Optimal Transport and Optimal Patterns

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Abstracts

Benamou, Jean-David
Sinkhorn Algorithm and Stochastic Mean-Field Games
I will review the relationship between Sinkhorn Algorithm and the Schroedinger problem.
This shows that, via a detour with Multi-Marginal Optimal Transport, the Sinkhorn algorithm is well adapted to the numerical resolution of variational problems governed by Fokker-Planck equations.
This is typically the case for a class of Variational Mean Field Games.

Bucur, Dorin
Optimal partition problems and the honeycomb conjecture
In 2005-2007 Burdzy, Caffarelli and Lin, Van den Berg conjectured in different contexts that the sum (or the maximum) of the first eigenvalues of the Dirichlet-Laplacian associated to arbitrary cells partitioning a given domain of the plane, is asymptomatically minimal on honeycomb structures, when the number of cells goes to infinity. I will discuss the history of this conjecture, giving the arguments of Toth and Hales on the classical honeycomb problem, and I will prove the conjecture (of the maximum) for the Robin-Laplacian eigenvalues. The results have been obtained with I. Fragala, B. Velichkov and G. Verzini.

Cagnetti, Filippo
Optimal Lattice Quantizers and Best Approximation in the Wasserstein Metric
We will discuss the problem of the best approximation of the three-dimensional Lebesgue measure on a domain of volume 1 by a discrete probability measure supported on a Bravais lattice.

Choksi, Rustum
Optimal Centroidal Voronoi Tessellations: Gersho's Conjecture in 3D and Navigating the Energy Landscape
Nonconvex and nonlocal variational problems are pervasive in energy-driven pattern formation.
Two central issues are:

(Q1) can one conjecture and prove asymptotic statements on the (geometric) nature of global minimizers.

(Q2) can one develop systematic, hybrid numerical algorithms to navigate (or probe) the energy landscape and access low energy states whose basin of attraction might be ``tiny";

In this talk, we explore both (Q1) and (Q2) in the context of the simple, yet rich, paradigm of optimal quantization and centroidal Voronoi tessellations (CVT). We begin with (Q1) via the 3D Gersho's conjecture. Gersho's conjecture may be viewed as a crystallization conjecture and asserts the periodic structure, as the number of generators tends to infinity, of the optimal CVT. In joint work with Xin Yang Lu (Lakehead University), we present certain bounds which, combined with a 2D approach introduced by P. Gruber, reduce the resolution of the 3D Gersho's conjecture to a finite (albeit very large) computation of an explicit convex problem in finitely many variables.

In ongoing work with Ivan Gonzales and JC Nave (McGill University), we address (Q2) by presenting a new hybrid algorithm which alternates gradient descent (or Lloyd's method) with movement away from the closest generator.
We also address and partially explain some interesting observations about defect structures and optimal CVTs for a small number of generators on the 2D flat torus.

Cotar, Codina

Universality class of Coulomb and Riesz costs

We consider two sharp next-order asymptotics problems, namely the asymptotics for the minimum energy for optimal point configurations and the asymptotics for the many-marginals Optimal Transport, in both cases with Riesz costs with inverse power-law long-range interactions. The first problem describes the ground state of a Coulomb or Riesz gas, while the second appears as a semiclassical limit of the Density Functional Theory energy modelling a quantum version of the same system. Recently the second-order term in these expansions was precisely described, and corresponds respectively to a Jellium and to a Uniform Electron Gas model. The present work shows that for inverse-power-law interactions with power s\in [d-2,d), d\ge 2 dimensions, the two problems have the same minimum value asymptotically. For the Coulomb case in d= 3, our result verifies the physicists long-standing conjecture regarding the equality of the second-order terms for these two problems.
Furthermore, our work implies that, whereas minimum values are equal, the minimizers may be different. Moreover, provided that the crystallization hypothesis in d= 3 holds, which is an extension of Abrikosovs conjecture originally formulated in d= 2, then our result verifies the physicists conjectured \approx 1.4442 lower bound on the famous Lieb- Oxford constant. Our work also rigorously confirms some of the predictions formulated by physicists, regarding the optimal value of the Uniform Electron Gas second-order asymptotic term. Additionally, we show that on the whole range s\in (0,d), the Uniform Electron Gas second-order constant is continuous in s. Besides, our method provides a novel and robust alternative technique to the screening method of Sandier and Serfaty for the next order term in the Coulomb and Riesz gases problems. Our results can be extended to a larger class of models than power-law-type radial costs, such as non-rotationally invariant costs.

(This is based on joint works with Mircea Petrache).

