Approximation of OT problems with marginal moments contraints

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2 Alternative discretization: Moments Constrained Optimal Transport Problem – and numerical interest

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Kantorovich problem with two marginal laws

For any (open or compact) subset $\mathcal{X} \subset \mathbb{R}^d$ ($d \in \mathbb{N}^*$), let us denote by $\mathcal{P}(\mathcal{X})$ the set of probability measures on $\mathcal{X}$.

- Let $d_1, d_2 \in \mathbb{N}^*$, $\mathcal{X}_1 \subset \mathbb{R}^{d_1}$ and $\mathcal{X}_2 \subset \mathbb{R}^{d_2}$ be open or compact subsets.
- For $\nu_1 \in \mathcal{P}(\mathcal{X}_1)$ and $\nu_2 \in \mathcal{P}(\mathcal{X}_2)$, let

$$\Pi(\nu_1, \nu_2) = \left\{ \begin{array}{c} \gamma \in \mathcal{P}(\mathcal{X}_1 \times \mathcal{X}_2), \\ \int_{\mathcal{X}_2} \mathrm{d}\gamma(x_1, x_2) = \mathrm{d}\nu_1(x_1), \int_{\mathcal{X}_1} \mathrm{d}\gamma(x_1, x_2) = \mathrm{d}\nu_2(x_2) \end{array} \right\}$$

- Let $c : \mathcal{X}_1 \times \mathcal{X}_2 \to \mathbb{R}_+ \cup \{+\infty\}$ be lower semi-continuous (l.s.c) cost function.

The Kantorovich optimal transport problem reads:

$$\boxed{\inf_{\gamma \in \Pi(\nu_1, \nu_2)} \int_{\mathcal{X}_1, \mathcal{X}_2} c(x_1, x_2) \mathrm{d}\gamma(x_1, x_2).}$$

Multi-marginal Kantorovich problem

- Let $N \in \mathbb{N}^*$, and for all $1 \leq i \leq N$, let $d_i \in \mathbb{N}^*$, $\mathcal{X}_i \subset \mathbb{R}^{d_i}$ be an open or compact subset.
- For all $1 \leq i \leq N$, let $\nu_i \in \mathcal{P}(\mathcal{X}_i)$, and let

$$\Pi^N((\nu_i)_{1\leq i\leq N}) := \left\{\gamma \in \mathcal{P}(\mathcal{X}_1, ..., \mathcal{X}_N), \mathrm{d}\mu_\gamma^i(x_i) = \mathrm{d}\nu_i(x_i), \forall 1 \leq i \leq N\right\},$$

where $\mu_\gamma^i \in \mathcal{P}(\mathcal{X}_i)$ denotes the i^{th} marginal law of γ, defined by

$$\mathrm{d}\mu_\gamma^i(x_i) := \int_{\mathcal{X}_1\times...\mathcal{X}_{i-1}\times\mathcal{X}_{i+1}\times...\times\mathcal{X}_N} \mathrm{d}\gamma(x_1, ..., x_N).$$

- Let $c : \mathcal{X}_1 \times ... \times \mathcal{X}_N \to \mathbb{R}_+ \cup \{+\infty\}$ be lower semi-continuous (l.s.c.) cost function.

The multi-marginal Kantorovich optimal transport problem reads:

$$I = \inf_{\gamma\in\Pi^N((\nu_i)_{1\leq i\leq N})} \int_{\mathcal{X}_1\times...\times\mathcal{X}_N} c\mathrm{d}\gamma.$$

discretization

Let $M \in \mathbb{N}^*$, we discretize the measure $\nu_i \in \mathcal{P}(\mathcal{X}_i)$ on a fixed discretization grid of $\mathcal{X}_i$, $x_i^1, \ldots, x_i^M \in \mathcal{X}_i$.

$$\mathrm{d}\nu_i(x) \approx \sum_{j=1}^{M} \bar{\nu}_i^j \delta_{x_i^j},$$

for some $\bar{\nu}_i^j \in \mathbb{R}_+$ such that $\sum_{j=1}^{M} \bar{\nu}_i^j = 1$.

