Optimal Transport in Natural and Data Sciences
La théorie du transport dans les sciences naturelles et informatiques
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FANCH COUDREUSE, ENS de Lyon
Quantum Optimal Transport and applications to Quantum Gaussian states

Optimal Transport has proven to be a powerful tool in a wide range of mathematical subjects, and its application to the non-commutative and Quantum setting has attracted significant interest in recent years. In this seminar, we will provide a comprehensive introduction to the different formulations of Quantum Optimal Transport, from basic transport to regularized optimal transport. We will discuss the advantages and limitations of each formulation. In particular, we will focus on the transport of Gaussian states, which are commonly used in quantum information theory and quantum optics. Through this example, we will explore the key concepts and techniques involved in Quantum Optimal Transport, and discuss open research questions and future directions in the field.

ROBERT DE KEIJZER, Eindhoven University of Technology
Pulse based Variational Quantum Optimal Control for hybrid quantum computing

In this talk we discuss pulse based variational quantum algorithms (VQAs), which are designed to determine the ground state of a quantum mechanical system by combining classical and quantum hardware. In contrast to more standard gate based methods, pulse based methods aim to directly optimize the laser pulses interacting with the qubits, instead of using some parametrized gate based circuit. Using the mathematical formalism of optimal control, these laser pulses are optimized. This method has been used in quantum computing to optimize pulses for quantum gate implementations, but has only recently been proposed for full optimization in VQAs. Pulse based methods have several advantages over gate based methods such as faster state preparation, simpler implementation and more freedom in moving through the state space.

Based on these ideas, we present the development of a novel adjoint based variational method. This method can be tailored towards and applied in neutral atom quantum computers. This method of pulse based variational quantum optimal control is able to approximate molecular ground states of simple molecules up to chemical accuracy and is able to compete with the gate based variational quantum eigensolver in terms of total number of quantum evaluations. The total evolution time T and the form of the control Hamiltonian are important factors in the convergence behavior to the ground state energy, having influence on the quantum speed limit. Our VQOC method is able to converge to ground states of molecular problems for lower T than gate based algorithms can, mitigating decoherence effects.

DMITRY EVDOKIMOV, University of Ottawa
Computational aspects of Optimal Transport: classical and quantum

In this talk, I will discuss the computational aspects of the classical and quantum optimal transport problems. Starting from the entropy-regularized Kantorovich problem and Sinkhorn algorithm implementations, I proceed with a quantum analog of this problem and show the experiments for solving it in the particular case of Gaussian states.

MOHAMMAD ALI AHMADPOOR JADEHKENARY, Carleton University
Uniqueness of optimal plans for multi-marginal mass transport problems via a reduction argument

In this paper, by introducing a reduction argument, we investigate the relation between an optimal mass transport problem with N-marginals and its associated lower dimensional problems that consist of $k-$marginal problems for $k \in \mathcal{N} = \{1, \dots, N\}$. Namely, for a family of probability spaces $\{(X_k, \mathcal{B}_{X_k}, \mu_k)\}_{k=1}^N$ and a cost function $c : X_1 \times \cdots \times X_N \to \mathbb{R}$ we consider the

Monge-Kantorovich problem

$$\inf_{\lambda\in\Pi(\mu_1,\dots,\mu_N)}\int_{\prod_{k=1}^N X_k} c\,d\lambda. \tag{MKP}$$

Then for each ordered subset $\mathcal{P}=\{i_1,\dots,i_p\}\subsetneq\mathcal{N}$ we create a new cost function $c_{\mathcal{P}}$ corresponding to the original cost function c defined on $\prod_{k=1}^p X_{i_k}$. This new cost function $c_{\mathcal{P}}$ enjoys many of the features of the original cost c while it has the property that any optimal plan λ of (MKP) restricted to $\prod_{k=1}^p X_{i_k}$ is also an optimal plan to the problem

$$\inf_{\tau\in\Pi(\mu_{i_1},\dots\mu_{i_p})}\int_{\prod_{k=1}^p X_{i_k}} c_{\mathcal{P}}\,d\tau. \tag{RMKP}$$

Then, for appropriate choices of index set $\mathcal{P}$, we show that one can recover the optimal plans of (MKP) from (RMKP). Particularly, we determine situations in which the problem (MKP) admits a unique solution depending on the uniqueness of the solution to (RMKP). This allows us to prove many uniqueness results for multi-marginal problems when the unique optimal plan is not necessarily induced by a map. To this end, we extensively benefit from disintegration theorems and the c-extremality notion. Moreover, by employing the reduction method, besides recovering many standard results on the subject including the pioneering work of Gangbo-Swiech, several new applications will be demonstrated to evince the applicability of this method.

ADOLFO-VARGAS JIMENEZ, University of Ottawa

Dispersion Interactions in the Strictly Correlated Electron Limit of DFT via Multi-Marginal Optimal Transp

Multi-marginal optimal transport (MMOT) is the general problem of aligning a finite collection of probability measures to minimize some notion of overall cost. Due to its own substantial group of applications MMOT has attracted a great deal of attention. In particular, this problem with the well-known Coulomb cost has allowed the development of a mathematical framework to the strongly correlated systems in Density Functional Theory (DFT). In this talk, I will briefly introduce the mathematical settings for both MMOT and strongly correlated systems in DFT, and connect them with the dissociation limit in DFT.

This is joint work with Augusto Gerolin and Mircea Petrache.

ANNINA LIEBERHERR, University of Oxford

Optimal Transport distances for classifying electronic excitations

In chemistry, electronic excitations may be seen as an electron moving from one energy level to another. They are heuristically divided into three groups based on certain characteristics of the involved energy levels. Knowing which group an excitation belongs to can be useful, because calculated excitation energies can vary greatly in accuracy depending on which group the excitation belongs to. On the quest to finding a systematic classification, we introduce a diagnostic based on the Sinkhorn divergence from Optimal Transport and compare it to an existing one which uses the overlap. We then apply both to a selected set of molecules and study the quality of the resulting classifiers.

NATALIIA MONINA, University of Ottawa

Multimarginal Optimal Transport with Neural Networks

Optimal Transport problems arise naturally in many different fields such as Economics, Biology or Quantum Physics. In this talk, I will introduce the classical two-marginal optimal transport problem, and then generalize it to the problem with finitely many marginals. Finally, we will discuss computational algorithms solving the Entropy-Regularized Optimal Transport using Sinkhorn algorithm, and a novel one using Neural Networks.

BRENDAN PASS, Alberta