The strong correlation limit of DFT: What's known, what's new, what's open

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Electronic Schrödinger equation

Dirac 1929: Chemically specific behaviour of atoms and molecules captured, "in principle", by quantum mechanics.

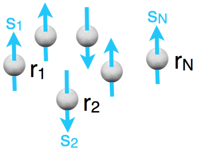
Emission/absorption spectra, binding energies, equilibrium geometries, interatomic forces ($\rightarrow$ materials science),...

Born-Oppenheimer approximation, statics, N electrons –> need to find E_0, Ψ_0 = lowest e-value/e-state of Schrödinger operator

$$H = \underbrace{-\frac{1}{2}\sum_{i=1}^{N} \Delta_{\mathbf{r}_i}}_{T} + \underbrace{\sum_{1 \le i < j \le N} \frac{1}{|\mathbf{r}_i - \mathbf{r}_j|}}_{V_{ee}} + \underbrace{\sum_{i=1}^{N} v(\mathbf{r}_i)}_{V_{ne}}$$

acting on $\Psi \in L^2_{anti}((\mathbb{R}^3 \times \mathbb{Z}_2)^N; \mathbb{C})$, $||\Psi||_{L^2} = 1$.
$v : \mathbb{R}^3 \to \mathbb{R}$ external potential, e.g. $v(\mathbf{r}) = -\sum_{\alpha=1}^{M} Z_\alpha / |\mathbf{r} - R_\alpha|$.

$|\Psi(\mathbf{r}_1, s_1, .., \mathbf{r}_N, s_N)|^2$ = N-point probability density of positions and spins (Born formula)



Key collective variable: electron density

$$\rho(\mathbf{r}_1) = N \sum_{s_1,..,s_N \in \mathbb{Z}^2} \int |\Psi(\mathbf{r}_1, s_1, .., \mathbf{r}_N, s_N)|^2 d\mathbf{r}_2..d\mathbf{r}_N$$

Curse of dimension $\rightarrow$ DFT

Pb. with N-electron Schrödinger equation: curse of dimension
discretize $\mathbb{R} \rightarrow$10 gridpts
single CO_2 molecule: $L^2(\mathbb{R}^{3N}) = L^2(\mathbb{R}^{66}) \rightarrow 10^{3N} = 10^{66}$ gridpts.

DFT: approximate the Schrödinger eq. by systems of equations / variational principles based on the single-particle density.

Physics community: idea of constrained search

Levy 1979: assuming that a lowest e-value/e-state of H exists,

$$\begin{aligned} E_0 &= \min_{||\Psi||^2=1} \left\langle \Psi, T + V_{ee} + V_{ext} | \Psi \right\rangle \quad \text{(Rayleigh-Ritz)} \\ &= \min_{\rho} \min_{\Psi \mapsto \rho} \left\langle \Psi | T + V_{ee} + V_{ext} | \Psi \right\rangle \\ &= \min_{\rho} \Bigg(\underbrace{\min_{\Psi \mapsto \rho} \langle \Psi | T + V_{ee} | \Psi \rangle}_{\substack{\text{Levy-Lieb functional } F^{LL}[\rho] \\ \text{universal part}}} + \underbrace{\int_{\mathbb{R}^3} v(\mathbf{r}) \rho(\mathbf{r}) \, d\mathbf{r}}_{\text{chemically specific part}} \Bigg) \end{aligned}$$

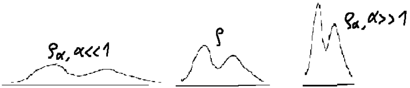
Lieb 1983: rigorous formulation in function spaces; proof that the inner minimum is attained

inner min. over $\{\Psi \in H^1((\mathbb{R}^3 \times \mathbb{Z}_2)^N) : \Psi \text{ antisymm.}, \Psi \mapsto \rho\}$

outer min. over $\{\rho : \sqrt{\rho} \in H^1(\mathbb{R}^3), \rho \geq 0, \int \rho = N\}$

Density scaling

For any given density ρ, consider its dilation $\rho_\alpha(\mathbf{r}) := \alpha^d \rho(\alpha \mathbf{r})$ $(\alpha > 0)$



Levy/Perdew '85: density scaling doesn't commute with constrained search.

