Moment constrained optimal transport: application to quantum chemistry

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Outline of the talk

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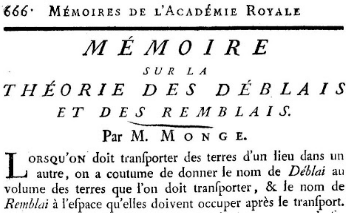
Introduction to optimal transport

Density functional theory and optimal transport

Moment constrained optimal transport problem

Monge's problem

Gaspard Monge (1746-1818)



666· MÉMOIRES DE L'ACADÉMIE ROYALE

MÉMOIRE

SUR LA

THÉORIE DES DÉBLAIS

ET DES REMBLAIS.

Par M. MONGE.

LORSQU'ON doit tranſporter des terres d'un lieu dans un autre, on a coutume de donner le nom de *Déblai* au volume des terres que l'on doit tranſporter, & le nom de *Remblai* à l'eſpace qu'elles doivent occuper après le tranſport.

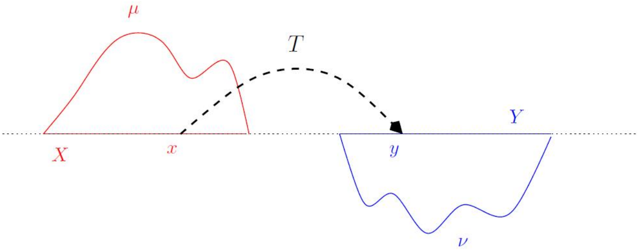
Mémoires sur la théorie des déblais et remblais (1781)

Monge's problem

Question: what is the most economical way to fill a hole with a heap of sand?

$X, Y \subset \mathbb{R}^d$: sand heap is located on the set X, hole located on the set Y

$\mu(x) \geq 0$: represents the height of the heap of sand (source measure)
$\nu(y) \geq 0$: represents the depth of the hole (target measure)



Assumption: the cost of transporting a unit mass of sand from a point $x \in X$ to a point $y \in Y$ is equal to $c(x, y)$ with $c : X \times Y \to \mathbb{R}_+$

Conservation of the total volume/mass of sand:

$$\int_X \mu(x)\, dx = \int_Y \nu(y)\, dy$$

Monge's problem

Monge's optimal transport problem: find a map $T : X \to Y$ which "transports μ onto ν with minimal cost".

What does it mean?

- A map $T : X \to Y$ is said to "transport μ onto ν" if for all bounded functions $f : Y \to \mathbb{R}$, it holds that

$$\int_Y f(y)\nu(y)\,dy = \int_X f(T(x))\mu(x)\,dx$$

$\nu = T\#\mu$ is the pushforward measure of μ by T, i.e.

$$\mu(x) = \nu(T(x))|\det \nabla T(x)|$$

- The cost associated to the map T is defined as

$$\int_X c\,(x, T(x))\,\mu(x)\,dx$$

Monge's problem

More generally, μ and ν can be chosen as probability measures on the sets X and Y respectively.

Let $\mathcal{P}(X)$ and $\mathcal{P}(Y)$ denote the set of probability measures on X and Y respectively.

Monge's optimal transport problem

Given $\mu \in \mathcal{P}(X)$, $\nu \in \mathcal{P}(Y)$ and $c : X \times Y \to \mathbb{R}_+ \cup \{+\infty\}$,

find a map $T : X \to Y$ which minimizes the cost

$$\int_X c\,(x, T(x))\, \mu(x)\, dx$$

under the constraint that T transports μ onto ν.

Monge's optimal transport problem

Monge's optimal transport problem

Given $\mu \in \mathcal{P}(X)$, $\nu \in \mathcal{P}(Y)$ and $c : X \times Y \to \mathbb{R}_+ \cup \{+\infty\}$,

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under the constraint that T transports μ onto ν.

This is an ill-posed problem in general.

Kantorovich problem

Leonid Kantorovich (1912-1986),
Economy Nobel prize in 1975

introduced a generalization of the Monge's problem with much better mathematical properties!

Coupling

An important aspect of this generalisation is that it is symmetric with respect to μ and ν, and is based on the notion of coupling between μ and ν.

