Optimal Transport and Dynamics (24w5198)

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1 Overview of the Field

The *optimal transport* (OT) or *Monge-Kantorovich* problem is a variational problem where one attempts to couple two mass distributions in some optimal manner. The original formulation of the problem, proposed by Gaspard Monge in 1781 ([43]), is as follows: given two probability measure spaces, (X, μ) and (Y, ν), and a measurable *cost function* $c : X \times Y \to \mathbb{R}$, minimize the functional $\int_X c(x, T(x))d\mu(x)$ over the set of measurable mappings $T : X \to Y$ satisfying the push-forward condition $T_{\#}\mu = \nu$. Such a minimizer is known as a *Monge solution*. In the 1950s, Kantorovich introduced a relaxation of the problem and a related dual problem ([30]), henceforth the problem has also been known as the Monge-Kantorovich problem. This is a stationary problem, but turns out to have many important ties to dynamics.

Interest in the relations between OT and dynamics broadly falls into two categories. The first is the use of dynamical methods to analyze the solutions of the optimal transport problem itself: these are methods such as parabolic OT, fluids based numerical algorithms, and the Benamou-Brenier dynamical formulation. The second is the use of the structure induced by optimal transport in order to rigorously define dynamics in more singular situations: the framework of gradient flows on metric spaces and Lagrangian models for diffusions and congested dynamics, along with various geometric flows fall within this category.

2 Recent Developments and Open Challenges

Monge-Ampère equations.

In many physical and geometric applications, one is interested in finding a mapping between spaces whose Jacobian satisfies some prescribed equation. In certain cases, one expects the map to be determined by some scalar potential function (and its derivatives). Such a situation yields a partial differential equation of Monge-Ampère type for the potential function. In the simplest example of cyclically monotone mappings in Euclidean space, the mappings are the gradient of a scalar convex potential and this results in the classical real Monge-Ampère equation: the determinant of the Hessian of the (convex) potential is prescribed. More sophisticated examples include the *optimal transport map* in the Monge-Kantorovich problem; the *ray tracing map* in geometric optics problems involving reflection / refraction; and the *Gauss map* in the classical Minkowski problem. The study of these problems is relevant to many fields, including nonlinear optimization and calculus of variations, differential geometry, geometric optics, probability, and economics (stable matching problems).

Starting with Brenier's work [7], it has been observed that, for a large class of cost functions defined on products of smooth manifolds, a Monge solution can be obtained from the gradient of a real-valued potential function u that solves an elliptic PDE of Monge-Ampère type coupled with the so-called second boundary condition, which encodes the act of transporting mass from the source to the target. The regularity theory for such PDEs leads directly to smoothness results for Monge solutions of OT, and a robust theory has been developed in a fairly general setting ([9, 19, 10, 51, 39, 21, 17, 25]). Based on this connection between OT and Monge-Ampère equations, a natural dynamical approach to solving the OT problem is to find solutions of this elliptic PDE as stationary states for a related *parabolic* PDE of the form

$$\partial_t u - \log\det(D^2 u + A(x, \nabla u)) = \psi(x, \nabla u),$$

for some matrix-valued function A and a scalar-valued function ψ determined by the cost function and source and target measures. A number of existence, global regularity, and asymptotic convergence results are known for the parabolic OT problem in the high regularity setting for various costs ([49, 48, 33]). It is also known that, when the data are sufficiently regular, solutions of the parabolic OT equation converge *exponentially fast* to the stationary elliptic solution, as shown in [32, 1]. Recently there has been interest in using the parabolic approach to develop fast numerical methods: an implementation in a single spatial dimension can be found in [6].

Existing results for this parabolic Monge-Ampère equation are only valid in the regime where the data involved possess a large amount of a priori regularity. A recent interesting approach due to Berman [4] suggests a weak formulation for the parabolic OT equation by capitalizing on a connection with scaling limits of the so-called Sinkhorn algorithm for doubly stochastic matrices [50]. In the setting of OT, the Sinkhorn algorithm provides a method for computing approximate minimizers of a regularized version of the OT problem between discrete measures. This regularization involves by adding an *entropy* term to the total cost functional [16]. In [4], Berman shows that, given iterates generated by the Sinkhorn algorithm for a sequence of entropy regularized problems on the torus, if the size of the spatial discretization and the regularization parameter for the entropy term both approach zero in a prescribed manner, then one recovers a solution of the parabolic OT equation in the limit, assuming the source and target measures are sufficiently regular. It may be possible to use this observation as a starting point for the definition of a weak solution of the parabolic OT problem for less regular data.

