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Applications of Optimal Transportation in the Natural Sciences (online meeting)

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Abstract. Concepts and methods from the mathematical theory of optimal transportation have reached significant importance in various fields of the natural sciences. The view on classical problems from a "transport perspective" has lead to the development of powerful problem-adapted mathematical tools, and sometimes to a novel geometric understanding of the matter. The natural sciences, in turn, are the most important source of ideas for the further development of the optimal transport theory, and are a driving force for the design of efficient and reliable numerical methods to approximate Wasserstein distances and the like.

The presentations and discussions in this workshop have been centered around recent analytical results and numerical methods in the field of optimal transportation that have been motivated by specific applications in statistical physics, quantum mechanics, and chemistry.

Mathematics Subject Classification (2010): 28-XX, 35-XX, 81-XX, 92-XX.

Introduction by the Organizers

This workshop has been devoted to the recent developments in the mathematical theory of optimal transport (OT for short) that have been motivated by specific applications in the naural sciences. This has been a purely virtual event, with more than fifty registered participants mostly from Germany, France and the United States; about half of them have been given a presentation, among them five young researchers in the narrow sense.

The broad mixture of topics in the presentations underlined that the range of OT applications has become extremely diverse. The presented applications ranged from density functional theory in quantum chemistry to full waveform inversion in geophysics, from vortex dynamics in fluid mechanics to fast reaction limits in chemistry, etc. Numerical methods for fluid simulations, statistical evaluation and machine learning played a significant role as well. The focus of this workshop was thus complementary to the majority of the numerous OT-related mathematical events that have taken place in the past years, since most of these conferences and meetings were concerned *either* with the very topical applications of OT in all variants of data sciences (and have a strong emphasis on fast numerical algorithms), *or* with the progress in pure theory, primarily in differential geometry. Specific recent developments in the theory, like multi-marginal transport with concave costs or unbalanced mass transport, that are rather exotic at the majority of OT events, have been central in this workshop.

In comparison to the workshop with a similar topic by the same organizers in 2017, a stronger connection in the mathematical theory behind the diverse applications could be noticed. Specifically the topic of entropic regularization was a recurrent theme, clearly in connection with mean field games or the Sinkhorn algorithm, but also for instance for the transport on networks. For the numerical methods, an impressive development — also in the analysis of the methods — could be observed in comparision to four years ago, particularly for the efficient computation of optimal transport maps and multi-marginal plans, but also for the simulation of Wasserstein gradient flows.

Gradient flows in the Wasserstein distance have since long been a topic of central interest in OT, and this was also reflected in this workshop. The geometry and stability of crystal-like steady states in a gradient flow modeling biological aggregation was the topic of Robert McCann's presentation. In a similar spirit, Andre Schlichting performed a bifurcation analysis in the McKean-Vlasov equation and also developed tools to study metastability in gradient flows. Another aspect, namely the micro-macro passage, in same general class of gradient flows was considered by Maria Bruna. On the more general level, Giuseppe Savare presented ideas to extend elements from the AGS theory to dissipative evolutions that are *not* of gradient type, while Mark Peletier demonstrated a structural instability of variational flows. In his, as usual, extremely vivid presentation, Filippo Santambrogio discussed possibilities to define a gradient flow for a very non-convex functional that is minimized by segregated states. Flows were also used by Jean Dolbeault, who proved functional inequalities of GNS-type with their aid. Last but not least, Andrea Natale presented a provably convergent Lagrangian discretization for numerical solution not only of Wasserstein gradient flows, but also of the Euler equations.

Transport distances have been used recently to attack the problem of *full seismic waveform inversion*. This is a well-known nonlinear inverse problem where one tries to recover the underground parameters of a 'forward' wave propagation model mapping a wave source to a 'seismogram' (time $\times$ surface signal recordings at fixed

receivers). Yang and Métivier explained how the classical least-squares misfit is known to lead to an ill-posed minimization problem with many local minima. This pathology is called 'cycle skipping' and linked to phase shifts in the oscillatory signals. At least for simple models transport distances convexify the problem. This is an important paradigm shift for the geophysical community which has been considering mostly the least squares misfit for more than 50 years. I Time signals are, however, not probability measures and some data transformation is needed. There is little understanding of the interpretation of time oscillatory signals in terms of mass or probability measures and this question remains largely open. Métivier suggests for instance to interpret "lines" of receivers recording as shapes in the time $\times$ signal amplitude 'graph space'. After a discretization in time, they give empirical measures living in $\mathbb{R}_{\text{time}} \times \mathbb{R}_{\text{amplitude}}$ space.

Symmetric multimarginal optimal transport problems arise naturally in quantum chemistry applications as the semi-classical limit of the so-called Lévy-Lieb functional. This quantity plays a central role in Density Functional Theory for the calculation of the electronic structure of molecules, in particular for the computation of the ground states (states of lower energy) of the electrons within the molecule. Understanding and computing these states is of vital importance in order to accurately predict optical, electrical and chemical properties of these systems.

Gero Friesecke gave a nice introduction to this emerging topic and presented recent results in a new numerical method for the resolution of symmetric multimarginal optimal transport problem with a large number of marginals (which is equal to the number of electrons in the molecule) which successfully enables to bypass the curse of dimensionality. Maria Colombo presented new theoretical results about the semi-classical limit of electronic ground states and the link with the solutions of the multimarginal optimal transport problem. Codina Cotar showed that the Jellium and Uniform Electron Gas next-order asymptotic terms (in the semi-classical limit) are equal for Coulomb and Riesz potentials and related their expressions to solutions of optimal transport problems.

Workshop (online meeting): Applications of Optimal Transportation in the Natural Sciences

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Abstracts

Scaling Optimal Transport for High Dimensional Learning

Gabriel Peyré

Optimal transport (OT) has recently gained lot of interest in machine learning (ML). It is a natural tool to compare in a geometrically faithful way probability distributions. It finds applications in both supervised learning (using geometric loss functions) and unsupervised learning (to perform generative model fitting). We refer to [1] for an overview of this rapidly growing field. OT is however plagued by the curse of dimensionality, since it might require a number of samples which grows exponentially with the dimension. A workaround, which is now the workhorse of many approaches to OT in ML, is to introduce entropic regularization. Given two probability distributions α, β on $\mathbb{R}^d$ (some of these results extend to more general spaces and distances), its entropic cost is

$$\mathrm{OT}_\varepsilon(\alpha,\beta)^p \triangleq \inf_{\pi\in\mathcal{M}_+(\mathbb{R}^d\times\mathbb{R}^d)} \int_{\mathbb{R}^d\times\mathbb{R}^d} \left(\|x-y\|^2 + \varepsilon \log\left(\frac{\mathrm{d}\pi}{\mathrm{d}\alpha\mathrm{d}\beta}(x,y)\right)\right)\mathrm{d}\pi(x,y)$$

where the minimization is performed over all joint probability distributions having marginals α and β. When $\varepsilon = 0$, one recovers the usual (un-regularized) OT, which suffers severely from the curse of dimensionality. Indeed, if one has only access to n samples $(x_i, y_i)_{i=1}^n$ drawn independently from the distributions α and β, one can consider the empirical distributions $\hat{\alpha} = \frac{1}{n}\sum_i \delta_{x_i}$, $\hat{\beta} = \frac{1}{n}\sum_i \delta_{y_i}$ and one has the following approximation result for the plugin estimator

$$\mathbb{E}(|\mathrm{OT}_0(\alpha,\beta) - \mathrm{OT}_0(\hat{\alpha},\hat{\beta})|) = O(1/n^{1/d}),$$

where the expectation is computed with respect to the samples, see [2] for more details. This shows that the rate is exponentially bad with the dimension d, and furthermore this upper-bound is tight and cannot be improved (as long as for instance α or β have density with respect to the Lebesgue measure). It has been recently shown in [3] that if $\alpha \neq \beta$, then the rate is actually better

$$\alpha \neq \beta \implies \mathbb{E}(|\mathrm{OT}_0(\alpha,\beta) - \mathrm{OT}_0(\hat{\alpha},\hat{\beta})|) = O(1/n^{2/d}), \tag{1}$$

but this is not true anymore if $\alpha = \beta$. In sharp contrast, it is shown in [5, 6] that the entropic cost enjoys a rate which is independent of the dimension

$$\mathbb{E}(|\mathrm{OT}_\varepsilon(\alpha,\beta) - \mathrm{OT}_\varepsilon(\hat{\alpha},\hat{\beta})|) = O(\varepsilon^{-d/2}/n^{1/2}), \tag{2}$$

the main issue being that the constant $\varepsilon^{-d/2}$ blows as $\varepsilon \to 0$, making questionnable its use to improve the estimation of OT distances.

Another issue is that for $\varepsilon > 0$, OT_ε is not a distance, and in particular $\mathrm{OT}_\varepsilon(\alpha,\alpha) > 0$. This is due to the presence of the entropy, which causes a "bias" which is problematic when using OT_ε as a loss function for machine learning purposes. This "bias" is studied in detailed in [8] and [7] who show the following

Taylor expansion (under strong regularity conditions on the measures and the Monge map to ensure a second order expansion)

$$\text{(3)}\quad \mathrm{OT}_\varepsilon(\alpha,\beta)^2 = \mathrm{OT}_0(\alpha,\beta)^2 + d\varepsilon\log\sqrt{2\pi\varepsilon} + \varepsilon(\mathrm{H}(\alpha)+\mathrm{H}(\beta)) + \varepsilon^2\mathrm{I}(\alpha,\beta) + o(\varepsilon^2)$$

where $\mathrm{H}(\alpha) = \int \log(\frac{\mathrm{d}\alpha}{\mathrm{d}x})\mathrm{d}\alpha$ is the differential entropy and

$$\mathrm{I}(\alpha,\beta) \triangleq \int_0^1 \int_{\mathbb{R}^d} \|\nabla \log(\rho_t(x))\|^2 \rho_t(x)\mathrm{d}x\mathrm{d}t$$

is the Fisher information of the OT geodesic ρ_t (so-called McCann interpolation) between the densities of α and β.

In order to remove as much as possible of this bias, [5] introduced the Sinkhorn divergence

$$\text{(4)}\qquad \overline{\mathrm{OT}}_\varepsilon(\alpha,\beta)^p \triangleq \mathrm{OT}_\varepsilon(\alpha,\beta)^p - \frac{1}{2}\mathrm{OT}_\varepsilon(\alpha,\alpha)^p - \frac{1}{2}\mathrm{OT}_\varepsilon(\beta,\beta)^p.$$

From the above Taylor expansion (3) of OT_ε, one sees that for regular enough distributions, one has second order accuracy in the sense that

$$\overline{\mathrm{OT}}_\varepsilon(\alpha,\beta) - \mathrm{OT}_0(\alpha,\beta) = O(\varepsilon^2)$$

where the constants are controlled by the relative Fisher information of α and β. Combinining this second order accuracy with the sample complexity (2) of the entropic cost ensures if $\alpha \neq \beta$

$$\mathbb{E}(|\mathrm{OT}_\varepsilon(\hat{\alpha},\hat{\beta}) - \mathrm{OT}_\varepsilon(\hat{\alpha},\hat{\beta})|) = O(1/n^{2/d}),$$

as long as one selects $\varepsilon \sim 1/n^{1/d}$. One thus retrieves the rate (1) of the plugin estimator, but using entropic regularization. While this might seem deceiving at first, a chief advantage is that $\mathrm{OT}_\varepsilon(\hat{\alpha},\hat{\beta})$ can be computed very efficiently using the highly parallizable Sinkhorn algorithm (see [1] for an overview), with a complexity of $O(n^2/\varepsilon^2)$ to reach ε accuracy [9].

An important open question is to be able to lift the curse of dimensionality by leveraging strong smoothness hypotheses on the distributions. If these distributions have very smooth densities (with of order d derivatives), this could be achieved by using more powerful "debiasing" formula than (4) in order to reach an accuracy of order ε^d instead of ε^2. A computational approach to achieve this using Richardson extrapolation is explained in [3], but this approach is unstable and thus induces constants which explode with d. A more straightforward a way to achieve this is to consider a smoothing of the empirical measures using a convolution against a smooth kernel $k_\varepsilon(x) = k(x/\varepsilon)$

$$k_\varepsilon \star \hat{\alpha} = \frac{1}{n}\sum_i k((x-x_i)/\varepsilon),$$

since then one has for $\varepsilon \sim 1/n^{1/d}$

$$\mathbb{E}(|\mathrm{OT}_0(k_\varepsilon\star\hat{\alpha}, k_\varepsilon\star\hat{\beta}) - \mathrm{OT}_\varepsilon(\hat{\alpha},\hat{\beta})|) = O(1/n^{1/2}).$$

This approach has been developed, generalized and studied in [10]. Unfortunately there is no efficient algorithm to estimate $\mathrm{OT}_0(k_\varepsilon\star\hat{\alpha}, k_\varepsilon\star\hat{\beta})$ in high dimension,

since approximating this quantity typically requires re-sampling $k_\varepsilon \star \hat{\alpha}$ using $\sim n^d$ points. Another approach has been proposed in [11], which bypass this direct spacial smoothing by imposing instead the smoothness of the dual variable (so-called Kantorovitch potential), which can itself be enforced numerically using a sum-of-square method and semi-definite programming.

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Domain decomposition for entropic optimal transport

Bernhard Schmitzer

(joint work with Mauro Bonafini, Ismael Medina)

Optimal transport has become a highly relevant numerical tool in data analysis applications. Consequently the development of increasingly efficient computational methods is of great importance. In recent years entropic regularization and the Sinkhorn algorithm have become a standard method. Despite its tremendous success, solving large problems with low regularization remains challenging due to memory limitations, numerical instabilities and slow convergence. Combining this method with a domain decomposition algorithm due to Benamou [1] will require only the solution of smaller partial problems at each iteration. This could remedy issues with memory and stability while also allowing for large-scale parallelization.

Let X, Y be compact, convex subsets of $\mathbb{R}^d$, let $c : X \times Y \to \mathbb{R}_+$ be a continuous cost function and let μ, ν be two probability measures on X and Y respectively. Further, denote by $\Pi(\mu, \nu)$ the set of transport plans, i.e. the probability measures

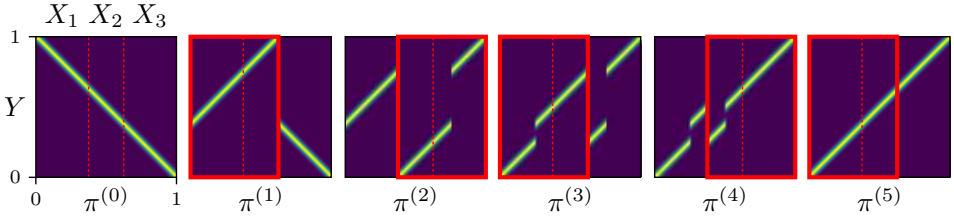

FIGURE 1. Illustration of the domain decomposition algorithm for $X = Y = [0, 1]$ with some entropic regularization. The 'diagonal' plan is optimal, we start with a sub-optimal 'anti-diagonal' plan.

on $X \times Y$ with marginals μ and ν, and by KL denote the Kullback–Leibler divergence. For some regularization parameter $\varepsilon \geq 0$ the (entropy regularized) optimal transport problem is then given by

$$\inf \left\{ \int_{X\times Y} c \, \mathrm{d}\pi + \varepsilon \cdot \mathrm{KL}(\pi | \mu \otimes \nu) \middle| \pi \in \Pi(\mu, \nu) \right\}. \tag{1}$$

For $\varepsilon > 0$, this can be solved by the Sinkhorn algorithm.

In its basic form, Benamou's algorithm works as follows: Let (X_1, X_2, X_3) be a partition of X into three sets and let $X_{12} := X_1 \cup X_2$, $X_{23} := X_2 \cup X_3$. Let $\pi^{(0)} \in \Pi(\mu, \nu)$ be an initial feasible transport plan. The first step is then to optimize $\pi^{(0)}$ on $X_{12} \times Y$, while keeping it fixed on $X_3 \times Y$, denote the result by $\pi^{(1)}$. The second step is to optimize $\pi^{(1)}$ on $X_{23} \times Y$ while keeping it fixed on $X_1 \times Y$, obtaining the next iterate $\pi^{(2)}$. Subsequently, these two steps are repeated until convergence. This is illustrated in Figure 1 for $X = Y = [0, 1]$.

For $\varepsilon = 0$, $c(x, y) = \|x - y\|^2$ and μ having a Lebesgue density, Benamou showed that this converges to the globally optimal solution if the partition satisfies a *convex overlap principle*, which essentially implies that a function $X \to \mathbb{R}$ that is convex on separately X_{12} and X_{23} must be convex on X. The proof hinges on Brenier's polar factorization which provides (in this setting) that optimal plans are unique and supported on the graph of the gradient of a convex map.

The algorithm can be generalized to finer partitions, such that at each iteration, many partial sub-problems could be solved in parallel. Unfortunately, convergence to the global minimizer fails for discretized problems and can only be recovered asymptotically as the discretization becomes increasingly finer. This makes adaptation as a distributed numerical method delicate.

The key observation of [2] is that for $\varepsilon > 0$ the algorithm converges to the global minimizer under very mild assumptions, even in the discretized setting. For the above 'three cell' example, the convergence rate is bounded by

$$\Delta(\pi^{(\ell)}) \leq \left(1 + \exp\left(-\frac{2\|c\|}{\varepsilon}\right) \frac{\mu(X_2)}{\mu(X_1 \cup X_3)}\right)^{-1} \cdot \Delta(\pi^{(\ell-1)}) \tag{2}$$

where $\Delta(\pi)$ denotes the sub-optimality of a plan with respect to the minimal value of (1) and $\|c\| := \max\{c(x, y) | (x, y) \in X \times Y\}$. In [2] the bound is also extended

to finer partitions. The contraction ratio in (2) tends to 1 exponentially as $\varepsilon \to 0$. This is reminiscent of the contraction ratio for the Sinkhorn algorithm in Hilbert's projective metric given in [4].

Exponentially slow convergence can be realized on malicious worst-case examples where convergence is entirely driven by the entropic smoothing. Conversely, on more geometric problems (such as those considered by Benamou) empirically much faster convergence is observed. Intuitively, this fast convergence is driven by the monotonicity properties of the cost function. On such problems [2] reports essentially log-linear scaling of the run-time with the number of pixels per image and inverse proportionality in the number of worker threads for a suitable efficient numerical implementation.

In $d = 1$ this 'geometric' convergence mechanism is related to the *odd-even transposition sort* algorithm which can be shown to converge in n parallelized iterations (where n is the number of partition cells). Unfortunately, an analogous analysis in higher dimensions is still lacking. As a first step in this direction we currently study [3] the convergence behaviour of the algorithm in the limit $n \to \infty$ where we find that the required number of iterations is proportional to n and asymptotically the iterates $\pi^{(\ell)}$ describe a smooth trajectory in the space $\Pi(\mu, \nu)$ which (under suitable assumptions on c) eventually concentrates on the graph of a map. However, this limit need not be globally optimal in general and identifying corresponding sufficient conditions remains an intriguing open question.

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Breaking the curse of dimensionality in statistical estimation of smooth optimal transport.

François-Xavier Vialard
(joint work with A. Vacher, B. Muzellec, A. Rudi, and F. Bach)

It is well-known that plug-in statistical estimation of optimal transport suffers from the curse of dimension. Despite recent efforts to improve the rate of estimation with the smoothness of the problem, the computational complexities of these recently proposed methods still degrade exponentially with the dimension. In this talk, thanks to a representation theorem, we derive a statistical estimator of smooth optimal transport which achieves in average a precision ϵ for a computational cost of $\tilde{O}(\epsilon^{-4})$ when the smoothness increases, hence yielding a dimension free rate. Even though our result is theoretical in nature due to the large constants

involved in our estimations, it settles the question of whether the smoothness of optimal solutions can be taken advantage of from a computational and statistical point of view.

Optimal transport is formulated as a constrained optimization problem on a space of functions. It is a linear optimization problem under an inequality constraint on a space of functions. Therefore, it can be interpreted as learning a function which has a particular structure, namely non-negativity. A particular case of optimizing on non-negative functions can be found in polynomial optimization [7]. A typical problem of interest is the optimization of a polynomial function on a set constrained by polynomial inequalities. Leveraging, when available, a representation theorem such as Putinar's Positivestellensatz, the optimization problem can be reduced to a hierarchy of SDP problems, see [3]. Using this approach for optimal transport was actually already proposed by Lasserre. Recent works address the problem of learning positive functions in more general spaces such as Reproducing Kernel Hilbert Space (RKHS). In [2], it is proposed to represent a positive function in a RKHS as a sum-of-squares. These ideas were further developed in [4] and exploited for non-convex optimization in [1] where the authors recast, as is standard, the problem of minimization of a function $f : D \subset \mathbb{R}^d \to \mathbb{R}$ defined on a domain D as a convex optimization problem, $\max c$ under the inequality constraint $c \leq f(x)$ for every $x \in D$. Obviously, this problem is computationally intractable in general and they propose to solve it under structural assumptions on $f(x) - c = \frac{1}{2}\langle \phi(x), A\phi(x) \rangle$ for a positive self-adjoint operator $A : \mathcal{H} \mapsto \mathcal{H}$ where $\mathcal{H}$ is a RKHS. The value of this new optimization problem is a priori less than the minimum value of f but it does coincide under the assumption that

$$f = \text{cste} + \frac{1}{2}\langle \phi(x), A_* \phi(x) \rangle \,, \tag{1}$$

for some A_*. The key point here is a representation result stating that a fairly large space of smooth functions (to be considered for optimization) can be represented by a sum of squares in RKHS, as in Equation (1). Indeed, they show that it is the case if the function f has at least one global minimizer and there is a *finite* number of global minimizers which all have a non-singular Hessian.

Optimal transport in its dual formulation for the quadratic cost also optimizes on a subset of non-negative functions. Under smoothness assumption of the optimizer, one is tempted to formulate a result on the computational-statistical efficiency of the problem. However, while leveraging regularity can be done using sampling inequalities for a given smooth function, see [6], it is not possible in general for functions for which only inequality constraints are available. As shown in [1], it is possible though when more structure on the minimizers is available. Therefore, the key issue is the representation formula of the minimizers with the additional sum-of-squares structure. In the dual formulation of OT, the minimizers do not define a *finite* number of saturation points for the inequality constraint, on the contrary to the hypothesis in [1]. Rather the saturation set of the constraint defined by the optimizers is a *continuous* set of points, the graph of the optimal

transport map. Based on a second order Taylor expansion, we prove a representation result of the optimizer for smooth OT, which is actually a special case of the Morse lemma with parameter. This allows to formulate an (infinite dimensional) SDP-SOCP formulation for OT which is tight. By a standard "kernel trick", this problem admits a finite dimensional representation which can be solved by convex optimization algorithms, leading to polynomial computational bounds which are independent of the dimension of the ambient space.

For further details, we refer to [5]. Among future works, we mention the development of efficient numerical methods to solve the SDP problem, taking into account the particular structure of the transport problem and second the study of the convergence of the optimal potentials for which we expect almost optimal statistical rates to be obtain by our method.

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Lagrangian discretizations of compressible fluids and porous media flow with semi-discrete optimal transport

Andrea Natale

(joint work with Thomas O. Gallouët, Quentin Mérigot)

The Euler equations describing the evolution of a barotropic fluid in a compact domain $M \subset \mathbb{R}^d$ and on a time interval $[0, T]$ are given by the following system of equations:

$$\begin{cases} \partial_t u + (u \cdot \nabla)u + \nabla U'(\rho) = 0\,, \\ \partial_t \rho + \operatorname{div}(\rho u) = 0\,, \end{cases} \tag{1}$$

where $\rho(t, x) \geq 0$ is the fluid density, $u(t, x) \in \mathbb{R}^d$ is the Eulerian velocity and $U : [0, \infty) \to \mathbb{R}$ defines the internal energy as a function of the density. The system is supplemented by the initial conditions $\rho(0, \cdot) = \rho_0$, $u(0, \cdot) = u_0$, and boundary conditions $u \cdot n_{\partial M} = 0$. Let $S_0 \subseteq M$ be the support of ρ_0 and $X : [0, T] \times S_0 \to M$ be the flow associated to the (smooth) vector field u, i.e. satisfying $\dot{X}_t = u(t, X_t)$.

Then, $\rho(t,\cdot) = (X_t)_{\#}\rho_0$, and at least formally, the flow evolution is described by Newton's second law on the space $\mathbb{X} := L^2_{\rho_0}(M;\mathbb{R}^d)$:

$$\ddot{X}_t = -\nabla_{\mathbb{X}}\mathcal{F}(X_t)\,, \quad \mathcal{F}(X) := \mathcal{U}(X_{\#}\rho_0)\,, \tag{2}$$

where $\mathcal{U}(\rho) := \int_M U(\rho)\mathrm{d}x$ is the internal energy functional, which we set to $+\infty$ whenever ρ is not a.c. with respect to $\mathrm{d}x|_M$.

The dissipative counterpart to the Euler system (1) is given by the equation

$$\partial_t\rho - \operatorname{div}(\rho\nabla U'(\rho)) = 0\,, \tag{3}$$

with the initial conditions $\rho(0,\cdot) = \rho_0$, and boundary conditions $\nabla U'(\rho)\cdot n_{\partial M} = 0$. In this case, given a solution ρ to (3), the flow X associated with the vector field $-\nabla U'(\rho)$ solves the following gradient flow equation:

$$\dot{X}_t = -\nabla_{\mathbb{X}}\mathcal{F}(X_t)\,, \tag{4}$$

which the Lagrangian version of the Wasserstein gradient flow interpretation of system (3). Note that for the classical choice $U(r) = r^m/(m-1)$ with $m > 1$, systems (1) and (3) yield the isentropic Euler and the porous media equations, respectively.

