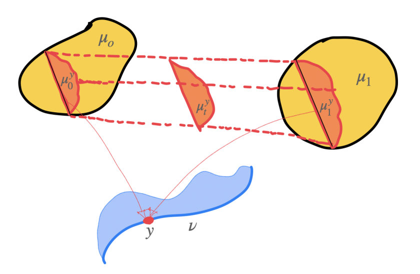

- This is only a **semi-metric** in general, that is the triangle inequality fails.
- If we restrict to the class $\mathcal{P}_\nu^u(X) \subseteq \mathcal{P}(X)$ of probability measures on X for which optimal transport is unique, then it is a metric. If $\boldsymbol{m} = \boldsymbol{n}$ it coincides with the Linear Optimal Transport distance introduced in **[Wang,Slepčev, Basu, Ozolek, and Rohde '13]**.

Characterisations of $\mathcal{W}_\nu^2(\mu_1, \mu_2)$

- Via **conditional probabilities**

$$\mathcal{W}_\nu^2(\mu_1, \mu_2) = \inf \left\{ \int_X \mathcal{W}_2^2(\mu_1^y, \mu_2^y) \mathrm{d}\nu(y) \mid \pi_i \in \Pi_O(\mu_i, \nu),\ i = 1, 2 \right\},$$

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Via Multi-Marginal OT

any weak limit point $\bar{\gamma}$ as $\eta \to 0$ of minimizers γ_η of the multi-marginal problem

$$\inf_{\gamma \in \Pi(\nu, \mu_1, \mu_2)} \int_{X^3} (\eta|x_1 - x_2|^2 + |x_1 - y|^2 + |x_2 - y|^2)\mathrm{d}\gamma(y, x_1, x_2)$$

is an optimal coupling between μ_1 and μ_2 for the problem defining $\mathcal{W}^2_\nu(\mu_1, \mu_2)$.

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Consider

- $m \geq 2$ probability measures μ_i compactly supported on $\mathcal{C}^2$ submanifolds $X_i \subseteq \mathbb{R}^N$ of dim d_i ;
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Entropic Multi-Marginal Optimal Transport problem

It reads as:

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where

- $\Pi(\mu_1, \dots, \mu_m)$ is the set of *couplings* $\gamma \in \mathcal{P}(\mathsf{X})$ having μ_i as marginals
- $\mathrm{Ent}(\gamma \,|\, \pi)$ is the Boltzmann-Shannon entropy, that is

$$\mathrm{Ent}(\gamma \,|\, \pi) = \int \rho \log \rho \mathrm{d}\pi, \text{ if } \gamma = \rho\pi.$$

Some useful remarks

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- It admits a dual problem

$$\mathrm{MOT}_\varepsilon = \sup_{\varphi_i \in \mathcal{C}_b(X_i)} \Psi(\varphi) := \sum_{i=1}^{m} \int_{X_i} \varphi_i(x_i) \mathrm{d}\mu_i - \varepsilon \log \left(\int_{\boldsymbol{X}} e^{\frac{\sum_{i=1}^m \varphi_i(x_i) - c(\boldsymbol{x})}{\varepsilon}} \mathrm{d} \otimes_{i=1}^m \mu_i \right).$$

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$$\varphi_1^{k+1} = -\varepsilon \log \left(\int_{X_2} e^{\frac{\varphi_2^k - c}{\varepsilon}} \mathrm{d}\mu_2 \right), \quad \varphi_2^{k+1} = -\varepsilon \log \left(\int_{X_1} e^{\frac{\varphi_1^{k+1} - c}{\varepsilon}} \mathrm{d}\mu_1 \right).$$

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- **More on entropic transport on Friday!**

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2. Some assumptions to make it simple:
   2.1 **(Equal marginals and discrete set)** All the marginals are equal $\mu_i = \rho = \sum_{x \in X} \rho_x \delta_x$, where X is a finite subset.
   2.2 **(Pair-wise cost)** $c_\eta(x_1, \dots, x_m) := \eta \sum_{i=2}^{m} \sum_{j=i+1}^{m} w(x_i, x_j) + \boldsymbol{\sum_{i=2}^{m} w(x_1, x_i)}$.
   2.3 **(Symmetric cost)** The two body cost w is symmetric $w(x, y) = w(x, y)$.
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Rmk: We can drop hypothesis 2.1→2.3.

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$$\frac{\mathrm{d}\varphi}{\mathrm{d}\eta}(\eta) = -[D^2_{\varphi,\varphi}\Psi(\varphi(\eta), \eta)]^{-1} \frac{\partial}{\partial \eta} \nabla_{\varphi}\Psi(\varphi(\eta), \eta).$$

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Step 3: The following well-posedness theorem then holds.