A probability measure $\gamma \in \mathcal{P}(X \times Y)$ is said to be a coupling between μ and ν if it satisfies

$$\int_Y \gamma(x, y)\, dy = \mu(x), \quad \int_X \gamma(x, y)\, dx = \nu(y)$$

γ is said to be the x-marginal of γ and ν is said to be the y-marginal of γ.

Couplings with transport maps

Example: Let $T : X \to Y$ and assume that μ is very regular.
Define $\gamma^T(x,y) \in \mathcal{P}(X \times Y)$ a probability measure on $X \times Y$ such that

$$\gamma^T(x,y) = \mu(x)\delta_{(x,T(x))}(x,y)$$

Then, γ^T is a coupling between μ and ν if and only if T transports μ onto ν.

Besides, in this case, it holds that

$$\int_X c(x,T(x))\mu(x)\,dx = \int_{X\times Y} c(x,y)\gamma^T(x,y)\,dx\,dy$$

Kantorovich problem

Monge's optimal transport problem using couplings

Given $\mu \in \mathcal{P}(X)$, $\nu \in \mathcal{P}(Y)$ and $c : X \times Y \to \mathbb{R}_+ \cup \{+\infty\}$,

find a map $T : X \to Y$ which minimizes the cost

$$\int_{X \times Y} c(x, y)\gamma^T(x, y)\, dx\, dy$$

under the constraint that γ^T is a coupling between μ and ν .

Kantorovich optimal transport problem

Given $\mu \in \mathcal{P}(X)$, $\nu \in \mathcal{P}(Y)$ and $c : X \times Y \to \mathbb{R}_+ \cup \{+\infty\}$,

find a probability measure $\gamma \in \mathcal{P}(X \times Y)$ which minimizes the cost

$$\int_{X \times Y} c(x, y)\gamma(x, y)\, dx\, dy = \int_{X \times Y} c\gamma$$

under the constraint that γ is a coupling between μ and ν.

Kantorovich optimal transport problem with two marginals

Given $\mu \in \mathcal{P}(X)$, $\nu \in \mathcal{P}(Y)$ and $c : X \times Y \to \mathbb{R}_+ \cup \{+\infty\}$,

find a probability measure $\gamma \in \mathcal{P}(X \times Y)$ which minimizes the cost

$$\int_{X \times Y} c\gamma$$

under the constraint that the x-marginal of γ is μ and the y-marginal of γ is ν.

$$\int_Y \gamma(x,y)\,dy = \mu(x), \quad \int_X \gamma(x,y)\,dx = \nu(y)$$

Example: $X = Y \subset \mathbb{R}^d$ and $c(x,y) = |x-y|^2$

Wasserstein distance between μ and ν:

$$W_2^2(\mu,\nu) := \inf_{\gamma \in \Pi(\mu,\nu)} \int_{X \times Y} c\gamma$$

Multi-marginal optimal transport Kantorovich problem

Let $N \in \mathbb{N}^*$, $X_1, \cdots, X_N \subset \mathbb{R}^d$.

Given $\mu_1 \in \mathcal{P}(X_1), \cdots, \mu_N \in \mathcal{P}(X_N)$, and $C : X_1 \times \cdots \times X_N \to \mathbb{R}_+ \cup \{+\infty\}$,

find a probability measure $\gamma \in \mathcal{P}(X_1 \times \cdots \times X_N)$ which minimizes the cost

$$\int_{X_1 \times \cdots \times X_N} C\gamma$$

under the constraint that, for all $1 \leq i \leq N$, the i^{th} marginal of γ is μ_i.

$$\int_{X_1 \times \cdots \times X_{i-1} \times X_{i+1} \times \cdots \times X_N} \gamma = \mu_i$$

Symmetric multi-marginal (classical) optimal transport problem

- $X_1 = \cdots = X_N = X \subset \mathbb{R}^d$.
- $\mu_1 = \cdots = \mu_N = \rho$
- $C : X^N \to \mathbb{R}_+$ symmetric function

Given $\rho \in \mathcal{P}(X)$, and $C : X^N \to \mathbb{R}_+ \cup \{+\infty\}$ symmetric,

find a symmetric probability measure $\gamma \in \mathcal{P}_{\mathrm{sym}}(X^N)$ which minimizes the cost

$$\int_{X^N} C\gamma$$

under the constraint that the marginal of γ is ρ.

$$\int_{X_2 \times \cdots \times X_N} \gamma = \rho$$

And DFT?

