Smoothing operators in multi-marginal Optimal Transport

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Optimal Transport Methods in Density Functional Theory
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Summary

1. Multi-marginal Optimal Transport
2. A smoothing operator
   - Definition
   - Properties
3. Applications to Density Functional Theory
   - The semiclassical limit
   - Lieb's *open map* problem

Multi-marginal Optimal Transport

Given $\rho_1, \dots, \rho_N$ probability measures over $\mathbb{R}^d$, and a cost function $c : (\mathbb{R}^d)^N \to [0, +\infty]$, the Kantorovich formulation for the multi-marginal optimal transport problem is to minimize

$$\int_{(\mathbb{R}^d)^N} c(x_1, \dots, x_N) dP(x_1, \dots, x_N)$$

where $P \in \Pi(\rho_1, \dots, \rho_N) := \left\{ P \in \mathcal{P}\left((\mathbb{R}^d)^N\right) \mid \pi^j_\#(P) = \rho_j \text{ for all } j \right\}$.

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$$\left(\frac{\mathrm{d}\rho}{\mathrm{d}\mathcal{L}^d}\right)^{1/p} \in W^{1,p}(\mathbb{R}^d).$$

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When $p = 2$ we recover the well-known space

$$\mathcal{R} := \left\{\rho \mid \rho \geq 0, \int_{\mathbb{R}^d} \rho = 1, \sqrt{\rho} \in H^1(\mathbb{R}^d)\right\}.$$

H. Lieb, *Density Functionals for Coulomb Systems* (1983)

Multi-marginal Optimal Transport

The space $\mathcal{P}^{1,p}$ is a metric space with distance

$$\delta^{1,p}(\rho_1, \rho_2) = \left\| \left(\frac{\mathrm{d}\rho_1}{\mathrm{d}\mathcal{L}^d} \right)^{1/p} - \left(\frac{\mathrm{d}\rho_2}{\mathrm{d}\mathcal{L}^d} \right)^{1/p} \right\|_{W^{1,p}}.$$

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Theorem

If $P \in \mathcal{P}^{1,p}\left((\mathbb{R}^d)^N\right)$, then its marginals belong to $\mathcal{P}^{1,p}(\mathbb{R}^d)$. Moreover, the map

$$\begin{aligned} \pi \colon \mathcal{P}^{1,p}\left((\mathbb{R}^d)^N\right) &\longrightarrow \mathcal{P}^{1,p}(\mathbb{R}^d)^N \\ P &\longmapsto (\rho_1, \dots, \rho_N) \end{aligned}$$

is continuous w.r.t. the $\delta^{1,p}$ metrics.

Goal

Let $\rho_1, \dots, \rho_N \in \mathcal{P}^{1,p}(\mathbb{R}^d)$ and $P \in \Pi(\rho_1, \dots, \rho_N)$.

If P is not regular, we want to approximate P with $(P_\varepsilon)_{\varepsilon>0}$ such that:

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Since P in general is only a measure, the "suitable sense" is the weak convergence of measures (in duality with C_b).

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For every $\varepsilon > 0$ consider a Gaussian kernel on $\mathbb{R}^d$

$$\eta^\varepsilon(z) = \frac{1}{(2\pi\varepsilon)^{d/2}} \exp\left(-\frac{|z|^2}{2\varepsilon}\right),$$

and define

$$P_\varepsilon(X) := \Theta^\varepsilon[P](X) = \iint \prod_{j=1}^N \frac{\rho_j(x_j)\eta^\varepsilon(y_j - x_j)\eta^\varepsilon(y_j - z_j)}{(\rho_j * \eta^\varepsilon)(y_j)} \mathrm{d}P(Z)\,\mathrm{d}Y.$$

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<u>Remark</u> The marginals are recovered: $\Theta^\varepsilon[P] \in \Pi(\rho_1, \ldots, \rho_N)$.

Properties of Θ^ε: regularity

$\Theta^\varepsilon[P]$ is $W^{1,p}$-regular, with a kinetic energy control:

$$T(\Theta^\varepsilon[P]) \leq \sum_{j=1}^{N} \left(T(\rho_j)^{\frac{1}{p}} + \frac{c(d,p)}{\sqrt{\varepsilon}} \right)^p .$$

