Optimal transport with Coulomb cost: theory and applications to electronic structure of atoms & molecules (lecture 3)

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(Young European Probabilists)

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Recall

$$(\mathcal{P}_N) \quad \min_{\substack{\gamma \in \mathcal{P}^N_{sym}(\mathbb{R}^3) \\ \gamma \to \rho}} C_N[\gamma] = \int_{\mathbb{R}^{3N}} \sum_{i<j} \frac{1}{|x_i - x_j|} \, d\gamma(x_1, \ldots, x_N)$$

$N = 2$ Monge min's, !que

$N \geq 3$ $\exists$ non Monge min's B. Pass 2013

- $\neq$ physics ansatz
$$\gamma(x_1, \ldots, x_N) = \left(\rho(x_1)\, \delta_{T_2(x_1)}(x_2) \cdots \delta_{T_N(x_1)}(x_N)\right)_{sym.}$$
- $\neq$ math. results for positive power costs Gangbo - Święch

5. large N

Infinite-body OT

$$C_\infty[\gamma] := \lim_{N \to \infty} \binom{N}{2}^{-1} \int_{(\mathbb{R}^d)^\infty} \sum_{1 \leq i < j \leq N} c(x_i, x_j) \, d\gamma(x_1, \ldots, x_N, \ldots)$$

(cost per particle pair)

$$(\mathcal{P}_\infty) \quad \min_{\substack{\gamma \in \mathcal{P}^\infty_{sym}(\mathbb{R}^d) \\ \gamma \mapsto \mu}} C_\infty[\gamma] \qquad \begin{array}{l} \mu \in \mathcal{P}(\mathbb{R}^d) \\ c \in L^1(\mu \otimes \mu) \end{array}$$

<u>Q's</u>

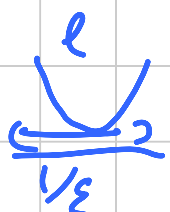
- Behaviour of $(\mathcal{P}_\infty)$
- Rel'nship $(\mathcal{P}_N) \leftrightarrow (\mathcal{P}_\infty)$

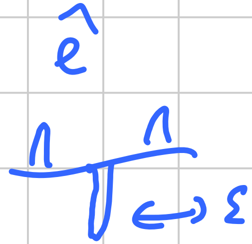
<u>Thm</u> ((Cotar, GF, B. Pass, arXiv 2013) Spse $c(x,y) = \ell(x-y)$, ℓ has <u>positive Fourier trf</u>. Then

$$\gamma_{opt} = \mu \otimes \mu \otimes \dots = \mu^{\otimes \infty}$$

is the unique minimizer of $(\mathcal{P}_\infty)$.

eg $\ell(x-y) = |x-y|^p$, $p>0$ $\qquad \hat{\ell} \not> 0$





$\ell(x-y) = |x-y|^{-p}$, $p>0$, $p<d$ $\qquad \hat{\ell} = c(p,d)\,\frac{1}{|z|^{d-p}} > 0$

Pf (formal) Let $\gamma \in \mathcal{P}^{\infty}_{sym}(\mathbb{R}^d)$, arbitrary

$$\gamma \to \mu_2 \in \mathcal{P}^2_{sym}(\mathbb{R}^d) \to \mu \in \mathcal{P}(\mathbb{R}^d)$$

- De Finetti Hewett Savage $\gamma \in \mathcal{P}^{\infty}_{sym}(X)$ ($\sim$ exch. seq. r.v.'s $X_1, X_2, \ldots$) $\Rightarrow \exists!\, \nu \in \mathcal{P}(\mathcal{P}(X))$ s.th.

$$\gamma = \int_{\mathcal{P}(X)} Q^{\otimes\infty}\, d\nu(Q) \qquad \left(\Rightarrow \mu_2 = \int Q\otimes Q\, d\nu(Q)\right)$$

- Fourier calculus $\hat{\ell}(z) = \int_{\mathbb{R}^d} e^{-iz\cdot x}\, \ell(x)\, dx$