In another direction, questions of *partial regularity* for Monge-Ampère equations are an active and difficult area of interest. Results such as [20, 18] address how small the closure of the singular set of a Monge-Ampère equation can be in terms of measure, while delicate questions about the Hausdorff dimension are rather open (see [44] for certain developments). Another recent approach to this partial regularity problem is an ϵ-regularity based method ([23, 24, 42, 47]) which is a direction rich for exploration.

Gradient flows. OT plays a significant role in the development of a rich theory of gradient flows for functionals defined on (possibly singular) metric spaces. If (X, d) is a Polish space, then for $\mu_1, \mu_2 \in \mathcal{P}_2(X)$ (the space of probability measures on X with bounded second moment) the 2-*Wasserstein metric* $W_2(\mu_1, \mu_2)$ is defined by the square root of the minimum value in the Kantorovich problem between μ_1 and μ_2 with cost function d^2. The Wasserstein metric lifts the metric structure of X to $\mathcal{P}_2(X)$, which in some sense has "better regularity" than the original space X. One can then consider gradient flows of a functional F on $\mathcal{P}_2(X)$ as defined by *curves of maximal slope* (see [3]).

The seminal paper of Jordan, Kinderlehrer, and Otto [29] shows that the heat equation on Euclidean space can be viewed as the gradient flow of the Boltzmann entropy on $\mathcal{P}_2(\mathbb{R}^n)$ equipped with the 2-Wasserstein metric W_2. This is shown in [29] by using an implicit Euler scheme in $\mathcal{P}_2(\mathbb{R}^n)$, considering the sequence of probability measures $\{\rho_k\}$ (the Moreau-Yosida approximations) generated via the iterative procedure

$$\rho_{k+1} = \operatorname*{argmin}_{\rho} F(\rho_k) + \frac{1}{2h} W_2(\rho, \rho_k)^2.$$

Taking an appropriate scaling limit in h yields a gradient flow of F in $\mathcal{P}_2(\mathbb{R}^n)$.

The ideas in [29] are robust enough to be applied to a diverse family of dissipative evolution evolutions, such as the porous medium equation [46], thin film equations [40], and the Keller-Segel system [5]. More recently the JKO scheme was successfully modified to address problems with more general energy structure. The scheme, in particular, provides a general variational approach to approximate and generate physically meaningful weak solutions for problems that typically lack classical solutions. One example of recent progress is on interface motions for incompressible fluids, such as the Hele-Shaw flow with drift ([41, 2, 15]), the Muskat problem with surface tension ([27]) and the Mullins-Sekerka flow ([45, 14]). Another set of results concerns systems of multi-species equations, such as cross-diffusion systems in population dynamics ([8, 31]), multi-fluid systems in porous media ([22, 11, 12]), and systems of tumor growth ([28]). Most of the established results so far focus on achieving global-in-time existence of weak solutions with energy dissipation structure. Much remains to be achieved in order for the scheme to successfully address qualitative properties of continuum solutions, such as stability and long time behavior. The general challenge for further qualitative analysis lies in capturing sufficient compactness in the scheme that survives in the continuum limit. For the aforementioned systems the difficulty lies in tracking different population densities in the evolution to rule out infinitesimal mixing phenomena. A Lagrangian point of view may prove useful in this regard ([13, 26]).