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In the two marginal laws case, introduce

$$\Gamma := \left\{ \begin{array}{c} (\bar{\gamma}^{j_1,j_2}) \in \mathbb{R}_+^{M^2} \\ \forall 1 \leq j \leq M, \sum_{j_1=1}^M \bar{\gamma}^{j_1,j} = \bar{\nu}_2^j, \sum_{j_2=1}^M \bar{\gamma}^{j,j_2} = \bar{\nu}_1^j \end{array} \right\}$$

so that

$$\gamma \approx \sum_{j_1,j_2} \bar{\gamma}^{j_1,j_2} \delta_{x_1^{j_1},x_2^{j_2}}$$

and we solve the **linear problem under linear constraints in** $\mathbb{R}^{M^2}$

$$\inf_{(\bar{\gamma}_{j_1,j_2}) \in \Gamma} \sum_{j_1,j_2}^{M} c(x_1^{j_1}, x_2^{j_2}) \bar{\gamma}^{j_1,j_2}.$$

discretization

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for some $\bar{\nu}_i^j \in \mathbb{R}_+$ such that $\sum_{j=1}^M \bar{\nu}_i^j = 1$.
In the multi-marginal case with N marginal laws, introduce

$$\Gamma := \left\{ \begin{array}{c} (\bar{\gamma}^{j_1,\dots,j_N}) \in \mathbb{R}_+^{M^N} \\ \sum_{1 \le j_1,\dots,j_{i-1},j_{i+1},\dots,j_N \le M} \bar{\gamma}^{j_1,\dots,j_{i-1},j,j_{i+1},\dots,j_N} = \bar{\nu}_i^j, \ \forall i,j \end{array} \right\}$$

so that

$$\gamma \approx \sum_{1 \le j_1,\dots,j_N \le M} \bar{\gamma}^{j_1,\dots,j_N} \delta_{x_1^{j_1},\dots,x_N^{j_N}}$$

and we solve the **linear problem under linear constraints in** $\mathbb{R}^{M^N}$

$$\inf_{(\bar{\gamma}_{j_1,\dots,j_N}) \in \Gamma} \sum_{1 \le j_1,\dots,j_N \le M} c(x_1^{j_1}, ..., x_N^{j_N}) \bar{\gamma}^{j_1,\dots,j_N}.$$

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$$\mathrm{d}\nu_i(x) \approx \sum_{j=1}^{M} \bar{\nu}_i^j \delta_{x_i^j},$$

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so that

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$$\inf_{(\bar{\gamma}_{j_1,\dots,j_N}) \in \Gamma} \sum_{1 \le j_1,\dots,j_N \le M} c(x_1^{j_1}, \dots, x_N^{j_N}) \bar{\gamma}^{j_1,\dots,j_N}.$$

Curse of dimensionality!

Numerical methods for multi-marginal optimal transport problems

Several numerical methods have been introduced in the literature for the resolution of the multi-marginal optimal transport problems. We mention here two of them in the context of the symmetric multimarginal Kantorovich problem with Coulomb Cost:

- [Benamou,Carlier,Cuturi,Nenna,Peyre,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, and clever treatment of the (infinite-dimensional) inequality constraint.

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Alternative discretization: Moments Constrained Optimal Transport Problem

Let $M \in \mathbb{N}^*$ and $\phi_1^i, ..., \phi_M^i \in \mathcal{C}_b(\mathcal{X}_i)$ be some continuous bounded functions on $\mathcal{X}_i$. They will be called hereafter **test functions**.

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For all $1 \leq i \leq N$, the marginal constraint

$$\mathrm{d}\mu_\gamma^i(x_i) = \mathrm{d}\nu_i(x_i)$$

is then approximated by the M moment constraints: for all $1 \leq j \leq M$,

$$\int_{\mathcal{X}_i} \phi_j^i(x_i)\mathrm{d}\mu_\gamma^i(x_i) = \int_{\mathcal{X}_1 \times \ldots \times \mathcal{X}_N} \phi_j^i(x_i)\mathrm{d}\gamma(x_1, ..., x_N) = \int_{\mathcal{X}_i} \phi_j^i(x_i)\mathrm{d}\nu_i(x_i) =: \bar{\nu}_i^j$$