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If in addition $P \in \mathcal{P}^{1,p}\left((\mathbb{R}^d)^N\right)$, then

$$T(\Theta^\varepsilon[P]) \leq \sum_{j=1}^N \left(\left\| \nabla_{x_j} (P * \eta^\varepsilon)^{\frac{1}{p}} \right\|_p + c_p \Delta(\varepsilon, p, \rho_j) \right)^p$$

where

$$\Delta(\varepsilon, p, \rho) = \begin{cases} \left[(T(\rho) + T(\rho * \eta^\varepsilon))^{\frac{1}{p-1}} - 2T(\rho * \eta^\varepsilon)^{\frac{1}{p-1}} \right]^{\frac{p-1}{p}} & 1 < p < 2 \\ (T(\rho) - T(\rho * \eta^\varepsilon))^{\frac{1}{p}} & p \geq 2. \end{cases}$$

Properties of Θ^ε: continuity I

Proposition

Let $P \in \mathcal{P}\left((\mathbb{R}^d)^N\right)$*. Then* $\Theta^\varepsilon[P] \rightharpoonup P$*, i.e., for every* $\phi \in C_b\left((\mathbb{R}^d)^N\right)$

$$\lim_{\varepsilon \to 0} \int \phi(X)\Theta^\varepsilon[P](X)dX = \int \phi(X)dP(X).$$

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If P is itself $W^{1,p}$-regular, then we get:

Proposition

Let $P \in \mathcal{P}^{1,p}\left((\mathbb{R}^d)^N\right)$. Then

$$\lim_{\varepsilon \to 0} \delta^{1,p}(\Theta^\varepsilon[P], P) = 0.$$

Properties of Θ^{ε}: continuity II

Consider Θ as an operator

$$\Theta : (0, +\infty) \times \mathcal{P}\left((\mathbb{R}^d)^N \right) \longrightarrow \mathcal{P}^{1,p}\left((\mathbb{R}^d)^N \right).$$

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Theorem

Let $P_n \in \Pi(\rho_1^n, \ldots, \rho_N^n)$ and $P \in \Pi(\rho_1, \ldots, \rho_N)$ such that $P_n \rightharpoonup P$. Suppose moreover that $\rho_j^n, \rho_j \in \mathcal{P}^{1,p}(\mathbb{R}^d)$, and $\delta^{1,p}(\rho_j^n, \rho_j) \to 0$. Then, for every $\varepsilon > 0$,

$$\lim_{n\to\infty} \delta^{1,p}(\Theta^\varepsilon[P_n], \Theta^\varepsilon[P]) = 0.$$

Applications: the semiclassical limit of the HK functional

Consider the Hohenberg-Kohn functional

$$\mathcal{F}_{\hbar}^{HK}(\rho) = \inf_{\psi \mapsto \rho} \langle \psi | \hbar^2 T + V_{ee} | \psi \rangle .$$

Theorem

As $\hbar \to 0$, the functional $\mathcal{F}_{HK}^{\hbar}$ Γ-converges to the Optimal Transport functional

$$\mathcal{C}(\rho) = \inf \left\{ \int \sum_{i<j} \frac{1}{|x_i - x_j|} \mathrm{d}P(X) \,\Big|\, P \in \Pi(\rho, \ldots, \rho) \right\} .$$

Cotar-Friesecke-Klüppelberg (2013), B-De Pascale (2017), Cotar-Friesecke-Klüppelberg (2018), Lewin (2018)

Applications: Lieb's *open map* question

Consider the map from $H^1_{Sym}\left((\mathbb{R}^d)^N\right)$ to $\mathcal{R}$ which sends ψ to its marginal

$$\rho^{\psi}(x) = \int |\psi(x, x_2, \ldots, x_N)|^2 \, dx_2 \cdots dx_N.$$

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Question 2. Although the map is not invertible (since it is not 1 : 1), we can ask the following: Given a sequence $\rho_i^{1/2}$ that converges to $\rho^{1/2}$ in the above $H^1(\mathbb{R}^3)$ since, and given some ψ satisfying (1.6) for ρ, does there exist a sequence ψ_i [related to ρ_i by (1.6)] that converges to ψ in the above $H^1(\mathbb{R}^3)$ sense? [This is equivalent to the statement that the map $\psi \mapsto \rho^{1/2}$ is "open," that is, the map takes open sets in $H^1(\mathbb{R}^{3N})$ into open sets in $H^1(\mathbb{R}^3)$.]

Applications: Lieb's *open map* question

Theorem (B-De Pascale 2019, to appear)

Let $\psi \in H^1_{Sym}\left((\mathbb{R}^d)^N\right)$ *(real-valued), and* $\rho_n \in \mathcal{R}$ *such that* $\rho_n \to \rho^\psi$*.*
Then there exist $(\psi_n)_{n\in\mathbb{N}}$ *such that:*

1. ψ_n *maps to* ρ_n*;*
2. $\psi_n \to \psi$ *in* $H^1_{Sym}\left((\mathbb{R}^d)^N\right)$ *(complex-valued).*

Thanks for your attention!