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

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joint work with B. Pass

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    - Classical Optimal transport
    - Multi-marginal optimal transport
2. Entropic Multi-Marginal Optimal Transport
3. The ODE
4. The algorithm and some numerical results
5. An extension to general (entropic) multi-marginal problem

A crash introduction to (multi-marginal) Optimal Transport

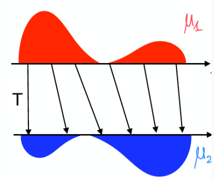
Classical Optimal Transportation Theory

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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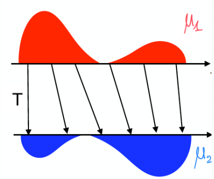

- Duality:

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

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?
Example: $m = 3$, $d = 1$, $\mu_i = \mathcal{L}_{[0,1]}$ $\forall i$ and $c(x_1, x_2, x_3) = |x_1 + x_2 + x_3|^2$.

- Uniqueness fails **(Simone Di Marino, Gerolin, and Luca Nenna 2017)**;
- $\exists$ T_i optimal, are not differentiable at any point and they are fractal maps **ibid., Thm 4.6**

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- Martingale transport (JD's talk), etc

Entropic Multi-Marginal Optimal Transport

Definition of the problem

Consider **(1)** m probability measures μ_i on $X_i \subseteq \mathbb{R}^d$ of dimension d_i; **(2)** a cost function $c : \boldsymbol{X} \to \mathbb{R}_+$ (e.g. continuous or lsc) where $\boldsymbol{X} := \times_i^m X_i$;

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It reads as:

$$\mathrm{MOT}_\varepsilon := \inf_{\gamma \in \Pi(\mu_1,\dots,\mu_m)} \left\{ \int_{\mathsf{X}} c(x_1,\dots,x_m)\,\mathrm{d}\gamma(x_1,\dots,x_m) + \varepsilon \mathrm{Ent}(\gamma \mid \otimes_{i=1}^m \mu_i) \right\},$$

where the infimum is taken among all *couplings* γ having μ_i as marginals ($\gamma \in \Pi(\mu_1,\dots,\mu_m)$), and $\varepsilon > 0$ is a small temperature parameter.

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- Asymptotics as $\varepsilon \to 0$

Theorem ((Luca Nenna and Pegon 2023))

Let μ_i be compactly supported measures over X_i with L^∞ densities. Assume that $c \in \mathcal{C}^2(\mathrm{X})$ and satisfying a signature condition on second mixed derivatives. Then

$$\mathrm{MOT}_\varepsilon = \mathrm{MOT}_0 + \frac{1}{2}\left(\sum_{i=1}^m d_i - \max_i d_i\right)\varepsilon \log(1/\varepsilon) + O(\varepsilon).$$

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$$\begin{cases} \dfrac{\mathrm{d}\phi}{\mathrm{d}\eta}(\eta) = -[D^2_{\phi,\phi}\tilde{\Phi}(\phi(\eta), \eta)]^{-1} \dfrac{\partial}{\partial \eta} \nabla_\phi \tilde{\Phi}(\phi(\eta), \eta), \\ \phi(0) = \phi_w, \end{cases}$$

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Remark: This method is actually inspired by the one introduced in **(G. Carlier, Galichon, and Santambrogio 2009/10)** to compute the Monge solution of the two marginal problem, starting from the Knothe-Rosenblatt rearrangement.

The ODE

How to derive the differential equation

Some assumptions to make it simple:

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. **(Pair-wise cost)** $c_\eta(x_1, \ldots, x_m) := \eta \sum_{i=2}^{m} \sum_{j=i+1}^{m} w(x_i, x_j) + \boldsymbol{\sum_{i=2}^{m} w(x_1, x_i)}$.
3. **(Symmetric cost)** The two body cost w is symmetric $w(x, y) = w(x, y)$.
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Step 1: Consider the dual problem (it is convex!);

$$\inf_{\phi} \left\{ \tilde{\Phi}(\phi, \eta) \right\}, \tag{4}$$

where

$$\tilde{\Phi}(\phi, \eta) := -(m-1) \int_X \phi \mathrm{d}\rho + \varepsilon \int_X \underbrace{\log \left(\int_{X^{m-1}} \exp \left(\frac{\sum_{i=2}^{m} \phi - c_\eta}{\varepsilon} \right) \mathrm{d} \otimes^{m-1} \rho \right)}_{\text{Log-Sum-Exp}} \mathrm{d}\rho.$$

Step 2: Thanks to convexity we have that the minimizers are characterized by $\nabla_\phi \tilde{\Phi}(\phi, \eta) = 0$. Then, by differentiate w.r.t. η we obtain

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

Theorem

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

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Sketch of the proof:

- The pure second derivatives with respect to ϕ as well as the mixed second derivatives with respect to ϕ and η exist and are Lipschitz;
- The Hessian with respect to ϕ is invertible: since the cost is bounded then the potentials are bounded too (**(Guillaume Carlier 2021)**). So one can restrict the study of the well-posedness of the ODE on the set

$$U := \{\phi \mid \phi_{x_0} = 0, \ ||\phi||_\infty \leq C\}.$$

On this set the functional $\tilde{\Phi}$ is now **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 $||\phi^{(k+1)} - \phi^{(k)}|| < \text{tol}$ **do**

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

  $b^{(k)} := -\frac{\partial}{\partial \epsilon}\nabla_{\phi}\tilde{\Phi}(\phi^{(k)}, kh)$