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and we consider the following approximate problem (**MCOT problem**)

$$I^M = \inf_{\substack{\gamma \in \mathcal{P}(\mathcal{X}_1 \times \ldots \times \mathcal{X}_N) \\ \forall 1 \leq i \leq N, \forall 1 \leq j \leq M, \\ \int_{\mathcal{X}_1 \times \ldots \times \mathcal{X}_N} \phi_j^i(x_i)\mathrm{d}\gamma(x_1, \ldots, x_N) = \bar{\nu}_i^j \\ \int_{\mathcal{X}_1 \times \ldots \times \mathcal{X}_N} \sum_{i=1}^N \theta_{\nu_i}(|x_i|)\mathrm{d}\gamma(x_1, \ldots, x_N) \leq A_0}} \int_{\mathcal{X}_1 \times \ldots \times \mathcal{X}_N} c\mathrm{d}\gamma. \quad (1)$$

Alternative discretization: Moments Constrained Optimal Transport Problem

Remark

$$I^M \leq I$$

Alternative discretization: Moments Constrained Optimal Transport Problem

Remark

$$I^M \leq I$$

Under appropriate conditions on the test functions,

Theorem ([Alfonsi, C., Ehrlacher, Lombardi, 2019])

For all $M \in \mathbb{N}^*$, *it holds that* $I^M \leq I$ *and* $I^M \xrightarrow[M \to +\infty]{} I$.

Besides, there exists an integer $1 \leq K \leq MN + 2$, *and for all* $1 \leq k \leq K$, *points* $z^k = (x_1^k, ..., x_N^k) \in \mathcal{X}_1 \times ... \times \mathcal{X}_N$ *and weights* $w_k > 0$ *such that*

$$\gamma^M = \sum_{k=1}^{K} w_k \delta_{x_1^k, \dots, x_N^k}$$

is a minimizer of the MCOT Problem (1).

$MN + 2$ bound on the number of charged points

Theorem (Tchakaloff [Bayer & Teichmann, 2006])

Let $d \in \mathbb{N}^*$ and let γ be a measure on $\mathbb{R}^d$ concentrated on a Borel set $A \in \mathcal{F}$, i.e. $\gamma(\mathbb{R}^d \setminus A) = 0$. Let $M_0 \in \mathbb{N}^*$ and $\Lambda : \mathbb{R}^d \to \mathbb{R}^{M_0}$ a Borel measurable map. Assume that the first moments of $\Lambda \# \gamma$ exist, i.e.

$$\int_{\mathbb{R}^{M_0}} \|u\| \mathrm{d}\Lambda\#\gamma(u) = \int_{\mathbb{R}^d} \|\Lambda(z)\| \mathrm{d}\gamma(z) < \infty,$$

where $\|\cdot\|$ denotes the Euclidean norm of $\mathbb{R}^{M_0}$. Then, there exist an integer $1 \leq K \leq M_0$, points $z_1, \ldots, z_K \in A$ and weights $w_1, \ldots, w_K > 0$ such that

$$\forall 1 \leq j \leq M_0, \quad \int_{\mathbb{R}^d} \Lambda_j(z) \mathrm{d}\gamma(z) = \sum_{k=1}^{K} w_k \Lambda_j(z_k),$$

where Λ_j denotes the j-th component of Λ.

This suggests to consider the following problem (**particle problem**) as a numerical scheme

$$\inf_{\substack{w_1,\dots,w_{MN+2}\geq 0\\ \sum_{k=1}^{MN+2} w_k=1\\ (x_1^k,\dots,x_{MN+2}^k)_{1\leq k\leq MN+2}\in(\mathcal{X}_1\times\dots\times\mathcal{X}_N)^{MN+2}\\ \forall 1\leq i\leq N,\,\forall 1\leq j\leq M,\sum_{k=1}^{MN+2} w_k\phi_j^i(x_i^k)=\bar{\nu}_i^j}} \sum_{k=1}^{MN+2} w_k c(x_1^k,\dots,x_N^k). \tag{2}$$

Numerical Interest

This suggests to consider the following problem (**particle problem**) as a numerical scheme

$$\inf_{\substack{w_1,\dots,w_{MN+2}\geq 0 \\ \sum_{k=1}^{MN+2} w_k=1 \\ (x_1^k,\dots,x_{MN+2}^k)_{1\leq k\leq MN+2}\in(\mathcal{X}_1\times\dots\times\mathcal{X}_N)^{MN+2} \\ \forall 1\leq i\leq N,\, \forall 1\leq j\leq M,\, \sum_{k=1}^{MN+2} w_k\phi_j^i(x_i^k)=\bar{\nu}_i^j}} \sum_{k=1}^{MN+2} w_k c(x_1^k,\dots,x_N^k). \tag{2}$$

Remark

The number of particles grows linearly with the number of marginal laws, as well as the number of coordinates of those particles.