Cosmology. Related to the dynamical formulation of OT by Benamou and Brenier, there has been independent interest in computational modeling of the dynamics of the early universe using OT. A major goal of astrophysicists is to accurately reconstruct the state of the early universe based on the observed current state of the universe. It is too difficult to reconstruct the evolution of all particles to any semblance of accuracy, as this corresponds to an N-body problem for a horrendously large N. However, the current universe can be viewed as a collection of high density structures of relatively small (on the order of a few Megaparsecs) diameter. By collapsing such structures into singular parts of a mass distribution, and making the widely accepted ansatz that the initial universe consisted of an almost constant distribution of mass (both visible and dark matter), the Benamou-Brenier dynamical formulation can be used to give a unique reconstruction of early states for the universe.

Recently there has been development of higher precision instruments such as the James Webb Space Telescope, and the release of newer, more comprehensive data through efforts such as the European Space Agency's Gaia mission. This has led to a renewed interest in the use of OT for early universe reconstruction, for example [37]. However, these more recent data sets are very large and require the development of more robust and efficient numerical methods, an effort in this direction is the damped Newton method in [34] in the semi-discrete case, as implemented and utilized in [35, 38, 36].

3 Presentation Highlights

The workshop presentations provided updates on several recent applications of optimal transport theory to problems in dynamics, as well as on developments in the theory of optimal transport itself, which may have future application to tackling open problems in dynamics.

- **Cristian Gutiérrez: Fine Properties of Monotone Maps arising in Optimal Transport for non quadratic costs.**

  Gutiérrez's talk focused on recent results concerning various properties of mappings arising in optimal transport problems for non quadratic costs. The cost functions considered have the form $c(x, y) = h(x - y)$, where $h \in C^2(\mathbb{R}^n)$ is convex, positively homogeneous of degree $p \geq 2$, and $D^2h(x)$ has eigenvalues bounded away from zero and infinity for all $x \in \mathbb{S}^{n-1}$. A multivalued mapping $T : \mathbb{R}^n \to \mathcal{P}(\mathbb{R}^n)$ is c-monotone if $c(\xi, x) + c(\zeta, y) \leq c(\xi, y) + c(\zeta, x)$ for all $\xi \in Tx, \zeta \in Ty$ for all $x, y \in \mathbb{R}^n$. Optimal maps with respect to the cost c are c-monotone. If $h(x) = |x|^2$, then c-monotonicity is the standard monotonicity $(\xi - \zeta) \cdot (x - y) \geq 0$ having a large number of applications to optimization and nonlinear evolution PDEs. Gutiérrez presented recent work with Annamaria Montanari (U. of Bologna) where, motivated by recent results of M. Goldman and F. Otto concerning partial regularity of optimal transport maps for the quadratic cost, they show that c-monotone mappings T are single valued a.e. as well as establish local L^∞-estimates on balls for $u(x) = Tx - Ax - b$ for each matrix

A and each vector b in terms of averages of u on a slightly larger ball. As a consequence, their work deduces differentiability of T a.e., shows that these maps are related to maps of bounded deformation, and derives further differentiability and Hölder continuity properties.

- **Alfred Galichon: A model of dynamic matching.**

  Galichon's talk drew from their working paper "Repeated Matching Games: An Empirical Framework" with Pauline Corblet and Jeremy Fox, where they introduce a model of dynamic matching with transferable utility, extending the static model of Shapley and Shubik (1971). Forward-looking agents have individual states that evolve with current matches. Each period, a matching market with market-clearing prices takes place. Galichon and co-authors prove the existence of an equilibrium with time-varying distributions of agent types and show it is the solution to a social planner's problem. They also prove that a stationary equilibrium exists and introduce econometric shocks to account for unobserved heterogeneity in match formation. Galichon proposed two algorithms to compute a stationary equilibrium and adapt both algorithms for estimation. Finally, Galichon estimated a model of accumulation of job-specific human capital using data on Swedish engineers.

- **Will Feldman: A rate-independent model of droplet evolution.**

  Feldman's talk explained the phenomenon of contact angle pinning/hysteresis at a heuristic level and then discussed some models for rate independent motion of capillary drops under the effects of pinning/hysteresis. Feldman presented work with Inwon Kim, Norbert Pozar, and Carson Collins, studying the regularity and other fine properties of solutions, including uniqueness using energy and comparison based formulations.

