The dual charge method for the multimarginal optimal transport with Coulomb cost

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Motivation from statistical physics (1/2)

- N identical particles with positions $x_1, \ldots, x_N$ in $\mathbb{R}^d$
- $x_1, \ldots, x_N$ distributed along $\mathbb{P}(x_1, \ldots, x_N) \in \mathscr{P}_{sym}((\mathbb{R}^d)^N)$
- Two-body interaction potential $w(|x - y|)$ with $w : \mathbb{R}_+ \to \mathbb{R}_+$ lsc

$$c_w(x_1, \ldots, x_N) := \sum_{1 \leq i < j \leq N} w(|x_i - x_j|)$$

- One-body external potential $V_{\mathrm{ex}}(x)$, *e.g.* confining potential

Ground-state/free energy

$$F_N^{(T)}(V_{\mathrm{ex}}) := \inf_{\mathbb{P} \in \mathscr{P}_{sym}((\mathbb{R}^d)^N)} \left\{ \int_{\mathbb{R}^{dN}} \left(c_w + \sum_{i=1}^{N} V_{\mathrm{ex}}(x_i) \right) \mathrm{d}\mathbb{P} + T \cdot Ent(\mathbb{P}) \right\}$$

where $T \geq 0$ is temperature and $Ent(\mathbb{P}) = \int_{\mathbb{R}^{dN}} \mathbb{P} \log \mathbb{P}$ is entropy.

Motivation from statistical physics (2/2)

$$F_N^{(T)}(V_{\text{ex}}) := \inf_{\mathbb{P}} \left\{ \int_{\mathbb{R}^{dN}} \Big(c_w + \sum_{i=1}^N V_{\text{ex}}(x_i) \Big) \mathrm{d}\mathbb{P} + T \cdot Ent(\mathbb{P}) \right\}$$

- Computing $F_N^{(T)}(V_{\text{ex}})$ complicated $N \gg 1$: many local minima

<u>**Two-step minimisation**</u> : split *infimum* into two *infima*

$$F_N^{(T)}(V_{\text{ex}}) = \inf_{\mathbb{P} \in \mathscr{P}_{sym}((\mathbb{R}^d)^N)} \{\cdots\} = \inf_{\rho \in \mathscr{P}(\mathbb{R}^d)} \ \inf_{\mathbb{P} \in \mathscr{P}_{sym}((\mathbb{R}^d)^N) \ s.t. \ \pi_1^\sharp \mathbb{P} = \rho} \{\cdots\}$$

<u>**Multimarginal OT:**</u> rewrite ground-state/free energy as

$$F_N^{(T)}(V_{\text{ex}}) = \inf_{\rho} \left\{ OT_N^{(T)}(\rho) + \int_{\mathbb{R}^{dN}} V_{\text{ex}} \rho \right\}, \quad OT_N^{(T)}(\rho) := \inf_{\mathbb{P} \text{ s.t. } \pi_1^\sharp \mathbb{P} = \rho} \left\{ \int_{\mathbb{R}^{dN}} c_w \mathrm{d}\mathbb{P} + T \cdot Ent(\mathbb{P}) \right\}$$

- $OT_N^{(T)}(\rho)$ complicated, *but* indep. of V_{ex} $\implies$ use approximations (DFT & chemists)

What is my problem ?

$$\boxed{OT_N^{(T)}(\rho) := \inf_{\mathbb{P} \text{ s.t. } \pi_1^\sharp \mathbb{P} = \rho} \left\{ \int_{\mathbb{R}^{dN}} c_w \mathrm{d}\mathbb{P} + T \cdot Ent(\mathbb{P}) \right\}}$$

- We want to solve numerically $OT_N^{(T)}(\rho)$ when $N \gg 1$
- *E.g.* for small $0 < T \ll 1$, in order to approximate the unregularized OT, *i.e.* $OT_N^{(0)}(\rho)$

Kantorovich duality ($T > 0$)

$$OT_N^{(T)}(\rho) = \sup_{V:\mathbb{R}^d \to \mathbb{R}} \left\{ F_N^{(T)}(V) - N \int_{\mathbb{R}^d} V\rho \right\}$$