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Symmetric multi-marginal OT problem with Coulomb Cost and DFT

Hohenberg-Kohn theorem : the ground state energy of a system can be obtained by minimizing

$$E[\rho] = F[\rho] + \int v_{\text{ext}}(x)\rho(x)dx, \tag{3}$$

where v_{ext} is an external potential and

$$F[\rho] = \min_{\Psi \to \rho} \langle \Psi | -\frac{1}{2}\sum_{i=1}^{N} \Delta_i + \sum_{i \neq j=1}^{N} \frac{1}{|x_i - x_j|} | \Psi \rangle. \tag{4}$$

In the "strictly correlated electrons" limit,

$$F[\rho] \approx \min_{\Psi \to \rho} \langle \Psi | -\frac{1}{2}\sum_{i=1}^{N} \Delta_i | \Psi \rangle + \underbrace{\min_{\Psi \to \rho} \langle \Psi | \sum_{i \neq j=1}^{N} \frac{1}{|x_i - x_j|} | \Psi \rangle}_{V_{ee}^{\text{SCE}}[\rho]}. \tag{5}$$

Symmetric multi-marginal OT problem with Coulomb Cost

This problem arises in quantum chemistry applications [Seidl, 1999], [Seidl, Gori-Giorgi, Savin, 2007], [Cotar, Friesecke, Klüppelberg, 2011], [Lewin, 2017], [Cotar, Friesecke, Klüppelberg, 2018], where N is a number of electrons. (see M. Seidl, C. Cotar, G. Friesecke, M. Lewin, A. Gerolin and L. Nenna talks)

- Let $d = d_1 = ... = d_N$ and $\mathcal{X}_1 = ... = \mathcal{X}_N = \mathbb{R}^d$.
- Let $\rho = \nu_1 = ... = \nu_N$, and $\Pi^N(\rho) := \Pi(\rho, ..., \rho)$
- Let

$$c : \begin{cases} (\mathbb{R}^d)^N & \to & \mathbb{R}_+ \cup \{+\infty\} \\ (x_1, ..., x_N) & \mapsto & \sum_{1 \leq i < j \leq N} \frac{1}{|x_i - x_j|} \end{cases}$$

  be the Coulomb Cost.

The problem considered is

$$I = \inf_{\gamma \in \Pi^N(\rho)} \int_{(\mathbb{R}^d)^N} c d\gamma.$$

Symmetric multi-marginal OT problem with Coulomb Cost

Recall the associated MCOT Problem, where $\rho_j = \int_{\mathbb{R}^d} \phi_j(x) \mathrm{d}\rho(x)$

$$I^M_{A_0} = \inf_{\substack{\gamma \in \mathcal{P}((\mathbb{R}^d)^N) \\ \forall 1 \leq i \leq N, \forall 1 \leq j \leq M, \\ \int_{(\mathbb{R}^d)^N} \phi_j(x_i) \mathrm{d}\gamma(x_1,\dots,x_N) = \rho_j \\ \int_{(\mathbb{R}^d)^N} \sum_{i=1}^N \theta_\rho(|x_i|) \mathrm{d}\gamma(x_1,\dots,x_N) \leq A_0}} \int_{(\mathbb{R}^d)^N} c \mathrm{d}\gamma. \tag{6}$$

Symmetric multi-marginal OT problem with Coulomb Cost

Recall the associated MCOT Problem, where $\rho_j = \int_{\mathbb{R}^d} \phi_j(x)\mathrm{d}\rho(x)$

$$I_{A_0}^M = \inf_{\substack{\gamma\in\mathcal{P}((\mathbb{R}^d)^N) \\ \forall 1\leq i\leq N, \forall 1\leq j\leq M, \\ \int_{(\mathbb{R}^d)^N} \phi_j(x_i)\mathrm{d}\gamma(x_1,\dots,x_N)=\rho_j \\ \int_{(\mathbb{R}^d)^N} \sum_{i=1}^N \theta_\rho(|x_i|)\mathrm{d}\gamma(x_1,\dots,x_N)\leq A_0}} \int_{(\mathbb{R}^d)^N} c\mathrm{d}\gamma. \tag{6}$$