  $\hat{Q}(z) = \qquad \ldots\ldots\, dQ(x)$ (bdd cts fctn)

- elementary pos. th. (error splitting)

$$(1) \qquad C_\infty[\gamma] = \int_{(\mathbb{R}^d)^\infty} c(x_1,x_2)\, d\gamma(x_1,x_2,\dots)$$

$$= \int c(x,y)\, d\mu_2(x,y)$$

$$= \int_{\mathcal{P}(\mathbb{R}^d)} \Big(\underbrace{\int_{\mathbb{R}^{2d}} \ell(x-y)\, dQ(x)\, dQ(y)}_{= \int_{\mathbb{R}^d} (\ell * Q)(x)\, dQ(x)} \Big)\, d\nu(Q)$$

$$\underset{\text{Plancherel}}{=} (2\pi)^{-d} \int_{\mathbb{R}^d} \underbrace{\widehat{\ell * Q}(z)}_{= \hat{\ell}\, \hat{Q}}\, \overline{\hat{Q}(z)}\, dz$$

$$= (2\pi)^{-d} \int_{\mathbb{R}^d} \hat{\ell}(z)\, |\hat{Q}(z)|^2\, dz$$

$$(1) \qquad = (2\pi)^{-d} \int_{\mathbb{R}^d} \hat{\ell}(z) \int_{\mathcal{P}(\mathbb{R}^d)} |\hat{Q}(z)|^2\, d\nu(Q)$$

Similarly

(2) $$\underbrace{\int c(x,y)\, d\mu(x)\, d\mu(y)}_{\substack{\| \\ C_\infty[\mu\otimes\mu\otimes\ldots] \\ \text{mean field cost}}} = \underbrace{(2\pi)^{-d}}_{=:c} \int_{\mathbb{R}^d} \hat{\ell}(z) \left| \int_{\mathcal{P}(\mathbb{R}^d)} \hat{Q}(z)\, d\nu(Q) \right|^2 dz$$

$$(1)-(2) = c \cdot \int_{\mathbb{R}^d} \hat{\ell}(z)\, \mathrm{var}_{\nu(dQ)}\, \hat{Q}(z)\, dz$$

$$\Rightarrow C_\infty[\gamma] = \int_{\mathbb{R}^{2d}} \underbrace{\ell(x-y)\, d\mu(x)\, d\mu(y)}_{\text{mean field term}} + c \cdot \int_{\mathbb{R}^{2d}} \underbrace{\hat{\ell}(z)}_{>0} \mathrm{var}_{\nu(dQ)}\, \hat{Q}(z)\, dz$$

$>0 \Rightarrow$ minimized iff $\nu = \delta_{Q_0}$
$$\delta_{Q_0} = \delta_\mu$$

Sub. this ν into de Finetti $\Rightarrow \gamma = \mu^{\otimes\infty}$.

(Argument rigorous up to justifying Fourier calculus steps for costs that are not bdd & cts; for that see our paper)

$\mathcal{P}_N$ vs $\mathcal{P}_\infty$

C_N & C_∞ dep. only on μ_2 (if pair interact. only)

Def. A symm. $\mu_2 \in \mathcal{P}^2_{sym}(\bar{X})$ is <u>N-representable</u> if $\exists\ \gamma_N \in \mathcal{P}^N_{sym}(\bar{X})$ s.th. $\gamma_N \to \mu_2$, & <u>infinitely representable</u> if $\exists\ \gamma_\infty \in \mathcal{P}^\infty_{sym}(\bar{X})$ s.th. $\gamma_\infty \to \mu_2$

<u>Reformulation of many-body OT as 2-body OT with representability constraint</u>

$(\mathcal{P}_N)$ $\qquad \min\limits_{\substack{\mu_2\ N\ \text{repr} \\ \mu_2 \to \mu}} \int c(x,y)\, d\mu_2$