The Hamiltonian structure of system (2) and the gradient flow structure of (4) can be exploited to construct stable Lagrangian numerical schemes. Here we consider particle discretizations which correspond to constraining the flow X to be piecewise constant on a given partition $\mathcal{P}_N := (P_i)_{1\le i\le N}$ of M, with $N \in \mathbb{N}^*$. In particular, introducing

$$\mathbb{X}_N := \{X_N \in \mathbb{X} \,:\, X_N(\omega) = X_N^i \in \mathbb{R}^d \quad \text{for } \rho_0\text{-a.e. } \omega \in M\},$$

a discrete flow is a curve $X_N : [0,T] \to \mathbb{X}_N$, which is then characterized by the trajectories of N particles $t \in [0,T] \mapsto (X_N^i(t))_i \in \mathbb{R}^{dN}$. In turn, the fluid density is given by the empirical measure

$$\rho_N(t) := X_N(t)_{\#}\rho_0 = \sum_{i=1}^N \rho_0[P_i]\delta_{X_N^i(t)}\,.$$

This setting is common to most Lagrangian approaches for the discretization of the systems above. However, since the energy is not well-defined on singular measures, one must define a discrete version of it, which is where the various existing methods differ. Convolution procedures are the most common approaches for both systems (see, e.g., Smoothed Particle Hydrodynamics methods for the Euler system, or the review article [2] for gradient flows). We consider instead a discretization based on the Moreau-Yosida regularization, proposed in [1, 5, 3], i.e. we define for any $X_N \in \mathbb{X}_N$, with $\rho_N := (X_N)_{\#}\rho_0$,

$$\mathcal{F}_\varepsilon(X_N) := \inf_{X\in\mathbb{X}} \frac{\|X_N - X\|^2_{\mathbb{X}}}{2\varepsilon} + \mathcal{F}(X) = \inf_{\rho\in\mathcal{P}_{ac}(M)} \frac{W_2^2(\rho_N,\rho)}{2\varepsilon} + \mathcal{U}(\rho). \tag{5}$$

Note in particular that the L^2 regularization in the definition of $\mathcal{F}_\varepsilon$ corresponds to a Wasserstein regularization at the Eulerian level, which can be computed efficiently using semi-discrete optimal transport tools [4].

Let $N_T \in \mathbb{N}^*$, $\tau := T/N_T$ be a fixed time step and $t_n := n\tau$ for $0 \le n \le N_T$. On each time interval $[t_n, t_{n+1})$ we define the discrete dynamics as the Hamiltonian (resp. gradient flow) dynamics on $\mathbb{X}_N$ associated with the energy

$$X_N \in \mathbb{X}_N \mapsto \frac{\|X_N - X_N^\varepsilon(t_n)\|^2}{2\varepsilon} + \mathcal{F}(X_N^\varepsilon(t_n)) \in \mathbb{R}\,.$$

where

$$X_N^\varepsilon(t_n) \in \operatorname*{argmin}_{X\in\mathbb{X}} \frac{\|X_N(t_n) - X\|_{\mathbb{X}}^2}{2\varepsilon} + \mathcal{F}(X)$$

More precisely, the discrete version of problem (2) consists in finding a C^1 curve $X_N : [0,T] \to \mathbb{X}_N$ which satisfies for all $0 \le n < N_T$,

$$\ddot{X}_N(t) = -\frac{X_N(t) - P_{\mathbb{X}_N} X_N^\varepsilon(t_n)}{\varepsilon}\,, \quad \forall t \in [t_n, t_{n+1})\,, \tag{6}$$

where $P_{\mathbb{X}_N}$ is the L^2 projection onto $\mathbb{X}_N$. Similarly, the discrete version of problem (4) consists in finding a C^0 curve satisfying for all $0 \le n < N_T$,

$$\dot{X}_N(t) = -\frac{X_N(t) - P_{\mathbb{X}_N} X_N^\varepsilon(t_n)}{\varepsilon}\,, \quad \forall t \in [t_n, t_{n+1})\,. \tag{7}$$

This time discretization is an adaptation of the one proposed by Brenier in [1], and it has the remarkable feature of guaranteeing stability for the regularized energy (5), despite being fully explicit.

Our main results give the convergence of the schemes described above towards smooth solutions of the Euler system (1) and the gradient flow (3). The proof relies on a classical modulated energy (or relative entropy) argument. Importantly, the proof is fundamentally Eulerian, which is natural since the energy $\mathcal{F}$ is not convex on $\mathbb{X}$ in general, and it requires the definition of a discrete modulated energy which is to be interpreted a discretization of its continuous counterpart:

$$\int_M U(\rho|\bar{\rho})\mathrm{d}x\,, \quad U(r|s) := U(r) - U(s) - U'(s)(r-s)\,.$$

Moreover, we require that there exists $A > 0$ such that

$$|P(r|s)| \le AU(r|s) \quad \forall r, s > 0\,, \tag{8}$$

where $P(r|s) := P(r) - P(s) - P'(s)(r-s)$, and $P(r) = rU'(r) - U(r)$ defines the pressure as a function of the density. We state here the precise result only for the Euler system, but a similar statement holds in the gradient flow case.

Theorem 1. *Suppose that (ρ, u) is a strong solution to (1) with $U : [0,\infty) \to \mathbb{R}$ being a smooth strictly convex and superlinear function such that (8) holds. Suppose that u and ρ are respectively of class $C^{2,1}$ and $C^{1,1}$ on $[0,T]\times M$; and that either $\rho \ge \rho_{min} > 0$ or that $|U''_+(0)| < \infty$. Suppose in addition that $X_N : [0,T] \to \mathbb{X}_N$ is a C^1 curve which satisfies (6), with initial conditions $X_N(0) = P_{\mathbb{X}_N}\mathrm{Id}$ and $\dot{X}_N(0) = u(0, P_{\mathbb{X}_N}\mathrm{Id}(\cdot))$. Then, denoting by X the Lagrangian flow associated with u satisfying $X(0) = \mathrm{Id}$,*

$$\max_{t\in[0,T]} \|\dot{X}_N(t) - u(t, X_N(t))\|_{\mathbb{X}}^2 + \|X_N(t) - X(t)\|_{\mathbb{X}}^2 \le C\Big(\frac{h_N^2}{\varepsilon} + h_N + \varepsilon + \frac{\tau}{\varepsilon}\Big)\,, \tag{9}$$

where $h_N = \max_i \mathrm{diam}(P_i)$*, and* $C > 0$ *depends only on the Lipschitz norm (in space) of* u*,* $\partial_t u$*,* ∇u*,* $\nabla \mathrm{div}\, u$*,* $\nabla U'(\rho)$*,* $P'(\rho)$ *and* $U'(\rho(0))$*, on the* L^∞ *norm of* u *and* $P'(\rho)$*, on the initial energy* $\mathcal{U}(\rho(0))$*, and on* M *and* T*.*

We remark that differently from [5] we prove convergence of the discrete scheme without assuming any a priori bounds on the discrete solution, but rather relying on the smoothness of the exact one. It is an open question whether convergence holds for less regular solutions and in particular in the case where the $-\nabla U'(\rho)$ is non zero at the boundary of the support of ρ, which is the case for the Barenblatt solution of the porous media equation. Nonetheless, numerically we generally observe convergence with even better rates compared to (9). Finally, we observe that due to ε, our estimates imply a CFL-type condition linking τ and h_N, and it is open whether this can be avoided by a different choice of regularization or time discretization, while maintaining the main features of the scheme.

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Point vortex dynamics for the Euler equation

Christian Seis

(joint work with Stefano Ceci)

Coherent flow structures are widely observed in turbulent fluid motions. Typical examples are isolated regions of concentrated vorticity, such as those observed, for instance, as small eddies in rivers after bridge piers or as spectacular whether phenomena such as tornados. In many situations, the fluid motion in the vortex regions is approximately two-dimensional and the vortex centers can be idealized as points.

The evolution of coherent vortex structures can thus, at least for small times and heuristically, be modelled both on the level of an integrable vorticity distribution and by a system of singular point vortices. The mathematical model from the first point of view is, in the simplest case, the Euler equation

$$\partial_t \omega + u \cdot \nabla \omega = 0, \tag{1}$$

which we consider on $\mathbb{R}^2$ in order to neglect the effect of boundaries. Here, $\omega = \omega(t,x) \in \mathbb{R}$ is the vorticity of the fluid and $u = u(t,x) \in \mathbb{R}^2$ its velocity. At any

instant of time, the velocity can be computed from the vorticity with the help of the Biot–Savart law, $u = K * \omega$, where

$$K(z) = \frac{1}{2\pi}\frac{z^\perp}{|z|^2}$$

is the Biot–Savart kernel, and $z^\perp$ represents the counter-clockwise rotation of a vector z about the origin. A first formal derivation of a point vortex model goes back to the pioneering work of Helmholtz [4], in which he predicted that a set of idealized point vortices $X_1, \dots, X_N$ in $\mathbb{R}^2$ evolves by a simple system of ordinary differential equations,

$$\frac{d}{dt}X_i = \sum_{j\neq i} \lambda_j K(X_i - X_j). \tag{2}$$

Here, λ_i is the circulation or strength of the ith vortex, which is preserved during the evolution.

The connection between Euler equations (1) and the point vortex system (2) was made rigorous for the first time about fourty years ago by Marchioro and Pulvirenti [5], and there have been many improvements since then. The results hold true for initial data which separate into N regions of disjoint supports and distinguished signs,

$$\omega^0 = \sum_{i=1}^N \omega_i^0,$$

and the corresponding intensities and initial vortex centers are

$$\lambda_i = \int \omega_i \, dx, \qquad X_i^0 = \frac{1}{\lambda_i}\int x\omega_i^0(x)\, dx.$$

Marchioro and Pulvirenti (and also the later contributors) futhermore imposed strong vorticity concentration in the sense that

$$\text{spt } \omega_i^0 \subset B_\varepsilon(X_i^0), \tag{3}$$

for some small $\varepsilon > 0$, and uniform scaling assumptions of the form

$$0 \leq \frac{\omega_i^0}{\lambda_i} \lesssim \varepsilon^{-\gamma},$$

for some $\gamma \geq 2$. The prototype vortex region is a constant patch, for instance, $\omega_i^0 = \frac{\lambda_i}{\pi\varepsilon^2}\chi_{B_\varepsilon(X_i^0)}$. If $\omega_i(t)$ denotes the vortex patch at later times, which is simply advected by the flow of the velocity field u, it can be proved that the patches remain sharply concentrated around solutions to the point vortex system (2). More precisely, it holds that

$$\text{spt } \omega_i(t) \subset B_{C\varepsilon^\beta}(X_i(t)) \tag{4}$$

for some $\beta \in (0, 1/2)$, see [5].

The key estimate in the derivation of (4) is a bound on the second moment function

$$\int |x - X_i(t)|^2 \frac{\omega_i(t,x)}{\lambda_i}\, dx \lesssim e^{\frac{Ct}{a^2}} \int |x - X_i^0|^2 \frac{\omega_i^0(x)}{\lambda_i}\, dx,$$

where d is the minimal distance between the point vortices and C some universal constant (dependent on the ciruclations). This estimate can be interpreted as a bound on the 2-Wasserstein distance,

$$W_2\left(\frac{\omega_i(t)}{\lambda_i}, \delta_{X_i(t)}\right) \lesssim e^{\frac{Ct}{d^2}} W_2\left(\frac{\omega_i^0}{\lambda_i}, \delta_{X_i^0}\right).$$

Under the strong concentration assumptions (3), the right-hand side is of the order ε, and an application of the triangle inequality yields

$$W_1(\omega(t), \sum_i \lambda_i \delta_{X_i(t)}) \lesssim e^{\frac{Ct}{d^2}} \varepsilon. \tag{5}$$

We remark that choosing the W_1 distance here is necessary because the latter can be extended to unsigned densities thanks to the Kantorovich–Rubinstein theorem. Moreover, because Wasserstein distances metrize weak convergence, the latter can be understood as an estimate on the rate of weak convergence of Euler solutions to the point vortex system,

$$\omega = \omega^\varepsilon \longrightarrow \sum_i \lambda_i \delta_{X_i} \quad \text{weakly with rate } \varepsilon.$$

In a recent work [2], we derived Marchioro and Pulvirenti's result under a weaker concentration hypothesis. Moreover, we managed to handle unbounded vorticity fields.

Theorem 1. *Suppose that ω_i^0 is such that*

$$W_2\left(\frac{\omega_i^0}{\lambda_i}, \delta_{X_i^0}\right) \lesssim \varepsilon, \quad \|\omega_i^0\|_{L^p} \lesssim \varepsilon^{-\gamma} \quad \textit{with } \gamma = 2(1 - \frac{2}{p}).$$

Then (5) *holds for any $t \in (0, T)$ for some $T \gtrsim 1$.*

The result can be easily extended to (multiply connected) domains (as considered in [2]) and to the viscous setting [3].

The theorem is remarkable because in the setting under consideration, there is no uniqueness result known for the Euler equations. Nevertheless, since solutions to the point vortex system can be formally considered as solutions to the Euler equations, the result provides a stability estimate between a weak, possibly non-unique, solution and a singular solution with more structure.

We finally remark that by combining the methods of this works with the techniques developed in [1], the above result can be easily generalized to *any* γ, provided that the weak concentration assumption is traded for the strong concentration assumption. A control of the L^p seems to be necessary, however, as is guarantees that the velocity field is bounded.

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Convergence of a gradient flow to a non-gradient-flow

Mark A. Peletier
(joint work with Mikola Schlottke)

We study the limit $\varepsilon \to 0$ for the family of Fokker-Planck equations in one dimension defined by

$$\partial_t \rho_\varepsilon = \varepsilon \tau_\varepsilon \left[\partial_{xx} \rho_\varepsilon + \partial_x \left(\rho_\varepsilon \frac{1}{\varepsilon} \partial_x V \right) \right], \quad \text{on } \mathbb{R}_+ \times \mathbb{R}. \tag{1}$$

Here we take an *asymmetric* double-well potential $V : \mathbb{R} \to \mathbb{R}$ as depicted in Figure 1.

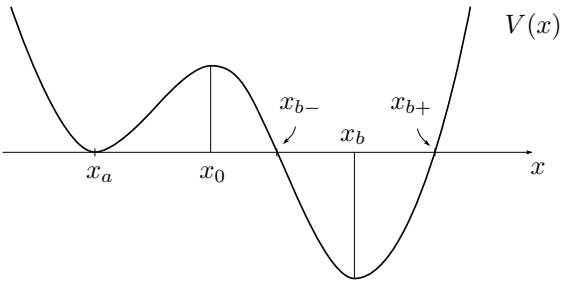

Figure 1. A typical asymmetric potential $V(x)$.

A typical solution $\rho_\varepsilon(t, x)$ is displayed in Figure 2, showing mass flowing from left to right: as time increases, the mass shifts from the left to the right well.

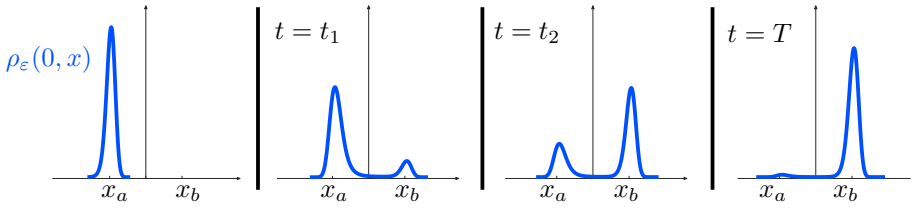

Figure 2. The time evolution of a solution $\rho_\varepsilon(t, x)$ to (1) whose initial distribution is supported on the left. Time increases from left to right. The smaller the value of ε, the sharper the equilibrium distribution concentrates around the global minimum x_b.

There are two parameters, $\varepsilon > 0$ and $\tau_\varepsilon > 0$. The parameter ε controls how sharply the mass is concentrated around x_a and x_b, and how fast mass can move between the potential wells. The second parameter τ_ε sets the global time scale, and is chosen such that transitions from the local minimum x_a to the global minimum x_b happen at rate of order one as $\varepsilon \to 0$:

$$\tau_\varepsilon := \frac{2\pi}{\sqrt{V''(x_a)|V''(x_0)|}} \exp\{\varepsilon^{-1}(V(x_0) - V(x_a))\}.$$

As $\varepsilon \to 0$, we expect the mass to be concentrated at x_a and x_b, and we expect the limiting dynamics to be characterized by mass being transferred at rate one from the local minimum x_a to the global minimum x_b, with no mass moving in the opposite direction. In terms of the solution ρ_ε, therefore, we expect

$$\rho_\varepsilon \rightharpoonup \rho_0 = z\delta_{x_a} + (1-z)\delta_{x_b},$$

where the limit density $z = z(t)$ of particles at x_a satisfies $\partial_t z = -z$, corresponding to left-to-right transitions happening at rate 1. This is illustrated in Figure 3.

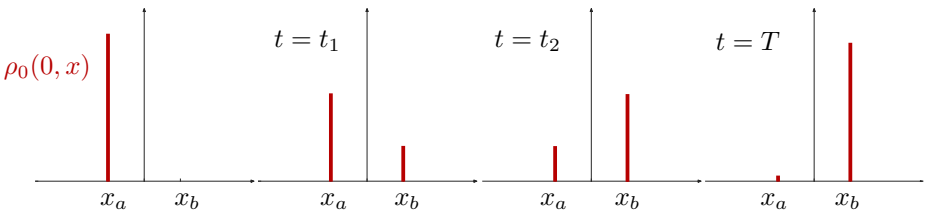

FIGURE 3. The time evolution of ρ_0, defined as the $\varepsilon \to 0$ limit of the solution $\rho_\varepsilon(t,x)$ to (1).

Equation (1) is a Wasserstein gradient flow [AGS08] of the functional

$$E_\varepsilon(\rho) := \mathcal{H}(\rho|\gamma_\varepsilon) \quad \text{where} \quad \gamma_\varepsilon(\mathrm{d}x) := \frac{1}{Z_\varepsilon} e^{-V(x)/\varepsilon}\,\mathrm{d}x,$$

where $\mathcal{H}(\mu|\nu)$ is the relative entropy of μ with respect to ν. This structure was used in [AMPSV12, LMPR17] to prove 'EDP-convergence' of this gradient system to a limiting gradient system, in the case of a *symmetric* potential V.

For a non-symmetric potential V we show in [PS21] that no EDP-convergence is possible. The main reason for this is that the gradient structure is 'lost' in the limit. One indication of this is the singular behaviour of the energy E_ε:

$$E_\varepsilon \xrightarrow{\Gamma} E_0(\rho) := \mathcal{H}(\rho|\delta_{x_b}) = \begin{cases} 0 & \text{if } \rho = \delta_{x_b} \\ +\infty & \text{otherwise,} \end{cases}$$

while

$$\varepsilon E_\varepsilon \xrightarrow{\Gamma} \int \rho V.$$

This shows that for any $\rho \neq \delta_{x_b}$, $E_\varepsilon(\rho)$ diverges at rate $1/\varepsilon$, and any gradient system driven by the limit functional E_0 only admits constant solutions $\rho(t) = \delta_{x_b}$ for all t.

Instead, we follow the idea of variational convergence but for more general formulations. The starting point is the following reformulation of equation (1). For pairs $(\rho_\varepsilon, j_\varepsilon)$ satisfying the continuity equation $\partial_t \rho_\varepsilon + \partial_x j_\varepsilon = 0$, equation (1) can formally be written as $\mathcal{I}_\varepsilon(\rho_\varepsilon, j_\varepsilon) \le 0$, where

$$\mathcal{I}_\varepsilon(\rho_\varepsilon, j_\varepsilon) := \frac{1}{2}\int_0^T \int_{\mathbb{R}} \frac{1}{\varepsilon\,\tau_\varepsilon}\frac{1}{\rho(t,x)}\big|j(t,x) - J_\varepsilon^\rho(t,x)\big|^2 \,\mathrm{d}x\mathrm{d}t$$
$$\text{and } J_\varepsilon^\rho := -\tau_\varepsilon\left[\varepsilon\,\partial_x\rho_\varepsilon + \rho_\varepsilon \partial_x V\right].$$

In the context of EDP-convergence, one would split this functional into energetic and dissipation parts,

$$\mathcal{I}_\varepsilon(\rho_\varepsilon, j_\varepsilon) \;=\; E_\varepsilon(\rho)\Big|_{t=0}^{t=T} + \underbrace{\int_0^T \Big[R_\varepsilon(\rho, j) + R_\varepsilon^*\big(\rho, -\mathrm{D}E_\varepsilon(\rho)\big)\Big]\,\mathrm{d}t}_{(*)}$$

and one would proceed to characterize the Γ-convergence of the terms separately. Because of the singularity of E_ε this fails, and both $E_\varepsilon(\rho)|_{t=0}^{t=T}$ and the term $(*)$ diverge as $1/\varepsilon$. Instead we keep the terms together, and study the Γ-convergence of the combined functional $\mathcal{I}_\varepsilon$.

Theorem 1 (Main result)**.** *Let V satisfy a number of technical assumptions that encode the 'two-well' nature. Then*

(1) *Sequences $(\rho_\varepsilon, j_\varepsilon)$ for which there exists a constant C such that*

$$\mathcal{I}_\varepsilon(\rho_\varepsilon, j_\varepsilon) \le C \qquad \textit{and} \qquad E_\varepsilon(\rho_\varepsilon(0)) \le \frac{C}{\varepsilon}$$

are compact in a distributional sense;

(2) *Along sequences $(\rho_\varepsilon, j_\varepsilon)$ satisfying*

$$\rho_\varepsilon(t=0) \rightharpoonup \rho_0^\circ(\mathrm{d}x) := z^\circ \delta_{x_a}(\mathrm{d}x) + (1-z^\circ)\delta_{x_b}(\mathrm{d}x) \qquad \textit{as } \varepsilon \to 0,$$

the functional $\mathcal{I}_\varepsilon$ Γ-converges to a limit $\mathcal{I}_0$.

The limit functional $\mathcal{I}_0$ is defined by

$$\mathcal{I}_0(\rho, j) := 2\int_0^T S(j(t)|z(t))\,\mathrm{d}t,$$

provided $\rho(t, \mathrm{d}x) = z(t)\delta_{x_a}(\mathrm{d}x) + (1-z(t))\delta_{x_b}(\mathrm{d}x)$ with $z(0) = z^\circ$, and $j(t,x) = j(t)\mathbb{1}_{(x_a,x_b)}(x)$. Here the function $S : \mathbb{R}^2 \to [0,\infty]$ is given by

$$S(a|b) := \begin{cases} a\log\dfrac{a}{b} - a + b, & a, b > 0, \\ b, & a = 0,\ b > 0, \\ +\infty, & \text{otherwise.} \end{cases}$$

Lemma 2 (Characterization of minimizers of $\mathcal{I}_0$)**.** *If $\mathcal{I}_0(\rho, j) = 0$, then z satisfies $z'(t) = -z(t)$ for all t.*

Details can be found in the forthcoming publication [PS21].

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A cross-diffusion equation obtained by convexification

Filippo Santambrogio

(joint work with R. Ducasse, H. Yoldaş)

In a recent paper, [3], Barbaro, Rodriguez, Yoldaş, and Zamponi study a very simple cross-diffusion system given by

$$\begin{cases} \partial_t \rho = \Delta \rho + \nabla \cdot (\rho \nabla \mu), \\ \partial_t \mu = \Delta \mu + \nabla \cdot (\mu \nabla \rho), \end{cases}$$

which is a system of Fokker-Planck equations where each density acts as a potential for the other (in a given domain $\Omega \subset \mathbb{R}^d$ with no-flux boundary conditions, or in the d-dimensional torus). Local existence under the condition $\rho\mu < 1$ is proven in [3]. Indeed, this condition is not surprising. One can see that this system is, formally, the gradient flow in $W_2(\Omega) \times W_2(\Omega)$ of the functional F^0 given by

$$F^0(\rho, \mu) := \int_\Omega f^0(\rho(x), \mu(x)) dx, \qquad f^0(a, b) := a \log a + b \log b + ab.$$

It can easily be seen that the Hessian $D^2 f^0$ is positive semi-definite if and only if $ab \leq 1$, and that hence f^0 is in general not convex. This has two consequences: on the one hand from the point of view of the PDE system, if one had a soluton with $\rho\mu > 1$, then it would be possible to locally find suitable combinations of ρ and μ (for instance, take $u = \rho - \mu$ in the neighborhood of a point where $\rho = \mu > 1$) which approximtely solve a backward heat equation, which is a serious difficulty for existence; on the other hand, the functional F^0 is not l.s.c. for the weak convergence, and this prevents the JKO scheme

$$\min_{\rho,\mu} F^0(\rho, \mu) + \frac{W_2^2(\rho, \rho_k) + W_2^2(\mu, \mu_k)}{2\tau}$$

from having, in general, a solution. Actually, since the W_2 terms are continuous for the weak convergence, in the above minimization the functional F^0 is automatically replaced with a new functional F, which is the l.s.c. envelope of F^0. This l.s.c. envelope is easy to characterize, it is given by $F(\rho, \mu) := \int_\Omega f(\rho(x), \mu(x)) dx$ where f is the convex envelope of f^0.