And let us introduce

$$\tilde{I}_{A_0}^M = \inf_{\substack{\gamma\in\mathcal{P}((\mathbb{R}^d)^N) \\ \forall 1\leq j\leq M, \\ \int_{(\mathbb{R}^d)^N} \left(\frac{1}{N}\sum_{i=1}^N \phi_j(x_i)\right)\mathrm{d}\gamma(x_1,\dots,x_N)=\rho_j \\ \int_{(\mathbb{R}^d)^N} \sum_{i=1}^N \theta_\rho(|x_i|)\mathrm{d}\gamma(x_1,\dots,x_N)\leq A_0}} \int_{(\mathbb{R}^d)^N} c\mathrm{d}\gamma. \tag{7}$$

Symmetric multi-marginal OT problem with Coulomb Cost

Theorem

For all $M \in \mathbb{N}^*$, it holds that $I^M_{A_0} = \tilde{I}^M_{A_0}$.
Besides, there exists an integer $1 \leq K \leq M+2$, and for all $1 \leq k \leq K$, points $z^k = (x^k_1, ..., x^k_N) \in \mathcal{X}_1 \times ... \times \mathcal{X}_N$ and weights $w_k > 0$ such that

$$\gamma^M_{\mathrm{sym}} := \frac{1}{N!} \sum_{\sigma \in \mathcal{S}_N} \sum_{k=1}^{K} w_k \delta_{x^k_{\sigma(1)}, \dots, x^k_{\sigma(N)}}$$

is a minimizer of MCOT Problems (6) and (7).

Symmetric multi-marginal OT problem with Coulomb Cost

Theorem

For all $M \in \mathbb{N}^*$, *it holds that* $I_{A_0}^M = \tilde{I}_{A_0}^M$.
Besides, there exists an integer $1 \leq K \leq M + 2$, *and for all* $1 \leq k \leq K$, *points* $z^k = (x_1^k, ..., x_N^k) \in \mathcal{X}_1 \times ... \times \mathcal{X}_N$ *and weights* $w_k > 0$ *such that*

$$\gamma_{\mathrm{sym}}^M := \frac{1}{N!} \sum_{\sigma \in \mathcal{S}_N} \sum_{k=1}^{K} w_k \delta_{x_{\sigma(1)}^k, \dots, x_{\sigma(N)}^k}$$

is a minimizer of MCOT Problems (6) *and* (7).

Remark

To compute a minimizer of the MCOT problem, one only needs to find at most $M + 2$ scalars w_k and points $z^k = (x_1^k, ..., x_N^k) \in (\mathbb{R}^d)^N$: $\mathcal{O}(3(M + 2)N)$.
In [Friesecke, Vögler, 2018], a different result (but in the same spirit) was obtained by the authors in the case when the OT problem is discretized in a finite state space.

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1D example

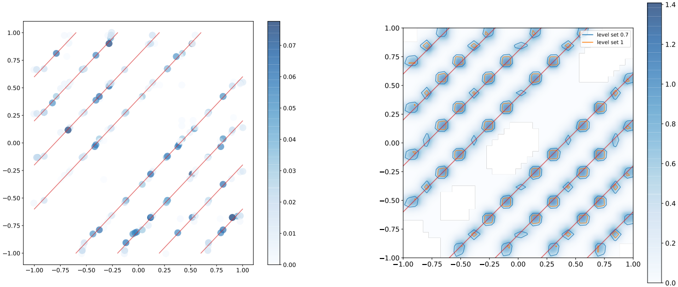

Figure: Optimal coupling measure for the MCOT problem $\left(\frac{1}{20}\sum_{k=1}^{60}\sum_{n\neq n'=1}^{5} w_k \delta_{x_{k,n},x_{k,n'}}\right)$.The optimal OT coupling measure support is represented in red. On the left graph are represented the particles coordinates $(x_{k,n}, x_{k,n'})$, the color of which is indexed on their weight (w_k). On the right graph is represented $\frac{1}{20}\sum_{k=1}^{60}\sum_{n\neq n'=1}^{5} w_k g(x_{k,n}, x_{k,n'})$, where $g(x,y) \sim \mathcal{N}(\begin{pmatrix} x \\ y \end{pmatrix}, \eta \mathrm{Id}_2)$, with $\eta = 1.5e^{-3}$.