$$\rho \xrightarrow{\text{scale}} \rho_\alpha(\mathbf{r}) = \alpha^{-d}\rho(\alpha\mathbf{r})$$

$$\rho \;\xrightarrow{\min_{\Psi\mapsto\rho} \langle\Psi|\alpha^2 T + \alpha V_{ee}|\Psi\rangle}\; \underbrace{\alpha^{-\frac{Nd}{2}}\Psi[\rho_\alpha](\tfrac{\mathbf{r}}{\alpha}, s)}_{=:\Psi_\alpha}$$

$$\rho_\alpha \;\xrightarrow{\min_{\Psi\mapsto\rho_\alpha} \langle\Psi|T + V_{ee}|\Psi\rangle}\; \Psi[\rho_\alpha]$$

$$\alpha^{-\frac{Nd}{2}}\Psi[\rho_\alpha](\tfrac{\mathbf{r}}{\alpha}, s) \xleftarrow{\text{scale back}} \Psi[\rho_\alpha]$$

High-density regime $(\alpha \gg 1)$ Kinetic energy dominates

$$F_{LL}[\rho] \approx \alpha^2 \min_{\Psi\mapsto\rho} \left\langle \Psi \middle| T \middle| \Psi \right\rangle.$$

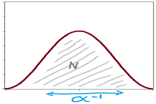
Low-density regime $(\alpha \ll 1)$ Interaction energy dominates

$$F_{LL}[\rho] \approx \alpha \inf_{\Psi\mapsto\rho} \left\langle \Psi \middle| V_{ee} \middle| \Psi \right\rangle.$$

The optimal wavefunctions look completely different in both regimes.

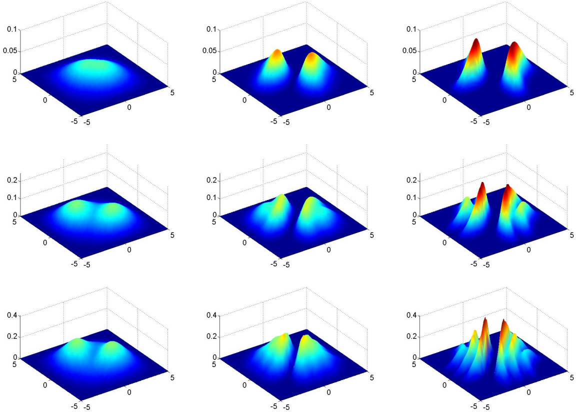
What does the constrained-search wavefunction look like?

Simulation, H.Chen/GF, Multisale Model. Simul., 2015 (Quasi-Newton + FEM-FCI)



ρ 1D 'lump', width α^{-1}, N electrons,
$\rho(x) = \alpha \frac{N}{2L}(1 + \cos(\alpha \frac{\pi}{2L} x)), \ x \in [-L/\alpha, L/\alpha]$

Shown: Pair density
$\rho_2(x_1, x_2) = \sum_{s_1,\dots,s_N \in \mathbb{Z}_2} \int .. \int |\Psi(x_1, .., x_N, s_1, .., s_N)|^2 dx_3..dx_N$



N=2

N=3

N=4

$\alpha = 100$ $\alpha = 1$ $\alpha = 0.1$

Sparsity

Recall ρ arbitrary density, $\rho_\alpha(\mathbf{r}) = \alpha^3\rho(\alpha\mathbf{r})$, $\Psi_\alpha = \underset{\Psi\mapsto\rho}{\mathrm{argmin}}\langle\Psi|\alpha T + V_{ee}|\Psi\rangle$

High-density (weak-interaction) limit $\alpha \to \infty$ (implicit Kohn/Sham 1965)

$$\text{expect } \lim_{\alpha\to\infty}\Psi_\alpha = \text{antisymmetriz. of } \varphi_1(\mathbf{r}_1, s_1)\cdots\varphi_N(\mathbf{r}_N, s_N)$$

maths: N scalar functions $\varphi_i : \mathbb{R}^3 \times \mathbb{Z}_2 \to \mathbb{C}$ which are L^2-orthonormal
physics: N Kohn-Sham orbitals, i.e. minimal kin.en. s/to $\sum_{i,s}|\varphi_i|^2 = \rho$
Data/storage complexity: $N\cdot\ell$, ℓ=no. of single-particle basis functions

Low-density (strong-interaction) limit $\alpha \to 0$ (Seidl 1999)

$$\text{hope } \lim_{\alpha\to 0}\sum_{s_1,..,s_N}|\Psi_\alpha|^2 = \text{symmetriz. of } \frac{\rho(\mathbf{r}_1)}{N}\delta(\mathbf{r}_2 - T_2(\mathbf{r}_1))\cdots\delta(\mathbf{r}_N - T_N(\mathbf{r}_1))$$

maths: N maps $T_i : \mathbb{R}^3 \to \mathbb{R}^3$ which transport ρ to ρ
physics: N co-motion functions, strictly correlated electrons (SCE)
Data/storage complexity (if ansatz justified): $N\cdot\ell$, ℓ=no. equi-mass cells