The main goal of the talk and of the work-in-progress with R. Ducasse and H. Yoldaş is to study the system of PDEs arising as a gradient flow for F. This requires first to compute or characterize the function f. It is possible to prove that f can be obtained in the following way: fix $s = a + b$. If $s \leq 2$ then f^0 is convex on $\{a + b = s\}$ and we have $f = f^0$. If $s > 2$ then f^0 has a double well on $\{a + b = s\}$ and f will coincide, on this segment, with the convexification of f^0 on the same segment, i.e. a function which joins the two equal-value wells of f^0 with a straight line. The position of the two wells can be characterized through a system of equations but not given explicitly, and we find the existence of a boundary $ab = P(s)$ (with $P(2) = 1$ and $P(s) < 1$ for $s > 2$) such that $f = f^0$ on $\{ab < P(a+b)\}$ (the *below region* B) and $f = \tilde{f}(a+b)$ on $\{ab \geq P(a+b)\}$ (the *above region* A).

The cross-diffusion system that we obtain recalls some studies which have been done for diffusion depending on the sum of two densities, because of what happens on the region A. These systems are gradient flows of a functional including a term of the form $\int \tilde{f}(\rho(x) + \mu(x))dx$; they are very difficult to study in case two different potentials ($+\int V d\rho + \int W d\mu$) are added, and the only available result proving existence of a solution can be currently found in dimension 1 under very stringent restrictions on the data ([7]). In the absence of exterior potentials but with different reaction terms there are results in 1D ([4, 6], both based on BV bounds which only apply in 1D) or in arbitrary dimension under restrictive assumptions on the reaction terms ([5], whose result could also be obtained with a similar technique to the one of our work). On the other hand, if neither reaction nor potentials distinguish the two species, the situation is much simpler, since the sum $S = \rho + \mu$ solves a porous-medium–type PDE. Here the situation is similar to the "simple" case (no potential nor reaction), but mixes two different behaviors: the sum-dependent diffusion on A and strict convexity in ρ and μ on B.

First, we need to be precise about the notion of solution. We define the admissible class $\mathcal{A}$ as follows:

$$\mathcal{A} = \{(\rho, \mu) \in \mathcal{P}(\Omega)\times\mathcal{P}(\Omega) \ : \ \sqrt{\rho + \mu} \in H^1(\Omega) \text{ and } \forall \chi \in C^1_c(B) \ \chi(\rho, \mu) \in H^1(\Omega)\}.$$

For $(\rho, \mu) \in \mathcal{A}$ we can define the gradient of the two partial derivatives $f_a(\rho, \mu)$ and $f_b(\rho, \mu)$ in the following way: on each point x s.t. $(\rho(x), \mu(x)) \in B$ we can use the condition $\eta(\rho, \mu) \in H^1$ for arbitrary $\eta \in C^1_c(B)$ to define $\nabla\rho(x)$ and $\nabla\mu(x)$ and hence $\nabla(f_a(\rho, \mu))$ and $\nabla(f_b(\rho, \mu))$; on each point x s.t. $(\rho(x), \mu(x)) \in A$ we can use the condition $\sqrt{S} \in H^1$ (with $S = \rho + \mu$) to define $\nabla S(x)$ and then $\nabla(f_a(\rho, \mu)) = \nabla(f_b(\rho, \mu)) = \tilde{f}''(S)\nabla S$.

We then look for a pair of curves (ρ_t, μ_t) with their velocity fields (v_t, w_t) solving

$$\partial_t\rho + \nabla \cdot (\rho v) = 0, \quad \partial_t\mu + \nabla \cdot (\mu w) = 0$$

such that $(\rho_t, \mu_t) \in \mathcal{A}$ for a.e. t and $v = -\nabla f_a(\rho, \mu)$ and $w = -\nabla f_b(\rho, \mu)$.

From the formal computation

$$\frac{d}{dt}F(\rho_t, \mu_t) = \int_\Omega \nabla f_a(\rho, \mu) \cdot v d\rho + \int_\Omega \nabla f_b(\rho, \mu) \cdot w d\mu, \tag{1}$$

and a classical application of the Young inequality coming from the so-called Energy Dissipation Inequality (see [1, 2]) it is enough to find a curve satisfying

$$(2)\quad F(\rho_T,\mu_T) \;+\; \frac{1}{2}\int_0^T\int_\Omega |\nabla f_a(\rho,\mu)|^2 d\rho + \frac{1}{2}\int_0^T\int_\Omega |v|^2 d\rho \\ +\; \frac{1}{2}\int_0^T\int_\Omega |\nabla f_b(\rho,\mu)|^2 d\mu + \frac{1}{2}\int_0^T\int_\Omega |w|^2 d\mu \;\le\; F(\rho_0,\mu_0).$$

We then prove the following results

- The quantity Slope$F$ defined via
$$\text{Slope}F(\rho,\mu) := \int_\Omega |\nabla f_a(\rho,\mu)|^2 d\rho + \int_\Omega |\nabla f_b(\rho,\mu)|^2 d\mu$$
is l.s.c. for the weak convergence of probability measures on the class $\mathcal{A}$ (this requires a fine discussion of the behavior in A and B separately);
- Using a flow-interchange technique (see [8]) any limit as $\tau \to 0$ of any suitable interpolation of the sequence (ρ_k, μ_k) obtained through the JKO scheme for F satisties $(\rho_t, \mu_t) \in \mathcal{A}$ for a.e. t;
- Using De Giorgi's variational interpolation and the above semi-continuity, any limit as $\tau \to 0$ of any suitable interpolation of the sequence (ρ_k, μ_k) obtained through the JKO scheme for F satisties (2).

The only remaining difficulty is to rigorously prove (1) for curves which only satisfy $(\rho_t, \mu_t) \in \mathcal{A}$ for a.e. t with some integrability conditions on the H^1 norms. This can be done by regularizing by convolution but we only have a complete proof in the case $d = 1$. Indeed, the regularization strategy passes through a statement of the form "if $u \in L^1$ is such that $u_+ \in H^1 \cap L^\infty$ and η_ε is a sequence of standard mollifiers (with possible assumptions on the shape of the mollifier) then for every $\alpha > 0$ the sequence $(\eta_\varepsilon * u - \alpha)_+$ is bounded in H^1 by $C(||u_+||_{L^\infty}, \alpha)||u_+||_{H^1}$", which can be obtained in dimension 1 but not in higher dimension.

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Dissipative evolution of measures

Giuseppe Savaré
(joint work with G. Cavagnari, G. Sodini)

A dissipative (multivalued) operator in a separable Hilbert space H (endowed with the scalar product $\langle\cdot,\cdot\rangle$ and the norm $|\cdot|$) is a subset $B \subset \mathsf{H}\times\mathsf{H}$ satisfying

$$\langle w-v, y-x\rangle \le 0 \quad \text{for every } (x,v),(y,w)\in B. \tag{1}$$

Using the identity

$$\frac{1}{2\tau}\Big(|y+\tau w-(x+\tau v)|^2-|x-y|^2\Big) = \langle w-v,y-x\rangle + \frac{1}{2}\tau|w-v|^2, \tag{2}$$

a dissipative operator can be equivalently characterized by the properties

$$\lim_{\tau\downarrow 0}\frac{|y+\tau w-(x+\tau v)|^2-|x-y|^2}{2\tau}\le 0 \quad \text{for every } (x,v),(y,w)\in B \tag{3}$$

or

$$|y+\tau w-(x+\tau v)|^2 \ge |x-y|^2 \quad \text{for every } \tau<0,\ (x,v),(y,w)\in B. \tag{4}$$

B is m- (or maximal) dissipative if for every $x\in\mathsf{H}$ and $\tau>0$ there exists a (unique, by (4)) $x_\tau = J_\tau(x)\in\mathsf{H}$ such that

$$x_\tau - \tau v_\tau = x, \quad (x_\tau, v_\tau)\in B. \tag{5}$$

(5) can be interpreted as one step of the Implicit Euler Method associated to the evolution equation driven by B, whose strong solutions $x:[0,\infty)\to\mathsf{H}$ satisfy

$$(x(t),\dot x(t))\in B \quad \text{for a.e. } t>0, \quad x(0)=x_0 \text{ given in } D(B); \tag{6}$$

here $D(B)$ is the proper domain $\{x\in\mathsf{H}:(x,v)\in B \text{ for some } v\in\mathsf{H}\}$ of B. The celebrated Crandall-Liggett Theorem [3] shows that for every $x_0\in\overline{D(B)}$ the limit $\lim_{n\to\infty}\big(J_{t/n}\big)^n(x_0)$ exists for every $t>0$ and defines a continuous curve x which is the unique integral solution to (7) according to Bénilan [2]

$$\frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}|x(t)-y|^2 \le -\langle w, x(t)-y\rangle \text{ in } \mathscr{D}'(0,\infty) \quad \text{for every } (y,w)\in B. \tag{7}$$

Moreover, whenever $(x_0,v_0)\in B$, x is Lipschitz continuous, it solves (6), and $|x(t)-(J_{t/n})^n(x_0)|\le 2\sqrt{t\tau}|v_0|$. The family of maps $S(t):x_0\mapsto x(t)$, $t\ge 0$, is a contraction semigroup in $\overline{D(B)}$.

It is natural to investigate if the above results can be at least partially extended to the generation of contraction semigroups in $\mathscr{P}_2(\mathsf{H})$, the Wasserstein space of Borel probability measures in H with finite quadratic moment. $\mathscr{P}_2(\mathsf{H})$ can be endowed with the Kantorovich-Rubinstein-Wasserstein distance W_2 induced by the norm of H and ii is a complete and separable metric space. A good indication of the feasibility of this approach relies in the case of the (opposite) subdifferential of

a proper, lower semicontinuous and (geodesically) convex functional $\Phi : \mathscr{P}_2(\mathsf{H}) \to (-\infty, +\infty]$, see [1].

A (multivalued) *probability vector field* (MPVF) can be defined as a subset $\mathfrak{F}$ of $\mathscr{P}_2(\mathsf{H} \times \mathsf{H})$ (see also [5]). If $\mathsf{x}, \mathsf{v} : \mathsf{H} \times \mathsf{H} \to \mathsf{H}$ denote the projections of a point $(x, v) \in \mathsf{H} \times \mathsf{H}$ on its first and second component, every $\boldsymbol{F} \in \mathfrak{F}$ gives raise to a curve

$$\boldsymbol{F}(\tau) := (\mathsf{x} + \tau\mathsf{v})_\sharp \boldsymbol{F}, \quad \tau \in \mathbb{R}.$$

As in (2), starting from $\boldsymbol{F}, \boldsymbol{G} \in \mathfrak{F}$ we can consider the squared distance map

$$D(\tau; \boldsymbol{F}, \boldsymbol{G}) := \frac{1}{2} W_2^2(\boldsymbol{F}(\tau), \boldsymbol{G}(\tau)),$$

which however is not quadratic nor convex w.r.t. τ. Due to the particular structure of the Wasserstein distance, $\tau \mapsto D(\tau; \boldsymbol{F}, \boldsymbol{G})$ is in fact a semi-concave map, i.e.

$$\tau \mapsto D(\tau; \boldsymbol{F}, \boldsymbol{G}) - C\tau \quad \text{is concave for a constant } C \geq 0 \text{ depending on } \boldsymbol{F}, \boldsymbol{G},$$

so that (3) and (4) are not equivalent in the Wasserstein setting. In order to define dissipativity, we rely on (3) and we first introduce the partial right derivatives of D at $\tau = 0$: if $\mu = \mathsf{x}_\sharp \boldsymbol{F} = \boldsymbol{F}(0)$ and $\nu = \mathsf{x}_\sharp \boldsymbol{G} = \boldsymbol{G}(0)$ we set

$$\begin{aligned} [\boldsymbol{F}, \nu]_r &:= \lim_{\tau \downarrow 0} \frac{W_2^2(\boldsymbol{F}(\tau), \nu) - W_2^2(\mu, \nu)}{2\tau}, \\ [\boldsymbol{G}, \mu]_r &:= \lim_{\tau \downarrow 0} \frac{W_2^2(\mu, \boldsymbol{G}(\tau)) - W_2^2(\mu, \nu).}{2\tau} \end{aligned} \tag{8}$$

Definition 1. We say that a MPVF $\mathfrak{F}$ is metrically dissipative if

$$[\boldsymbol{F}, \nu]_r + [\boldsymbol{G}, \mu]_r \leq 0 \quad \text{for every } \boldsymbol{F}, \boldsymbol{G} \in \mathfrak{F},\ \mu = \mathsf{x}_\sharp \boldsymbol{F},\ \nu = \mathsf{x}_\sharp \boldsymbol{G}. \tag{9}$$

(8) admits an equivalent representation in terms of plans: denoting by (x, v, y) a generic point in H^3 and by $(\mathsf{x}, \mathsf{v}, \mathsf{y})$ the corresponding projections, we set

$$\Gamma(\boldsymbol{F}, \nu) := \Big\{ \gamma \in \mathscr{P}_2(\mathsf{H}^3) : (\mathsf{x}, \mathsf{v})_\sharp \boldsymbol{\gamma} = \boldsymbol{F}, \quad \mathsf{y}_\sharp \boldsymbol{\gamma} = \nu, \\ (\mathsf{x}, \mathsf{y})_\sharp \boldsymbol{\gamma} \text{ is an optimal coupling between } \mathsf{x}_\sharp \boldsymbol{F} \text{ and } \nu \Big\}.$$

We have

$$[\boldsymbol{F}, \nu]_r = \min \Big\{ \int \langle v, x - y \rangle \, \mathrm{d}\boldsymbol{\gamma}(x, v, y) : \boldsymbol{\gamma} \in \Gamma(\boldsymbol{F}, \nu) \Big\}. \tag{10}$$

Using (10), the dissipativity inequality (9) can be interpreted as a suitable version of (1) at the level of probability measures. It is worth noticing that if $\Phi : \mathscr{P}_2(\mathsf{H}) \to (-\infty, +\infty]$ is a geodesically convex functional, then its Wasserstein subdifferential [1] satisfies (9). However, differently from the subdifferential case where the JKO-Minimizing Movement method is available [4, 1], for a general dissipative MPVF it is not clear how to define the resolvent and to apply the Implicit Euler method.

We can then consider the Explicit Euler method, assuming that $\mathfrak{F}$ is semi-bounded.

Definition 2. We say that a MPVF $\mathfrak{F}$ is semi-bounded if $\mathsf{x}_\sharp(\mathfrak{F}) = \mathscr{P}_2(\mathsf{H})$ and for every $R > 0$ there exists a constant $S = S(R) > 0$ such that

$$\boldsymbol{F} \in \mathfrak{F}, \quad \int |x|^2 \,\mathrm{d}F(x,v) \le R \quad \Rightarrow \quad \int |v|^2 \,\mathrm{d}\boldsymbol{F}(x,v) \le S.$$

If $\mathfrak{F}$ is a semi-bounded MPVF, for every initial measure $\mu_0 \in \mathscr{P}_2(\mathsf{H})$ and every time step $\tau > 0$ we can define recursively the sequence $(\mu_\tau^k)_{k\in\mathbb{N}}$ by

$$\mu_\tau^0 := \mu_0, \quad \mu_\tau^{k+1} := \boldsymbol{F}^k(\tau) \quad \text{for some } \boldsymbol{F}^k \in \mathfrak{F},\ \mathsf{x}_\sharp \boldsymbol{F}^k = \mu_\tau^k.$$

We can then consider the piecewise constant interpolant $\mu_\tau : [0,\infty) \to \mathscr{P}_2(\mathsf{H})$ of the sequence $(\mu_\tau^k)_{k\in\mathbb{N}}$, defined by

$$\mu_\tau(t) := \mu_\tau^k \quad \text{if } t \in [k\tau, (k+1)\tau).$$

The next Theorem collects our main generation result.

Theorem 3. *Let $\mathfrak{F}$ be a semi-bounded dissipative* MPVF*. For every $\mu_0 \in \mathscr{P}_2(\mathsf{H})$ and every $t \ge 0$ there exists the limit $\mu(t) := \lim_{\tau\downarrow 0} \mu_\tau(t)$. $\mu : [0,\infty) \to \mathscr{P}_2(\mathsf{H})$ is a Lipschitz curve and it is the unique solution of the dissipative Evolution Variational Inequality*

$$\frac{\mathrm{d}}{\mathrm{d}t}\frac{1}{2}W_2^2(\mu(t),\nu) \le -[\boldsymbol{F},\mu(t)]_r \quad \textit{a.e. in } (0,\infty), \textit{ for every } \boldsymbol{F} \in \mathfrak{F},\ \nu = \mathsf{x}_\sharp \boldsymbol{F}.$$

The family of maps $S(t) : \mu_0 \mapsto \mu(t)$ defines a contraction semigroup in $\mathscr{P}_2(\mathsf{H})$ and for every $T > 0$ there exists a constant $C > 0$ such that

$$\sup_{t\in[0,T]} W_2^2(\mu_\tau(t),\mu(t)) \le C\tau.$$

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Coarse graining of a Fokker-Planck equation with excluded volume effects preserving the gradient flow structure

Maria Bruna

(joint work with Martin Burger, José Antonio Carrillo)

We consider the topic of propagation of gradient flow structures from microscopic to macroscopic models. An interesting feature of many partial differential equations (PDEs) describing dissipative mechanisms in particle systems is that they can be seen as gradient flows (or steepest descents) of an associated free-energy functional. This is the case of the linear Fokker–Planck equation [6], and many other nonlinear Fokker–Planck equations including nonlinear diffusions and McKean–Vlasov like equations. For example, the set of N Brownian particles moving under an external potential $V(\mathbf{x})$,

$$\mathrm{d}\mathbf{X}_i(t) = \sqrt{2}\,\mathrm{d}\mathbf{W}_i(t) - \nabla V_{\mathbf{x}}(\mathbf{X}_i(t))\mathrm{d}t, \qquad 1 \le i \le N, \tag{1}$$

where $\mathbf{W}_i(t)$ are independent Brownian motions, can be described by a Fokker–Planck equation for its joint probability density $P(\vec{x},t)$, where $\vec{x} = (\mathbf{x}_1, \dots, \mathbf{x}_N)$:

$$\frac{\partial P}{\partial t}(\vec{x},t) = \nabla_{\vec{x}} \cdot \left[\nabla_{\vec{x}} P + \nabla_{\vec{x}} V_N(\vec{x}) P\right]. \tag{2}$$

Here $\nabla_{\vec{x}}$ and $\nabla_{\vec{x}}\cdot$ respectively stand for the gradient and divergence operators with respect to the N-particle position vector $\vec{x}$ and $V_N(\vec{x}) = \sum_{i=1}^N V(\mathbf{x}_i)$. Equation (2) can be seen as a gradient flow

$$\frac{\partial P}{\partial t}(\vec{x},t) = \nabla_{\vec{x}} \cdot \left(P \nabla_{\vec{x}} \frac{\delta \mathcal{E}_N}{\delta P} \right),$$

with respect to the 2-Wasserstein metric and the free energy

$$\mathcal{E}_N(P) = \int \left[P(\vec{x},t)\log P(\vec{x},t) + V_N(\vec{x})P\right] \mathrm{d}\vec{x}. \tag{3}$$

The connections between (1), (2) and (3) are well understood in the case of noninteracting particles, where essentially the macroscopic limit of a set of N particles coincides with the case of a single Brownian particle [6], leading to the linear Fokker–Planck equation for the one-particle probability density $p(\mathbf{x},t)$

$$\frac{\partial p}{\partial t}(\mathbf{x},t) = \nabla_{\mathbf{x}} \cdot \left[\nabla_{\mathbf{x}} p + \nabla_{\mathbf{x}} V(\mathbf{x}) p\right], \tag{4}$$

which is again 2-Wasserstein gradient flow with respect to the low-dimensional version of the energy (3), that is, $E(p) = \int [p\log p + V(\mathbf{x})p]\mathrm{d}\mathbf{x}$.

Interactions between particles can make the passage from microscopic to macroscopic challenging. In particular, the Fokker–Planck equation for the one-particle marginal density $p(\mathbf{x},t) = \int P(\vec{x},t)\delta(\mathbf{x}-\mathbf{x}_1)\mathrm{d}\vec{x}$ becomes in general coupled to higher-order marginals, leading to a BBGKY-type hierarchy, and its relation to the N-particle probability density becomes much more complicated due to correlations between particles. From a physical perspective, a desirable or even required condition on the macroscopic model might be that, if the microscopic model has an underlying gradient flow structure, this is preserved by the coarse-graining.

However, in general this is not guaranteed unless the coarse-graining procedure is such that it respects the structure. In particular, it is common to obtain the macroscopic model independently of the underlying gradient flow structure, and to establish a suitable energy and metric at the macroscopic level. This may lead to difficulties in identifying a suitable macroscopic energy and/or non-physical energies and mobilities [4]. Some strategies to obtain the macroscopic model are:

- truncating the BBGKY hierarchy using a closure approximation (e.g. mean field or Kirkwood superposition),
- proving a mean-field limit as $N \to \infty$ to obtain a closed equation for the one-particle marginal [5],
- Dynamical Density Functional Theory (DDFT), which by construction provides a macroscopic gradient-flow structure but relies on a good approximation of the excess free energy (steaming from particle interactions),
- using a large deviation principle and Γ-convergence to associate the stochastic process with its macroscopic gradient-flow structure [1].

To address these issues, in [3] we consider a coarse-graining approach starting from the time-discrete microscopic gradient flow (JKO scheme). We apply it to the problem of Brownian particles with short-range repulsive interactions, which are used to model excluded-volume effects between individuals (e.g. cells, animals). Consider a set of N pairwise interacting particles in a bounded domain $\Omega \subset \mathbb{R}^d$ with $|\Omega| = 1$:

$$\mathrm{d}\mathbf{X}_i(t) = \sqrt{2}\,\mathrm{d}\mathbf{W}_i(t) - \nabla_{\mathbf{x}} V(\mathbf{X}_i(t))\mathrm{d}t - \chi \sum_{j \neq i} \nabla_{\mathbf{x}} u((\mathbf{X}_i(t) - \mathbf{X}_j(t))/\ell)\mathrm{d}t, \tag{5}$$

for $1 \leq i \leq N$, where χ and ℓ represent the strength and the range of the potential u, respectively. Unlike the mean-field scaling ($\chi = 1/N, \ell = 1, N \to \infty$), here we consider strong short-range repulsive interactions, $\chi = 1, \ell = \epsilon \ll 1$ with N such that $\delta := (N-1)\epsilon^d$ is a small parameter (this corresponds to a low density regime). In particular, in what follows we describe the coarse-graining when u is a hard-core potential, $u(r) = +\infty, r < 1$, and 0 otherwise. In this case, the microscopic model coincides with (1), (2) and (3) except that the domain of $\vec{x}$ is not Ω^N as for noninteracting particles but the perforated domain

$$\Omega_\epsilon^N = \Omega^N \setminus \mathcal{B}_\epsilon, \quad \mathcal{B}_\epsilon = \left\{ \vec{x} \in \Omega^N : \exists i \neq j \text{ s.t. } \|\mathbf{x}_i - \mathbf{x}_j\| \leq \epsilon \right\}.$$

No-flux boundary conditions on the internal boundaries of this domain correspond to the hard-core interactions present between particles. The more general case of a repulsive short-range potential is described in [3].

The starting point is to write down the time-discrete variational formulation of the N-particle Fokker-Planck equation (2), which using the Benamou–Brenier formulation [2] leads to

$$\inf_{P_k} \inf_{(P,\vec{U})} \left\{ \frac{1}{2} \int_0^{\Delta t} \int_{\Omega_\epsilon^N} P \|\vec{U}\|^2 \mathrm{d}\vec{x}\mathrm{d}s + \mathcal{E}_N(P_k) \right\}, \tag{6}$$

where $(P, \vec{U}) \in CE_{\Delta t}(P_{k-1}, P)$ if it solves

$$\text{(CE)} \qquad \begin{aligned} \frac{\partial P}{\partial s} + \nabla_{\vec{x}} \cdot (P\vec{U}) &= 0, && \text{in } \Omega_\epsilon^N \times (0, \Delta t), \\ \vec{U} \cdot \vec{n} &= 0, && \text{on } \partial\Omega_\epsilon^N \times (0, \Delta t), \\ P &= P_{k-1}(\vec{x}), && \text{in } \Omega_\epsilon^N \times \{0\}, \\ P_k(\vec{x}) &= P, && \text{in } \Omega_\epsilon^N \times \{\Delta t\}. \end{aligned}$$

The scheme is initialised with $P_0(\vec{x})$ invariant to permutations of particle labels.

