Distance calculations in quantum optimal transport

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Electronic structure calculations in quantum chemistry are currently numerically very demanding, as they require the resolution of high-dimensional nonlinear eigenvalue partial differential equations. The aim of this work is to propose fast approximations for the solutions of such equations by computing barycenters in the framework of quantum optimal transport. As a first step, we aim at computing distances between density matrices based on the Carlen–Mass distance [2]. The Carlen–Mass distance consists in generalizing the classical optimal transport formulation, namely the dynamical formulation in the quantum setting. This means that we replace integrals with traces, functions with operators or matrices, and we seek analogous results. The goal is to numerically compute these "quantum" distances between matrices.
In this poster, we first recall the classical optimal transport problem formulated by Bénamou and Brenier, using a dynamic formulation inspired by fluid mechanics [1]. This formulation serves as a bridge to noncommutative mathematics, where functions are replaced by operators. However, this noncommutative formulation remains quite abstract - only few authors have attempted to explicitly compute such distances. We then we present numerical methods for computing these distances between density matrices, including a method by Chen et al. [3] and a method directly inspired by Bénamou and Brenier [1]. The following step would be to compute barycenters of density matrices.

[1] J.-D. Benamou, Y. Brenier. *A computational fluid mechanics solution to the monge-kantorovich mass transfer problem.* Numerische Mathematik, **84(3)**, 375–393, 2000.

[2] E. A. Carlen, J. Maas. *Non-commutative calculus, optimal transport and functional inequalities in dissipative quantum systems.* Journal of Statistical Physics, **178(2)**, 319–378, 2019.

[3] Y. Chen, E. Haber, K. Yamamoto, T. T. Georgiou, A. Tannenbaum. *An efficient algorithm for matrix-valued and vector-valued optimal mass transport*, 2017.

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