Plugging the sparse ansatz into the constrained-search

Weak interaction limit: Kohn-Sham ansatz reduces $\min_{\Psi\mapsto\rho}\langle\Psi|T|\Psi\rangle$ to

$$\min\{\sum_{i=1}^{N}\int_{\mathbb{R}^3\times\mathbb{Z}_2}\tfrac{1}{2}|\nabla\varphi_i|^2 \,:\, \int_{\mathbb{R}^3\times\mathbb{Z}_2}\varphi_i^*\varphi_j=\delta_{ij},\ \sum_{i=1}^{N}\sum_{s}|\varphi_i(\mathbf{r},s)|^2=\rho(\mathbf{r}) \text{ for all } \mathbf{r}\}.$$

Minimum value: Kohn-Sham kinetic energy functional $T_s[\rho]$.

Strong interaction limit: SCE ansatz reduces $\inf_{\Psi\mapsto\rho}\langle\Psi|V_{ee}|\Psi\rangle$ to

$$\inf\{\int_{\mathbb{R}^3}\frac{\rho(\mathbf{r})}{N}\sum_{1\le i<j\le N}\tfrac{1}{|T_i(\mathbf{r})-T_j(\mathbf{r})|}\,d\mathbf{r} \,:\, T_1,..,T_N \text{ push } \rho \text{ forward to } \rho\}.$$

Infimum value: SCE functional $V_{ee}^{SCE}[\rho]$. Mathematically, this is a very challenging optimal transport problem (multi-marginal; non-convex cost; Monge form).

Rigorous formulation of strong-interaction limit

Cotar/GF/Klüppelb. arXiv 2011, CPAM 2013; Buttazzo/Gori-Giorgi/DePascale, PRA 2012

The problem

$$\inf_{\Psi \mapsto \rho} \langle \Psi | V_{ee} | \Psi \rangle \tag{1}$$

on $L^2_{anti}((\mathbb{R}^3 \times \mathbb{Z}_2)^N)$ (square-integrable functions) has no minimizer, as Ψ tries to concentrate on lower-dimensional sets.

Way out: consider the interaction energy

$$\langle \Psi | V_{ee} | \Psi \rangle = \int_{\mathbb{R}^{3N}} \underbrace{\sum_{s_1,..,s_N \in \mathbb{Z}_2} |\Psi(\mathbf{r}_1,..,\mathbf{r}_N, s_1,..,s_N)|^2}_{=:\gamma} \sum_{1 \le i < j \le N} \frac{1}{|\mathbf{r}_i - \mathbf{r}_j|} d\mathbf{r}_1..d\mathbf{r}_N$$

as a function of the N-point position density $\gamma \in L^1(\mathbb{R}^{3N})$, and enlarge $L^1(\mathbb{R}^{3N})$ (integrable functions) to measures (e.g., delta functions on curves/surfaces):

$$\min_{\gamma \mapsto \rho} \int_{\mathbb{R}^{3N}} \sum_{1 \le i < j \le N} \frac{1}{|\mathbf{r}_i - \mathbf{r}_j|} d\gamma(\mathbf{r}_1,..,\mathbf{r}_N) \tag{2}$$

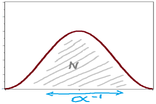
on $\mathcal{P}_{sym}(\mathbb{R}^{3N})$ (symmetric probability measures on $\mathbb{R}^{3N}$), where $\gamma \mapsto \rho$ means $\int_{(\mathbb{R}^3)^{i-1} \times A_i \times (\mathbb{R}^3)^{N-i}} d\gamma = \int_{A_i} \frac{\rho}{N}$ for all $A_i \subseteq \mathbb{R}^3$ (equal marginals ρ/N).

Problem (2) is well-posed, and a Kantorovich optimal transport problem.