Starting from the N-particle problem (6), we derive an analogous problem for the one-particle density and the associated flow using the method of matched asymptotic expansions in the limit of the volume fraction δ small. In general there might be a uniqueness issue in the determination of the flow, which is related to the problem of tilting gradient flows [7]. However, we have a natural convention in our case, since we can enforce consistency with the non-interacting particles case ($\delta = 0$). We obtain the following result from the optimality conditions of (6): the macroscopic density p and associated flow ϕ satisfy the following equations up to order δ:

$$\begin{aligned} \frac{\partial p}{\partial s} + \nabla_{\mathbf{x}} \cdot (p \nabla_{\mathbf{x}} \phi) &= 0, && \text{in } \Omega \times (0, \Delta t), \\ \frac{\partial \phi}{\partial s} + \frac{1}{2} \|\nabla_{\mathbf{x}} \phi\|^2 &= 0, && \text{in } \Omega \times (0, \Delta t), \\ \nabla_{\mathbf{x}} \phi \cdot \mathbf{n} &= 0, && \text{on } \partial\Omega \times (0, \Delta t), \\ p &= p_{k-1}(\mathbf{x}), && \text{in } \Omega \times \{0\}, \\ \phi &= -\left(\log p + V + \alpha \delta p\right), && \text{in } \Omega \times \{\Delta t\}. \end{aligned}$$

with $\alpha = V_d(1)$ the volume of the unit ball in $\mathbb{R}^d$. The final-time condition allows us indentify the macroscopic entropy as

$$E_\delta(p) = \int_\Omega \left[p \log p + pV(\mathbf{x}) + \tfrac{1}{2} \alpha \delta p^2 \right] \mathrm{d}\mathbf{x},$$

leading to the nonlinear Fokker–Planck equation

$$\frac{\partial p}{\partial t}(\mathbf{x}, t) = \nabla_{\mathbf{x}} \cdot \left[(1 + \delta p) \nabla_{\mathbf{x}} p + \nabla_{\mathbf{x}} V(\mathbf{x}) p \right]. \tag{7}$$

This result is consistent with the macroscopic model obtained via matched asymptotic expansions as the level of the Fokker–Planck equation.

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Remarks on MFG and Initial Value Problems

Yann Brenier

A typical example of MFG (à la Lasry-Lions) is

$$\partial_t \rho + \nabla \cdot (\rho \nabla \theta) = \nu \Delta \rho, \;\; \partial_t \theta + \frac{1}{2}|\nabla \theta|^2 + \nu \Delta \theta = f(\rho),$$

$\rho = \rho(t,x) \geq 0$, $\theta = \theta(t,x) \in \mathbb{R}$ being respectively prescribed at $t = 0$ and $t = T$, and $x \in D$ with, say, $D = \mathbb{T}^d$. Here $T > 0$ and $f : \mathbb{R}_+ \to \mathbb{R}$ are given. As long as $f' \geq 0$, these equations are "well-posed" with respect to the "backward-forward" time-boundary conditions. Indeed, they are just the optimality equations for the concave maximization problem

$$\sup_{\theta(T,\cdot)=\theta_T} \; -\int_0^T \int_D G(\partial_t \theta + \nu \Delta \theta, \nabla \theta) - \int_D \rho_0 \, \theta(0,\cdot),$$

$$G(\sigma, w) = \sup_{\rho \geq 0, q \in \mathbb{R}^d} \; \sigma \rho + w \cdot q - \frac{|q|^2}{2\rho} - \int_0^\rho f(s) ds.$$

The same equations also correspond to the Euler equations of a gas (without vorticity) and pressure equal to

$$p(\rho) = -\int_0^\rho s f'(s) ds$$

with speed of sound $\sqrt{p'(\rho)}$. Then, the initial value problem (IVP) is well-posed precisely in the *opposite* situation when $f' \leq 0$. This indicates how MFG and IVP may differ! So it seems useless to use the MFG approach to solve IVP. Nevertheless, following [1], we may use a *generalized* version of MFGs to solve some IVPs, typically for "entropic system of conservation laws"

$$\partial_t U + \nabla \cdot (F(U)) = 0, \; U = U(t,x) \in \mathbb{R}^m, \; x \in \mathbb{T}^d,$$

admitting a strictly convex "entropy" function $\mathcal{E} : \mathbb{R}^m \to \mathbb{R}$. We may as well consider their viscous version $\partial_t U + \nabla \cdot (F(U)) = \nu \Delta U$, with viscosity $\nu > 0$. It turns out that, at least for smooth solutions and sufficiently short time intervals $[0, T]$, we may reduce the IVP to the concave maximization problem

$$\sup_{A(T,\cdot)=0} \; -\int_0^T \int_D G(\partial_t A + \nu \Delta A, \nabla A) - \int_D A(0,\cdot) \cdot U_0$$

involving a *vector-potential* $A = A(t,x) \in \mathbb{R}^m$, where G is the convex function defined by

$$G(E,B) = \sup_{V \in \mathbb{R}^m} E \cdot V + B \cdot F(V) - \mathcal{E}(V).$$

Furthermore, when $\nu = 0$, the optimal vector-potential A is directly related to the solution U of the IVP through the very simple formula $A(t,x) = (t-T)\mathcal{E}'(U(t,x))$. The similarity of this concave problem with the MFG we started with is striking.

Just to quote a concrete example, let us consider the (viscous) "template matching equation", for use in data sciences and image processing,

$$\partial_t v + \nabla \cdot (v \otimes v) + \nabla(\frac{|v|^2}{2}) = \nu \Delta v, \quad v(0,\cdot) = v_0,$$

for which we obtain the "generalized" MFG

$$\sup_{M,q} \int_{[0,T]\times D} (-\frac{1}{2} M^{-1} : (q - \nu \nabla \cdot M)^{\otimes 2} + q \cdot v_0) dx dt$$

where the matrix-valued field $M = M^T = M(t,x) \geq 0$ and the vector field $q = q(t,x)$ are subject to

$$\partial_t M + \nabla q + \nabla q^T = (\nabla \cdot q)\, I_d, \quad M(T,\cdot) = I_d.$$

This problem may also be seen as a kind of Schrödinger/MFG variant of a matrix-valued optimal transport problem, in the sense of [2].

Let us finally mention that, as $d = 1$, we may recover, for arbitrarily large $T > 0$, the exact smooth solution $v(t,x)$ of the IVP for all $t \in [0,T]$, as $\nu > 0$, and, in the limit case $\nu = 0$, the exact "entropy" solution $v(t,x)$ (à la Kružkov) but only at the final time $t = T$!

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Convergence of some Mean Field Games systems to aggregation and flocking models

Pierre Cardaliaguet

(joint work with Martino Bardi)

The aim of this research project is to show a rigorous connection between two different mathematical theories modeling the dynamics of large populations of individuals: Mean Field Games (MFG) (in which the individual control a system and have a high degree of rationality), and agent-based models (in which they are

myopic). Following ideas of Degond and al.[1] and of Bertucci and al.[2], we show how some MFG systems degenerate into kinetic models as individuals become more and more impatients and as their control become cheaper. Our first result says that solutions (u_λ, m_λ) of the MFG system

$$\begin{cases} -\partial_t u_\lambda - \nu_\lambda \Delta u_\lambda + \lambda u_\lambda + \dfrac{\lambda}{2}|Du_\lambda|^2 = F(x, m_\lambda(t)) \qquad \text{in } \mathbb{R}^d \times (0, +\infty) \\ \partial_t m_\lambda - \nu_\lambda \Delta m_\lambda - \operatorname{div}(m_\lambda \lambda Du_\lambda) = 0 \qquad \text{in } \mathbb{R}^d \times (0, +\infty) \\ m_\lambda(0) = m_0, \qquad \text{in } \mathbb{R}^d, \qquad u_\lambda \text{ bounded}, \end{cases}$$

converges to the solution of the aggregation model

$$\begin{cases} \partial_t m - \operatorname{div}(m D_x F(x, m)) = 0 \qquad \text{in } \mathbb{R}^d \times (0, +\infty) \\ m(0) = m_0, \qquad \text{in } \mathbb{R}^d. \end{cases}$$

as $\lambda \to +\infty$ and $\nu_\lambda \to 0$. In this result we assume that the coupling $F = F(x, m)$ is uniformly continuous with respect to the first variable, uniformly with respect to the measure m. The result relies on careful semiconcavity estimates of the value function u_λ, which allows to bound the L^∞ norm of the density m_λ and to pass to the limit in the equation.

For second order MFG models, we establish the convergence of the system

$$\begin{cases} -\partial_t u_\lambda + \lambda u_\lambda - v \cdot D_x u_\lambda + \dfrac{\lambda}{2}|D_v u_\lambda|^2 = F(x, v, m_\lambda(t)) \text{ in } \mathbb{R}^{2d} \times (0, T) \\ \partial_t m_\lambda + v \cdot D_x m_\lambda - \operatorname{div}_v(m_\lambda \lambda D_v u_\lambda) = 0 \qquad \text{in } \mathbb{R}^{2d} \times (0, T) \\ m_\lambda(0) = m_0, \quad u_\lambda(x, v, T) = 0 \qquad \text{in } \mathbb{R}^{2d}, \end{cases}$$

to the solution of the kinetic equation

$$\begin{cases} \partial_t m + v \cdot D_x m - \operatorname{div}_v(m D_v F(x, v, m)) = 0 \qquad \text{in } \mathbb{R}^{2d} \times (0, T), \\ m(0) = m_0, \qquad \text{in } \mathbb{R}^{2d}, \end{cases}$$

as $\lambda \to +\infty$. For this second result, and to fix the ideas, we work in the case where the coupling term F corresponds to the Cucker-Smale model

$$F(x, v, m(t)) = k * m(x, v, t), \qquad k(x, v) = \frac{|v|^2}{(\alpha + |x|^2)^\beta}, \quad \alpha > 0, \beta \geq 0.$$

The second result is based on variational techniques and shows surprising connexions with "Weighted Energy-Dissipation" techniques, recently revisited by Rossi and al.[3], the main difference being that our system is not a gradient flow.

There remains several natural questions on the topic: The simplest one is the convergence rate, which is probably relatively simple to establish in the case of the first convergence result but much more challenging for the second one. Perhaps the most intriguing open question is to understand the link (if any) between the

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long time behavior of the MFG systems and the one for the aggregation/kinetic equation.

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Homogenisation of discrete dynamical optimal transport

Jan Maas
(joint work with Eva Kopfer, Peter Gladbach, Lorenzo Portinale)

In the past decades there has been intense research activity in the area of optimal transport. In continuous settings, a central result in the field is the Benamou–Brenier formula [1], which provides a dynamical formulation of the classical Monge–Kantorovich problem. In discrete settings, the equivalence between static and dynamical optimal transport breaks down, and it turns out that the dynamical formulation (introduced in [5, 6]) is essential in applications to evolution equations, discrete Ricci curvature, and functional inequalities.

The limit passage from discrete dynamical transport to continuous optimal transport turns out to be nontrivial. In fact, seemingly natural discretizations of the Benamou–Brenier formula do not necessarily converge to the Kantorovich distance $\mathbb{W}_2$, even in one-dimensional settings [3]. The main result in [2] asserts that, for a sequence of meshes on a bounded convex domain in $\mathbb{R}^d$, an isotropy condition on the meshes is required to obtain the convergence of the discrete dynamical transport distances to $\mathbb{W}_2$.

In this talk we present recent work in which we identify the limiting behaviour of the discrete metrics on $\mathbb{Z}^d$-periodic graphs where the isotropy condition fails to hold.

For an (undirected) graph $(\mathcal{X}, \mathcal{E})$ and probability measure $m^0, m^1 \in \mathcal{P}(\mathcal{X})$, we consider the dynamical transport cost given by

$$\mathcal{C}(m^0, m^1) = \inf_{(m,J)\in \mathrm{CE}(m^0,m^1)} \Big\{ \int_0^1 \sum_{(x,y)\in\mathcal{E}} c_{xy}\big(m_t(x), m_t(y), J_t(x,y)\big)\,\mathrm{d}t \Big\},$$

where $\mathrm{CE}(m^0, m^1)$ denotes the class of all solutions to the discrete continuity equation connecting m^0 and m^1, i.e., all curves of probability measures $m : [0,1] \to \mathcal{P}(\mathcal{X})$ and all time-dependent discrete vector fields (i.e., anti-symmetric functions) $J : [0,1] \to \mathbb{R}^{\mathcal{E}}$ satisfying the discrete continuity equation

$$\frac{\mathrm{d}}{\mathrm{d}t} m_t(x) + \sum_{y:y\sim x} J_t(x,y) = 0, \qquad m_0 = m^0,\ m_1 = m^1.$$

The cost functions $c_{xy} : \mathbb{R}_+ \times \mathbb{R}_+ \times \mathbb{R} \to \mathbb{R}_+$ are assumed to be lower-semicontinuous and convex.

In [3, 4] we fix a $\mathbb{Z}^d$-periodic graph $(\mathcal{X}, \mathcal{E})$ embedded in $\mathbb{R}^d$. For any $\varepsilon > 0$ with $1/\varepsilon \in \mathbb{N}$, we consider the rescaled graphs $(\mathcal{X}_\varepsilon, \mathcal{E}_\varepsilon)$ defined by

$$\mathcal{X}_\varepsilon = \varepsilon \mathcal{X}/Z^d \quad \text{and} \quad \mathcal{E}_\varepsilon = \varepsilon \mathcal{E}/\{(z,z) : z \in \mathbb{Z}^d\}.$$

The rescaled transport cost is given by

$$\mathcal{C}_\varepsilon(m^0, m^1) = \inf_{(m,J)\in \mathrm{CE}(m^0,m^1)} \left\{ \int_0^1 \sum_{(x,y)\in\mathcal{E}_\varepsilon} \varepsilon^d c_{xy}\left(\frac{m_t(x)}{\varepsilon^d}, \frac{m_t(y)}{\varepsilon^d}, \frac{J_t(x,y)}{\varepsilon^{d-1}} \right) \mathrm{d}t \right\}.$$

Loosely speaking, our main result asserts that these discrete transport problems converge to a continuous transport problem with a homogenized cost function, as $\varepsilon \to 0$. Namely, for any weakly converging sequences of probability measures $m^0_\varepsilon \rightharpoonup \mu^0$ and $m^1_\varepsilon \rightharpoonup \mu^1$, we have convergence $\mathcal{C}_\varepsilon(m^0_\varepsilon, m^1_\varepsilon) \to \mathbb{C}(\mu^0, \mu^1)$, where the limiting transport problem is given by

$$\mathbb{C}(\mu^0, \mu^1) = \inf_{\mu, j} \left\{ \int_0^1 \int_{\mathbb{T}^d} c_{\mathrm{hom}}\left(\frac{\mathrm{d}\mu_t}{\mathrm{d}\mathcal{L}^d}, \frac{\mathrm{d}j_t}{\mathrm{d}\mathcal{L}^d} \right) \mathrm{d}x\, \mathrm{d}t \ : \ \partial_t \mu + \nabla \cdot j = 0,\ \mu_{0,1} = \mu^{0,1} \right\}.$$

The homogenized cost $c_{\mathrm{hom}} : \mathbb{R}_+ \times \mathbb{R}^d \to \mathbb{R}$ is given by the cell formula

$$c_{\mathrm{hom}}(\rho, u) = \inf_{m,J} \left\{ \sum_{x\in\mathcal{X}\cap[0,1)^d} \sum_{y\sim x} c_{xy}\big(m(x), m(y), J(x,y)\big) \right\},$$

where the infimum runs over all $\mathbb{Z}^d$-periodic functions $m : \mathcal{X} \to \mathbb{R}_+$ and all $\mathbb{Z}^d$-periodic discrete vector fields (i.e., all anti-symmetric functions $J : \mathcal{E} \to \mathbb{R}$ with $\sum_{y:y\sim x} J(x,y) = 0$ for all $x \in \mathcal{X}$) satisfying

$$\sum_{x\in\mathcal{X}\cap[0,1)^d} m(x) = \rho \quad \text{and} \quad \frac{1}{2} \sum_{x\in\mathcal{X}\cap[0,1)^d} \sum_{y\sim x} J(x,y)(y-x) = u$$

for $(\rho, u) \in \mathbb{R}_+ \times \mathbb{R}^d$. This cell formula describes how the limiting transport cost is affected by the geometry of the periodic graph. The rigorous formulation of our main result is given in terms of Γ-convergence for curves in the space of probability measures.

In the special case where the discrete transport cost is associated to a Riemannian gradient flow structure for a Markov chain (as in [5, 6]), our result implies that the limiting metric is a 2-Wasserstein metric associated to a (not necessarily Riemannian) Finsler metric.

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Stability of optimal transport maps: the compact and non-compact cases

Quentin Mérigot
(joint work with Alex Delalande)

In this presentation, we establish quantitative stability of the quadratic optimal transport map between a fixed probability density ρ and a probability measure μ on $\mathbb{R}^d$. We assume that ρ is absolutely continuous with respect to the Lebesgue measure, supported over a compact convex set X, and that it is is bounded from above and below by positive constants on X. Given $\mu \in \mathcal{P}_2(\mathbb{R}^d)$, we call *Brenier map* the unique quadratic optimal transport map T_μ between ρ and μ and we call *Brenier potential* the unique convex function $\phi_\mu \in L^2(X)$ such that $T_\mu = \nabla\phi_\mu$ and which satisfies $\int_X \phi_\mu d\rho = 0$.

The map $\mu \mapsto T_\mu$ has been used to embed the metric space $(\mathcal{P}_2(\mathbb{R}^d), W_2)$ into the Hilbert space $L^2(\rho, \mathbb{R}^d)$. This approach is often referred to as the *Linearized Optimal Transport* framework [1] and has shown great results in applications. A practical benefit of the embedding is to enable the use of the classical Hilbertian statistical toolbox on families of probability measures while keeping some features of the Wasserstein geometry. Working with this embedding is equivalent to replacing the Wasserstein distance by the distance

$$W_{2,\rho}(\mu, \nu) = \|T_\mu - T_\nu\|_{L^2(\rho,\mathbb{R}^d)}.$$

We note that the geodesic curves with respect to the distance $W_{2,\rho}$ are called the *generalized geodesics* in the book of Ambrosio, Gigli, Savaré [2]. The choice of the Brenier map between a reference measure ρ and a measure μ as an embedding of μ may also be motivated by the Riemannian interpretation of the Wasserstein geometry, the map $\mu \mapsto T_\mu$ being the inverse of the exponential map based at ρ.

It is quite natural to expect that the embedding $\mu \mapsto T_\mu$ retains some of the geometry of the underlying space, or equivalently that the metric $W_{2,\rho}$ is comparable, in some coarse sense, to the Wasserstein distance. The main difficulty, which we study in this article, is to establish quantitative (e.g. Hölder) continuity properties for the mappings $\mu \mapsto T_\mu$ and $\mu \mapsto \phi_\mu$. We note that such stability estimates are also important in numerical analysis and in statistics.

Existing results. We first note that explicit examples show that the mapping $\mu \mapsto T_\mu$ is in general not better than $\frac{1}{2}$-Hölder. A much stronger negative result comes from Andoni, Naor and Neiman [3, Theorem 7] showing that one cannot construct a bi-Hölder embedding of $(\mathcal{P}_2(\mathbb{R}^d), W_2)$, $d \geq 3$, into a Hilbert space.

Theorem 1 (Andoni, Naor, Neiman)**.** *$(\mathcal{P}_2(\mathbb{R}^3), W_2)$ does not admit a uniform, coarse or quasisymmetric embedding into any Banach space of nontrivial type.*

This theorem implies in particular that one cannot hope to prove that $\mu \mapsto T_\mu$ is bi-Hölder on the whole set $\mathcal{P}_2(\mathbb{R}^d)$ of probability measures with finite second moment.

The existing quantitative stability results can be summarized under the two following statements. A first result due to Ambrosio and reported in [4], shows a local 1/2-Hölder behaviour near probability densities μ whose associated Brenier map T_μ is Lipschitz continuous, a strong hypothesis. A second result, due to Berman [5], proves quantitative stability of the map $\mu \mapsto T_\mu$ under milder assumptions on the target probability measures. Berman assumes that the source measure ρ is the restriction of the Lebesgue measure on a compact convex set X with unit volume. Under this assumption, he proves a stability result on the inverse transport maps when the target measure remains in a fixed compact set. This result implies quantitative stability of the Brenier maps:

Theorem 2 (Berman)**.** *Let X be a compact convex subset with unit volume, let ρ be the restriction of the Lebesgue measure to X, and let $Y \subset \mathbb{R}^d$ be another compact set. Then there exists a constant C depending only on X and Y such that for any $\mu, \nu \in \mathcal{P}(Y)$,*

$$\|T_\mu - T_\nu\|_{L^2(\rho)} \leq C W_1(\mu,\nu)^{\frac{1}{2(d-1)(d+2)}}.$$

The Hölder behavior does not depend on the regularity of the transport map T_μ, but the Hölder exponent depends exponentially on the ambient dimension d.

Contributions. In this talk, we present a quantitative stability results for quadratic optimal transport maps between a probability density ρ and target measure μ. We do not assume that μ is compactly supported. Introducing $M_p(\mu) = \int_{\mathbb{R}^d} \|x\|^p d\mu(x)$ the p-th moment of μ, we prove in particular the following theorem.

Theorem 3. *Let X be a compact convex subset of $\mathbb{R}^d$ and let ρ be a probability density on X, bounded from above and below by positive constants. Let $p > d$ and $p \geq 4$. Assume that $\mu, \nu \in \mathcal{P}_2(\mathbb{R}^d)$ have bounded p-th moment, i.e. $\max(M_p(\mu), M_p(\nu)) \leq M_p < +\infty$. Then*

$$\|T_\mu - T_\nu\|_{L^2(\rho)} \leq C_{d,p,X,\rho,M_p} W_1(\mu,\nu)^{\frac{p}{6p+16d}},$$

$$\|\phi_\mu - \phi_\nu\|_{L^2(\rho)} \leq C_{d,p,X,\rho,M_p} W_1(\mu,\nu)^{1/2},$$

where $C_{a_1,\ldots,a_n}$ depends a non-negative constant which depends only on $a_1, \ldots, a_n$. If μ, ν are supported on a compact set Y, we have an improved Hölder exponent for the Brenier map:

$$\|T_\mu - T_\nu\|_{L^2(\rho)} \leq C_{d,p,X,Y,\rho} W_1(\mu,\nu)^{\frac{1}{6}}.$$

A large class of probability measures verifies the moment assumption, such as sub-Gaussian or sub-exponential measures.

To prove these stability estimates, we use the fact that the dual potentials solve a convex minimization problem involving Kantorovich's functional $\mathcal{K}(\psi) = \int \psi^* d\rho$.

We first prove a strong convexity estimate for K, relying on the Brascamp-Lieb inequality, and which holds under the assumption that the Brenier potentials are bounded. This strong convexity estimate is then translated into a stability estimate concerning the dual and Brenier potentials. The stability of Brenier maps is then deduced using a Gagliardo-Nirenberg type inequality for the difference of convex functions.

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Entropic spatially inhomogeneous evolutionary games: fast reaction limit and learnability

Mauro Bonafini

(joint work with M. Fornasier and B. Schmitzer)

In the course of the past two decades there has been an explosion of research on models of multi-agent interactions to describe phenomena beyond physics, e.g., in biology, such as cell aggregation and motility, coordinated animal motion, coordinated human and synthetic agent behaviour and interactions. Most of these models start from particle-like systems by including fundamental "social interaction" forces within classical systems of first or second order equations. Others build on a game theoretic setting or move within the realm of mean-field games.

Recently, new forms of spatially inhomogeneous evolutionary games have been proposed by Ambrosio et al. in [1]. These models couple an evolutionary game selection of mixed strategies via replicator dynamics alongside the choice of a transport field for the agent population. Differently from mean-field games, evolutionary games of this kind are not based on an underlying optimal control problem, but they realize an evolutionary, nearly instantaneous adaptation of the agents' strategies of motion.

We move our steps from these general models and modify them for the description of more realistic behaviours, including the possibility of fast adaptation of the strategies of each agent. Hence, we introduce a novel multi-agent interaction model which describes an (entropic) undisclosed fast reaction limit of the general framework. In particular, for a given set of pure strategies U, $0 < \eta \in P(U)$ a reference probability measure on U, an "entropic" parameter $\varepsilon > 0$, and maps

$e\colon \mathbb{R}^d \times U \to \mathbb{R}$ and $J\colon \mathbb{R}^d \times U \times \mathbb{R}^d \to \mathbb{R}$, we introduce the N-agents system described by

$$\text{(UFR-N)} \qquad \begin{aligned} \partial_t x_i(t) &= v_i^J(x_1(t), \dots, x_N(t)) \quad \text{for } i = 1, \dots, N \\ v_i^J(x_1, \dots, x_N) &= \int_U e(x_i, u)\, \sigma_i^J(x_1, \dots, x_N)(u)\ \mathrm{d}\eta(u) \\ \sigma_i^J(x_1, \dots, x_N) &= \frac{\exp\left(\frac{1}{\varepsilon N} \sum_{j=1}^N J(x_i, \cdot, x_j)\right)}{\int_U \exp\left(\frac{1}{\varepsilon N} \sum_{j=1}^N J(x_i, v, x_j)\right)\ \mathrm{d}\eta(v)} \end{aligned}$$

Here, each σ_i^J represents a probability density with respect to η and corresponds to the optimal mixed strategy which is obtained under the fast reaction assumption. The main parameter governing the evolution is the payoff function J: $J(x, u, x')$ is the payoff a player located at x obtains when playing strategy u against another player located at x'. First order Newtonian models can be viewed as a subclass of undisclosed fast reaction dynamics, taking $\varepsilon \to 0$ for a specific selection of J.

Under suitable regularity assumptions on e and J, one proves that the system admits well defined solutions for any initial conditions and in particular, as the number of players increases, a corresponding mean field analysis can be performed, with the mean field equation being a standard continuity equation describing the evolution of the continuous distribution of agents.