Strong duality & existence of a (unique) Kantorovich potential V_T proved in [Chayes, Chayes & Lieb, '84] in physics paper related to classical DFT

A simple idea

$$\boxed{OT_N^{(T)}(\rho) = \sup_{V:\mathbb{R}^d\to\mathbb{R}} \left\{ F_N^{(T)}(V) - N\int_{\mathbb{R}^d} V\rho \right\}}$$

Idea to solve $OT_N^{(T)}$ (with $0 < T \ll 1$ typically)

1. Decompose $V_T \in Span(\{\phi_i\}_{i=1,\dots,M})$ onto finite basis $\{\phi_i\}_{i=1,\dots,M}$
2. Solve concave maximization problem

$$OT_N^{(T)}(\rho) \simeq \sup_{V\in Span(\{\phi_i\}_{i=1,\dots,M})} \left\{ F_N^{(T)}(V) - N\int_{\mathbb{R}^d} V\rho \right\}$$

- Optimise with gradient ascent : gradient can be computed by MCMC methods
- Dual of Moment Constrained OT [Alfonsi, Coyaud, Ehrlacher & Lombardi, '21]

$$\pi_1^\sharp \mathbb{P}_T = \rho \qquad \text{v.s.} \qquad \int_{\mathbb{R}^{dN}} \sum_{j=1}^N \phi_i(x_j)\mathrm{d}\mathbb{P}_T = \int_{\mathbb{R}^d} \phi_i\rho \quad \forall i = 1,\dots,M.$$

How to choose ϕ_i's ? Special case of Coulomb interaction (1/2)

- Coulomb interaction $w(|x-y|) = |x-y|^{-1}$ in dimension $d = 3$
- If $\rho_N := \rho$ for fixed $\rho \in \mathscr{P}(\mathbb{R}^d)$, following mean-field limit holds

$$\frac{V_{0,N}}{N} \xrightarrow[N\to\infty]{} -\rho * |x|^{-1} \qquad \big(\text{formally by [Cotar, Friesecke \& Pass, '14]}\big)$$

where $V_{0,N}$ Kantorovich potential for $OT_N^{(0)}(\rho)$.

Takeaway message : $V_{0,N}(x) = -N\rho * |x|^{-1} + \textit{correction terms} \quad (N \gg 1).$

How to choose the ϕ_i's ? Special case of Coulomb interaction (2/2)

Our idea to discretize V_T for $T \ll 1$ [L, '24] — also [Mendl & Lin, '14]

1. Write V_T as potential generated by an external dual charge $\rho_T^{(e)}$

$$V_T(x) = -\rho_T^{(e)} * |x|^{-1} := -\int_{\mathbb{R}^3} \rho_T^{(e)}(y)|x-y|^{-1}\mathrm{d}y.$$

Theorem : $\forall T \geq 0$, $\rho_T^{(e)}$ exists and can be assumed to be positive and s.t. $\int_{\mathbb{R}^{dN}} \rho_T^{(e)} = N-1$ as proved in [L, '24]

2. Decompose $\rho_T^{(e)} \in Span(\{\mu_i\}_{i=1,\ldots,M})$ onto a finite basis $\{\mu_i\}_{i=1,\ldots,M}$

- Otherwise stated : $V_T \in Span(\{\phi_i\}_{i=1,\ldots,M})$ with $\phi_i = \mu_i * |x|^{-1}$

Vague claim (formally by [Cotar, Friesecke & Pass, '14], true in $d=1$ [L, '24])

If $\rho_N := \rho$ with fixed $\rho \in \mathscr{P}(\mathbb{R}^d)$, then $\frac{\rho_0^{(e)}}{N} \xrightarrow[N\to\infty]{narrow} \rho$

Numerics of uniform droplets

- Uniform Droplets, *i.e.*

$$N \in \mathbb{N}, \quad \rho_N = N^{-1}\mathbb{1}_{B_N}, \quad \text{with } B_N := B(0, r_N) \subset \mathbb{R}^3 \text{ s.t. } |B_N| = N$$