Constraint-search wavefunctions vs. Opt.Tr./SCE

Huajie Chen, GF, Multiscale Model. Simul. 2015

ρ 1D 'lump', width α^{-1}, N electrons,
$\rho(x) = \alpha \frac{N}{2L}(1+\cos(\alpha \frac{\pi}{2L} x)),\ x \in [-L/\alpha, L/\alpha]$



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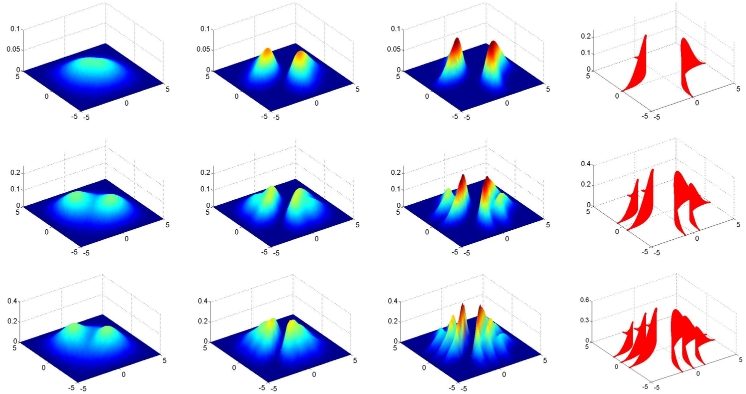

N=2

N=3

N=4

$\alpha = 100$ $\alpha = 1$ $\alpha = 0.1$ Opt.Tr./SCE

Constraint-search minimizers converge to optimal plans

physically expected, subtle maths (marginal-preserving smoothing of transport plans)

Cotar/GF/Klüppelberg 2013: N=2
Cotar/GF/Klüppelberg, Bindini/DePascale, Lewin (all arXiv 2017): general N
Our version:

Theorem: For any ρ, the constrained-search minimizers $\Psi_\alpha = \underset{\Psi \mapsto \rho}{\mathrm{argmin}} \langle \Psi | \alpha T + V_{ee} | \Psi \rangle$ satisfy, up to subsequences,

$$\lim_{\alpha \to 0} \sum_{s_1,..,s_N \in \mathbb{Z}_2} |\Psi_\alpha|^2 = \gamma$$

for some minimizer γ of optimal transport with Coulomb cost, the limit being weak* convergence of probability measures.

In fact, the constrained-search problem Gamma-converges to OT with Coulomb cost.

Different formulations of strongly correlated limit of DFT

Original constrained-search for electron repulsion

$$\inf_{\Psi \in L^2_{anti}((\mathbb{R}^3 \times \mathbb{Z}_2)^N)),\, \Psi \mapsto \rho} \langle \Psi | V_{ee} | \Psi \rangle \tag{1}$$

(ill-posed, curse of dimension),

$$\min_{\gamma \in \mathcal{P}_{sym}(\mathbb{R}^{3N}),\, \gamma \mapsto \rho} \int_{\mathbb{R}^{3N}} \sum_{1 \le i < j \le N} \frac{1}{|\mathbf{r}_i - \mathbf{r}_j|} d\gamma(\mathbf{r}_1, .., \mathbf{r}_N) \tag{2}$$

(Kantorovich OT, well posed [CFK, BDG], curse of dimension still there),

$$\max\{ N \int_{\mathbb{R}^3} v(\mathbf{r}) \rho(\mathbf{r}) \; : \; \sum_{i=1}^{N} v(\mathbf{r}_i) \le \sum_{1 \le i < j \le N} \frac{1}{|\mathbf{r}_i - \mathbf{r}_j|} \text{ for all } (\mathbf{r}_1, .., \mathbf{r}_N) \} \tag{3}$$

(dual Kantorovich, well posed [BDG], curse of dimension in constraint),

$$\inf\{ \int_{\mathbb{R}^3} \frac{\rho(\mathbf{r})}{N} \sum_{1 \le i < j \le N} \frac{1}{|T_i(\mathbf{r}) - T_j(\mathbf{r})|} d\mathbf{r} \; : \; T_1, .., T_N \text{ transport } \rho \text{ to } \rho \} \tag{4}$$

(SCE/Monge OT, not known if well-posed, curse of dimension gone).

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(SCE/Monge OT, not known if well-posed, curse of dimension gone).

Fundamental math question: When is the SCE/Monge ansatz exact, i.e. when does Kantorovich OT admit a minimizer of SCE/Monge form?