The idea is now to "reverse" the process: we are given observations $(x_1^N(t), \dots, x_N^N(t))$ and $(v_1^N(t), \dots, v_N^N(t))$, $t \in [0, T]$, for trajectories and velocities of a system of N evolving agents. The aim is to use an undisclosed fast reaction model to fit the data, under the assumption that every parameter is known except from J. Then, how is it possible to learn J from data? The general strategy, following [3], is to penalize some loss function measuring the mismatch between observations and predictions by the parametrized system. A possible choice is to penalize the mismatch between velocities, i.e., to consider the (non convex) energy

$$\mathcal{E}_v^N(J) = \frac{1}{T} \int_0^T \left[\frac{1}{N} \sum_{i=1}^N \left\| v_i^N(t) - v_i^J(x_1^N(t), \dots, x_N^N(t)) \right\|^2 \right] \mathrm{d}t.$$

This energy is directly linked to the discrepancy in trajectories, in the sense that for $(\hat{x}_1^N(t), \dots, \hat{x}_N^N(t))$ the solution of (UFR-N) induced by $\hat{J}$ for the same initial condition $(x_1^N(0), \dots, x_N^N(0)) \in [\mathbb{R}^d]^N$, one has

$$\frac{1}{N} \sum_{i=1}^N \|x_i^N(t) - \hat{x}_i^N(t)\| \le C \sqrt{\mathcal{E}_v^N(\hat{J})}$$

for all $t \in [0, T]$, with $C = C(T, \hat{J}, e, \varepsilon)$. Hence, payoff functions attaining small discrepancy in velocities are able to reproduce trajectories that are provably close to the observed ones. At this point, one can even use a minimal J (with respect to $\mathcal{E}_v^N$) to perform further data-driven simulations.

The whole learning process is stable in the limit: as $N \to \infty$, under the assumption that observations have a well defined mean field behaviour, suitable minimizers of the mismatch $\mathcal{E}_v^N$ at level N will converge to a minimizer of a limiting loss defined upon the mean field limit of the observations.

The abstract framework is fully constructive and numerically implementable. This is illustrated in [2] on computational examples where a ground truth payoff function is known and on examples where this is not the case, including a model for pedestrian movement, providing encouraging results for going in the direction of real-life data.

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Breaking the curse of dimension in multi-marginal optimal transport with Coulomb cost

Gero Friesecke

The multi-marginal OT problem with Coulomb cost is the following: Minimize

$$\int_{\mathbb{R}^d\times\ldots\times\mathbb{R}^d} \underbrace{\sum_{1\le i<j\le N} \frac{1}{|x_i-x_j|}}_{=:C[\gamma]}\, d\gamma(x_1,...,x_N) \quad \text{subj.to } \gamma\in\mathcal{P}(\mathbb{R}^d\times\ldots\times\mathbb{R}^d),\ \gamma\mapsto\mu,...,\mu.$$

Here $\mu \in \mathcal{P}(\mathbb{R}^d)$ is a given, typically absolutely continuous, marginal. All N marginals are equal, but the cost is repulsive, nonconvex, and (for $N \ge 3$) not twisted. Usually one is interested in symmetric minimizers (any nonsymmetric minimizer gives rise to a symmetric one, by symmetrization).

Motivation. In N-electron quantum mechanics, the following problem introduced from 1964 to 1983 by P.Hohenberg, W.Kohn, M.Levy, and E.Lieb plays an important role which contains an additional Fisher-information-type term: For bosons or fermions,

$$\min_{\gamma\mapsto\mu,...,\mu} \int_{\mathbb{R}^{dN}} \frac{1}{2}|\nabla\sqrt{\gamma}|^2 + C[\gamma] \quad \text{respectively} \quad \min \int_{\mathbb{R}^{dN}} \sum_{spins} \frac{1}{2}|\nabla\Psi|^2 + C\big[\sum_{spins}|\Psi|^2\big].$$

In the latter case, the square root of γ has to be introduced explicitly and has to be taken in $\mathbb{C}$; the minimization is over Ψ's in $H^1((\mathbb{R}^d\times\mathbb{Z}_2)^N;\mathbb{C})$ which are antisymmetric and satisfy $\sum_{spins}|\Psi|^2 \mapsto \mu,...,\mu$. The minimand is the kinetic plus interaction energy of the quantum state Ψ and the constraint means that Ψ

has single-particle density μ. MMOT with Coulomb cost is the low-density limit of both the above problems: replacing μ by $\mu_\alpha(x) = \alpha^d \mu(\alpha x)$ yields

$$\min\ \alpha \int_{\mathbb{R}^{dN}} \sum_{spins} \frac{1}{2}|\nabla\psi|^2 + C\big[\sum_{spins} |\Psi|^2\big]$$

which Gamma-converges as $\alpha \to 0$ to MMOT with Coulomb cost. The limit problem was introduced in the physics literature by Seidl (1999). Its interpretation as OT is due to Cotar, Friesecke, Klüppelberg (CFK) (arXiv 2011, CPAM 2013) and Buttazzo, DePascale, Gori-Giorgi (Phys.Rev.A 2012). Note N = #particles= #marginals, motivating the interest in large N. For the proof of Gamma convergence see CFK 2011/2013 ($N = 2$), Bindini and DePascale J. de l'Ecole Polyt. 2017 (simpler proof, extension to $N = 3$) and CFK ARMA 2018 (general case).

Sparsity of optimal plans. The beautiful theorems by Brenier and Gangbo-McCann showed us that for nice costs, optimal plans of two-marginal problems with absolutely continuous marginals μ_1, μ_2 are of Monge form,

$$\gamma = (id, T)_\sharp \mu_1.$$

For multi-marginal problems, the corresponding Monge ansatz

$$\gamma = (id, T_2, ..., T_N)_\sharp \mu_1$$

was justified by Gangbo-Swiech and Agueh-Carlier for, respectively, the maximum correlation problem

$$\min \int \sum_{i<j} |x_i - x_j|^2 \text{ subject to } \gamma \mapsto \mu_1, ..., \mu_N$$

and the Wasserstein barycenter problem

$$\min \int \frac{1}{N} \sum_{i=1}^N |x_i - B(x)|^2 \text{ subject to } \gamma \mapsto \mu_1, ..., \mu_N, \text{ with } B(x) = \frac{1}{N} \sum_{i=1}^N x_i;$$

in the latter case, $B_\sharp\gamma$ is the Wasserstein barycenter of the marginal measures. The story for the Coulomb cost turned out to be more complicated than originally expected. The Monge ansatz is known to be justified for $N = 2$ or $d = 1$ (work by, respectively, CFK 2011/2013 and Colombo, Di Marino, De Pascale (Canadian J. Math. 2015)). Pass (Nonlinearity 2012) has constructed an example for $N = d = 3$ with a nonunique minimizer of non-Monge form. Whether Monge-type minimizers always exist for the Coulomb cost is an open problem.

Sparsity after discretization; breaking the curse of dimension with respect to storage. In [2], the following slight generalization of the Monge ansatz was introduced. It is almost as sparse, yet – at least for discrete problems – sufficiently general to ensure existence of optimizers for any number of marginals and any cost. Let $X = \{a_1, ..., a_\ell\} \subset \mathbb{R}^d$ be any set of discretization points, or 'finite state space', and let $\Pi_\mu = \{\gamma \in \mathcal{P}(X^N) : \gamma \text{ symmetric}, \gamma \mapsto \mu, ..., \mu\}$ be the Kantorovich polytope for marginal μ. Below, $S_N\gamma$ denotes the symmetrization $(S_N\gamma)(A_1 \times ... \times A_N) = N!^{-1} \sum_{\text{permutations } \sigma} \gamma(A_{\sigma(1)} \times ... \times A_{\sigma(N)})$.

Theorem 1. [2] *For any $\mu \in \mathcal{P}(X)$, all extreme points of Π_μ are of 'Quasi-Monge' form:*

$$\gamma = S_N(T_1, ..., T_N)_\sharp \tilde{\mu}$$

for some $\tilde{\mu} \in \mathcal{P}(X)$ and some quasi-Monge maps $T_1, ..., T_N$ satisfying, instead of the classical Monge conditions $T_{i\sharp}\mu = \mu$, the average condition $\frac{1}{N}\sum_{i=1}^{N} T_{i\sharp}\tilde{\mu} = \mu$.

As a corollary, for any N, any cost function $c : X^N \to \mathbb{R}$, and any marginal μ, the discrete OT Problem 'Minimize $\int_{X^N} c\, d\gamma$ over $\gamma \in \Pi_\mu$' possesses an optimizer of quasi-Monge form. This breaks the curse of dimension with respect to storage, because – unlike a general Kantorovich plan in $\mathcal{P}(X^N)$ which needs ℓ^N coefficients to store – a quasi-Monge state only requires $\ell \cdot (N+1)$ coefficients (ℓ coefficients for each quasi-Monge map, of which there are N, and an extra ℓ for the measure $\tilde{\mu}$). Thus the storage cost goes down from exponential in N to linear in N. Sparsity is even more striking for MMOT than for two-marginal OT!

When μ is uniform (this is the analogue of absolute continuity in the discrete case), there is an important difference between two- and multi-marginal problems: for $N = 2$ the quasi-Monge ansatz can be replaced by the Monge ansatz (this is the content of the Birkhoff-Von Neumann theorem). When $N \geq 3$, the Monge ansatz is not enough and the extension to quasi-Monge states is really needed. For a proof of this via a simple counterexample with $N = \ell = 3$ see [1].

Alfonsi, Coyaud, Ehrlacher, and Lombardi (Math. Comp. 2021) established existence of sparse optimizers even in the situation when the state space is kept continuous and only the marginal constraints are discretized; moreover they proposed a constrained Lagrangian particle method for simulating the ensuing problem. Khoo and Ying (SIAM J. Sci. Comp. 2019) introduced and studied a semi-definite relaxation of a two-marginal formulation of MMOT from [2] and presented an algorithm for the relaxed problem.

Algorithm for breaking the curse of dimension: Genetic column generation. Very recently, in joint work with Andreas Schulz (TUM) and Daniela Vögler (TUM) [3] we finally figured out how to run an algorithm which finds such quasi-Monge states for, say, up to $N = 30$ marginals/electrons discretized by $\ell = 100$ gridpoints each, despite the ensuing Kantorovich polytope Π_μ having dimension about 10^{30}. In benchmark examples where the exact solution is known, the algorithm always found the exact optimizers, and was empirically observed to do this in polynomial time with respect to the system size, despite the fact that we prove rigorously that the key subproblem tackled by the algorithm is NP-complete. See Figure 5 of [3]. Our algorithm, called `GenCol`, is based on three ideas:

– exploit sparsity (in the 'quasi-Monge' version of [2]). For large N, one simply cannot afford to throw away the beautiful sparsity of optimal plans, revealed by many workers over may years (Brenier, Gangbo-McCann, Agueh-Carlier, ...).

– use the method of column generation (CG): replace the original LP by a small subproblem; solve it; add a new 'column' by solving a pricing problem; iterate. This is a standard method in discrete optimization, not hitherto used in MMOT,

which originated in integer programming ($\ell = 2$, N large). Note that this is the opposite regime to $N = 2$, ℓ large where Sinkhorn works best!

– the well known bottleneck in CG is that one needs to efficiently generate new candidate columns for the pricing problem; this is overcome by a genetic learning method tailormade for MMOT. In our context new columns represent intricately correlated spatial many-body configurations of the system, which are not known a priori; these are learned with the help of an "adversary" represented by the dual state within CG, in loose similarity to Wasserstein GANs.

For a more detailed description and numerical results see [3] sections 5 and 7.

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Equality of the Jellium and Uniform Electron Gas next-order asymptotic terms for Coulomb and Riesz potentialss

Codina Cotar

(joint work with Mircea Petrache)

Setting. We consider three minimization problems, and compare their asymptotics. In all three problems we will consider the energy of N-points configurations, in which the pairwise interaction $\mathsf{c}(x-y)$ between points $x, y \in \mathbb{R}^d$, depends upon the power-law potentials

$$\mathsf{c}(x) := \frac{1}{|x|^s} \text{ where } s > 0. \tag{1}$$

The first minimization which we consider is the *generalized Jellium* minimization problem, stated as follows. For a bounded domain $\Omega_N \subset \mathbb{R}^d$ with $|\Omega_N| = N$ (the most known case in the literature being that of $\Omega_N = K_R$, a cube of radius $R = N^{1/d}$), let

$$\mathrm{Jel}_{N,s}(\Omega_N) := \inf \Bigg\{ \sum_{\substack{1\le i,j\le N \\ i\neq j}} \mathsf{c}(x_i - x_j) - 2 \sum_{1\le i\le N} \int_{\Omega_N} \mathsf{c}(x_i - y)\mathrm{d}y + \int_{\Omega_N}\int_{\Omega_N} \mathsf{c}(x-y)\mathrm{d}x\mathrm{d}y : \; x_1, \dots, x_N \in \Omega_N \Bigg\}. \tag{2}$$

The second minimization which we consider is the closely-related *Coulomb and Riesz gases* minimization of energy

$$\mathcal{E}_{N,s}(V) := \inf \left\{ \sum_{1\le i\neq j\le N} \mathsf{c}(x_i - x_j) + N\sum_{i=1}^{N} V(x_i) : x_1, \dots, x_N \in \mathbb{R}^d \right\}, \tag{3}$$

where the external "confining" potential $V : \mathbb{R}^d \to \mathbb{R}$ satisfies

(V1) V is assumed to be bounded below, lower semicontinuous, such that $\{x : V(x) < \infty\}$ has positive c-capacity, and such that $V(x) \to \infty$ as $|x| \to \infty$. (Note that a set Ω has positive $\mathbf{c}$-capacity if there exists a positive measure supported on Ω such that $\int\int \mathsf{c}(x-y)d\mu(x)d\mu(y) < \infty$.)

The third problem which we consider is an *N-marginal optimal transport* (OT) problem with cost similarly given by pairwise interactions as above. For given $\mu \in \mathcal{P}(\mathbb{R}^d)$ we consider

$$\mathcal{F}_{N,s}(\mu) = \inf \left\{ \int_{(\mathbb{R}^d)^N} \sum_{i,j=1, i\neq j}^{N} \mathsf{c}(x_i - x_j)\mathrm{d}\gamma_N(x_1, \dots, x_N) : \gamma_N \in \mathcal{P}^N_{\mathrm{sym}}(\mathbb{R}^d), \gamma_N \mapsto \mu \right\}. \tag{4}$$

Here $\mathcal{P}^N_{sym}(\mathbb{R}^d) \subset \mathcal{P}((\mathbb{R}^d)^N)$ is the subset of probability measures which are invariant under the permutation of the N factors of the cartesian product $(\mathbb{R}^d)^N$ and the notation $\gamma_N \mapsto \mu$ means that γ_N has one-body density μ (physics terminology) or equivalently equal $\mathbb{R}^d$-marginals μ (probability terminology), i.e.

$$\gamma_N(\underbrace{\mathbb{R}^d \times \ldots \times \mathbb{R}^d}_{\text{i-1 times}} \times A_i \times \underbrace{\mathbb{R}^d \times \ldots \times \mathbb{R}^d}_{\text{N-i times}}) = \int_{A_i} \mathrm{d}\mu(x) \text{ for all Borel } A_i \subseteq \mathbb{R}^d \text{ and all } i = 1, \dots, N. \tag{5}$$

The case $s = 1, d = 3$, of (2) is the *classical Jellium problem* studied by Lieb and Narnhofer (1975), and it is of great interest in physics, where it has been extensively studied.

The problem (3) has its origin in numerical approximation questions, where it becomes important to study different measures of uniformity of large point configurations. Other motivations come from the study of interactions of vortices in supercondictivity. Important open problems closely linked to (3) are Smale's 7th problem, which in the case where the points are constrained to a submanifold in $\mathbb{R}^d$ requires to understand how to construct in polynomial time N-point configurations which are optimal to high accuracy and the mathematical understanding of large-N Abrikosov crystallization phenomena, especially in 2 dimensions. Tackling these long-open problems is the main motivation leading to the study of large-N asymptotics of the form (3).

The motivation for studying the problem (4) comes from Density Functional Theory (DFT). The functional $\mathcal{F}_{N,s}(\mu)$ appearing therein, in the particular case $s = 1, d = 3$, turns out to be a natural semiclassical limit to the famous *Hohenberg-Kohn (HK)* functional from quantum mechanics, originally introduced by Hohenberg-Kohn in the 1960s, and later rigorously proved by Levy and Lieb.

Main results. Concerning the $N \to \infty$ behavior of the problems (3) and (4), we are going first to note that the leading order term is in both cases a "mean field" term, and the only difference is that for the first problem we have imposed an external potential in order to confine the minimizing configurations, whereas in the second problem we did not (and the configurations are confined via the marginal constraint $\gamma_N \mapsto \mu$).

It seems that in both the (3) and (4) minimzation problems, a next-order asymptotics is available only for powers with long-range interactions, i.e. in the regime $s < d$, and therefore we restrict to this case. We also restrict here to the case $s > 0$.

Our first main result is the following:

Theorem 1. *Set $d \geq 1$. Assume that c is as in (1) with $0 < s < d$.*

(a) *(Asymptotics for the Jellium minimization problem (2))*
Let $\mu \in \mathcal{P}(\mathbb{R}^d)$ have continuous density ρ and $\mathrm{supp}(\rho) := U$ compact. Then

$$\lim_{N\to\infty} \frac{\mathrm{Jel}_{N,s}(\mu)}{N^{1+\frac{s}{d}}} = C_{\mathrm{Jel}}(s,d) \int_{\mathbb{R}^d} \rho^{1+\frac{s}{d}}(x)\mathrm{d}x, \tag{6}$$

where $C_{\mathrm{Jel}}(s,d) < 0$ depends only on s and d.

(b) *(Next-order term for the Coulomb and Riesz gases minimization problem (3))*
Assume that V is continuous, $\lim_{|x|\to\infty} V(x) = \infty$ and $\int_{\mathbb{R}^d} \exp(-V(x))\mathrm{d}x < \infty$. Then there exists a minimizer $\mu_V \in \mathcal{P}(\mathbb{R}^d)$ of the functional $I_{s,V}(\mu)$

$$\mathcal{I}_{s,V}(\mu) := \int_{\mathbb{R}^d}\int_{\mathbb{R}^d} \frac{1}{|x-y|^s}\mathrm{d}\mu(x)\ \mathrm{d}\mu(y) + \int_{\mathbb{R}^d} V(x)\mathrm{d}\mu(x), \tag{7}$$

where μ_V is compactly-supported and unique In particular, if μ_V has a continuous density ρ_V, we have the expansion

$$\lim_{N\to\infty} \frac{\mathcal{E}_{N,s}(V) - N^2\mathcal{I}_{s,V}(\mu_V)}{N^{1+\frac{s}{d}}} = \mathsf{C}_{\mathrm{Gas}}(s,d) \int_{\mathbb{R}^d} \rho_V^{1+\frac{s}{d}}(x)\,\mathrm{d}x, \tag{8}$$

where $C_{\mathrm{Gas}}(s,d) < 0$ depends only on s and d.

The asymptotics for the problems (2) and (3) have not been studied up to now in the cases $0 < s < d-2$. Theorem 1 (b) was previously proved by Petrache and Serfaty (2015) for c as in (1), with either $d \geq 3$ and $d-2 \leq s < d$, or $d = 2$ and $d-2 < s < d$, and with V satisfying (V1)

The main ingredient in the proof of Theorem 1 is the Fefferman-Gregg decomposition, as detailed in [1], which allows to reduce the original Riesz long-range interaction to a short-range interaction, greatly simplifying the problem.

Our second main result links the above three problems via the following result:

Main Theorem. *Let $d \geq 1$ and $0 < s < d$. We have*

$$\mathsf{C}_{\mathrm{Jel}}(s,d) = \mathsf{C}_{\mathrm{UEG}}(s,d) = \mathsf{C}_{\mathrm{Gas}}(s,d).$$

For $s = 1, d = 3$, our Main Theorem solves a controversy recently formulated by M. Lewin. More precisely, unlike what is implied by only looking at the case of crystals, we find that the Jellium and Uniform Electron Gas energies are the same, even in the Coulomb case. By comparison with the periodic (or more generally, homogeneous) case, we see that this must be due to important boundary effects, peculiar to the Coulomb case.

For our final result, we find the property of $\mathsf{C}_{\mathrm{UEG}}(s,d)$ being continuous in s across all the range of exponents $0 < s < d$.

Proposition 2. *Let $d \geq 1$. Then the value of $\mathsf{C}_{\mathrm{UEG}}(s,d)$ is left- and right-differentiable as a function of s, for $s \in (0,d)$. Furthermore, we have*

$$\lim_{s\to 0} \mathsf{C}_{\mathrm{UEG}}(s,d) = -1.$$

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Regularized unbalanced optimal transport and the large deviations of the branching Brownian motion

Aymeric Baradat

(joint work with Hugo Lavenant)

Let us give ourselves a dimension $d \in \mathbb{N}^*$, two positive parameters $\nu, \lambda > 0$ and a sequence of nonnegative numbers $(p_k)_{k\in\mathbb{N}} \in \mathbb{R}_+^{\mathbb{N}}$ satisfying $\sum_k p_k = 1$. Let us define the nonnegative convex function $\Psi : \mathbb{R} \to \mathbb{R}_+ \cup \{+\infty\}$ through its Legendre transform, as:

$$\Psi(r) := \sup_{s\in\mathbb{R}} rs - \Psi^*(s), \quad \forall r \in \mathbb{R},$$
$$\Psi^*(s) := \nu\lambda \sum_k p_k \left(e^{(k-1)\frac{s}{\nu}} - 1 \right), \quad \forall s \in \mathbb{R}.$$

The purpose of this work is to derive with probabilistic arguments the regularized unbalanced optimal transport problem aiming at finding, given two nonnegative finite Borel measures on the torus $\rho_0, \rho_1 \in \mathcal{M}_+(\mathbb{T}^d)$, the minimal value, denoted by $\mathrm{RUOT}(\rho_0, \rho_1)$, of

$$\int_0^1 \int \left\{ \frac{|v_t(x)|^2}{2} + \Psi(r_t(x)) \right\} \mathrm{d}\rho_t(x)\mathrm{d}t \tag{1}$$

among all triplets (ρ, v, r) satisfying in a weak sense

$$\begin{cases} \partial_t \rho_t + \operatorname{div}(\rho_t v_t) = \dfrac{\nu}{2}\Delta\rho_t + r_t\rho_t, \\ \rho_t|_{t=0} = \rho_0, \quad \rho_t|_{t=1} = \rho_1. \end{cases}$$

Here, ρ is a measurable curve in the set $\mathcal{M}_+(\mathbb{T}^d)$ of nonnegative finite Borel measures on $\mathbb{T}^d$, and $v = v_t(x)$ (resp. $r = r_t(x)$) is a measurable time-dependent vector fields (resp. scalar fields) with enough integrability for (1) to be finite.

1. Motivation

This study was motivated by a series of works, among which we cite [6, 4], which propose to interpolate between measurements coming from experiments in developmental biology using optimal transport methods.

These experiments focus on the mechanism of specialization of the cells of an individual during its development. For a given species, they aim at finding the typical evolution of the positions of the cells of individuals in the simplex of large dimension

$$\mathbb{S}^{N-1} := \{(x_1, \dots x_N) \in \mathbb{R}_+^N \ : \ x_1 + \cdots + x_N = 1\},$$

N being the number of genes in the DNA of this species. A cell is represented at position $(x_1, \dots x_N) \in \mathbb{S}^{N-1}$ if the proportion of RNA corresponding to gene $i = 1, \dots, N$ in this cell is x_i. Nowadays, its is possible to measure these proportions for a large number of cells of a large number of individuals at different stages of the development. The question is to get the whole movie of the development out of these measurements at discrete times.

The choice to use optimal transport is rather natural, and the need to consider unbalanced effects comes from the fact that the number of cells increase during the development of an individual. Our work suggests a specific cost for the growth of the population of cells. This cost can be computed in terms of parameters that can be at least approximately determined experimentally.

2. Entropic minimization w.r.t. the branching Brownian motion

Call R the law of of the branching Brownian motion of diffusivity ν, branching rate λ, and law of descendants $(p_k)_{k\in\mathbb{N}}$, that is, the process in which a population of independent Brownian particles of diffusivity ν die at independent random exponential times of parameter λ, and are replaced at these times by $k \in \mathbb{N}$ particles with probability p_k.

The law R is seen as a probability measure on $\Omega := \mathit{càdlàg}([0,1], \mathcal{M}_+(\mathbb{T}^d))$, the set of measure valued *càdlàg* curves: one realization of the branching Brownian motion is the time-dependent measure on the torus putting Dirac masses at the positions of the particles. Otherwise interpreted, this is a moving point cloud.

To characterize entirely R, one also needs an initial law, that is, a probability measure R_0 on the set $\Omega_0 := \mathcal{M}_+(\mathbb{T}^d)$, which concentrates on the set of finite sums of Dirac masses: R_0 is the law of a random point cloud.

For $t \in [0,1]$, we define $M_t : \Omega \to \mathcal{M}_+(\mathbb{T}^d)$ as the evaluation map at time t: this is the random variable on Ω whose value is the point cloud at time t. Also, we call $M : \Omega_0 \to \mathcal{M}_+(\mathbb{T}^d)$ the identity map.