Link between **Density Functional Theory** and **(classical and quantum) symmetric optimal transport** problems

Outline of the talk

Admissible electronic wavefunctions

For the sake of simplicity, atomic units are used and the influence of spin is neglected.

Consider a set of N electrons.

The set of admissible wavefunctions $\psi(x_1, \dots, x_N)$ (for all $1 \leq i \leq N$, $x_i \in \mathbb{R}^3$) for a system of electrons with **finite kinetic energy** is the set

$$\mathcal{A}_N := \left\{ \psi \in L^2(\mathbb{R}^{3N}; \mathbb{C}),\ \nabla_x \psi \in L^2(\mathbb{R}^{3N}; \mathbb{C}),\ \psi \text{ antisymmetric},\ \|\psi\|_{L^2} = 1 \right\}.$$

Antisymmetry: For all $\sigma \in \mathcal{S}_N$, the set of permutations of $\{1, \cdots, N\}$,

$$\psi(x_{\sigma(1)}, \cdots, x_{\sigma(N)}) = \epsilon(\sigma)\psi(x_1, \cdots, x_N), \quad \forall (x_1, \cdots, x_N) \in \mathbb{R}^{3N},$$

where $\epsilon(\sigma)$ is the signature of σ.

Many-body Schrödinger electronic problem

The ground state energy $E_g[v]$ is of a system of N electrons in the presence of an external potential v given by the many-body Schrödinger electronic problem:

$$E_g[v] = \inf_{\psi \in \mathcal{A}_N} \langle \psi | H_N^v | \psi \rangle$$

where

$$H_N^v = H_N^0 + \sum_{i=1}^N v(x_i)$$

with

$$H_N^0 = -\frac{1}{2} \sum_{i=1}^N \Delta_{x_i} + \sum_{1 \leq i < j \leq N} \frac{1}{|x_i - x_j|}$$

Example: External potential v generated by M nuclei at positions $R_1, \ldots, R_M \in \mathbb{R}^3$ and charges $Z_1, \ldots, Z_M > 0$ in the Born-Oppenheimer approximation:

$$v(x) := -\sum_{k=1}^M \frac{Z_k}{|R_k - x|}$$

Hohenberg-Kohn theorem and Density Functional Theory

For all $\psi \in \mathcal{A}_N$, the electronic density associated to ψ is defined by

$$\rho_\psi(x) := N \int_{\mathbb{R}^{3(N-1)}} |\psi(x, x_2, \cdots, x_N)|^2 \, dx_2 \cdots dx_N.$$

[Hohenberg,Kohn,1964], [Lévy,1979], [Lieb,1983]
It holds that

$$\mathcal{I}_N := \{\rho_\psi, \ \psi \in \mathcal{A}_N\} = \left\{ \rho \geq 0, \ \int_{\mathbb{R}^3} \rho = N, \ \int_{\mathbb{R}^3} |\nabla \sqrt{\rho}|^2 < +\infty \right\}$$

The Hohenberg-Kohn theorem states that

$$E_g[v] = \inf \left\{ F_{HK}[\rho] + \int_{\mathbb{R}^3} v\rho, \quad \rho \in \mathcal{I}_N \right\} \tag{1}$$

where the Hohenberg-Kohn functional $F_{HK}(\rho)$ is defined by

$$F_{HK}[\rho] := \inf \left\{ \langle \psi | H_N^0 | \psi \rangle, \quad \psi \in \mathcal{A}_N, \ \rho_\psi = \rho \right\}.$$

Density Functional Theory: approximations of $F_{HK}(\rho)$

Unfortunately, the functional $F_{HK}(\rho)$ is not known explicitly.