Rigorous results, optimal transport with Coulomb cost

Find optimal arrangement (N-body prob.distr.) of N particles in $\mathbb{R}^d$ given their 1-body density ρ

$$\min_{\substack{\gamma \in \mathcal{P}_{sym}(\mathbb{R}^{N\cdot d}) \\ \gamma \mapsto \rho/N}} \int_{\mathbb{R}^{Nd}} \sum_{1\le i<j\le N} |x_i - x_j|^{-\alpha} \, d\gamma(x_1, .., x_N) \quad (0 < \alpha < d)$$

Symmetric: $\gamma(A_1 \times \cdots \times A_N) = \gamma(A_{\sigma(1)} \times \cdots \times A_{\sigma(N)})$ for all perm's

$\gamma \mapsto \rho/N$: $\gamma(\mathbb{R}^d \times \cdots \times A_i \times \cdots \times \mathbb{R}^d) = \int_{A_i} \mu$ for all i, $\rho \in L^1(\mathbb{R}^d)$

	$d = 1$	$d = 3$
$N = 2$	unique min., of Monge form[1)]	
$2 < N < \infty$	unique min., Monge form[2)]	example of non-Monge min.[3)]
$N = \infty$	unique min., non-Monge[4)]	

Monge: $\gamma(x_1, .., x_N) =$symmetrization of $\frac{\rho(x_1)}{N} \delta_{T_2(x_1)}(x_2) \cdots \delta_{T_N(x_1)}(x_N)$
for $N-1$ maps $T_2, ..., T_N$ transporting ρ to itself

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Monge: $\gamma(x_1, .., x_N) =$symmetrization of $\frac{\rho(x_1)}{N} \delta_{T_2(x_1)}(x_2) \cdots \delta_{T_N(x_1)}(x_N)$ for $N-1$ maps T_2, ..., T_N transporting ρ to itself

1) Cotar, GF, Klüppelberg, 2011, 2013; Butazzo, Gori-Giorgi, DePascale 2012
2) Seidl 1999; Colombo, DiMarino, DePascale 2015
3) Pass 2014
4) Cotar, GF, Pass 2015

Trying to understand multi-marginal optimal transport
without having assigned three particles to three sites
is like trying to understand quantum many-body theory
without having solved the 1D harmonic oscillator.

The 3-particles-3-sites-assignment problem

GF, arXiv 1808.04318

$X = \{a_1, .., a_\ell\}$ finite state space (later: $\ell = 3$), $N = 3$ particles/marginals
uniform one-particle density $\rho(x) = \frac{N}{\ell} \sum_{i=1}^{\ell} \delta_{a_i}(x)$

Kantorovich OT, $\min_{\gamma \in \mathcal{P}_{sym}(X^3),\, \gamma \mapsto \rho} \int_{X^3} c(x,y,z)\, d\gamma(x,y,z)$, reduces to:

$$\min \sum_{i,j,k=1}^{\ell} c_{ijk} \gamma_{ijk}$$

over symmetric $\ell \times \ell \times \ell$ tensors (γ_{ijk}) of order 3 which are *tristochastic*,

$$\gamma_{ijk} \geq 0, \ \sum_{i,j} \gamma_{ijk} = 1 \text{ for all } k, \ \sum_{i,k} \mu_{ijk} = 1 \text{ for all } j, \ \sum_{j,k} \mu_{ijk} = 1 \text{ for all } i.$$

$T : X \to X$ transports ρ to ρ iff T a permutation ($T(a_i) = a_{\tau(i)}$).
SCE/Monge ansatz:

$$\gamma = S\gamma', \ \ \gamma' = \frac{1}{\ell} \sum_{\nu=1}^{\ell} \delta_{a_{\tau_1(\nu)}} \otimes \delta_{a_{\tau_2(\nu)}} \otimes \delta_{a_{\tau_3(\nu)}} \text{ for some permutations } \tau_1, \tau_2, \tau_3$$

Means γ' extremely sparse: each of the 3ℓ "planes" associated with the sum constraints contain exactly one 1 and $\ell^2 - 1$ zeros.

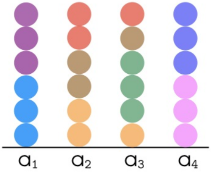
Kantorovich plans as molecular packings

Physics version of finite-state-space Kantorovich problem, GF, arXiv 1808.04318

Find the ground state of an ensemble of non-interacting molecules s.th.:
1) Each molecule is composed of 3 identical atoms.
2) All atoms must be confined to ℓ given sites $a_1, .., a_\ell \in \mathbb{R}^d$
3) All sites must be occupied equally often (marginal condition)
4) The cost to be minimized is the intramolecular interaction energy between the particles within a molecule.