If P_0 is a law on Ω_0, its *intensity* is the measure $\rho := \mathbb{E}_{P_0}[M] \in \mathcal{M}_+(\mathbb{T}^d)$. Correspondingly, if P is a law on Ω and $t \in [0,1]$, its *intensity* at time t is $\mathbb{E}_P[M_t]$.

Given $\rho_0, \rho_1 \in \mathcal{M}_+(\mathbb{T}^d)$, we call $\mathrm{H}(\rho_0, \rho_1)$ the optimal value of the relative entropy

$$H(P|R) := \begin{cases} \mathbb{E}_R[F \log R], & \text{if } P \ll R \text{ and } P = F \cdot R, \\ +\infty, & \text{otherwise,} \end{cases}$$

among laws P on Ω whose intensity at times $t = 0$ and 1 are ρ_0 and ρ_1 respectively. Due to Sanov's theorem, solving this entropic problem is like studying the large deviations of the space distribution of a large number of independent branching Brownian particles.

Finally, we call L the Legendre transform of the log-Laplace transform of the point cloud of law R_0, *i.e.*

$$\mathrm{L}(\rho) := \sup_{\varphi \in C^0(\mathbb{T}^d)} \int \varphi \, \mathrm{d}\rho - \log \mathbb{E}_{R_0} \left[\exp\left(\int \varphi \, \mathrm{d}M \right) \right].$$

Theorem 1. *Under mild technical assumptions*[1] *on* R_0 *and* $(p_k)_{k\in\mathbb{N}}$*, the map* $(\rho_0, \rho_1) \in (\mathcal{M}_+(\mathbb{T}^d))^2 \mapsto \nu \mathrm{L}(\rho_0) + \mathrm{RUOT}(\rho_0, \rho_1)$ *is the lower semi-continuous envelope of* H *for the topology of narrow convergence.*

Roughly speaking, the theorem indicates that

- To each competitor of the entropic problem corresponds a competitor for the regularized unbalanced optimal transport problem;
- To each competitor of the regularized unbalanced optimal transport problem corresponds a competitor of the entropic problem *up to regularization.*

We claim that this property is enough for both problems to be heuristically considered as the same one.

3. Open problems

3.1. **Other reference laws and small noise limit.** When R is the law of a branching Brownian motion with $p_0 = p_2 = 1/2$, in the regime where $\nu \to 0$ and $\lambda \sim \frac{1}{\nu} \exp(-1/\nu)$, we are able to show the Γ-convergence at the PDE level towards *optimal partial transport* (see *e.g.* [3]), that is, when $\Psi(r) = |r|$. Is it possible to get other unbalanced optimal transport models, especially the one where $\Psi(r) = r^2$ (see *e.g.* [5]) by using other kinds of branching processes as a reference law?

[1] The theorem holds *e.g.* when $p_k = 0$ for k large enough, and R_0 *(i)* exhibits a bounded number of points or *(ii)* is a Poisson point process of intensity proportional to Lebesgue.

3.2. **Fast algorithm?** The solutions of the regularized optimal transport are known to be calculable efficiently using the *Sinkhorn* algorithm [2, 1]. This algorithm relies heavily on the invariance of the Brownian motion through time reversal. The branching Brownian motion doesn't satisfy this property, so that there is no easy way to generalize the Sinkhorn algorithm in this case. Is it nevertheless possible to design a fast algorithm doing the job?

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On overrelaxation in the Sinkhorn algorithm

Max von Renesse

(joint work with Tobias Lehmann, Alexander Sambale, Andre Uschmajew)

Summary. We derive an a-priori parameter range for overrelaxation of the Sinkhorn algorithm, which guarantees global convergence and a strictly faster asymptotic local convergence. Guided by the spectral analysis of the linearized problem we pursue a zero cost procedure to choose a near optimal relaxation parameter.

Background and statement of the problem. The Sinkhorn algorithm is the benchmark approach to fast computation of the entropic regularization of optimal transportation [3]. Ultimately, one is faced with the following numerical problem: Given two probability vectors $a \in \mathbb{R}^m_+$, $b \in \mathbb{R}^n_+$ and a matrix $K \in \mathbb{R}^{m\times n}_+$, the goal is to find a pair of vectors $(u, v) \in \mathbb{R}^m_+ \times \mathbb{R}^n_+$ such that

$$u \circ Kv = a \quad \text{and} \quad v \circ K^{\mathsf{T}} u = b, \tag{1}$$

where $x \circ y$ denotes the component wise multiplication (Hadamard product) of vectors of equal dimension. We assume $\min(m, n) \geq 2$.

In the standard Sinkhorn algorithm an approximating sequence (u_ℓ, v_ℓ) starting from an initial vector $v_0 \in \mathbb{R}^n_+$ is constructed via the update rule

$$u_{\ell+1} = \frac{a}{Kv_\ell}, \qquad v_{\ell+1} = \frac{b}{K^{\mathsf{T}} u_{\ell+1}},$$

where $\frac{x}{y}$ denotes the component wise division of vectors of equal dimension. It is a classic result by Sinkhorn [13] that for any initial point $v_0 \in \mathbb{R}^n_+$ the algorithm converges to a solution (u^*, v^*) of (1). Moreover, the solution is unique modulo rescaling $(tu^*, t^{-1}v^*)$, $t > 0$. The rate of convergence, e.g. of suitably normalized iterates $u_\ell/\|u_\ell\|$ and $v_\ell/\|v_\ell\|$, or using other distance measures, is at least $O(\Lambda(K)^2)$, where $\Lambda(K) < 1$ is the Birkhoff contraction ratio defined in (3) below, c.f. [6, 12].

In this note we discuss a modified version of the Sinkhorn algorithm employing relaxation, which was recently proposed in [14] and [11]. It uses the update rule

$$u_{\ell+1} = u_\ell^{1-\omega} \circ \left(\frac{a}{Kv_\ell}\right)^\omega, \qquad v_{\ell+1} = v_\ell^{1-\omega} \circ \left(\frac{b}{K^\mathsf{T} u_{\ell+1}}\right)^\omega, \tag{2}$$

where $\omega > 0$ is are suitably chosen relaxation parameter, and exponentiation is understood component wise. In a log-domain formulation the relation to the classic concept of relaxation in (nonlinear) fixed point iterations will become immediately apparent. The iteration (2) still has the solution of (1) as its unique (modulo scaling) fixed point. As illustrated in op. cit., choosing the parameter ω larger than one can significantly accelerate the convergence speed compared to the standard Sinkhorn method, which sometimes can be slow. For optimal transport, such an improvement could be in particular relevant in the regime of small regularization, or when a high target precision is needed, such as in applications in density functional theory [2]. The main challenge of the approach, however, is a good choice of the overrelaxation of the parameter which depends on the linearisation of the spectral properties of the Sinkhorn iteration map at the fixed point, which is not known at the outset of the procedure. To deal with this issue, in [14] an adaptive approach is proposed. In our comment we address the question whether instead an a-priori choice of ω is possible and beneficial.

Main result. To state our main result let us recall the Birkhoff contraction ratio of a matrix with strictly positive entries which is defined as

$$\eta(K) = \max_{i,j,k,\ell} \frac{K_{ik}K_{j\ell}}{K_{jk}K_{i\ell}} \quad \text{and} \quad \Lambda(K) = \frac{\sqrt{\eta(K)}-1}{\sqrt{\eta(K)}+1}. \tag{3}$$

Secondly, given the data of the problem in form of a triple (K, a, b) we introduce the quantity

$$\delta_1 = \frac{a_{\min}}{b_{\max}} \cdot \frac{1-b_{\max}}{\left(\frac{\|K\|_\infty}{\sigma_{\min}(K)}\right)^2 - a_{\min}} > 0, \quad \delta_2 = \frac{b_{\min}}{a_{\max}} \cdot \frac{1-a_{\max}}{\left(\frac{\|K^\mathsf{T}\|_\infty}{\sigma_{\min}(K)}\right)^2 - b_{\min}} > 0, \quad \text{where}$$

$\sigma_{\min}(K)$ is the smallest positive singular value of K, $\|K\|_\infty = \max_{\|v\|_\infty=1} \|Kv\|_\infty$, and the subscripts min, max denote the smallest and largest entry of the corresponding vector and

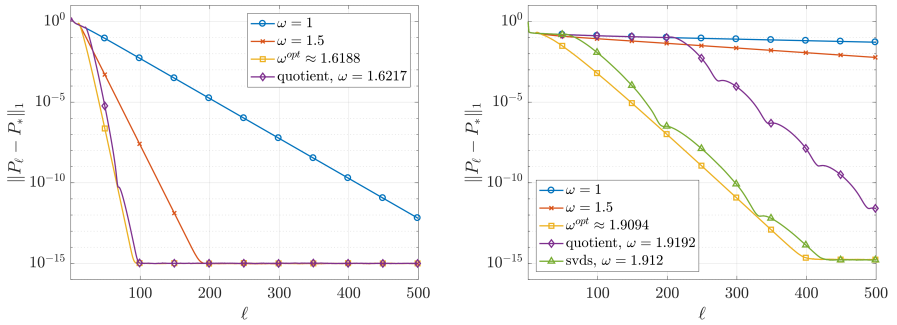
$$\delta_{K,a,b} := \begin{cases} \delta_1 & \text{if } m > n, \\ \delta_2 & \text{if } m < n, \\ \max(\delta_1, \delta_2) & \text{if } m = n. \end{cases}$$

Then our results can be summarized as follows.

Theorem. *Assume* $rank(K) = \min(m, n) \geq 2$. *Then for any* $1 < \omega < \min\left(1 + \delta_{K,a,b}, \frac{2}{1+\Lambda(K)}\right)$ *the modified method is both globally convergent and asymptotically faster than the standard method.*

This result is based on a global convergence guarantee which is obtained in the framework of so called compositional data space (c.f.[1]) and an a priori bound for the second largest eigenvalue of the linearized Sinkhorn iteration at the fixed point.

Numerical experiments and practical choice of ω In practice, the acceleration of our theoretically based a-priori choice for ω turns out to be only marginal. As a remedy we propose to estimate the critical spectral parameter only once after a few steps and then choose $\omega > 1$ once and for all based on this estimate. Below we present the empirical results for two model problems.



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Small- and long-time asymptotics of Entropic Optimal Transport

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(joint work with Giovanni Conforti, Léonard Monsaingeon, Dmitry Vorotnikov)

Entropic Optimal Transport and Schrödinger problem represent two (equivalent, in the Euclidean setting) ways to regularize the Monge-Kantorovich optimal transport problem. Because of this fact, they have gained a lot of attention in the recent years and have already shown to have far reaching consequences in various fields, ranging from machine learning to geometric analysis and functional inequalities. However, despite the equivalence, Entropic Optimal Transport and Schrödinger problem are very different in nature; the latter is more probabilistic and has a much stronger physical interpretation, which is still valid far beyond the Euclidean context. For this reason we shall adopt this second viewpoint and start by defining the Schrödinger problem as

$$\inf_{\pi\in\Pi(\mu_0,\mu_1)} H(\pi\,|\,\mathsf{R}_\varepsilon), \tag{1}$$

where $\Pi(\mu_0,\mu_1)$ denotes the set of couplings between μ_0 and μ_1, H the Boltzmann-Shannon relative entropy, and R_ε some reference measure (usually, the joint law at time 0 and ε of some diffusion process). The optimal value of (1) shall be denoted henceforth by $\mathscr{C}_\varepsilon(\mu_0,\mu_1)$ and called *entropic cost*. After [7, 8] the 'static' formulation of the Schrödinger problem is in fact equivalent to the following dynamical (à la Benamou-Brenier) one

$$\varepsilon\mathscr{C}_\varepsilon = \frac{\varepsilon}{2}\Big(H(\mu_0\,|\,\mathfrak{m})+H(\mu_1\,|\,\mathfrak{m})\Big)+\inf\iint_0^1\Big(\frac{|v_t|^2}{2}+\frac{\varepsilon^2}{8}|\nabla\log\rho_t|^2\Big)\rho_t\mathrm{d}t\mathrm{d}\mathfrak{m}, \tag{2}$$

where the infimum runs over all distributional solutions (ρ_t,v_t) of the continuity equation.

In this talk we shall investigate the entropic cost on weighted manifolds, studying its behaviour as $\varepsilon\downarrow 0$ (thus recovering optimal transport and the Wasserstein distance) and as $\varepsilon\to\infty$ (in this case, $\mathscr{C}_\varepsilon$ is related to information theory and approximates MMD divergences). More precisely, our framework will be a weighted smooth Riemannian manifold (M,g) with reference measure $\mathfrak{m}:=e^{-V}\mathrm{vol}$, where vol is the volume form and V is a smooth function such that $\mathrm{Ric}_g+\mathrm{Hess}(V)\geq\kappa g$

for some $\kappa \in \mathbb{R}$. As a first step, one has to observe that $\mathscr{C}_\varepsilon$ regularly depends on the 'temperature' parameter ε and its first derivative can be explicitly computed as

$$\frac{\mathrm{d}}{\mathrm{d}\varepsilon}\mathscr{C}_\varepsilon(\mu_0,\mu_1) = -\mathcal{E}_\varepsilon(\mu_0,\mu_1) := -\int \Big(\frac{|v_t^\varepsilon|^2}{2\varepsilon^2} - \frac{1}{8}|\nabla \log \rho_t^\varepsilon|^2\Big)\rho_t^\varepsilon \mathrm{d}\mathfrak{m},$$

$\mathcal{E}_\varepsilon(\mu_0,\mu_1)$ being the total energy of the system: indeed, it coincides with the Hamiltonian associated with (2) evaluated along the unique critical solution $(\rho_t^\varepsilon, v_t^\varepsilon)$. Although this elegant (from a physical standpoint) identity is rather elementary, since it is a consequence of (2) and of the envelope theorem, its consequences are extremely important, both for the long- and small-time asymptotics of the entropic cost. Indeed, as regards the former, once it is known that $\mathscr{C}_\varepsilon(\mu_0,\mu_1) \to H(\mu_0\,|\,\mathfrak{m}) + H(\mu_1\,|\,\mathfrak{m})$ as $\varepsilon \to \infty$ (and this can be seen by Γ-convergence arguments), this information can be improved into a quantitative version by leveraging on an 'energy-transport' inequality [1, 3] of the form '$|\mathcal{E}_\varepsilon(\mu_0,\mu_1)| \le C(\kappa,\varepsilon)\mathscr{C}_\varepsilon(\mu_0,\mu_1)$' and on an 'entropic' version of the celebrated Talagrand inequality (see [2]). In this way, the first main result of [3] reads as follows.

Theorem 1. *If $\kappa > 0$, then $\mathscr{C}_\varepsilon(\mu_0,\mu_1) \to H(\mu_0\,|\,\mathfrak{m}) + H(\mu_1\,|\,\mathfrak{m})$ as $\varepsilon \to \infty$ with*

$$|\mathscr{C}_\varepsilon(\mu_0,\mu_1) - H(\mu_0\,|\,\mathfrak{m}) - H(\mu_1\,|\,\mathfrak{m})| \le \frac{2}{e^{\kappa\varepsilon/2}-1}\Big(H(\mu_0\,|\,\mathfrak{m}) + H(\mu_1\,|\,\mathfrak{m})\Big)$$

The rate $e^{-\kappa\varepsilon/2}$ is sharp.

As for the short-time asymptotics, by the pioneering works of Mikami [10] and Léonard [9] it is well known that the rescaled entropic cost $\varepsilon\mathscr{C}_\varepsilon(\mu_0,\mu_1)$ converges to the halved squared Wasserstein distance between μ_0 and μ_1, and another step forward was made with the computation of the first derivative of the rescaled entropic cost at $\varepsilon = 0$, see [6, 12]. The importance of continuing this research line by determining the second derivative is evident and, in contrast to the 'static' approach used in the long-time regime, in this case our strategy heavily relies on the dynamical representation (2). For technical reasons that will not be discussed here, we restrict ourselves to weighted manifolds with Bakry-Émery Ricci tensor satisfying the curvature-dimension condition $\mathsf{CD}(\kappa, N)$ for some $N < \infty$.

Theorem 2. *If M satisfies $\mathsf{CD}(\kappa,N)$ and $\iint_0^1 |\nabla \log \rho_t^0|^2 \rho_t^0 \mathrm{d}t\mathrm{d}\mathfrak{m} < \infty$, where $(\rho_t^0\mathfrak{m})_{t\in[0,1]}$ is the unique Wasserstein geodesic between μ_0 and μ_1, then*

$$\varepsilon\mathscr{C}_\varepsilon(\mu_0,\mu_1) = \frac{1}{2}W_2(\mu_0,\mu_1)^2 + \frac{\varepsilon}{2}\Big(H(\mu_0\,|\,\mathfrak{m}) + H(\mu_1\,|\,\mathfrak{m})\Big) + \frac{\varepsilon^2}{8}\iint_0^1 |\nabla \log \rho_t^0|^2 \rho_t^0 \mathrm{d}t\mathrm{d}\mathfrak{m} + o(\varepsilon^2)$$

After this discussion, the reader may wonder whether these properties are peculiar to the structure of the Schrödinger problem, and thus of the choice of the Boltzmann-Shannon entropy in (1) and of the Fisher information as penalization term in (2), or if instead they are a particular case of a more general paradigm. In [11] this problem is addressed and studied for the small-time asymptotics. Since the proof of Theorem 2 relies on (2), the first step consists in generalizing the

Benamou-Brenier-like representation formula both at the level of setting and penalization term. To this end, note that the kinetic part in (2) can be interpreted as the metric speed with respect to the Wasserstein distance of the curve $t \mapsto \rho_t \mathfrak{m}$, whereas the Fisher information coincides with the slope of the relative entropy. Therefore, (2) can be seen as a particular case of

$$\inf_{\gamma:\gamma_0=x,\gamma_1=y} \frac{1}{2}\int_0^1 \Big(|\dot\gamma_t|^2 + \varepsilon^2 |\partial \mathsf{E}|^2(\gamma_t)\Big)\mathrm{d}t, \tag{3}$$

which can be formulated on any metric space (X,d) for any functional $\mathsf{E}: X \to \mathbb{R}\cup\{+\infty\}$. Under certain assumptions (the existence of a suitable 'weak' topology σ on X and the existence of an EVI_λ-gradient flow associated with E), the main results of [11] can be summarized as follows.

Theorem 3. *Problem* (3) Γ*-converges to the geodesic problem (i.e.* (3) *with* $\varepsilon = 0$*) as* $\varepsilon \downarrow 0$ *for the pointwise-in-time* σ*-convergence on* $C([0,1],X)$*.*

If there exists ω^* *optimal for* (3) *with* $\varepsilon = 0$ *such that* $\int_0^1 |\partial \mathsf{E}|^2(\omega_t^*)\mathrm{d}t < \infty$*, then*

$$\tilde{\mathscr{C}}_\varepsilon(x,y) = \tilde{\mathscr{C}}_0(x,y) + \varepsilon^2 \inf \int_0^1 |\partial \mathsf{E}|^2(\omega_t)\mathrm{d}t + o(\varepsilon^2),$$

where $\tilde{\mathscr{C}}_\varepsilon(x,y)$ *denotes the optimal value of* (3) *and the infimum runs over all minimizers of* (3) *with* $\varepsilon = 0$*.*

Although the hypotheses mentioned above may appear quite demanding, several interesting and not yet explored examples are covered: for instance, the 'mean field Schrödinger problem [1], Rényi entropies on the Wasserstein space over $\mathsf{CD}(0,N)$ manifolds and on the space of probability measures over convex Euclidean domains endowed with transport distances induced by 'non-linear mobilities' (see [5]).

Open questions. It would be interesting to see if also Theorem 1 holds for variational problems more general than (1). In this respect, generalizations of 'static' entropic optimal transport have recently appeared (in particular, it is worth mentioning [4]). However, Theorem 1 can not be extended to them in an easy way, since both ingredients mentioned above (the 'energy-transport' and the 'entropic' Talagrand inequalities) implicitly rely on dynamical aspects of (1).

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Mitigating non-convexity in full waveform inversion: optimal transport approaches

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(joint work with Romain Brossier, Andrzejt Górszczyk, Quentin Mérigot, Edouard Oudet, Arnaud Pladys, Jean Virieux)

High resolution seismic imaging is crucial in various field of applications, at multiple scales. Understanding the Earth's global structure, studying specific lithospheric targets such as subduction zones, volcanic areas, faults, prospecting the crust for hydrocarbon resources, monitoring CO2 storage zones, imaging the near surface at few meters depth for geotechnical engineering are instances of such applications where detailed information about the mechanical properties of the subsurface is required.

To access this information, geophysicists rely on the recording of mechanical waves using sensors deployed at the surface. Depending on the target scale, these waves are triggered either by earthquakes (global and regional scale imaging) or by controlled sources (explorations and near-surface scale imaging). From these recording, the mechanical properties of the subsurface are inferred in an inverse problem fashion.

Modern high resolution seismic imaging is based upon Full Waveform Inversion (FWI). This method has been introduced by [Lailly, 1983] and [Tarantola, 1984] as a PDE-constrained optimization problem. The least-squares distance between observed and calculated data is minimized iteratively starting from an initial guess of the subsurface model. The calculated data is obtained through the solution of a PDE system representing the propagation of mechanical wave within the subsurface. This problem is solved through local optimization (*ie* quasi-Newton l-BFGS [Nocedal, 1980]). At each iteration, the gradient of the misfit function measuring the discrepancy between calculated and observed data is computed. The adjoint-state strategy, [Lions, 1968] is used to compute this gradient. It is

obtained by the time-correlation of an incident field emitted from the source and an adjoint field backpropagated from the receivers position. The time-signature of the source for this adjoint field is given by the derivative of the misfit function measurement with respect to the calculated data [Plessix, 2006].

One main limitation of FWI remains the non-convexity of the least-squares distance with respect to model parameters, especially wave velocities, which are the parameters of primary interest. To overcome this difficulty, a recent proposition is to modify the misfit measurement function using an optimal transport (OT) distance [Engquist and Froese, 2014]. The motivation is that such distances are convex with respect to dilation and translation of the measures they compare. Large-scale velocity changes mainly affect the kinematic of the mechanical waves and as a result shift in time the recorded seismic events. Using a misfit measurement function convex with respect to translation (time-shifts) thus is a good proxy towards convexity with respect to wave velocities.

However, using an OT distance to compare seismic data is not straightforward as seismic data is signed, while OT theory is developed in the frame of probability measures. One possibility is to apply nonlinear transforms to the data to make it positive and normalized, so as to satisfy the positivity and mass conservation assumption required by OT [Yang et al., 2016, Yang and Engquist, 2018]. While satisfactory results have been obtained on synthetic data using these techniques, altering the signal shape might yield specific difficulties in the frame of field data inversion.

A first alternative discussed is the use of a specific instance of OT distance, namely the 1-Wasserstein distance [Métivier et al., 2016]. Its dual form can be extended to signed data with mass conservation, a condition satisfied "naturally" by seismic data, mass conservation being related to the zero frequency of the signal which is equal to 0 in practice. A fast numerical method can be designed to solve this dual problem. The specific choice of the ℓ_1 ground distance reduces the number of linear constraints from N^2 to $2N$ where N is the size of the discrete data. The proximal splitting algorithm ADMM is used to solve the corresponding problem [Combettes and Pesquet, 2011]. Each iteration of the ADMM algorithm requires to solve a linear system associated with the discretization of the constraints, equivalent to the second-order finite-difference discretization of the Laplacian operator. Fast Fourier transform based linear solvers can thus be used, yielding an overall complexity in $O(N \log N)$ at each iteration of the ADMM algorithm.

The development of this fast solver makes it possible to apply this distance to the comparison of 2D and 3D data: seismic gathers which collect the time-signal depending on the spatial position of the receivers. The coherency of the data in this representation space can thus be taken into account, a very interesting feature compared to standard L^p distances which operate in a point-to-point comparison. However, one main drawback of this method is that the convexity with respect to time-shifts is lost. This loss is due to the direct application of the 1-Wasserstein distance to signed data.

To overcome this difficulty, a second alternative consist in a graph-space lift of the data [Métivier et al., 2019]. Each seismic time-signal is associated with its discrete graph, yielding a 2D point cloud in a time/amplitude 2D space. This ensures simultaneously mass conservation and positivity of the compared quantities, without altering the signal shape. The comparison of point clouds through OT amounts to the solution of a linear assignment problem [Birkhoff, 1946], which we solve through the celebrated "auction" algorithm [Bertsekas and Castanon, 1989].

Computing the sensitivity of this graph-space based OT misfit measurement with respect to the calculated data is more involved. A theorem shows that given one input and one target point clouds, the optimal assignment is locally constant *almost everywhere*. The misfit measurement is thus differentiable *almost everywhere*. Its derivative resembles the one which would be obtained with a classical L^p norm, except that instead of a point-by-point comparison, the sampled which are compared are the ones connected through the optimal assignment computed through the solution of the OT problem.

In this graph-space comparison, the ground distance defining the distance between two points of the cloud needs also to be defined with care. Especially, a normalization between the time and amplitude axis needs to be applied. We show how, based on an estimation of the maximum expected time shifts, we can design this normalization.

The two proposed methods are applied on 2D and 3D synthetic and field data. The convexity associated with the OT distance makes it possible to start the inversion from crude initial models, while conventional least-squares norm converges towards non-informative local minima starting from these models. The graph-space lift strategy appears as more promising, however, due to its intrinsic computation cost, it is limited to the comparison of the data receiver by receiver, without taking into account the spatial coherency of the data in a 2D or 3D representation space. The perspective of this work is thus the possible reconciliation between both methods, to extend the graph space strategy to the comparison of whole 2D/3D seismic data. This would require the comparison of point clouds containing millions of points, in a repeatable thus stable manner. In addition the gradient computation step requires not only the evaluation of the OT problem but also the computation of its sensitivity with respect to the input data.

