Density Functional Theory meets (Multi-Marginal) Optimal Transportation

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The chemical behaviour of atoms and molecules is described by quantum mechanics.
Quantum mechanics for a molecule with N electrons boils down to the many-electron Schrödinger equation for a function $\psi \in L^2((\mathbb{R}\times\mathbb{Z}_2)^{3N};\mathbb{C})$, namely the wavefunction . The main drawback of this approach is computational. In order to predict the chemical behaviour of H_2O (10 electrons) using a 10 gridpoints discretization of $\mathbb{R}$, we need to solve the Schrödinger equation on 10^{30} gridpoints. Hohenberg, Kohn and Sham introduced, in [**?**] and [**?**], the Density Functional Theory as an approximate computational method for solving the Schrödinger equation at a more feasible cost.
The main idea of the DFT is to compute only the marginal $\rho(x_1) = \int \gamma_N dx_2 \cdots dx_N$, where $\gamma_N = \sum_{s_1,\cdots,s_N\in\mathbb{Z}_2} |\psi(x_1,s_1,\cdots,x_N,s_N)|^2$ is the joint probability density of electrons at positions $x_1,\cdots,x_N \in \mathbb{R}^3$ (and s_i is the spin variable), instead of the full wavefunction ψ. One of the scenario of interest for the DFT is when the repulsion between the electrons largely dominates over the kinetic energy. In this case we can reformulate it as an Optimal Transport problem.

Optimal transportation theory dates back to 1781 when Monge posed the problem of finding the optimal way to move a pile of dirt to a hole of the same volume. Kantorovich provided a generalised relaxed version in 1942. It is today known as the Monge-Kantorovich problem . Here we focus on the extension of the Monge-Kantorovich problem to the multi-marginal framework and its application to the DFT proposed in [**?**] and [**?**]. We propose to adapt a recently introduced [**?**] numerical method to solve it.

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