Cristoferi, Riccardo

Clustering of Big Data: consistency of a nonlocal Ginzburg-Landau type model The analysis of Big Data is one of the most important challenges of the modern era. A first step in order to extract some information from a set of data is to partition it according to some notion of similarity. When only geometric features are used to define such a notion of similarity and no a priori knowledge of the data is available, we refer to it as the clustering problem.

Typically this labeling task is fulfilled via a minimization procedure. Of capital importance for evaluating a clustering method is whether it is consistent or not; namely it is desirable that the minimization procedure approaches some limit minimization method when the number of elements of the data set goes to infinity.

In this talk the consistency of a nonlocal anisotropic Ginzburg-Landau type functional for clustering is presented. In particular, it is proved that the discrete model converges, in the sense of Gamma-convergence, to a weighted anisotropic perimeter.

The talk is based on a work in collaboration with Matthew Thorpe (Cambridge University).

De Luca, Lucia

Crystallization results for pairwise interaction energies in two dimensions

I will present some recent crystallization results concerning pairwise interaction energies.
First, I will focus on minimizers and quasi-minimizers of the so-called Heitmann-Radin sticky disc functional. I will show that, renormalizing the Heitmann-Radin potential by subtracting the minimal energy per particle (i.e., the kissing number), configurations scaling like a perimeter converge to a polycrystal. More precisely, the empirical measure converges - as the number of particles diverges - to a set of finite perimeter, and a microscopic variable, representing the orientation of the underlying lattice, converges to a locally constant function.
Such a compactness result is accompanied by a Gamma-convergence result in the case that the

limit configuration is a single crystal, namely it has a constant orientation.

In the second part of the talk, I will consider a new pairwise interaction potential inspired by the Heitmann-Radin one for which I show a crystallization result in the square lattice in the thermodynamic limit. Time permitting, I will show how such a crystallization result can be extended to smooth and long range potentials satisfying suitable growth and convexity assumptions.
Finally, I will illustrate some open problems.

The results I will present are obtained in several works in collaboration with L. Bétermin (Copenaghen), G. Friesecke (Muenchen), M. Novaga (Pisa), M. Petrache (Santiago), M. Ponsiglione (Rome).

Mérigot, Quentin
Particle discretization of evolution equations through semi-discrete optimal transport
We will show how to approximate numerically some evolution equations which can be obtained as the evolution of a probability density under the gradient flow of an energy functional, with respect to the Wasserstein distance. Such equations
include the Fokker-Planck equation, or equations describing the movement of a crowd in a situation of emergency evacuation. The main novel idea is to use the Moreau-Yosida regularization of the energy functional, which is finite for all probability measures, and can be computed efficiently when the measure is a finite sum of Dirac masses.

Joint work with Hugo Leclerc, Filippo Santambrogio and Federico Stra.

Peletier, Mark
Continuum limit of a hard-sphere particle system by large deviations
Many stochastic particle systems have well-defined continuum limits: as the number of particles tends to infinity, the density of particles converges to a deterministic limit that satisfies a partial differential equation. In this talk I will discuss one example of this.

The particle system consists of particles that have finite size: in two and three dimensions they are spheres, in one dimension rods. The particles cannot overlap each other, leading to a strong interaction with neighbouring particles.

Such systems of particles have been much studied, but for the continuum limit in dimensions two and up there is currently no rigorous result. There are conjectures about the form of the limit equation, often in the form of Wasserstein gradient flows, but to date there are no proofs.

We also cannot give a proof of convergence in higher dimensions, but in the one-dimensional situation we can give a complete picture, including both the convergence and the gradient-flow structure that derives from the large-deviation behaviour of the particles. This gradient-flow structure shows clearly the role of the free energy and the Wasserstein-metric dissipation, and how they derive from the underlying stochastic particle system.

The proof is based on a special mapping of the particle system to a system of independent particles, that is unique to the one-dimensional setup. This mapping is an isometry for the Wasserstein metric, leading to a beautiful connection between limit equations for interacting and non-interacting particle systems.

This is joint work with Nir Gavish and Pierre Nyquist.

Pelloni, Beatrice
Optimal transport techniques in geophysical fluid dynamics
I will survey the use and potential of these techniques for solving the semi-geostrophic equations.

Roper, Steven
Centroidal power diagrams and control of microstructure.
We present an approach to obtain representative volume elements for modelling the grain structure of metals, using optimal transport and centroidal power diagrams (Laguerre Voronoi diagrams).