  Solve $D^{(k)}z = b^{(k)}$

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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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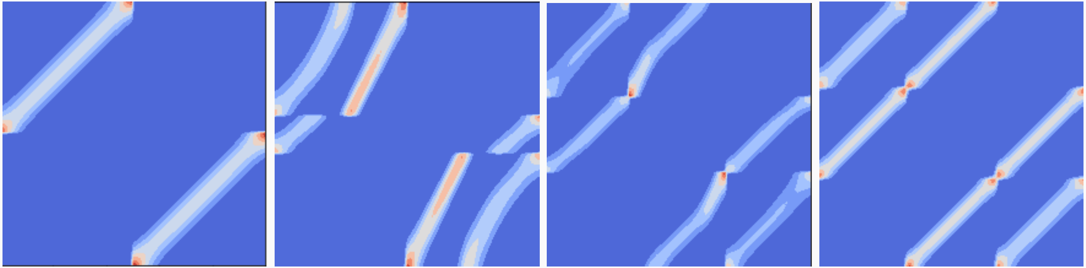
- Thanks to the regularity of the RHS of the ODE one can apply high order methods.
- At each step k we obtaine the solution of the entropic multi-marginal problem with cost c_{kh}!

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

- Log cost and support of the coupling $\gamma^{\eta}_{1,2}$.



$\eta = 0$ $\eta = 0.25$ $\eta = 0.75$ $\eta = 1$

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$$c(x_1, \dots, x_m) = \frac{m^2}{2T^2} \sum_{i=1}^{m-1} |x_{i+1} - x_i|^2 + \beta |F(x_1) - x_m|^2,$$

where $\beta > 0$ is a penalization parameter in order to enforce the initial-final constraint.

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- If we consider a uniform discretization of $[0, T]$ (where T is the final time) with m steps in time, we recover a multi-marginal formulation of the Brenier principle with the specific cost function

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where $\beta > 0$ is a penalization parameter in order to enforce the initial-final constraint.
- If we consider now the ODE setting, we have now to deal with a non symmetric case and so to solve a system, still well posed, of ODEs. In particular we consider the following c_η cost

$$\boxed{c_\eta(x_1, \dots, x_m) = \frac{m^2}{2T^2} |x_2 - x_1|^2 + \eta \left(\frac{m^2}{2T^2} \sum_{i=2}^{m-1} |x_{i+1} - x_i|^2 \right) + \beta |F(x_1) - x_m|^2.}$$

At $\eta = 1$ we plot the coupling $\gamma_{1,i}$ giving the probability of finding a generalized particle initially at x_1 to be at x_i at time i.

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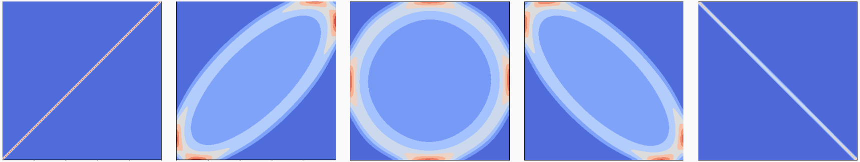

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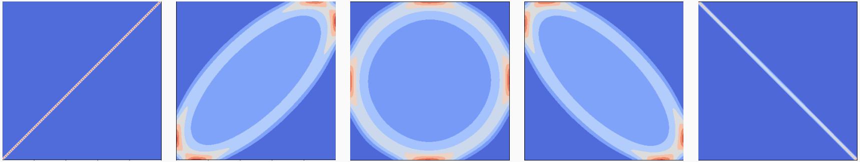

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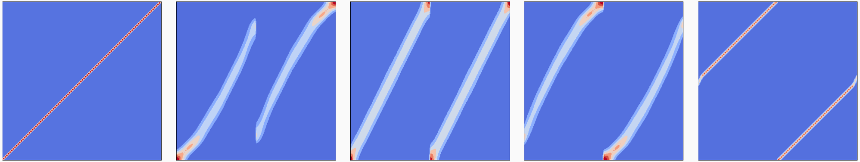
- $F(x) = (x + 1/2) \bmod 1$



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An extension to general (entropic) multi-marginal problem

Extension to general multi-marginal problems (joint work with B. Pass and J. Zoen-Git Hiew)

Consider the following "1st" generalization

$$\boxed{\mathrm{MOT}_\varepsilon := \inf_{\gamma\in\Pi(\mu_1,\ldots,\mu_m)} \left\{ \int_X c(\boldsymbol{\eta}, x_1,\ldots,x_m)\,\mathrm{d}\gamma(x_1,\ldots,x_m) + \varepsilon \mathrm{Ent}(\gamma \mid \otimes_{i=1}^m \mu_i) \right\},}$$

where the cost function is not anymore symmetric but such that $c(0, x_1, \ldots, x_m)$ give a MOT easy to solve:

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4. $c(\eta, x_1, \ldots, x_m, z) = \sum_{i=1}^m \lambda_i(\eta)|x_i - z|^2$ such that $\sum_{i=1}^m \lambda_i(\eta) = 1$ for every η and γ is an $m+1$ coupling with m fixed marginals. Then at for every η the $z-$marginal of γ is the **Wasserstein barycenter** with weights $\lambda_i(\eta)$.

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$$\boxed{\mathrm{MOT}_\varepsilon := \inf_{\gamma \in \boldsymbol{\Pi^Q(\mu_1,\ldots,\mu_m)}} \left\{ \int_X c(\eta, x_1, \ldots, x_m)\, \mathrm{d}\gamma(x_1, \ldots, x_m) + \varepsilon \mathrm{Ent}(\gamma \,|\, \otimes_{i=1}^m \mu_i) \right\},}$$

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$$\int [q(x_1)(x_2 - x_1) + h(x_1, x_2)(x_3 - x_2)]\mathrm{d}\gamma = 0, \quad \forall q \in \mathcal{C}_b(X_1), \forall h \in \mathcal{C}_b(X_1 \times X_2).$$

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Thank You!!