All DFT models rely on approximations of this functional in order to obtain computable models (Kohn-Sham LDA, GGA, hybrid functionals, machine-learnt exchange-correlation ...)

Besides, the functional $F_{HK}(\rho)$ is not convex! As a consequence, even if F_{HK} was known, the computation of $E_g(v)$ out of (1) might be a complicated task.

Lieb functional

To alleviate the second point, Lieb [Lieb, 1983] introduced the so-called Lieb functional $F_L[\rho]$, which is actually a **convexification** of the Hohenberg-Kohn functional $F_{HK}[\rho]$.

$$F_L[\rho] = \inf_{\substack{\alpha_i \geq 0,\ \rho_i \in \mathcal{I}_N,\ i \in \mathbb{N}^* \\ \sum_{i\in\mathbb{N}^*} \alpha_i \rho_i = \rho}} \sum_{i\in\mathbb{N}^*} \alpha_i F_{HK}[\rho_i]$$

In particular, it still holds that

$$E_g[v] = \inf \left\{ F_L[\rho] + \int_{\mathbb{R}^3} v\rho, \quad \rho \in \mathcal{I}_N \right\} \tag{2}$$

Mixed states

The Lieb functional can also be seen as a minimization problem defined over the set of mixed states (instead of pure states like in the Hohenberg-Kohn functional).

- $\mathcal{H}_0^N := \{\psi \in L^2(\mathbb{R}^{3N};\mathbb{C}),\ \psi$ antisymmetric $\}$
- $\mathfrak{S}_1^+(\mathcal{H}_0^N)$: Set of non-negative trace-class operators on $\mathcal{H}_0^N$, that is the set of operators Γ of the form:

$$\Gamma = \sum_{i=1}^{+\infty} \alpha_i |\psi_i\rangle\langle\psi_i|$$

for some

- $\alpha_i \geq 0$ s.t. $\sum_{i=1}^{+\infty} \alpha_i < +\infty$,
- $(\psi_i)_i$ orthonormal basis of $\mathcal{H}_0^N$

Associated electronic density:

$$\rho_\Gamma(x) = \sum_{i=1}^{+\infty} \alpha_i \rho_{\psi_i}(x)$$

Lieb functional: a quantum optimal transport problem

$$F_L[\rho] = \inf_{\substack{\Gamma \in \mathfrak{S}_1^+(\mathcal{H}_0^N) \\ \rho_\Gamma = \rho}} \mathrm{Tr}\left(H_N^0 \Gamma\right)$$

$$\mathrm{Tr}\left(H_N^0 \Gamma\right) = \sum_{i=1}^{+\infty} \alpha_i \langle \psi_i | H_N^0 | \psi_i \rangle$$

Strictly Correlated Electrons (SCE) limit of the Hohenberg-Kohn functional

The SCE limit of the HK functional was first considered in the series of work:
[Seidl,1999], [Seidl,Gori-Giorgi,Savin,2007]

$$H_N^0 = T + C$$

where

$$T = -\frac{1}{2}\sum_{i=1}^{N}\Delta_{x_i} \quad \text{and} \quad C(x_1,\ldots,x_N) = \sum_{1\leq i<j\leq N}\frac{1}{|x_i - x_j|}$$

Let $h > 0$ and consider

$$F^h{}_{HK}[\rho] := \inf\left\{h\langle\psi|T|\psi\rangle + \langle\psi|C|\psi\rangle, \quad \psi \in \mathcal{A}_N,\ \rho_\psi = \rho\right\}.$$

SCE limit of the Hohenberg-Kohn functional:

$$\boxed{F_{SCE}[\rho] = \lim_{h\to 0} F^h{}_{HK}(\rho)}$$

SCE functional: a classical optimal transport problem

If $\psi \in \mathcal{A}_N$, $\gamma_\psi := |\psi|^2$ is a symmetric probability measure on $\mathbb{R}^{3N}$, and

$$\langle \psi | C | \psi \rangle = \int_{\mathbb{R}^{3N}} C \gamma_\psi$$

For all $\gamma \in \mathcal{P}_{\rm sym}(\mathbb{R}^{3N})$ symmetric probability measure on $\mathbb{R}^{3N}$, let ρ_γ be its marginal

$$\rho_\gamma(x) = N \int_{(\mathbb{R}^3)^{N-1}} \gamma(x, x_2, \ldots, x_N)\, dx_2 \ldots dx_N \qquad (\rho_{\gamma_\psi} = \rho_\psi)$$