Theorem

Let $\varphi(\eta)$ be the solution to the dual problem above for all $\eta \in [0, 1]$. Then $\eta \mapsto \varphi(\eta)$ is $\mathcal{C}^1$ and is the unique solution to the Cauchy problem with $\varphi(0) = \varphi_0$.

Idea of the proof: fix the value of the potential in one point and then show that Ψ is strongly convex.

The algorithm and some numerical results

The algorithm to compute the ODE solution

- Algorithm to compute the ϕ via explicit Euler method takes the following form:

Require: $\phi(0) = \phi_w$

while $||\phi^{(k+1)} - \phi^{(k)}|| <$tol **do**

$\quad D^{(k)} := D^2_{\phi,\phi}\tilde{\Phi}(\phi^{(k)}, kh)$

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The algorithm to compute the ODE solution

- Algorithm to compute the ϕ via explicit Euler method takes the following form:

Require: $\phi(0) = \phi_w$

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- The Euler scheme converges linearly and the uniform error between the discretized solution obtained via the scheme and the solution to the ODE is $O(h)$;
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- At each step k we obtaine the solution of the entropic multi-marginal problem with cost c_{kh}!

Comparison with Sinkhorn

Consider $\varepsilon = 0.006$, $m = 3$, the uniform measure on $[0,1]$ uniformily discretized with 400 gridpoints, the pairwise interaction $w(x,y) = -\log(0.1 + |x-y|)$ and a reference solution φ_ε computed via a gradient descent algorithm. Then we have the following comparison between the ODE approach and Sinkhorn in terms of performances

	3rd RK	5th RK	8th RK	Sinkhorn
relative error	1.47×10^{-5}	7.8×10^{-6}	7.62×10^{-6}	5.46×10^{-6}
iterations	87	87	87	820
CPU time (sec)	72.39	158.9	385.1	102.8

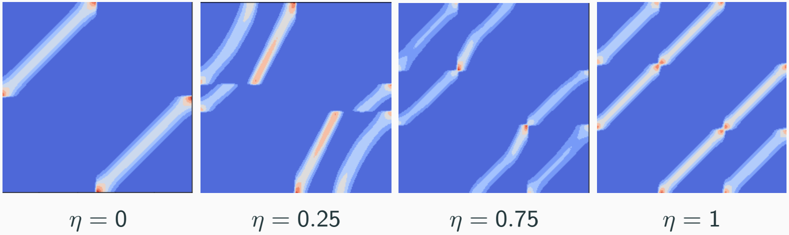

Figure 1: Support of the coupling $\gamma_{1,2}^{\eta}$.

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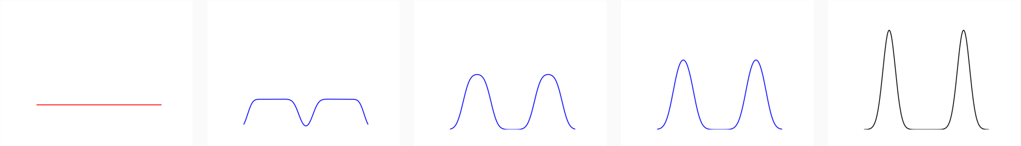

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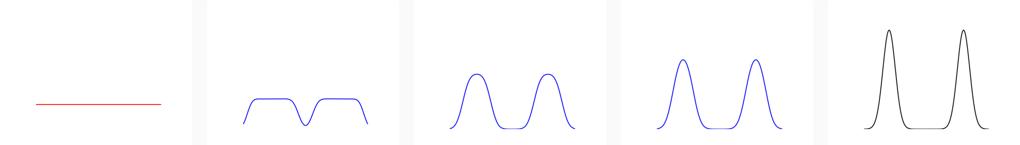

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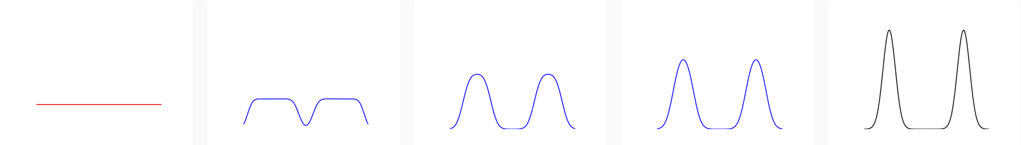

3. One can also compute the **Wasserstein barycenter**.
4. We can add extra linear constraints to treat other generalization of optimal transport: e.g. martingale OT, etc

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Thank You!!