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Dimension reduction for measures in position velocity space

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(joint work with Martin Holler, Alexander Schlüter)

In the field of inverse problems, both the reconstruction of measure-valued objects as well as the reconstruction of temporally changing quantities are gaining importance. This has recently led to several approaches using some version of optimal transport as a regularizer, often in a dynamic formulation: one reconstructs a Radon measure at every time point at which one has an observation or a measurement and penalizes the transport distance between the reconstructions at consecutive time steps. The motivation is twofold: First, the optimal transport plan yields information about the evolution or the motion of the reconstructed quantity. Second, the temporal consistency ensured by optimal transport may improve the reconstruction at each single time point.

The problem with optimal transport-based regularization approaches is the associated computational cost. If one just considers the standard Wasserstein-p distance between consecutive time points, then the dynamic Benamou–Brenier formulation alleviates this issue, leading to a feasible optimization of measures in spacetime (where the time interval extends over all the observation time points). However, if a stronger temporal regularization is desired which simultaneously considers more than just two consecutive time points, then one is led to multi-marginal transport problems which are typically numerically prohibitive. Since in

this field the regularizing effect of optimal transport-type functionals is more important than the exact calculation of a transport plan, we suggest to remedy the issue of computational intractability by a dimension reduction which only considers certain projections of optimal transport couplings. We describe the idea below for an existing model of dynamic particle reconstruction, showing that the favourable regularization properties do not suffer under the dimension reduction.

To introduce the setting, let us first recapitulate a model for reconstructing stationary particles (without optimal transport-type regularization). Given a measure $u^\dagger = \sum_{i=1}^n m_i \delta_{x_i} \in \mathcal{M}_+(\Omega)$, describing n particles of masses $m_i > 0$ at locations $x_i \in \Omega \subset \mathbb{R}^d$, $d \in \{2, 3\}$, one takes a measurement $f^\dagger = \mathrm{Ob}u^\dagger$ of the configuration via a linear observation operator $\mathrm{Ob} : \mathcal{M}_+(\Omega) \to \mathbb{R}^m$. An exemplary case is a Fourier series expansion, truncated at some maximum frequency f,

$$\mathrm{Ob}u = \big(\langle u, x \mapsto e^{i\xi\cdot x}\rangle\big)_{\xi\in\mathbb{Z}^d, |\xi|<f} \text{ for } \Omega = (-\pi, \pi]^d \text{ with periodic boundary.}$$

This setting is closely related to superresolution microscopy (for which a Nobel prize was awarded in 2014), where the particles represent fluorescent molecules and the observation y is just the Fourier transform of a flourescence microscopy image (it is truncated at some maximum frequency due to the limited microscope resolution). The task now is to reconstruct $u^\dagger$ from $f^\dagger$. Remarkably, for the above measurement operator this is possible exactly.

Theorem 1 (Candès & Fernandez-Granda, 2013)**.** *There exists a constant $C > 0$ such that the following holds. If the minimum particle distance in $u^\dagger$ is no smaller than $\frac{C}{f}$, then $u^\dagger$ is the unique minimizer of*

$$\min_{u\in\mathcal{M}_+(\Omega)} \|u\|_{\mathcal{M}} \text{ such that } \mathrm{Ob}u = f^\dagger. \tag{1}$$

The result is proved by constructing dual certificates for $u^\dagger$ and is in principle not restricted to Ob being a truncated Fourier series. If the measurements are corrupted by noise, the constraint $\mathrm{Ob}u = f^\dagger$ can be replaced by a penalty term, and one can derive some error estimate of the reconstruction (Candès and Fernandez-Granda consider some type of maximum mean discrepancy norm of $u - u^\dagger$).

Next consider the dynamic setting, where the particles move over time. Denote the particle configuration at time t by $u_t^\dagger$ and assume that we have observations $f_j^\dagger = \mathrm{Ob}u_{t_j}^\dagger$, $j = 1, \dots, k$, from which we aim to reconstruct the dynamic particle configuration. The latter could for instance be described by a multimarginal coupling $\eta^\dagger = \sum_{i=1}^n m_i \delta_{x_i^1,\dots,x_i^k}$, where m_i represents the ith particle mass as before and x_i^j its position at time t_j. Thus, $\mathrm{proj}_j \eta^\dagger = u_{t_j}^\dagger$, where proj_j denotes the jth marginal. The natural extension of (1) to the dynamic problem now reads

$$\min_{\eta\in\mathcal{M}_+(\Omega\times\ldots\times\Omega)} \int_\Omega \dots \int_\Omega c(x_1, \dots, x_k)\, \mathrm{d}\eta(x_1, \dots, x_k)$$
$$\text{such that } \mathrm{Ob}(\mathrm{proj}_j \eta) = f_j^\dagger \text{ for } j = 1, \dots, k.$$

The cost c can be chosen to achieve a desired temporal regularization. For instance, one could require constant particle velocities by choosing

$$c(x_1, \dots, x_k) = \begin{cases} 1 & \text{if there exist } x, v \in \mathbb{R}^d \text{ with } x_j = x + t_j v,\ j = 1, \dots, k, \\ \infty & \text{else.} \end{cases}$$

This case of particles with linear trajectories was considered by Alberti, Ammari, Romero and Wintz. Due to its enforced high temporal consistency, the coupling $\eta^\dagger$ can here actually be reduced to just a measure in $\Lambda = \{(x, v) \in \mathbb{R}^d \times \mathbb{R}^d \,|\, x + t_j v \in \Omega \text{ for } j = 1, \dots, k\} \subset \mathbb{R}^d \times \mathbb{R}^d$. Indeed, the dynamic particle configuration can be represented as a measure $\lambda^\dagger = \sum_{i=1}^n m_i \delta_{(x_i, v_i)}$, where x_i denotes the initial position and v_i the velocity of the ith particle. The configuration u_{t_j} at time t_j is now obtained from $\lambda^\dagger$ via a "move" operator (a simple pushforward),

$$u_{t_j} = \mathrm{Mv}_{t_j}^d \lambda^\dagger \text{ for } \mathrm{Mv}_t^d \lambda = [(x, v) \mapsto x + tv]_\# \lambda.$$

In analogy to theorem 1 one can reconstruct $\lambda^\dagger$ exactly from the measurements.

Theorem 2 (Alberti, Ammari, Romero & Wintz, 2018)**.** *Let C be the constant from theorem 1. If there exists a set of "good times" $\mathcal{T} \subset \{t_1, \dots, t_k\}$ such that*

- *the minimum particle distance in $u_t^\dagger$ is no smaller than $\frac{C}{f}$ for all $t \in \mathcal{T}$,*
- *there are no ghost particles with respect to $\mathcal{T}$,*

then $\lambda^\dagger$ is the unique minimizer of

$$\min_{\lambda \in \mathcal{M}_+(\Lambda)} \|\lambda\|_{\mathcal{M}} \text{ such that } \mathrm{Ob}(\mathrm{Mv}_{t_j}^d \lambda) = f_j^\dagger \text{ for } j = 1, \dots, k. \tag{2}$$

Above, the notion of ghost particles refers to pairs (x, v) of initial position and velocity that do not correspond to any real particle, but nevertheless satisfy $x + tv \in \mathrm{support}(u_t^\dagger)$ for all $t \in \mathcal{T}$. Again, the result is not restricted to Ob being a truncated Fourier series, but we stick to that case for simplicity of exposition.

Finally, let us introduce our dimension reduction. For $\theta \in S^{d-1}$ we define the Radon transform and the "joint Radon transform" as the pushforwards

$$\mathrm{Rd}_\theta u = [x \mapsto \theta \cdot x]_\# u, \quad \mathrm{Rj}_\theta \lambda = [(x, v) \mapsto (\theta \cdot x, \theta \cdot v)]_\# \lambda.$$

The essential intuition is that the move operator and the joint Radon transform yield quite complementary projections of spacetime, so $\gamma^\dagger = (\mathrm{Rj}_\theta \lambda^\dagger)_{\theta \in \Theta}$ and $u^\dagger = (\mathrm{Mv}_t^d \lambda^\dagger)_{t \in \Sigma}$ contain complementary information (where we shall fix $\Theta = S^{d-1}$ and $\Sigma = [-1, 1]$, but other choices are possible as well). Hence it may be reasonable to use new variables γ and u instead of λ. Since γ can be viewed as a measure on $\mathbb{R} \times \mathbb{R} \times S^{d-1}$ and u as a measure on $\mathbb{R}^d \times \mathbb{R}$, the dimensions of the new variables are indeed lower than those of λ. In particular, for three-dimensional particle configurations ($d = 3$), γ and u live in a four-dimensional space, which can still be discretized. (Note that one may actually reduce the dimension even further by taking finite Θ and Σ.) Of course, γ and u are not completely independent due to the compatibility relation $\mathrm{Rd}_\theta u_t^\dagger = \mathrm{Rd}_\theta \mathrm{Mv}_t^d \lambda^\dagger = \mathrm{Mv}_t^1 \mathrm{Rj}_\theta \lambda^\dagger = \mathrm{Mv}_t^1 \gamma_\theta^\dagger$ for all $\theta \in \Theta$, $t \in \Sigma$. We prove that the favourable reconstruction properties persist after

this dimension reduction, and we even obtain error estimates in the unbalanced transport dissimilarity measure (in which W_2 denotes the Wasserstein-2 distance)

$$W_{2,r}^2(\rho,\nu) = \inf_{\eta} W_2^2(\rho,\eta) + r^2\|\eta-\nu\|_{\mathcal{M}}.$$

Theorem 3. *Under the same conditions as in theorem 2,* $(\gamma^\dagger, u^\dagger)$ *is the unique minimizer of*

$$\min_{\substack{\gamma\in\mathcal{M}_+(\mathbb{R}\times\mathbb{R})^\Theta\\ u\in\mathcal{M}_+(\Omega)^\Sigma}} \sup_{\theta\in\Theta}\|\mu_\theta\|_{\mathcal{M}} \text{ such that } \begin{cases}\mathrm{Rd}_\theta u_t = \mathrm{Mv}_t^1\gamma_\theta \text{ for all } \theta\in\Theta, t\in\Sigma,\\ \mathrm{Ob}u_{t_j} = f_j^\dagger \text{ for } j=1,\dots,k.\end{cases}$$

Now let Δ *be the largest distance by which particle locations in* $\lambda^\dagger$ *can be shifted without producing a collision or ghost particle in the projected configurations* $\{\mathrm{Rd}_\theta u_t^\dagger \mid t\in\mathcal{T}\}$. *If* $f_1^\delta,\dots,f_k^\delta$ *are noisy measurements with* $\sum_{j=1}^k |f_j^\delta - f_j^\dagger|^2 \le \delta^2$, *then there exist* $c, r>0$ *(depending on* $\lambda^\dagger$*) such that the minimizer* $(\gamma^\delta, u^\delta)$ *of*

$$\min_{\substack{\gamma\in\mathcal{M}_+(\mathbb{R}\times\mathbb{R})^\Theta\\ u\in\mathcal{M}_+(\Omega)^\Sigma}} \sup_{\theta\in\Theta}\|\mu_\theta\|_{\mathcal{M}} + \frac{1}{\delta}\sum_{j=1}^k |\mathrm{Ob}u_{t_j} - f_j^\delta|^2 \text{ s. t. } \mathrm{Rd}_\theta u_t = \mathrm{Mv}_t^1\gamma_\theta \,\forall\theta\in\Theta, t\in\Sigma$$

satisfies, for almost all $\theta\in\Theta$ *and all* $t\in\Sigma$,

$$W^2_{2,\min\{r,\Delta/(3\sqrt{1+\max_{t\in\mathcal{T}} t^2})\}}(\gamma_\theta^\delta,\gamma_\theta^\dagger) \le c\delta, \quad W_{2,r}^2(u_t^\delta,u_t^\dagger)\le c\delta.$$

The proof again is essentially a careful construction of dual certificates: first for all $u_t^\dagger$ with $t\in\mathcal{T}$ in the set of good times, then based on that for all $\mu_\theta^\dagger$, and finally (with the help of those new dual certificates) for all $u_t^\dagger$.

The implicit regularization of the quadratic Wasserstein metric in data-fitting problems and Bayesian inference

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(joint work with Björn Engquist, Matt Dunlop, Kui Ren)

In recent years, the quadratic Wasserstein metric (W_2) is proposed as an alternative for the L^2 metric in solving such inverse data matching problems. Numerical experiments suggest that the W_2 metric has attractive properties for some inverse data matching problems that the classical L^2 metric does not have, such as nonlinear full-waveform inversion [3, 7, 8, 12] and parameter identification for nonlinear dynamical systems [6]. Here, we summarize the mathematical properties of the W_2 metric in inverse data matching problems into the following three aspects.

1. Convexity with respect to data translation and dilation. Optimal transport-related techniques are nonlinear as they explore the model through both signal intensities and their locations. The geometry of optimal transport has been instrumental in tackling applied problems, such as capturing the essential continuous dependence between the model parameter m and the data $f(m)$. The W_2 distance is ideal for dealing with this type of problem as it has perfect convexity

with respect to translation and dilation, which was the original motivation for us to introduce W_2 as the misfit function in seismic inversion [2]. We improve our result in [3] with a stronger convexity proof in the following Theorem 1, which states a joint convexity in multiple variables with respect to both translation and dilation changes in the data. Assume that $s_k \in \mathbb{R},\ k = 1, \dots, d$ is a set of translation parameters and $\{e_k\}_{k=1}^d$ is the standard basis of the Euclidean space $\mathbb{R}^d$. $A = \mathrm{diag}(1/\lambda_1, \dots, 1/\lambda_d)$ is a dilation matrix where $\lambda_k \in \mathbb{R}^+, k = 1, \dots, d$. We define f_Θ as jointly the translation and dilation transformation of function g

$$f_\Theta(x) = \det(A) g(A(x - \sum_{k=1}^{d} s_k e_k)). \tag{1}$$

Theorem 1 [5] [Convexity of W_2 in translation and dilation]
Let $g = d\nu$ be a probability density function with finite second moment and f_Θ is defined by (1)*. If, in addition, g is compactly supported on convex domain $Y \subseteq \mathbb{R}^d$, the optimal transport map between $f_\Theta(x)$ and $g(y)$ is $y = T_\Theta(x)$ where $\langle T_\Theta(x), e_k\rangle = \frac{1}{\lambda_k}(\langle x, e_k\rangle - s_k), k = 1, \dots, d$. Moreover, $I(\Theta) = W_2^2(f_\Theta(x), g)$ is a strictly convex function of the multivariable Θ.*

2. Robustness to high-frequency perturbations. It is well-known that the W_2 metric between f and g is connected to a weighted $\dot{\mathcal{H}}^{-1}$ distance between them. If μ is the probability measure and $d\pi$ is an infinitesimal perturbation that has zero total mass, then [11, Section 7.6]

$$W_2(\mu, \mu + d\pi) = \|d\pi\|_{\dot{\mathcal{H}}^{-1}_{(d\mu)}} + o(d\pi). \tag{2}$$

For two positive probability measures μ and ν with densities f and g that are sufficiently regular, we have the following *non-asymptotic* equivalence [10]:

$$\mathfrak{c}_1 \|\mu - \nu\|_{\dot{\mathcal{H}}^{-1}_{(d\mu)}} \le W_2(\mu, \nu) \le \mathfrak{c}_2 \|\mu - \nu\|_{\dot{\mathcal{H}}^{-1}_{(d\mu)}}, \text{ for some } \mathfrak{c}_1, \mathfrak{c}_2 > 0. \tag{3}$$

We seek the solution of the inverse problem as the minimizer of the $\mathcal{H}^s$ functional

$$\Phi_{\mathcal{H}^s}(m) \equiv \frac{1}{2}\|f(m) - g\|^2_{\mathcal{H}^s} := \frac{1}{2}\int_{\mathbb{R}^d} \langle\xi\rangle^{2s} |\widehat{f}(m)(\xi) - \widehat{g}(\xi)|^2 d\xi, \tag{4}$$

with $\langle\xi\rangle := \sqrt{1 + |\xi|^2}$, $f(m) = Am$ and g replaced with the noisy datum g_δ. Here, we use a linear inverse problem as an example. Please refer to [4] for the analysis of nonlinear inverse problems. The solution at frequency ξ is therefore

$$\widehat{m}(\xi) = \Big(\widehat{A}^*(\xi)\big(\langle\xi\rangle^{2s}\widehat{A}\big)\Big)^{-1} \widehat{A}^*(\xi)\Big(\langle\xi\rangle^{2s}\widehat{g_\delta}(\xi)\Big).$$

Performing an inverse Fourier transform gives the solution in the physical space

$$m = \Big(A^* P A\Big)^{-1} A^* P g_\delta, \qquad P := (\mathcal{I} - \Delta)^{s/2}, \tag{5}$$

where the operator $(\mathcal{I} - \Delta)^{s/2}$ is defined through the relation $(\mathcal{I} - \Delta)^{s/2} m := \mathcal{F}^{-1}(\langle\xi\rangle^s \widehat{m})$, with $\mathcal{F}^{-1}$ being the inverse Fourier transform.

When $s < 0$, P is a (smoothing) integral operator. Applying P to g_δ suppresses its high-frequency components. The implicit regularization property regarding $s = -1$ naturally applies to the W_2 metric as a result of (2) and (3).

3. The W_2 metric as the likelihood function in Bayesian inference. The shape and curvature of the likelihood surface represent information about the estimates' stability, whose analogy in the deterministic approach of solving inverse problems is the objective function in PDE-constrained optimization. In [9], the W_2 metric was first used in Bayesian seismic inversion as the likelihood function, which motivates us to further analyze the W_2 metric under the framework of Bayesian seismic inversion. We first study its underlying noise model, which is compared with other common choices of likelihood functions in the table below.

ϕ	Likelihood function	Noise model assumption
Φ_{L^2}	$\|\mathcal{G}(u)(x,\cdot) - y(x,\cdot)\|^2_{L^2}$	$y = \mathcal{G}(u) + \eta,\ \eta \sim N(0, I)$
$\Phi_{H^{-1}}$	$\|\mathcal{G}(u)(x,\cdot) - y(x,\cdot)\|^2_{\dot{H}^{-1}}$	$y = \mathcal{G}(u) + \eta,\ \eta \sim N(0, -\Delta)$
Φ_{W_2}	$W_2^2\left(\widetilde{\mathcal{G}(u)}(x,\cdot), \widetilde{y}(x,\cdot)\right)$	$\widetilde{y} = \eta \cdot \widetilde{\mathcal{G}(u)},\ \eta \| u \sim N(1, \mathcal{L}(u))$
Φ_M	$\left\|\frac{\mathcal{G}(u)(x,\cdot) - y(x,\cdot)}{y(x,\cdot)}\right\|^2_{L^2}$	$y = \eta \cdot \mathcal{G}(u),\ 1/\eta \sim N(1, I)$

Here, u is the state parameter, $\mathcal{G}$ is the forward operator, $\mathcal{G}(u)$ is the synthetic output, and y is the observed data. The $\widetilde{y}$ denotes the normalized function, which is then a probability density. The operator $\mathcal{L}(u)$ is defined by

$$\mathcal{L}(u)\phi = -\frac{1}{\widetilde{\mathcal{G}(u)}} \nabla \cdot \left(\widetilde{\mathcal{G}(u)} \nabla \phi\right),$$

Thus, the W_2 metric as a likelihood function can be regarded as asymptotically coming from **the state-dependent multiplicative noise data model**.

We also state an informal version of [1, Theorem 6] demonstrating the better robustness of the W_2 metric as the likelihood function compared to the conventional choice of L^2-type likelihood function.

Theorem 2 [Well-posedness] *For $\Phi \in \{\Phi_{L^2}, \Phi_{W_2}\}$, under mild assumptions, there exists $C_\Phi(r) > 0$ such that for any $\|y\|_{L^\infty}, \|y'\|_{L^\infty} < r$, with π^y_Φ and $\pi^{y'}_\Phi$ denoting the corresponding posterior distributions, we have*

$$d_{\mathrm{H}}(\pi^y_{\Phi_{W_2}}, \pi^{y'}_{\Phi_{W_2}}) \le C_{W_2}(r)\|y - y'\|_{H^{-1}}, \quad d_{\mathrm{H}}(\pi^y_{\Phi_{L^2}}, \pi^{y'}_{\Phi_{L^2}}) \le C_{L^2}(r)\|y - y'\|_{L^2}.$$

d_{H} represents the Hellinger distance.

We remark that If $y - y' \approx \sin(kx)$, $\|y - y'\|_{H^{-1}} \approx \mathcal{O}(\frac{1}{k})$, while $\|y - y'\|_{L^2} \approx \mathcal{O}(1)$. Thus, Theorem 2 is another result demonstrating the noise insensitivity of the W_2 metric in a Bayesian inference framework in the context of solving Bayesian inverse problems. The result is well-aligned with the analysis for the deterministic approach of solving the same inverse problem.

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Stability in Gagliardo-Nirenberg-Sobolev inequalities

Jean Dolbeault

(joint work with Matteo Bonforte, Bruno Nazaret, Nikita Simonov)

Optimal constants and optimal functions are known in some functional inequalities. The next question is the stability issue: is the difference of the two terms controlling a distance to the set of optimal functions ? A famous example is provided by Sobolev's inequalities: in 1991, G. Bianchi and H. Egnell proved that the difference of the two terms is bounded from below by a distance to the manifold of the Aubin-Talenti functions. They argued by contradiction and gave a very elegant although not constructive proof. Since then, estimating the stability constant and giving a constructive proof has always been a challenge.

This contribution focuses on Gagliardo-Nirenberg-Sobolev inequalities. The main tool is based on entropy methods and nonlinear flows. In our method, proving stability amounts to establish, under some constraints, a version of the entropy – entropy production inequality with an improved constant. In simple cases, for instance on the sphere, rather explicit results have been obtained by the *carré du champ* method introduced by D. Bakry and M. Emery. In the Euclidean space, results based on constructive regularity estimates for the solutions of the nonlinear

flow have been obtained in a joint research project with Matteo Bonforte, Bruno Nazaret, and Nikita Simonov.

According to [1], on $\mathbb{R}^d$, $d \ge 3$, there is a positive constant α such that

$$\mathsf{S}_d \, \|\nabla f\|^2_{\mathrm{L}^2(\mathbb{R}^d)} - \|f\|^2_{\mathrm{L}^{2^*}(\mathbb{R}^d)} \ge \alpha \inf_{\varphi \in \mathcal{M}} \|\nabla f - \nabla \varphi\|^2_{\mathrm{L}^2(\mathbb{R}^d)} \,, \tag{1}$$

where the left-hand side is the difference of the two terms in Sobolev's inequality, with optimal constant S_d, and $\mathfrak{M}$ denotes the manifold of the optimal Aubin-Talenti functions. Various improvements as, *e.g.*, in [4, 7] have been obtained but the question of *constructive* estimates is still widely open: α is obtained by compactness estimates and contradiction arguments, and no good stability estimate is known so far at least with a strong notion of distance as in the right-hand side of (1). See [6] for a result with a weaker norm.

We consider the family of *Gagliardo-Nirenberg-Sobolev inequalities*

$$\|\nabla f\|_2^\theta \, \|f\|_{p+1}^{1-\theta} \ge \mathcal{C}_{\mathrm{GNS}}(p) \, \|f\|_{2\,p} \tag{2}$$

with $\theta = \frac{d\,(p-1)}{(d+2-p\,(d-2))\,p}$, $p \in (1, +\infty)$ if $d = 1$ or 2, $p \in (1, p^*]$ if $d \ge 3$, $p^* = \frac{d}{d-2}$. It is known from [5] that equality is achieved if and only if, up to a multiplication by a constant, a translation and a scaling, $f = \mathsf{g}$ where $\mathsf{g}(x) := \big(1 + |x|^2\big)^{-1/(p-1)}$. We shall denote the corresponding manifold by $\mathfrak{M}$ as when $p = p^*$. Sobolev's inequality when $d \ge 3$, $p = p^*$, the Euclidean Onofri inequality obtained for $d = 2$ by taking the limit as $p \to +\infty$ with $f(x) = \mathsf{g}(x)\,\big(1 + \frac{1}{2\,p}\,(h(x) - \overline{h})\big)$,

$$\log\left(\int_{\mathbb{R}^2} e^{h-\overline{h}}\,\tfrac{dx}{\pi\,(1+|x|^2)^2}\right) \le \frac{1}{16\,\pi}\int_{\mathbb{R}^2} |\nabla h|^2\,dx \quad \text{with} \quad \overline{h} = \int_{\mathbb{R}^2} \tfrac{h(x)\,dx}{\pi\,(1+|x|^2)^2}$$

and, as $p \to 1_+$, the (scale invariant) *Euclidean logarithmic Sobolev inequality*

$$\frac{d}{2}\,\log\left(\frac{2}{\pi\,d\,e}\int_{\mathbb{R}^d} |\nabla f|^2\,dx\right) \ge \int_{\mathbb{R}^d} |f|^2\,\log|f|^2\,dx$$

are all limit cases of (2). Let us define the *deficit functional*

$$\delta[f] := (p-1)^2\,\|\nabla f\|_2^2 + 4\,\frac{d - p\,(d-2)}{p+1}\,\|f\|_{p+1}^{p+1} - \mathcal{K}_{\mathrm{GNS}}\,\|f\|_{2\,p}^{2\,p\,\gamma}$$

with $\mathcal{K}_{\mathrm{GNS}} = C(p,d)\,\mathcal{C}_{\mathrm{GNS}}^{2\,p\,\gamma}$, $\gamma = \frac{d+2-p\,(d-2)}{d-p\,(d-4)}$ for some explicit positive constant $C(p,d)$. A scale optimization shows that (2) is equivalent to the inequality $\delta[f] \ge 0$. Stability results for (2) with non-constructive estimates are known from [3, 10].