[Cotar,Friesecke, Klüppelberg, 2011], [Lewin, 2017], [Cotar,Friesecke, Klüppelberg, 2018]

$$F_{SCE}[\rho] = \inf_{\substack{\gamma \in \mathcal{P}_{\rm sym}(\mathbb{R}^{3N}) \\ \rho_\gamma = \rho}} \int_{\mathbb{R}^{3N}} C \gamma$$

Recap'

Lieb functional

$$F_L[\rho] = \inf_{\substack{\Gamma \in \mathfrak{S}_1^+(\mathcal{H}_0^N) \\ \rho_\Gamma = \rho}} \mathrm{Tr}\left(H_N^0 \Gamma\right)$$

- Γ mixed state (trace-class non-negative s.a. operator)
- $\rho_\Gamma = \rho$: partial trace constraint
- Cost functional: $\mathrm{Tr}\left(H_N^0 \Gamma\right)$

Quantum optimal transport

SCE functional

$$F_{SCE}[\rho] = \inf_{\substack{\gamma \in \mathcal{P}_{\mathrm{sym}}(\mathbb{R}^{3N}) \\ \rho_\gamma = \rho}} \int_{\mathbb{R}^{3N}} C\gamma$$

- γ symmetric probability measure on $\mathbb{R}^{3N}$
- $\rho_\gamma = \rho$: marginal constraint
- Cost functional: $\int_{\mathbb{R}^{3N}} C\gamma$

Classical optimal transport

Several recent efforts on the design of numerical schemes for the computation of the SCE functional.
Much less (at least up to my knowledge) for the computation of the Lieb functional.

Classical discretization: discrete state space

Let $y^1, \cdots, y^M \in \mathbb{R}^3$ and $Y = \{y^1, \cdots, y^M\}$ be a discretization grid of $\mathbb{R}^3$.

Classical discretization (for the SCE problem) approaches consist in approximating the solution γ as a discrete measure defined on Y^N:

$$\gamma \approx \sum_{1 \leq i_1, \ldots, i_N \leq M} \gamma_{i_1, \ldots, i_N} \delta_{(y^{i_1}, \ldots, y^{i_N})}$$

Linear problem of size M^N! Curse of dimensionality

Complexity is even worse for classical discretizations of the Lieb problem

Numerical methods for the SCE problem

- [Benamou,Carlier,Cuturi,Nenna,Peyré,2015], [Nenna,2016] : use of an entropic regularization (using the Kullback-Leibler entropy), together with an iterative algorithm called Sinkhorn algorithm.
- [Mendl,Lin,2013] : dual formulation of the Kantorovich problem: needs appropriate treatment of the (infinite-dimensional) inequality constraint.
- [Vögler,2019],[Friesecke, Schulz, Vögler,2021] : The Genetic column generation algorithm builds on the sparsity structure of minimizers of classical discretizations of the SCE problem
- [Alfonsi, Coyaud, VE, Lombardi,2021], [Alfonsi, Coyaud, VE,2022]: Moment constraints discretization also leads to sparse minimizers

[VE, Nenna,2023] Moment constraints discretization also leads to sparse minimizers for the **Lieb functional**