State of a single molecule: $\delta_{x_1} \otimes \delta_{x_2} \otimes \delta_{x_3}$, $x_1 \leq x_2 \leq x_3$
"$\leq$" from indistinguishability, "$=$" allowed as atoms can be on same site

State of ensemble: $\gamma = \sum_\nu p_\nu \delta_{x_1^{(\nu)}} \otimes \delta_{x_2^{(\nu)}} \otimes \delta_{x_3^{(\nu)}}$, p_ν occup. probab'ies

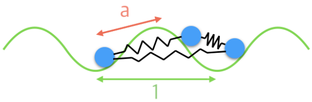


Example: $\gamma = \frac{1}{2}\delta_{a_2} \otimes \delta_{a_2} \otimes \delta_{a_3} + \frac{1}{3}\delta_{a_1} \otimes \delta_{a_1} \otimes \delta_{a_1} + \frac{1}{3}\delta_{a_4} \otimes \delta_{a_4} \otimes \delta_{a_4} + \frac{1}{6}\delta_{a_3} \otimes \delta_{a_3} \otimes \delta_{a_3}$

Simple counterexample to Monge ansatz

GF, arXiv 1808.04318

$X = \{1, 2, 3\} \subset \mathbb{R}$ three equi-spaced sites on the real line
Minimize $\int_{X^3} \big(v(|x-y|) + v(|y-z|) + v(|x-z|)\big)\, d\gamma(x,y,z)$
s/to $\gamma \mapsto \delta_1 + \delta_2 + \delta_3$
$v(r) = (r-a)^2$, $a = \frac{3}{4}$ (springs of bondlength 3/4)
Marginal condition + interaction ≈ Frenkel-Kontorova model



Unique minimizer $\gamma = S(\frac{1}{2}\delta_1 \otimes \delta_1 \otimes \delta_2 + \frac{1}{2}\delta_2 \otimes \delta_3 \otimes \delta_3)$
not Monge, not symmetrized Monge

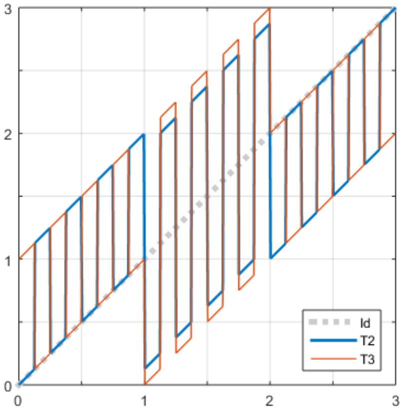
no. N of particles/marginals, no. ℓ of sites both minimal
N=2, any ℓ: Monge ansatz ok for *all* costs, Birkhoff-Von Neumann-theorem
any N, $\ell = 2$: follows from resuls of FMPCK, JCP 139,164109,2013

Continuous counterexample, formation of microstructure

partially inspired by DiMarino/Gerolin/Nenna fractal Monge map (2015)
Monge problem with no minimizer (GF, arXiv 2018): $\rho(x) \equiv 1/3$ on $[0,3]$,

$$\text{minimize} \int_0^3 \frac{\rho(x)}{3}\big(v(|x-T_2(x)|)+v(|T_2(x)-T_3(x)|)+v(|x-T_3(x)|)\big)\,dx$$

over T_2, T_3 transporting ρ to ρ, $v(r)=\frac{r^4}{4}-\frac{r^3}{3}$.



Convex geometry of the set of Kantorovich plans

Kantorovich polytope For finite $X = \{a_1, .., a_\ell\}$, any N, any given one-body density ρ, set of Kantorovich plans $\{\gamma \in \mathcal{P}_{sym}(X^N) : \gamma \mapsto \rho/N\}$ is a convex polytope.

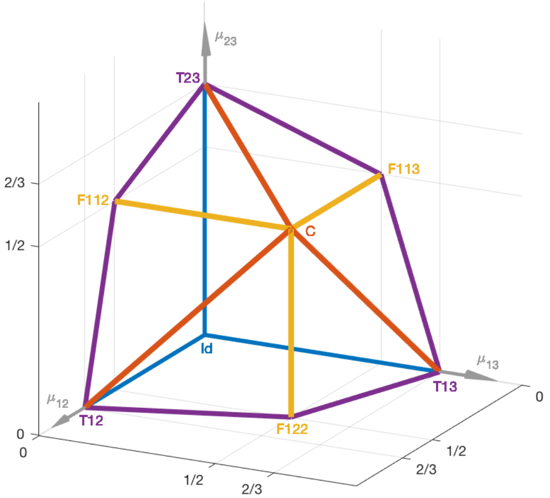
Typical costs (like Coulomb, springs from counterex., repulsive harmonic, ...) are 2-body, so cost depends only on 2-point marginal $\mu_{ij} = \sum_{k_3,..,k_N} \gamma_{ijk_3...k_N}$. Reduced Kantorovich polytope $= \mu's$ coming from γ's in the Kantorovich polytope.