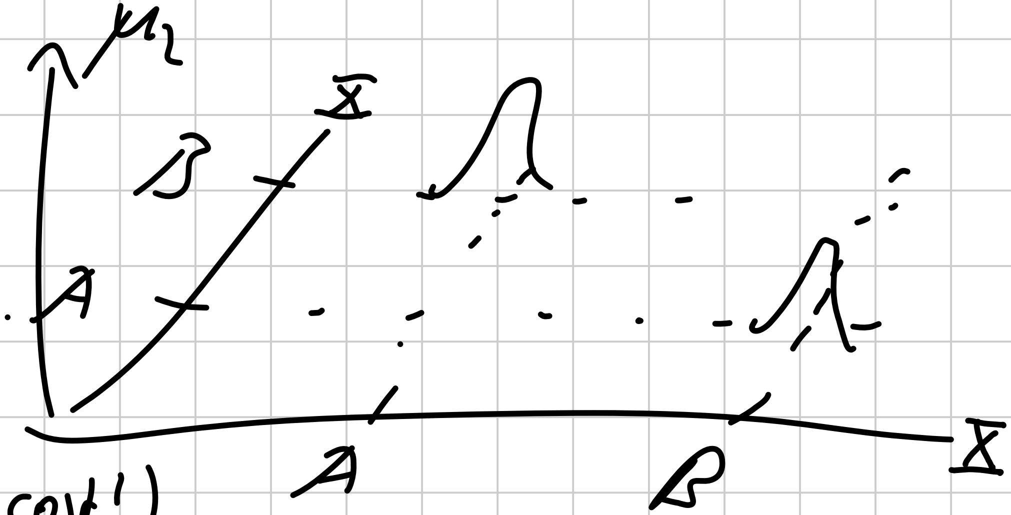
∞ $\qquad \infty$

$\gamma \in \mathcal{P}^\infty_{sym} \iff$ joint distr. of exchangeable seq. $X_1, X_2, \dots$ of rv's (i.e.
$(X_1, \dots, X_n) \sim (X_{\sigma(1)}, \dots, X_{\sigma(n)})\ \forall n,\ \forall \text{perm } \sigma)$

N-repr. $\iff$ (X_1, X_2) extendable to $(X_1, \dots, X_n)$

∞ repr. $\Leftrightarrow$ $(X_1, \dots, X_n, \dots)$

Aldous '85 (good reference in prob. th. lit.)



Ex. $A \neq B \in X$

$$\mu_2 = \frac{1}{2}\left(\delta_A \otimes \delta_B + \delta_B \otimes \delta_A\right)$$

(favoured by decreasing OT cost!)

not 3-representable !!

N-repr. fights against anticorrelation!

Diaconis, Freedman '80: μ_2 N-repr. $\Rightarrow$ $\exists\, \tilde{\mu}_2$ ∞ly rep.
$\| \mu_2 - \tilde{\mu}_2 \| \leq \frac{1}{N}$

Cor $\quad \dfrac{\inf(\mathcal{S}_N)}{\binom{N}{2}} \to \inf(P_\infty) \quad (N \to \infty)$

$$\inf(P_\infty) = J[\mu] = \int c \, d(\mu \otimes \mu)$$

[Diaconis-Freedman-construction: $\tilde{\mu}_2(A) = \displaystyle\int_{(\mathbb{R}^d)^N} \left(\frac{\delta_{\omega_1} + \dots + \delta_{\omega_N}}{N} \right)^{\otimes 2} (A) \, d\gamma_N(\omega)$

where $\gamma_N \to \mu_2$]

Other mathematical results (for references to our work see lecture 1 or http://www-m7.ma.tum.de)

B. Pass — Non Monge minimizers; general facts about ∞-body OT

G. Buttazzo, P. Gori-Giorgi, L. De Pascale — dual approach $\rightsquigarrow$ similar results to Sec. 2&3

$$\max \int \rho \, \psi \qquad \sum_i \psi(x_i) \le c(x_1, \dots, x_N)$$

M. Colombo, L. De Pascale, S. Di Marino — N-body, 1D