Outline of the talk

Assumptions

- **Assumption on ρ:** there exists $\theta : \mathbb{R}_+ \to \mathbb{R}_+$ continuous non-decreasing function such that $\theta(r) \underset{r\to+\infty}{\longrightarrow} +\infty$ and such that

$$C_0 := \int_{\mathbb{R}^3} \theta(|x|)\rho(x)\,dx < +\infty.$$

- **Assumption on moment functions:**
$(\varphi_m)_{m\in\mathbb{N}^*} \subset \mathcal{C}(\mathbb{R}^3) \cap \left(L^\infty(\mathbb{R}^3) + L^{3/2}(\mathbb{R}^3)\right)$ s.t.
  - $\varphi_1(x) = 1$;
  - for all $\widetilde{\rho} \in \mathcal{I}_N$ with $\int_{\mathbb{R}^3} \theta(|x|)\widetilde{\rho}(x)\,dx \leq C_0$,

$$\left(\forall m \in \mathbb{N}^*, \quad \int_{\mathbb{R}^3} \varphi_m \widetilde{\rho} = \int_{\mathbb{R}^3} \varphi_m \rho\right) \quad \Rightarrow \quad \widetilde{\rho} = \rho.$$

$$\forall m \in \mathbb{N}^*, \quad \rho^m := \int_{\mathbb{R}^3} \varphi_m \rho$$

the moment of ρ associated with the moment function φ_m

Alternative discretization: moment constraints

Let $M \in \mathbb{N}^*$ be a discretization parameter.

The marginal/partial trace constraint

$$\rho_\gamma = \rho \text{ (SCE case)} \qquad \rho_\Gamma = \rho \text{ (Lieb case)} \tag{3}$$

is replaced by the M moment constraints: for all $1 \leq m \leq M$,

$$\int_{\mathbb{R}^3} \varphi_m \rho_\gamma = \rho^m \text{ (SCE case)} \qquad \int_{\mathbb{R}^3} \varphi_m \rho_\Gamma = \rho^m \text{ (Lieb case)} \tag{4}$$

and the additional technical condition:

$$\int_{\mathbb{R}^3} \theta(|x|)\rho_\gamma \leq C_0 \text{ (SCE case)} \qquad \int_{\mathbb{R}^3} \theta(|x|)\rho_\Gamma \leq C_0 \text{ (Lieb case)} \tag{5}$$

$$F_{SCE}^M[\rho] = \inf_{\substack{\gamma \in \mathcal{P}_{\rm sym}(\mathbb{R}^{3N}) \\ \rho_\gamma \text{ satisfies} \\ (4) \text{ and } (5)}} \int_{\mathbb{R}^{3N}} C\gamma$$

$$F_L^M[\rho] = \inf_{\substack{\Gamma \in \mathfrak{S}_1^+(\mathcal{H}_0^N) \\ \rho_\Gamma \text{ satisfies} \\ (4) \text{ and } (5)}} \mathrm{Tr}\left(H_N^0 \Gamma\right)$$

Convergence and existence of minimizers

[Alfonsi, Coyaud, VE, Lombardi, 2021], [VE, Nenna, 2023]

Theorem

For all $M \in \mathbb{N}^*$, there exists at least one minimizer to both moment constraint optimal transport problems (SCE and Lieb case). In addition, it holds that

$$F_{SCE}^M[\rho] \underset{M\to+\infty}{\longrightarrow} F_{SCE}[\rho] \quad \text{and} \quad F_L^M[\rho] \underset{M\to+\infty}{\longrightarrow} F_L[\rho]$$

Tchakaloff's theorem

The following theorem is the backbone of our analysis to prove the existence of **sparse** minimizers.

[Bayer,Teichmann,2006]

Theorem

Let μ be a non-negative Borel measure on a Hilbert space $\mathcal{H}$ concentrated on a Borel set B, i.e. $\mu(\mathcal{H} \setminus B) = 0$. Let $M_0 \in \mathbb{N}^*$ and $\Lambda : \mathcal{H} \to \mathbb{R}^{M_0}$ be a continuous map. Assume that the first moments of $\Lambda\#\mu$ exist i.e.

$$\int_{\mathcal{H}} \|\Lambda(z)\| \, d\mu(z) < +\infty.$$

Then, there exists an integer $1 \leq K \leq M_0$, points $z^1, \cdots, z^K \in B$ and weights $w_1, \cdots, w_K > 0$ such that

$$\forall 1 \leq m \leq M_0, \quad \int_{\mathcal{H}} \Lambda_m(z) \, d\mu(z) = \sum_{k=1}^{K} w_k \Lambda_m(z^k),$$

where Λ_m denotes the m^{th} component of Λ.