- **Matias Delgadino: Generative Adversarial Networks: Dynamics and Mode Collapse.**

  Generative Adversarial Networks (GANs) was one of the first Machine Learning algorithms to be able to generate remarkably realistic synthetic images. In their presentation, Delgadino delved into the mechanics of the GAN algorithm and its profound relationship with optimal transport theory. Through a detailed exploration, Delgadino illuminated how a GAN approximates a system of PDE, particularly evident in shallow network architectures. Furthermore, Delgadino investigated the phenomenon of mode collapse, a well-known pathological behavior in GANs, and elucidated its connection to the underlying PDE framework through an illustrative example.

- **Caroline Moosmüller: Trajectory Inference in Wasserstein Space**

  Capturing data from dynamic processes through cross-sectional measurements is seen in fields from computer graphics to robot path planning and cell trajectory inference. This inherently involves the challenge of understanding and reconstructing the continuous trajectory of these processes from discrete data points, for which interpolation and approximation plays a crucial role. In their talk, Moosmüller presented joint work with Amartya Banerjee, Harlin Lee, and Nir Sharon, where they propose a method to compute measure-valued B-splines in the Wasserstein space through consecutive averaging. This method can carry out approximations with high precision and at a chosen level of refinement, including the ability to accurately infer trajectories in scenarios where particles undergo splitting (division) over time. In their paper, Moosmüller and co-authors rigorously evaluate their method using simulated cell data characterized by bifurcations and merges, comparing its performance against both state-of-the-art trajectory inference techniques and other interpolation methods. The results of their work not only underscore the effectiveness of their method in addressing the complexities of inferring trajectories in dynamic processes but also highlight its proficiency in performing spline interpolation that respects the inherent geometric properties of the data.

- **Seonghyeon Jeong: Optimal Transportation problem on a surface of a convex body without twisted condition.**

  Regularity of solutions of optimal transportation problems has been well studied with relation to Monge-Ampère type equations. There are several conditions such as the twist condition or MTW condition on the cost function, which one needs to use in the analysis of Monge-Ampère type equations to study the regularity of optimal transportation problems. However, one can easily come up with examples which do not satisfy such conditions. In their talk, Jeong considered the optimal transportation problem on a boundary of a convex body with Euclidean distance squared cost function, which does not satisfy the twist condition. Jeong discussed how to get regularity in this case.

- **Henok Mawi: Optimal Transport in the Design of Freeform Optical Surfaces**

  The theory of optimal transport has been used successfully to model several freeform lens design problems. A freeform optical surface, refers to an optical surface (lens or mirror) whose shape lacks rotational symmetry. The use of such surfaces allows design of spatially efficient optical devices. In their talk, Mawi exhibited the existence of a far field refracting lens between two anisotropic media by using the optimal transport framework.

- **René Cabrera: An optimal transport problem with interaction effects**

  Cabrera spoke about a modification of the Monge-Kantorovich problem taking into account interaction effects via path dependency between particles. Cabrera's work proves the existence of solutions under mild conditions on the data, and after imposing stronger conditions, characterizes the minimizers by relating them to an auxiliary Monge-Kantorovich problem of the more standard kind. With this notion of how particles interact and travel along paths, Cabrera produced a dual problem. The main novelty here is to incorporate an interaction effect to the optimal path transport problem. Lastly, Cabrera's results include an extension of Brenier's theorem on optimal transport maps and a formulation of the celebrated Benamou-Brenier theory with interaction effects.

- **Héctor Chang-Lara: A dynamic model of congestion**

  Chang-Lara addressed the problem of assigning optimal routes in a graph that transport two given densities over the nodes. The occupation of each edge at a given time defines a metric over this graph, for which the routes must be geodesics. This model may describe for example the congestion of a city and its solutions are known as Wardrop equilibria. Additionally, a central planner can require that the assignment is efficient, meaning it minimizes the Kantorovich functional arising from this metric. In their presentation, Chang-Lara characterized this problem in terms of a partial differential equation and illustrated a simple case. The results presented were from work in collaboration with Sergio Zapeta Tzul, a former MSc student at CIMAT and current PhD student at the University of Minnesota.

