M.A.G.A. days

Monge-Ampère et Géométrie Algorithmique

November 15, 2019

Program

Figure 1: G. Monge

Wednesday (room 2L8, building 307)

- 14h00-14h50 Paola Gori-Giorgi
  Beyond the optimal transport limit of density functional theory: different strategies to reconstruct the effect of the kinetic correlation energy

- 15h50-15h40 Andrea Natale
  Dynamical optimal transport for density reconstruction with mixed finite elements

- 15h45-16h15 break (room 2L15)

- 16h15-17h10 Quentin Berthet
  TBA

- 17h10-18h00 Giulia Luise **Regularity properties of Entropic Optimal Transport in applications to machine learning**

Thursday (room 3L8, building 307)

- 9h00-9h50 Giovanni Conforti
  Energy-Transport inequalities and applications
- 9h50-10h15 break (room 2L15)
- 10h15-11h05 Silvio Fanzon
  Optimal transport regularization for variational inverse problems
- 11h05-11h55 Clement Sarrazin
  A lagrangian discretization for mean field games with congestion
- 12h-14h Lunch (room 2L15)
- 14h00-15h00 Thierry Champion (ANEDP seminar)
  Relaxed multi-marginal costs in optimal transport and quantization effects
- 15h 15h30 break (room 2L15)
- 15h30-16h25 Hugo Leclerc
  High Performance Computing of Power Diagrams for Optimal Transport

Abstracts

Paola Gori-Giorgi

Beyond the optimal transport limit of density functional theory: different strategies to reconstruct the effect of the kinetic correlation energy
The optimal transport (OT) limit of the density functional theory (DFT) formulation of the many-electron problem has been the object of several studies in the last decade with many new results. In this talk I will outline some strategies to include the quantum effects due to kinetic energy that are missed by the strict OT limit. In particular, I will present a new approach to dispersion (a.k.a. van der Waals) interactions in which the diagonal of the density matrix (marginal) of the two interacting fragments is kept fixed. This defines a modified OT problem in which an anisotropic harmonic cost is corrected with a gradient term. Although the approach is not exact by construction (as in the exact case the marginals are known to change) it highly simplifies the problem and yields surprisingly accurate (and in some cases even exact) results. I will also discuss strategies based on the entropic regularisation of the OT problem and on a semiclassical expansion.

Andrea Natale

Dynamical optimal transport for density reconstruction with mixed finite elements
Optimal transport offers a useful framework to interpolate and reconstruct densities undergoing transport phenomena. This is a common task in oceanography, for example, when one needs to analyse complex data describing the time evolution of variables such as temperature (SST), height (SSH) etc. In this context algorithms based on dynamical optimal transport are particularly attractive, since they offer great flexibility to regularize the dynamics and avoid unphysical results. Relying on the recent work of Lavenant [1] on the convergence of discretizations for dynamical optimal transport, we will define a class of convergent mixed finite element discretizations for this problem which are simple to implement and manipulate. We will connect these to existing discretizations and discuss how to include regularization terms which are relevant to density interpolation problems.

[1] Hugo Lavenant. Unconditional convergence for discretizations of dynamical optimal transport. arXiv preprint arXiv:1909.08790, 2019.

Quentin Berthet

TBA

Giulia Luise

Regularity properties of Entropic Optimal Transport in applications to machine learning
The entropic regularization has proved to be a powerful tool to define approximations of optimal transport distances with improved computational and statistical aspects. In this talk we will focus on further advantages of such entropic regularization, in terms of smoothness. We discuss its regularity properties and their role in some machine learning problems where regularized optimal transport is used as discrepancy metric in supervised and unsupervised frameworks.

Giovanni Conforti

Energy-Transport inequalities and applications
The study of the Schrodinger problem as an entropic regularisation of the Monge-Kantorovich problem leads naturally to consider the entropic transportation cost as a noisy version of the squared Wasserstein distance. In this talk, we mainly focus on a much less studied quantity related to the Schrodinger problem that also serves as a probabilistic counterpart to the Wasserstein distance and may be called energy, owing to its geometrical interpretation. We will show how this quantity can be linked to the entropic transportation cost via a functional inequality and how to use such inequality to study the ergodic behaviour of a

class of (mean field) stochastic control problems that includes the Schrodinger problem.

Silvio Fanzon

Optimal transport regularization for variational inverse problems
We propose and study a novel optimal transport based regularization of linear dynamic inverse problems. The considered inverse problems aim at recovering a measure valued curve and are dynamic in the sense that (i) the measured data takes values in a time dependent family of Hilbert spaces, and (ii) the forward operators are time dependent and map, for each time, Radon measures into the corresponding data space. The variational regularization we propose bases on dynamic optimal transport. We apply this abstract framework to variational reconstruction in dynamic undersampled MRI. Further we will present some ideas on conditional gradient methods for sparse reconstruction. This is joint work with Kristian Bredies, Marcello Carioni and Francisco Romero

Clement Sarrazin

A lagrangian discretization for mean field games with congestion
When approximating the solutions of variational mean field games with particle distributions, congestion terms in the energy that are only semi-continuous can behave awkwardly. I will first present a way to define a weaker congestion term for these energies that can be computed using methods inspired by semi-discrete optimal transport. Then, I will present a result in the spirit of Gamma-convergence of these "discretized" differential games towards the mean field game. Finally, I will conclude by some numerical results and computations of discrete solutions.

Thierry Champion

Relaxed multi-marginal costs in optimal transport and quantization effects
In this talk, we present a relaxation formula and duality theory for the multi-marginal Coulomb cost that appears in optimal transport problems arising in Density Functional Theory. The related optimization problems involve probabilities on the entire space and, as minimizing sequences may lose mass at infinity, it is natural to expect relaxed solutions which are sub-probabilities. We first characterize the N-marginals relaxed cost in terms of a stratification formula which takes into account all interactions of k particles, with k lower than N. We then develop a duality framework and deduce primal-dual necessary and sufficient optimality conditions. Finally we apply these results to a minimization problem involving a given continuous potential and we give evidence of a mass quantization effect for the optimal solutions. This is a joint work with G. Bouchitté (Univ. Toulon), G. Buttazzo (Univ. Pisa) and L. De Pascale (Univ. Firenze)

Hugo Leclerc

High Performance Computing of Power Diagrams for Optimal Transport

High speed computations of power diagrams in general settings has been the focus of several important and successful works by previous authors. For the case where the power diagrams are only intended to compute spatial integrals – meaning notably that the exact connectivity is not fully required – different kinds of optimizations remained to be developed and tested. In this talk, we will focus on the specific context of semi-discrete optimal transport, paying special attention on scalability, notably for computations on distributed memory hardware.