Fruitful to analyze/visualize these polytopes and their extreme points

GF, arXiv 2018, $N = \ell = 3$
Vögler, arXiv 2019, larger N and ℓ, by computer
GF, Vögler, SIAM J.Math.Anal. 2018, sparse ansatz capturing all ext.pts

The reduced Kantorovich polytope for N=ℓ=3

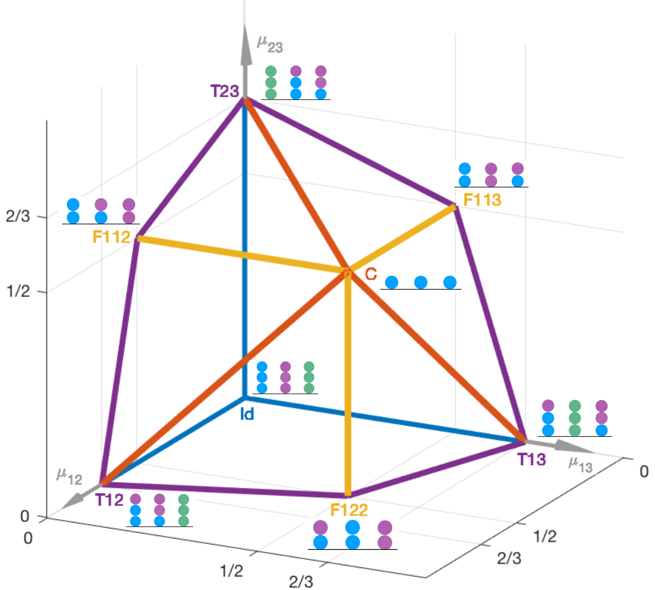
GF, arXiv 2018



8 extreme points, 5 Monge (blue, purple, red), 3 non-Monge (yellow)

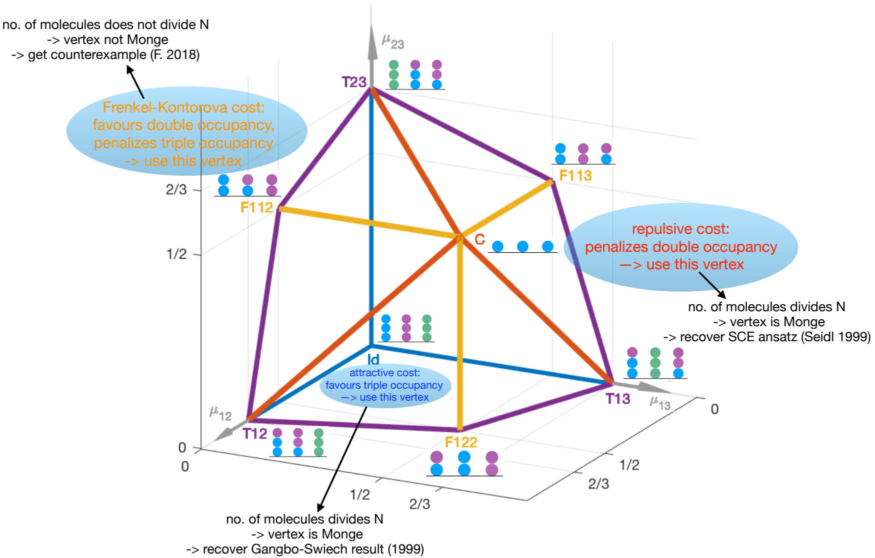
The reduced Kantorovich polytope for N=ℓ=3

GF, arXiv 2018



The reduced Kantorovich polytope for N=ℓ=3

GF, arXiv 2018



Breaking the curse of dimension

new ansatz replacing Monge: GF, Vögler, SIAM J.Math.Anal. 2018

finite state space $X = \{a_1, ..., a_\ell\}$, marginal $\mu = \sum_i \mu_i \delta_{a_i}$

Monge state $\in \mathcal{P}_{sym}(X^N)$:

$$\gamma = S \sum_{\nu=1}^{\ell} \mu_\nu \delta_{T_1(a_\nu)} \otimes \cdots \otimes \delta_{T_N(a_\nu)}$$