- **Alpár Mészáros: From the porous medium equation to the Hele-Shaw flow: an optimal transport perspective**

  Mészáros' talk, based on a recent joint work with Noemi David and Filippo Santambrogio, revisited the classical problem on the Hele-Shaw or incompressible limit for nonlinear degenerate diffusion equations. Mészáros demonstrated that the theory of optimal transport via gradient flows can bring new perspectives, when it comes to considering confining potentials or nonlocal drift terms within the problem. In particular, Mészáros provided quantitative convergence rates in the 2-Wasserstein distance for the singular limit, which are global in time thanks to the contractive property arising from the external potentials.

- **Sangmin Park: A variational perspective on the Vlasov-Fokker-Planck equation**

  It is well-known that the Vlasov-Fokker-Planck equation can be formally seen as a dissipative Hamiltonian system in the Wasserstein space of probability measures. In order to better understand this geometric formalism, Park proposed a time discrete variational scheme whose solution converges to the weak solution of the Vlasov-Fokker-Planck equation. Park discussed how the variational scheme can be seen as an implementation of the symplectic Euler scheme in the Wasserstein space. Moreover, Parks showed that the energy functionals involved in each variational problem are geodesically convex with respect to the metric.

- **Kerrek Stinson: Some geometric perspectives for adversarial training: Perimeters and Mean Curvature Flows.**

  Recent work views adversarial training for binary classification as the minimization of a fidelity term and a non-local perimeter, opening the door to geometric perspectives. Stinson presented joint work with Leon Bungert (Wuerzburg) and Tim Laux (Regensburg), where they showed that, as the adversarial budget vanishes, the non-local perimeter Gamma-converges to an anisotropic perimeter that reflects the stability of adversarial training. Interpreting the full adversarial training problem is a bit tricky. It is possible to rely on a source condition or, alternatively, take a dynamic approach. For the latter, Stinson and co-authors introduced a slight modification of the adversarial training scheme, which can be seen as a minimizing movements scheme for the non-local perimeter functional. From this, they draw rigorous connections to a weighted mean curvature flow, indicating that the efficacy of adversarial training may be due to locally minimizing the length of the decision boundary.

- **Zhonggan Huang: Regularity theory of a gradient degenerate Neumann problem.**

  Huang, in joint work with Will Feldman, studied the regularity and comparison principle for a gradient degenerate Neumann problem. This problem is a generalization of the Signorini or thin obstacle problem which appears in the study of certain singular anisotropic free boundary problems arising from homogenization. In scaling terms, the problem is critical since the gradient degeneracy and the Neumann PDE operator are of the same order. Huang showed the (optimal) $C^{1,\frac{1}{2}}$ regularity in dimension $d = 2$ and the same regularity result in dimension $d > 2$ conditional on the assumption that the degenerate values of the solution do not accumulate. Huang also proved a comparison principle characterizing minimal supersolutions, which may have applications to homogenization and other related scaling limits.

- **Nikhil Padmanabhan: Reconstructing the Initial Conditions of the Universe with Optimal Transport.**

  Padmanabhan began with an overview of some of the key questions in cosmology today and discussed the “reconstruction problem” – inferring the initial conditions of the Universe from our late time observations. Padmanabhan then discussed how optimal transport might provide an elegant solution to the reconstruction problem and concluded with open questions to potentially seed further discussion.

- **Bruno Lévy: Optimal Transportation: your round-trip ticket to the edge of the Universe.**

  Lévy presented on-going works in Optimal Transport for cosmology with Roya Mohayaee, Yann Brenier, Farnik Nikakhtar, Sebastian von Hausegger, Ravi Sheth, and Nikhil Padmanabhan. Lévy focused on the following aspects of their works:

  – Early Universe reconstruction, an inverse problem that aims at reconstructing the trajectories of galaxies, back in time.

  – Forward simulation of Monge-Ampére gravity, to test some non-linear models of Dark Matter and Dark Energy.