Santambrogio, Filippo
Weighted very fast diffusion equation arising in quantization of measures
The problem of the optimal quantization of probability measures consists in approximating a given density f with a finite number (N) of atoms. For fiwed N, this can be tackled by letting an initial configuration evolve in time by considering a continuous-time variant of the well-known Lloyd's algorithm, where every point points to the center f its Voronoi cell. When N tends to infinity, Gamma-convergence tells us which is the limit functional, and one can consider its gradient flow in the W_2 Wasserstein space. Since the functional includes a negative power of the density, the resulting PDE is similar to a porous-medium equation with negative exponent (ultrafast diffusion). Exploiting the gradient flow structure, in particular through the so-called JKO scheme, we introduce a notion of weak solutions, prove existence, uniqueness, BV and H^1 estimates, L^1 weighted contractivity, instantaneous regularisation, Harnack inequalities, and in some cases exponential convergence to a steady state. The talk will give a flavor of these questions, in particular insisting on the optimal transport techniques.

Scardia, Lucia
Equilibrium measures for nonlocal energies: The effect of anisotropy
Nonlocal energies are continuum models for large systems of particles with long-range interactions. Under the assumption that the interaction potential is radially symmetric, several authors have investigated qualitative properties of energy minimisers. But what can be said in the case of anisotropic kernels? Motivated by the example of dislocation interactions in materials science, we pushed the methods developed for nonlocal energies beyond the case of radially symmetric potentials, and discovered surprising connections with random matrices and fluid dynamics.

Schmitzer, Bernhard
Particle trajectories from dynamic PET via optimal transport regularization.
Positron emission tomography (PET) can measure the distribution of radiolabelled biomarkers in the body. For research and therapy it is desirable to trace small amounts of markers as they flow through the patient. Unfortunately conventional PET image reconstruction techniques break down in this regime due to particle motion and low signal intensity.
We propose a functional which explicitly models the flow of the biomarker and enforces temporal consistency by regularization with optimal transport.

Schönlieb, Carola-Bibiane
Wasserstein for learning image regularisers
In this talk I will present the results of our recent NeurIPS paper on adversarial regularisers for inverse problems which are trained with an objective function that approximates the 1-Wasserstein distance. I will discuss what we understand about this training procedure theoretically and showcase the performance of the learned regulariser for computed tomography imaging. This is joint work with Sebastian Lunz and Ozan Öktem.

Theil, Florian
Order in particle systems with randomness
We investigate the effect of randomness on optimal patterns in the context of particle systems. In a collaboration with Alessandro Giuliani (Roma Tre) we have obtained new results for a discrete microscopic model for an elastic crystal with dislocations in three dimensions, previously introduced by Ariza and Ortiz. The model is rich enough to support some realistic features of three-dimensional dislocation theory, most notably grains and the Read-Shockley law for grain boundaries. At sufficiently low temperatures the Gibbs distribution exhibits long range positional order, i.e. the translational invariance of the crystalline ground state remains intact.

Thorpe, Matthew

Continuum Limits in Semi-Supervised Learning

Given a data set $\{x_i\}_{i=1}^n$ with labels $\{y_i\}_{i\in Z_n}$, where $Z_n \subset \{1, \dots , n\}$ the goal of semi-supervised learning is to infer labels on the remaining $\{x_i\}_{i\not\in Z_n}$ data points. In this talk we use a random geometric graph model with connection radius ε_n. The framework is to consider objective functions which reward the regularity of the estimator function and impose or reward the agreement with the training data, more specifically we will consider discrete p-Laplacian regularization.

The talk concerns the asymptotic behaviour as $n \to \infty$. To compare labelling functions on different domains we use a metric based on optimal transport which then allows for the application of methods from the calculus of variation, in particular, Γ-convergence. We will consider two regimes. In the first regime the number of labelled points remains finite, i.e. $Z_n = \{1, \dots , N\}$ for some fixed N. The results are to uncover a delicate interplay between the regularizing nature of the functionals considered and the nonlocality inherent to the graph constructions. I will give almost optimal ranges on the scaling of ε_n for asymptotic consistency to hold. In the second regime we allow $|Z_n| \to\infty$. We give a lower bound on the rate at which $|Z_n| \to \infty$ sufficient for the case $p = 2$ to be asymptotically well-posed.

This is joint work with Jeff Calder (Minnesota) and Dejan Slepcev (CMU).

Wirth, Benedikt

Semi-discrete unbalanced optimal transport and qualtization

In applications, the requirement of optimal transport models to leave the total amount of mass invariant is often violated, which can be remedied by so-called unbalanced transport. We study the special case of semi-discrete unbalanced transport, where one of the masses is discrete and the other Lebesgue-continuous and which (as in the classical semi-discrete transport) is related to tesselation problems. As an application we consider the quantization problem and its asymptotics. This is joint work with David Bourne and Bernhard Schmitzer.