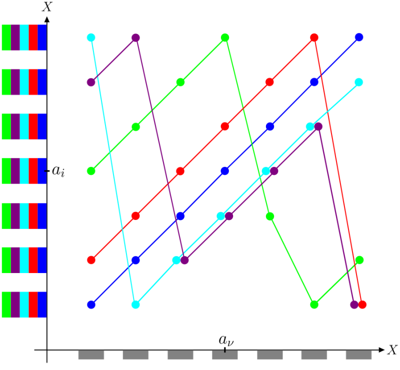
Each $T_1, ..., T_N : X \to X$ pushes μ forward to μ
(each map contributes one point to each site, $(T_i)_\sharp \mu = \mu$ for all i)

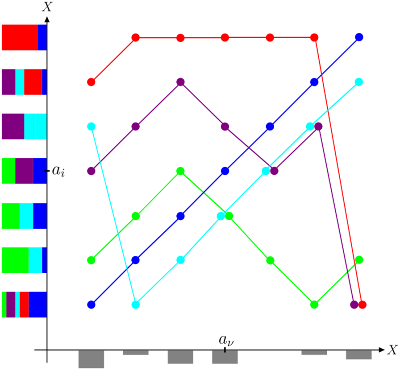
"Quasi-Monge" state $\in \mathcal{P}_{sym}(X^N)$: flexible site weights α_ν

$$\gamma = S \sum_{\nu=1}^{\ell} \alpha_\nu \delta_{T_1(a_\nu)} \otimes \cdots \otimes \delta_{T_N(a_\nu)}$$

Average push-forward of $\alpha = \sum_\nu \alpha_\nu \delta_{a_\nu}$ under the maps
$T_1, ..., T_N : X \to X$ is equal to to μ
(maps contribute unequally to different sites, $\frac{1}{N} \sum_{i=1}^{N} (T_i)_\sharp \alpha = \mu$)

Breaking the curse of dimension





Monge state:
each map contributes
one point to each site

"Quasi-Monge" state:
flexible site weights
maps contribute unequally to sites

Breaking the curse of dimension

Theorem (GF, Vögler, SIAM J.Math.Anal., 2018) For any number N of marginals, any cost $c : X^N \to \mathbb{R}$, and any marginal $\mu \in \mathcal{P}(X)$, the Kantorovich problem "Minimize $\int_{X^N} c\, d\gamma$ subject to $\gamma \to \mu$" admits a minimizer of "Quasi-Monge" form.

Breaking the curse of dimension

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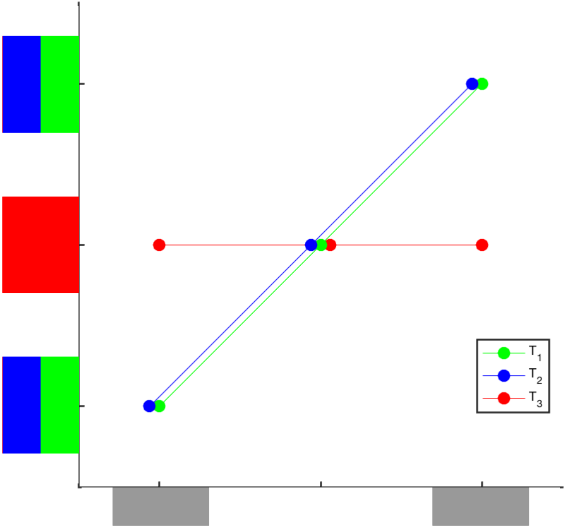
High-dimensional linear pb. $\longrightarrow$ low-dimensional nonlinear pb
$\binom{N+\ell-1}{\ell-1} \to \ell \cdot (N+1)$ DOF's.

The counterexample is quasi-Monge



Quasi-Monge problem formulated in terms of maps

GF, Vögler, SIAM J.Math.Anal. 2018

$$V_{ee}^{QSCE}[\rho] = \min_{\alpha,\, T_1,..,T_N} \int_{\mathbb{R}^3} \alpha(\mathbf{r}) \sum_{1 \le i < j \le N} \frac{1}{|T_i(\mathbf{r}) - T_j(\mathbf{r})|} d\mathbf{r}$$

subject to $\frac{1}{N}\sum_{i=1}^{N}(T_i)_\sharp \alpha = \rho$, α probability measure on $\mathbb{R}^3$

after discretiz.: minimizer exists, exactly same as Kantorovich pb., numerically nice

Summary

1) DFT in the strong correlation limit reduces to a highly nontrivial optimal transport problem.

2) Still not known whether, for this problem, Kantorovich = Monge

3) But, after discretization, Kantorovich = Quasi-Monge, thereby breaking the curse of dimension.

Thanks for your attention!

GF, arXiv 1808.04318

GF, Vögler, SIAM J.Math.Anal. 2018