- Ball B_N discretized into M concentric shells, *i.e.*

$$B_N = \cup_{i=1}^M S_i \quad \text{where } S_i := B(r_i) \setminus B(r_{i-1}), \quad 0 = r_0 < r_1 \leq \cdots \leq r_{M-1} < r_M = r_N$$

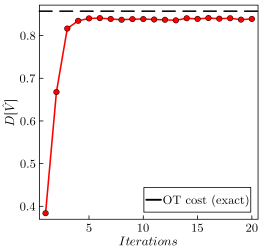
- μ_i are indicators of S_i's, *i.e.*

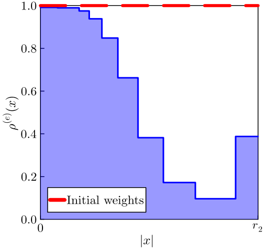
$$V_T \simeq \widehat{V}(\omega_1, \ldots, \omega_M) = \textstyle\sum_{i=1}^M \omega_i \mu_i * |x|^{-1} \text{ with } \quad \mu_i = \mathbb{1}_{S_i} \qquad (T \ll 1)$$

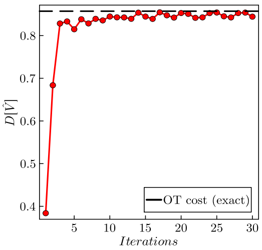
- Initialised on mean-field limit *i.e* $\omega_i^{(0)} = 1$ for $i = 1, \ldots, M$

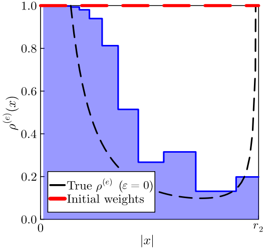
- **Parameters**: $N = 2$, with $M \in \{10, 20\}$ and $T \in \{50^{-1}, 500^{-1}\}$
- Optimised $\widehat{V}(\widehat{\omega_1}, \ldots, \widehat{\omega_M})$ is plugged into unregularized OT dual, *i.e.*

$$D_0(\widehat{V}) := \min_{x_1,\ldots,x_N} \left\{ c_w + \sum_{i=1}^N \widehat{V}(x_i) \right\} - \int_{\mathbb{R}^3} \widehat{V}\rho$$

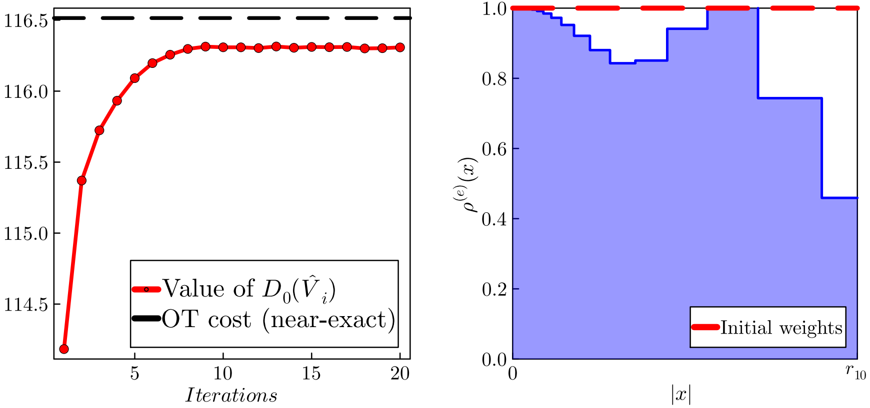








- **Parameters**: $N = 20$, with $M = 50$ and $T = 150^{-1}$
- Compared with upper bound of `[Räsänen, Gori-Giorgi & Seidl, '16]`



Conclusion

- Efficient discretisation of Kantorovich potentials for Coulomb-like cost
- Lots of room for optimisation improvement — gradient & MCMC methods
- Question : *In which sense* $V_0 \simeq -N\rho * |x|^{-1}$ *?* $1^{st}/2^{nd}$-order corrections ?
- [L, '24] : `An external dual charge approach to the multimarginal optimal transport with Coulomb cost, ESAIM COCV`

Thank you !