- **Farnik Nikakhtar: Reconstruction/Forward Modeling of Large-Scale Structures Using Optimal Transport Theory.**

  The universe we observe today is dotted with galaxy clusters separated by vast voids, in sharp contrast to its initial state, which was nearly uniform with only minor density fluctuations. The evolution from this early uniformity to today’s complex structure of galaxies is a profound transformation, with many intermediate processes still unexplained. Nikakhtar’s talk focused on this transformation, aiming to reconstruct both the initial density and the displacement fields of galaxies observed in spectroscopic surveys, and also suggesting a forward modeling approach based on optimal transport theory. This theory deals with moving objects from one place to another while conserving mass and minimizing effort. In a cosmological context, it involves mapping the observed galaxy distribution back to its initial uniform state, minimizing the displacement of galaxies. In this framework, Nikakhtar is able to reconstruct the position and shape of biased tracers in Lagrangian space, in addition to the displacement field, which can be used to reconstruct the initial overdensity fluctuation field. This algorithm also suggests an effective way for field-level inference with forward modeling.

- **Asuka Takatsu: Non-preservation of concavity properties by the Dirichlet heat flow on Riemannian manifolds.**

  It is known that the log-concavity is preserved by the Dirichlet heat flow in convex domains of Euclidean space. In their talk on joint work with Kazuhiro Ishige and Haruto Tokunaga (U. of Tokyo), Takatsu explained that no concavity properties are preserved by the Dirichlet heat flow in a totally convex domain of a Riemannian manifold unless the sectional curvature vanishes everywhere on the domain.

- **Micah Warren: Flows on the Kim-McCann metric.**

  Kim and McCann demonstrated the MTW curvature corresponds to the curvature of an (n, n) pseudo-Riemannian Kahler manifold. The metric turns out to have some interesting properties: the graph of an optimal transport map is a Lagrangian space-like submanifold of this manifold, and when given weights depending on the mass distributions, becomes a volume maximizing surface. This leads naturally to the question of flows toward optimal transport plans. When an initial graph is determined by a scalar, the mean curvature flow preserves the Lagrangian property and is controlled by a parabolic Monge-Ampère equation. One can also consider a gradient flow for volume, which is represented by a fourth order quasilinear parabolic equation. Warren offered a recent survey of this area, and some recent progress.

- **Jeremy Wu: Mean Field Limit for Congestion Dynamics in One Dimension.**

  In their talk, Wu presented recent joint work with Inwon Kim and Antoine Mellet in which they derive a model for congested transport (a PDE at a macroscopic scale) from particle dynamics (a system of ODEs at the microscopic scale). Such PDEs appear very naturally in the description of crowd motion, tumor growth, and general aggregation phenomena. Wu and co-authors begin with a system where the particle trajectories evolve according to a gradient flow constrained to some finite distance of separation from each other. This constraint leads to a Lagrange multiplier which, in the mean field limit (infinite number of particles), generates a pressure variable to enforce the hard-congestion constraint. Wu's results are confined to one spatial dimension and rely on both the Eulerian and Lagrangian perspectives for the continuum limit.

- **Matt Jacobs: Lagrangian solutions to PME and diffusion models.**

  There is a large body of recent work on the approximation of diffusion equations by particle systems. Most of this analysis approaches the problem from a stochastic perspective due to the difficulty of studying deterministic particle trajectories. This is largely due to the fact that in the continuous setting, it may be extremely hard to solve diffusion equations in Lagrangian coordinates. In fact, the existence of Lagrangian solutions to the Porous Media Equation (PME) with general initial data was open until 2022. In their talk, Jacob discussed how to construct Lagrangian solutions to PME and then sketched how this analysis can be used to obtain convergence rates for certain deterministic versions of score matching type algorithms.

4 Other outcomes of the Meeting

One nontraditional activity which was held as part of the workshop was a panel discussion on academic job searches. Leveraging the internationally diverse list of attendees, there was an hour long panel discussion on job search procedures in various countries (US, UK, Mexico, France, and Japan). Topics discussed included job search timelines, where to find postings, job application materials, interview procedures, academic position hierarchies, and typical faculty responsibilities in each country. The panel was very well received, with both postdoctoral researchers and graduate student participants in attendance; the organizers received multiple emails afterward stating the usefulness of the panel discussion.

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