Sparse structure of minimizers: SCE case

Using the Tchakaloff's theorem, [Bayer,Teichmann,2006]

Theorem ([Alfonsi, Coyaud, VE, Lombardi, 2021])

There exists an integer $1 \leq K \leq M+1$, and for all $1 \leq k \leq K$, points $X^k \in (\mathbb{R}^3)^N$ and weights $w_k > 0$ such that the symmetrized measure associated to

$$\gamma = \sum_{k=1}^{K} w_k \delta_{X^k} \tag{6}$$

is a minimizer to $F^M_{SCE}[\rho]$.

Complexity of this sparse representation: $\mathcal{O}(MN)$

Sparse structure of minimizers: Lieb case

Using the Tchakaloff's theorem, [Bayer,Teichmann,2006]

Theorem ([VE, Nenna, 2023])

There exists an integer $1 \leq K \leq M+1$*, and for all* $1 \leq k \leq K$*, functions* $\psi_k \in \mathcal{A}_N$ *and weights* $\omega_k > 0$ *such that*

$$\Gamma = \sum_{k=1}^{K} \omega_k |\psi_k\rangle\langle\psi_k| \tag{7}$$

is a minimizer to $F_L^M[\rho]$*.*

There exists at least a minimizer to $F_L^M[\rho]$ which has rank at most $M+1$.

Back to the SCE case: particle and weight optimization problem

Natural idea for a numerical method: Restrict the minimization set of problem $F^M_{SCE}[\rho]$ to measures γ that can be written under the form (7) for some weights w_k and points X^k.

$$F^{M,K}_{SCE}[\rho] = \inf_{\substack{Y := (X^k)_{1\leq k\leq K} \subset (\mathbb{R}^3)^N, \\ W := (w^k)_{1\leq k\leq K} \subset \mathbb{R}_+, \\ \sum_{k=1}^K w^k = 1, \\ \forall 1 \leq m \leq M, \\ \sum_{k=1}^K w^k \Phi_m(X^k) = \rho^m}} \sum_{k=1}^K w^k c(X^k). \tag{8}$$

where

$$\forall X = (x_1, \cdots, x_N) \in (\mathbb{R}^3)^N, \quad \Phi_m(X) := \frac{1}{N}\sum_{i=1}^N \varphi_m(x_i).$$

Non convex optimization problem under non convex constraints!
⇒ Stochastic gradient algorithm with constrained overdamped Langevin dynamics

SCE case: particle and weight optimization problem

Minimization set:

$$\mathcal{P}^K := \left\{ \begin{array}{c} (W,Y) \in \mathbb{R}_+^K \times ((\mathbb{R}^3)^N)^K, \quad W := (w^k)_{1\leq k\leq K},\ Y := (X^k)_{1\leq k\leq K}, \\ \sum_{k=1}^K w^k = 1, \\ \forall 1 \leq m \leq M,\ \sum_{k=1}^K w^k \Phi_m(X^k) = \rho^m \end{array} \right\}$$

$$F_{SCE}^{M,K}[\rho] = \inf_{(W,Y)\in\mathcal{P}^K} \mathcal{J}(W,Y), \tag{9}$$

with

$$\mathcal{J}(W,Y) := \sum_{k=1}^K w^k c(X^k).$$

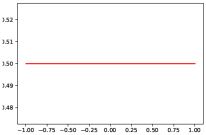
Theorem ([Alfonsi, Coyaud, VE, 2022])

If $K \geq 2M+6$, for any $(W_0,Y_0),(W_1,Y_1) \in \mathcal{P}^K$, there exists a continuous path $\zeta : [0,1] \to \mathcal{P}^K$ such that

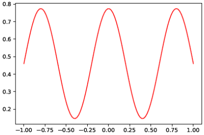
- $\zeta(0) = (W_0, Y_0)$;
- $\zeta(1) = (W_1, Y_1)$;
- $[0,1] \ni t \mapsto \mathcal{J}(\zeta(t))$ *is monotonous.*