- $N = 5$ marginal laws (electrons) in 1D
- regularized Coulomb cost $c(y_1,\dots,y_5) = \sum_{i\neq j=1}^{5} \frac{1}{\epsilon + |y_i - y_j|}$, $\epsilon = 1e^{-3}$, $\forall i = 1,\dots,5, y_i \in \mathbb{R}$.
- The marginal law is uniform over $[-1,1]$, $\rho \sim \mathcal{U}_{[-1,1]}$
- test functions : Legendre polynomials (that are orthogonal for ρ) up to degree $M = 30$.
- $K = 60$ particles $z^k = (x_1^k,\dots,x_5^k)$, $k = 1,\dots,60$.
- Solved using a projected gradient algorithm.

3D example

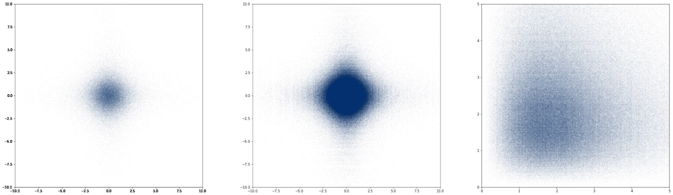

Figure: Projection of the optimal coupling measure for the MCOT problem at initialization and during optimization.

- left graph: $\frac{1}{10K}\sum_{k=1}^{K}\sum_{n=1}^{10}\delta_{x_{n,0}^k, x_{n,1}^k}$.
- middle graph: $\frac{1}{90K}\sum_{k=1}^{K}\sum_{n\neq n'=1}^{10}\delta_{x_{n,0}^k, x_{n',0}^k}$.
- right graph: $\frac{1}{90K}\sum_{k=1}^{K}\sum_{n\neq n'=1}^{10}\delta_{|x_n^k|,|x_{n'}^k|}$, where $|x_n^k| = \sqrt{\sum_{i=1}^{3}(x_{n,i}^k)^2}$.

- $N = 10$ marginal laws (electrons) in 3D
- regularized Coulomb cost $c(y_1, \dots, y_{10}) = \sum_{i\neq j=1}^{10}\frac{1}{\epsilon + |y_i - y_j|}$, $\epsilon = 1e^{-3}$, $\forall i = 1, \dots, 10$, $y_i \in \mathbb{R}^3$.
- The marginal law is gaussian, $\rho \sim \mathcal{N}(0_3, \mathrm{Id}_3)$
- test functions $M = 27$: polynomials $\phi_{a,b,c}(x) = P_a(x_0)P_b(x_1)P_c(x_2)$,where P_n are normalized Hermite polynomials, $x \in R^3$, and $(a+1)(b+1)(c+1) \leq 6$ (hyperbolic cross).
- $K = 10000$ particles $z^k = (x_{1,1}^k, x_{1,2}^k, x_{1,3}^k, x_{2,1}^k \dots, x_{10,3}^k)$, $k = 1, \dots, 10^4$.
- Solved using a projected gradient algorithm with fixed weights.

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Conclusion

- Alternative way of discretizing multi-marginal optimal transport problems, in particular for application in quantum chemistry, using test functions: MCOT problems;
- Convergence of MCOT problem towards the OT problem;
- Some minimizers of MCOT problems can be written as discrete measures charging a low number of points
- suggest the use of a particle numerical scheme for the resolution of the MCOT problem
- Preliminary results on simple OT problems on the rate of convergence of the MCOT problem towards the OT problem for piecewise constant and piecewise affine functions

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Thank you for your attention.

Summary

1 Introduction

2 Alternative discretization: Moments Constrained Optimal Transport Problem – and numerical interest

3 Symmetric multi-marginal OT problem with Coulomb Cost

4 Numerical Examples in the Symmetric multimarginal OT problem with Coulomb Cost

5 Conclusions

6 Rates of convergence

Sets of test functions

Let $M \in \mathbb{N}^*$ and let us define the intervals

$$T_1^M := \left[0, \frac{1}{M}\right], T_j^M := \left(\frac{j-1}{M}, \quad \frac{j}{M}\right], \forall 2 \leq j \leq M.$$

We consider three different sets of test functions:

- Piecewise constant ($\mathbb{P}_0$) test functions:

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Theorem

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$$|I - I^M| = |W_2^2(\nu_1, \nu_2) - I^M| \leq \frac{7}{3}\frac{\|\rho_1\|_{L^\infty} + \|\rho_2\|_{L^\infty}}{M^2}.$$