1D Numerical results

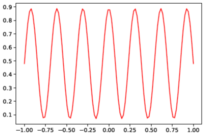
ρ_1



ρ_2



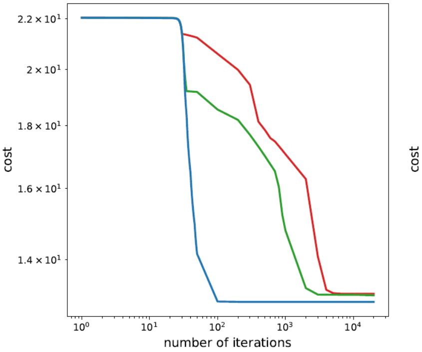
ρ_3



1D numerical tests presented with $N = 5$.

$X = [-1, 1]$ and Legendre polynomial test functions.

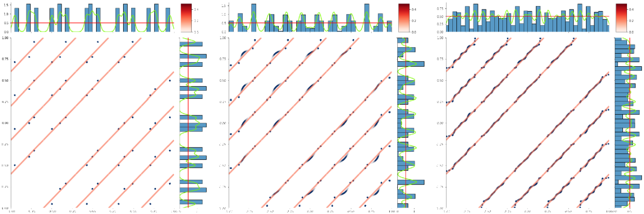
1D Numerical results



- blue curve: $M = 10$
- green curve: $M = 20$
- red curve: $M = 40$

1D Numerical results

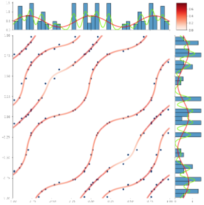
ρ_1

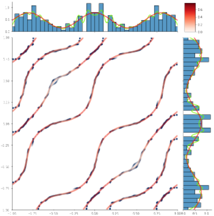


$M = 10$ $M = 20$ $M = 40$

1D Numerical results

ρ_2

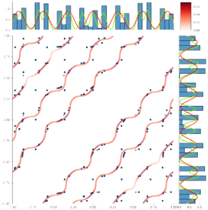




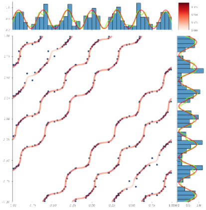
$M = 20$ $M = 40$

1D Numerical results

ρ_3



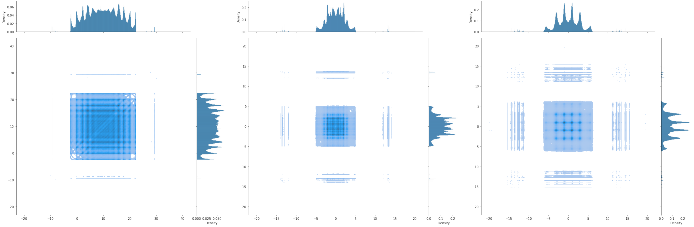
$M = 20$

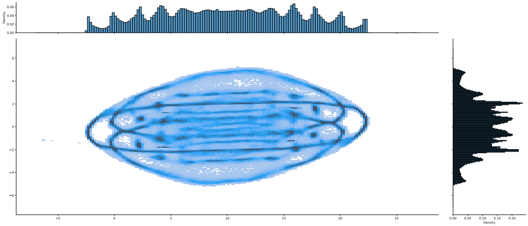


$M = 40$

3D numerical results

$N = 100$, $M = 52$ (polynomial test functions), ρ (normalized) sum of six gaussian functions defined on $\mathbb{R}^3$





Conclusion and perspectives

Conclusions:

- Alternative way of discretizing optimal transport problems from DFT with moment constraints: sparse minimizers
- Numerical particle scheme for the approximation of the SCE functional: encouraging numerical results

Perspectives:

- Numerical scheme for the approximation of the Lieb functional (work in progress with Luca Nenna)
- Numerical scheme which allows for more moment functions
- Choice of the moment functions and rates of convergence (preliminary results for the SCE functional, might be difficult to extend such results for the Lieb functional...)
- Proof of convergence of the numerical scheme (perhaps combining ideas with the GenCol algorithm of Friesecke and collaborators...): Very recent work with promising results in this direction [Friesecke, Penka, 2023]
- Learning the Lieb functional?

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