With $d \ge 1$, $m \in (1 - 1/d, 1)$, the *fast diffusion* equation in $\mathbb{R}^d$

$$\frac{\partial u}{\partial t} = \Delta u^m \tag{3}$$

with initial datum $u(t = 0, x) = u_0(x) \ge 0$, $u_0 \in \mathrm{L}^1\big(\mathbb{R}^d, (1 + |x|^2)\,dx\big)$, can be interpreted as the gradient flow of the *entropy* $\mathsf{E} := \int_{\mathbb{R}^d} u^m\,dx$ with respect to Wasserstein's distance, as it is known from [8]. By the *carré du champ method* (adapted from the work of D. Bakry and M. Emery), we can relate (2) and (3),

and obtain a proof of (2). The key property, inspired by the *Rényi entropy powers* of [9] is based on the one hand on the fact that

$$\mathsf{E}' = (1-m)\,\mathsf{I}$$

where $\mathsf{I} := \int_{\mathbb{R}^d} u\,|\nabla \mathsf{P}|^2\,dx$ is the *Fisher information* and $\mathsf{P} = \frac{m}{m-1}\,u^{m-1}$ is the *pressure variable*, and on the other hand on the identity

$$-\tfrac{d}{dt}\log\Big(\mathsf{I}^{\frac12}\,\mathsf{E}^{\frac{1-\theta}{\theta(p+1)}}\Big) = \int_{\mathbb{R}^d} u^m\,\big\|\mathrm{D}^2\mathsf{P} - \tfrac1d\,\Delta\mathsf{P}\,\mathrm{Id}\big\|^2\,dx + (m-m_1)\int_{\mathbb{R}^d} u^m\Big|\Delta\mathsf{P} + \tfrac{\mathsf{I}}{\mathsf{E}}\Big|^2\,dx\,.$$

Hence $\mathsf{I}^{\frac12}\,\mathsf{E}^{\frac{1-\theta}{\theta(p+1)}}$ is monotone with a limit given by self-similar *Barenblatt functions* or, equivalently by g^{2p}. With the relations $f = u^{m-1/2}$, $p = 1/(2\,m-1)$, so that $\int_{\mathbb{R}^d} u\,dx = \int_{\mathbb{R}^d} f^{2p}\,dx$, $\mathsf{E} = \int_{\mathbb{R}^d} f^{p+1}\,dx$ and $\mathsf{I} = (p+1)^2\int_{\mathbb{R}^d}|\nabla f|^2\,dx$, the role of (2) is easily recovered. A rigorous proof goes through the time-dependent rescaling

$$u(t,x) = \frac{1}{\kappa^d\,R^d}\,v\Big(\tau,\frac{x}{\kappa\,R}\Big) \quad \text{where} \quad \frac{dR}{dt} = R^{1-\mu}\,, \quad \tau(t) := \tfrac12\,\log R(t)$$

so that (3) is changed, with same initial datum u_0 and the choice $R(0)=1$, into the *Fokker-Planck type equation*

$$\frac{\partial v}{\partial\tau} + \nabla\cdot\Big[v\,\big(\nabla v^{m-1} - 2\,x\big)\Big] = 0\,. \tag{4}$$

With now $f = v^{m-1/2}$ such that $\int_{\mathbb{R}^d} f^{2p}\,dx = \int_{\mathbb{R}^d}\mathsf{g}^{2p}\,dx$ and again $p = \frac{1}{2\,m-1}$, with $\mathcal{Q}[v] := \mathcal{I}[v]/\mathcal{F}[v]$, $\delta[f]\ge 0$ is equivalent to $\mathcal{Q}[v]\ge 4$, where $\mathcal{B} := \mathsf{g}^{2p}$ and

$$\mathcal{F}[v] := \int_{\mathbb{R}^d}\big(\mathcal{B}^{m-1}\,(v-\mathcal{B}) - \tfrac1m\,(v^m-\mathcal{B}^m)\big)\,dx\,, \quad \mathcal{I}[v] := \int_{\mathbb{R}^d} v\,\big|\nabla v^{m-1} + 2\,x\big|^2\,dx\,.$$

For any $m\in(1-1/d,1)$, the main result in [2] is the fact that

$$\mathcal{Q}[v(\tau,\cdot)] > 4+\eta \quad \forall\,\tau>0\,, \tag{5}$$

for some $\eta>0$, under the conditions that $\int_{\mathbb{R}^d} v_0\,(1,x)\,dx = \int_{\mathbb{R}^d}\mathcal{B}\,(1,x)\,dx$ and

$$\mathsf{A}[v_0] := \sup_{r>0} r^{\frac{d-p\,(d-4)}{p-1}}\int_{|x|>r} v_0\,dx$$

is finite, with an explicit dependence of η on $\mathsf{A}[v_0]$ and $\mathcal{F}[v_0]$. The method involves:

(i) An *initial time layer* property: if $\mathcal{Q}[v(T,\cdot)]\ge 4+\eta$ for some $\eta>0$ and $T>0$, then $\mathcal{Q}[v(\tau,\cdot)]\ge 4+4\,\eta\,e^{-4\,T}/(4+\eta-\eta\,e^{-4\,T})$ for any $\tau\in[0,T]$.

(ii) *A threshold time.* Based on a *global Harnack Principle*, there exists some $T>0$ such that $(1-\varepsilon)\,\mathcal{B}\le v(\tau,\cdot)\le(1+\varepsilon)\,\mathcal{B}$ for any $\tau>T$.

(iii) An *asympotic time layer* property: as a consequence of an improved *Hardy-Poincaré* (spectral gap) inequality, (5) holds for $\eta=\eta(\varepsilon)$, for any $\tau\ge T$.

Rewritten in terms of f, the improved entropy – entropy production inequality $\mathcal{Q}[v]>4+\eta$ is a stability result.

Theorem 1. *Let $d\ge 1$ and $p\in(1,p^*)$. There is an explicit $\mathcal{C}=\mathcal{C}[f]$ such that, for any $f\in \mathrm{L}^{2p}\big(\mathbb{R}^d,(1+|x|^2)\,dx\big)$ such that $\nabla f\in\mathrm{L}^2(\mathbb{R}^d)$ and $\mathsf{A}\big[f^{2p}\big]<\infty$,*

$$\delta[f] \ge \mathcal{C}[f]\,\inf_{\varphi\in\mathfrak{M}}\int_{\mathbb{R}^d}\big|(p-1)\,\nabla f + f^p\,\nabla\varphi^{1-p}\big|^2\,dx\,.$$

The main point is that the dependence of $\mathcal{C}[f]$ on $\mathsf{A}\big[f^{2p}\big]$ and $\mathcal{F}\big[f^{2p}\big]$ is explicit and does not degenerate if $f \in \mathfrak{M}$. The critical case $p = p^*$ can also be covered up to an additional scaling. A major open issue is of course to remove the condition $\mathsf{A}\big[f^{2p}\big] < \infty$, which requires a new approach.

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Dynamic optimal transport on networks

Martin Burger, Jan-F. Pietschmann

Since the seminal paper by Benamou and Brenier, it is well known that the problem of optimal transport allows for a dynamic formulation.

The goal of this work is to extend this to a two-dimensional, planar network where edges can be identified with one-dimensional domains, for details see [1]. We denote the network by $\mathcal{G} = (\mathcal{V}, \mathcal{E})$ with $\mathcal{V} = \{V^1, \dots, V^n\}$ being the set of vertices for $n \in \mathbb{N}$ and $\mathcal{E} = \{E^1, \dots, E^m\}$ the set of edges for $m \in \mathbb{N}$. Every vertex is defined via its coordinates in the two-dimensional space $\mathbb{R}^2$, i.e. $V^i \in \mathbb{R}^2$ for every $i \in \{1, \dots, n\}$ and every edge is homeomorphic to a one-dimensional, open interval. To each edge we assign a starting and an end point and we define two functions $\alpha, \omega \colon \mathcal{E} \to \mathcal{V}$ that assign to every edge its starting or its end point thus determining an orientation. Furthermore $\bar{\alpha}, \bar{\omega} \colon \{1, \dots, m\} \to \{1, \dots, n\}$ assigns to the index of a given edge the indices of the vertices attached at the starting and end point, respectively. By $Z(V^i)$ we denote the indices of all edges originating or

ending at V^i for $i \in \{1, \dots, n\}$, i.e.

$$Z(V^i) = \big\{ j \in \{1, \dots, m\} \colon \alpha(E^j) = V^i \vee \omega(E^j) = V^i \big\}.$$

Finally, we denote by ν_j the outward normal at the j-th edge and for all $(i,j) \in \{(i,j) \,:\, i \in \{1,\dots,n\} \text{ and } j \in Z(V^i)\}$ by $\nu_{i,j}$ the outward normal vector of edge j at the point where it is connected to vertex i. With this notation, $\nu_{\bar{\alpha}(j),j}$ gives the normal at the starting point of E_j. Moreover, we denote by $\mathcal{M}_+(X)$ the set of non-negative bounded measures on a given space X and more precisely the set of non-negative measures on the set of edges (vertices) by

$$\mathcal{M}_+(\mathcal{E}) = \mathcal{M}_+(E^1) \times \ldots \times \mathcal{M}_+(E^m),$$
$$\mathcal{M}_+(\mathcal{V}) = \mathcal{M}_+(V^1) \times \ldots \times \mathcal{M}_+(V^n).$$

To formulate the dynamic optimal transport problem on the network let $\boldsymbol{\rho_0} = (\rho_0^1, \dots, \rho_0^m) \in \mathcal{M}_+(E^j)$, $\boldsymbol{\rho_1} = (\rho_1^1, \dots, \rho_1^m) \in \mathcal{M}_+(E^j)$ be given vectors containing the concentrations on edges at times $t = 0$, $t = 1$ and by $\boldsymbol{\gamma_0} = (\gamma_0^1, \dots, \gamma_0^n)\mathcal{M}_+(V^n)$, $\boldsymbol{\gamma_1} = (\gamma_1^1, \dots, \gamma_1^n)\mathcal{M}_+(V^n)$ the respective vectors of concentrations on the vertices. Next, on the closed set $\Omega_{\mathcal{G}} = \bigcup_{i=1}^n V^i \cup \bigcup_{j=1}^m E^j$ we define the measure that translates to the total density on the network by

$$\varsigma_l = \sum_{j=1}^m \rho_l^j + \sum_{i=1}^n \gamma_l^i, \quad l \in \{0,1\}, \tag{1}$$

and make the assumption that our initial and final data $(\boldsymbol{\rho_0}, \boldsymbol{\rho_1}, \boldsymbol{\gamma_0}, \boldsymbol{\gamma_1})$ are such that ς_0, $\varsigma_1 \in \mathcal{P}(\Omega_{\mathcal{G}})$ holds.

On every edge and every vertex, i.e. for every $j \in \{1, \dots, m\}$ and $i \in \{1, \dots, n\}$, we consider the following *continuity equation* on the network $\mathcal{G}$

$$\partial_t \rho_t^j + \partial_x F_t^j = 0 \text{ in } E^j, \quad \partial_t \gamma_t^i = f_t^i \text{ on } V^i \quad \text{with } f_t^i = \sum_{j \in Z(V^i)} F_t^j(V_i) \cdot \nu_{i,j}, \tag{2}$$

where $F_t^j \colon E^j \times (0,T] \to \mathbb{R}$, $f_t^i \in \mathbb{R}$, the space derivative $\partial_x F_t^j$ is calculated with respect to the orientation of the edge and $\nu_{i,j}$ denotes the normal outward of the edge E^j at the boundary point that is connected with the vertex V^i.

For a given network concentration $(\boldsymbol{\rho_0}, \boldsymbol{\rho_1}, \boldsymbol{\gamma_0}, \boldsymbol{\gamma_1}) \in \mathcal{M}_+(\mathcal{E}) \times \mathcal{M}_+(\mathcal{E}) \times \mathcal{M}_+(\mathcal{V}) \times \mathcal{M}_+(\mathcal{V})$ with ς_0, $\varsigma_1 \in \mathcal{P}(\Omega_{\mathcal{G}})$, we consider the *minimisation-problem* of an action being the combination of Wasserstein and the Fisher-Rao terms

$$\mathcal{W}_\kappa^2(\boldsymbol{\rho_0}, \boldsymbol{\rho_1}, \boldsymbol{\gamma_0}, \boldsymbol{\gamma_1}) = \inf_{(\boldsymbol{\rho_t}, \boldsymbol{F_t}, \boldsymbol{\gamma_t}, \boldsymbol{f_t}) \in \mathcal{CE}(\boldsymbol{\rho_0}, \boldsymbol{\rho_1}, \boldsymbol{\gamma_0}, \boldsymbol{\gamma_1})} \left\{ \sum_{j=1}^m \iint_{\overline{E^j} \times [0,1]} \frac{|F_t^j|^2}{2\rho_t^j} \, dxdt + \kappa^2 \sum_{i=1}^n \int_{[0,1]} \frac{|f_t^i|^2}{2\gamma_t^i} \, dt \right\}, \tag{3}$$

where $\kappa > 0$ is a given constant and with

$$\mathcal{CE}(\boldsymbol{\rho_0}, \boldsymbol{\rho_1}, \boldsymbol{\gamma_0}, \boldsymbol{\gamma_1}) = \Big\{ (\boldsymbol{\rho_t}, \boldsymbol{F_t}, \boldsymbol{\gamma_t}, \boldsymbol{f_t}) \text{ that fulfil (2) and } \boldsymbol{\rho_{t=0}} = \boldsymbol{\rho_0}, \boldsymbol{\rho_{t=1}} = \boldsymbol{\rho_1}, \, \boldsymbol{\gamma_{t=0}} = \boldsymbol{\gamma_0}, \boldsymbol{\gamma_{t=1}} = \boldsymbol{\gamma_1} \Big\}.$$

Remark 1. *It is important to note that in the case of a trivial graph consisting only of one edge and two vertices, our model coincides with the one-dimensional version of the model introduced by L. Monsaigneon in* [2]. *In this work, existence of minimizers is shown via duality and we adopt this strategy to our situation.*

Our main result is existence of minimizers using a duality argument. For $\phi_t^j \in C^1(\mathcal{Q}_{\overline{E^j}}), \psi_t^i \in C^1(Q_{V^i})$, $\boldsymbol{\phi_t} = (\phi_t^1, \dots, \phi_t^m), \boldsymbol{\psi_t} = (\psi_t^1, \dots, \psi_t^n)$ we define the primal functional

$$\mathcal{J}^\kappa(\boldsymbol{\phi_t}, \boldsymbol{\psi_t}) \coloneqq \sum_{j=1}^m \int_{\overline{E^j}} \left(\phi_1^j d\rho_1^j - \phi_0^j \, d\rho_0^j\right) + \sum_{i=1}^n (\psi_1^i \gamma_1^i - \psi_0^i \gamma_0^i)$$
$$+ \sum_{j=1}^m \iint_{\mathcal{Q}_{\overline{E^j}}} \iota_{S_E}(\partial_t \phi_t^j, \partial_x \phi_t^j) \, dxdt - \sum_{i=1}^n \int_0^1 \iota_{S^\kappa_{V^i}}(\partial_t \psi_t^i, \psi_t^i, \phi_t|_{V^i}) \, dt.$$

where the sets S_E and $S^\kappa_{V^i}$ are defined as

(4)

$$S_E \coloneqq \left\{(\alpha, \beta) \in \mathbb{R}^+ \times \mathbb{R} \colon \quad \alpha + \frac{|\beta|^2}{2} \le 0\right\},$$
$$S^\kappa_{V^i} \coloneqq \left\{(a, b, \boldsymbol{c}) \in \mathbb{R}^+ \times \mathbb{R} \times \mathbb{R}^{|Z(V^i)|} \colon \quad a + \frac{|b - \frac{1}{|Z(V^i)|}|\sum_{j \in Z(V^i)} c_j|^2}{2\kappa^2} \le 0\right\}$$

These definitions enable us to prove the duality theorem:

Theorem 2. *Given admissible* $(\boldsymbol{\rho_0}, \boldsymbol{\rho_1}, \boldsymbol{\gamma_0}, \boldsymbol{\gamma_1})$ *we have the duality*

$$\mathcal{W}^2_\kappa(\boldsymbol{\rho_0}, \boldsymbol{\rho_1}, \boldsymbol{\gamma_0}, \boldsymbol{\gamma_1}) = \sup_{\mathcal{C}} \mathcal{J}^\kappa(\boldsymbol{\phi_t}, \boldsymbol{\psi_t}) \tag{5}$$

where inf = min *is attained in* (3).

We also address the question of the behaviour of the model when the parameter κ tends to either $+\infty$ or zero. In the first case, the term in the action (3) that is multiplied by κ accounts for the cost of transporting mass onto (or off) the vertices. Thus as κ increases, this becomes more and more costly and in the limit we expect f_t^i to be zero. This is indeed the case and we have the following theorem: In the case of incompatible edge masses, but compatible overall mass, i.e.

$$\sum_j \|\rho_0^j\| = \sum_j \|\rho_1^j\|$$

we can introduce a Wasserstein metric on the edges only which, at the nodes, are connected via Kirchhoff's law, i.e.

$$\mathcal{W}^2_{\mathcal{E}}(\boldsymbol{\rho_0}, \boldsymbol{\rho_1}) = \min \left\{ \sum_{j=1}^m \iint_{\overline{E^j} \times [0,1]} \frac{|F_t^j|^2}{2\rho_t^j} \, dxdt \text{ s.t. } \begin{array}{ll} \partial_t \rho_t^j + \partial_x F_t^j = 0 & \text{in } E^j, \\ \sum_{j \in Z(V^i)} F_t^j \cdot \nu_j = 0 & \text{in } \partial\overline{E^j}, \end{array} \right\}$$

Proposition 3. *For fixed* $(\boldsymbol{\rho_0}, \boldsymbol{\rho_1}, \boldsymbol{\gamma_0}, \boldsymbol{\gamma_1})$ *we obtain*

$$\mathcal{W}^2_\kappa(\boldsymbol{\rho_0}, \boldsymbol{\rho_1}, \boldsymbol{\gamma_0}, \boldsymbol{\gamma_1}) \underset{\kappa \to +\infty}{\to} \begin{cases} \mathcal{W}^2_{\mathcal{E}}(\boldsymbol{\rho_0}, \boldsymbol{\rho_1}) & \text{if } \boldsymbol{\gamma_0} = \boldsymbol{\gamma_1}, \\ +\infty & \text{otherwise,} \end{cases} \tag{6}$$

Let moreover $\boldsymbol{\mu_t}^\kappa = (\boldsymbol{\rho_t}^\kappa, \boldsymbol{F_t}^\kappa; \boldsymbol{\gamma_t}^\kappa, \boldsymbol{f_t}^\kappa)$ *be any* $\mathcal{W}^2_\kappa(\boldsymbol{\rho_0}, \boldsymbol{\rho_1}, \boldsymbol{\gamma_0}, \boldsymbol{\gamma_1})$*-geodesic. If the node masses are compatible, i.e.* $\boldsymbol{\gamma_0} = \boldsymbol{\gamma_1}$*,* $\|\rho_0^j\| = \|\rho_1^j\|$ *for all* $j \in \{1, \dots, m\}$ *then up to a subsequence*

$$(\boldsymbol{\rho_t}^\kappa, \boldsymbol{F_t}^\kappa) \to (\boldsymbol{\rho_t}, \boldsymbol{F_t}), \quad \text{and} \quad \|f_t^\kappa\| \to 0$$

where $(\boldsymbol{\rho_t}, \boldsymbol{F_t})$ *is a* $\mathcal{K}^2$*-geodesic .*

Let us mention finally that in a similar way we can also analyze the limit of $\kappa^{-2}\mathcal{W}^2_\kappa$ as $\kappa \to 0$. Here we obtain that the edge fluxes $F^{j,\kappa}$ converge to zero and using the sandwich property

$$\kappa^{-2}\mathcal{W}^2_\kappa \le \mathcal{FR}^2_1(\boldsymbol{\gamma_0}, \boldsymbol{\gamma_1})$$

we finally obtain convergence to the Fisher-Rao metric $\mathcal{FR}^2_1(\boldsymbol{\gamma_0}, \boldsymbol{\gamma_1})$, i.e.,

$$\mathcal{FR}^2_\kappa(\boldsymbol{\gamma_0}, \boldsymbol{\gamma_1}) := \min \mathcal{A}^{\mathcal{FR}} = \min \left\{ \sum_{i=1}^n \int_0^1 \kappa^2 \frac{|f_t^i|^2}{2\gamma_t^i}\, dt \quad \text{s.t.} \quad \partial_t \gamma_t^i = f_t^i \text{ in } V^i \right\},$$

under the condition that $\rho_0^j = \rho_1^j$ for all j, while we have divergence otherwise. The study of gradient flows with respect to these resulting metrics is an interesting open problem.

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Phase transitions and a mountain pass theorem in the space of probability measures

André Schlichting

(joint work with José A. Carrillo, Rishabh Gvalani, Grigorios A. Pavliotis, Christian Seis)

We present results concerning the qualitative and quantitative description of mean-field interacting systems of McKean-Vlasov type

$$dX_t^i = -\frac{\kappa}{N} \sum_{i \neq j}^N \nabla W(X_t^i - X_t^j)\, dt + \sqrt{2\sigma}\, dB_t^i, \qquad \text{for} \qquad i = 1, \dots, N. \tag{1}$$

The particles X_t^i have the d-dimensional torus $\mathbb{T}^d_L \simeq [0, L)^d$ of size $L > 0$ as state space with B_t^i being independent Brownian motions on it. For many interaction potentials W, the model possesses phase transition by varying the interaction strength $\kappa > 0$ while keeping the diffusion constant $\sigma > 0$ fixed.

The mean-field limit $N \to \infty$ of this system is a classical result and many authors have shown for different classes of interaction potentials that the empirical

measure $\varrho^{(N)} := N^{-1} \sum_{i=1}^{N} \delta_{X_t^i}$ converges weakly to some measure ϱ which satisfies the following nonlocal parabolic equation

$$\partial_t \varrho = \sigma \Delta \varrho + \kappa \nabla \cdot (\varrho \nabla W \star \varrho)\,. \tag{2}$$

The equation (2) comes with a free energy functional consisting of entropy and interation energy

$$\mathcal{F}_\kappa(\varrho) = \sigma \int_{\mathbb{T}_L^d} \varrho \log \varrho \, dx + \frac{\kappa}{2} \iint_{\mathbb{T}_L^d \times \mathbb{T}_L^d} W(x-y)\varrho(y)\varrho(x)\, dy\, dx\,, \tag{3}$$

which is the driving functional for a gradient flow description in the Wasserstein space.

Let us note that the uniform state $\rho_\infty \equiv L^{-d}$ is always a stationary point, which at the same time is the global minima of $\mathcal{F}_\kappa$ for $\kappa > 0$ sufficiently small. Hence, we can consider the first transition point $\kappa_c > 0$ as the point where ρ_∞ loses its global stability. The transition can happen continuously (local bifurcation) or discontinuously for the L^1 topology. One of the main results of [2] is the classification of the kind of phase transitions in terms of the (real) Fourier modes $\tilde{W}(k) := (2/L)^{1/2} \int_{\mathbb{T}_L} W(x) \cos\left(\frac{2\pi k}{L} x\right)$ for $k \in \mathbb{N}$, here stated for the sake of presentation for $d = 1$.

Theorem [2]**.** *Let $W : \mathbb{T}_L \to \mathbb{R}$ be smooth and coordinate-wise even and let $\kappa_c < \infty$ be the first transition point of the free energy $\mathcal{F}_\kappa$:*

(1) near resonant modes*: If there exist non-zero $k^a, k^b, k^c \in \mathbb{N}$ with $\tilde{W}(k^a) \approx \tilde{W}(k^b) \approx \tilde{W}(k^c) \approx \min_k \tilde{W}(k) < 0$ such that $k^a = k^b + k^c$, then κ_c is a discontinuous transition point.*

(2) dominant mode*: Let $k^\sharp = \operatorname{argmin}_k \tilde{W}(k)$ be well-defined with $\tilde{W}(k^\sharp) < 0$. Then, if for some $\alpha \in (0, 1]$ small enough holds $\alpha \tilde{W}(k^\sharp) \le \tilde{W}(k)$ for all $k \neq k^\sharp$, then the transition point κ_c is continuous.*

Mathematically, the continuous phase transitions are accessible by local bifurcation analysis. However, the investigation of the discontinuous phase transition is more subtle. It exploits the free energy landscape by constructing appropriate competitor states, leading to the above theorem's resonance condition.

The identification of discontinuous phase transitions for the McKean–Vlasov dynamic raises the question if the free energy $\mathcal{F}_\kappa(\rho)$ for $\kappa = \kappa_c$ possesses, besides the two global minima, a third critical point. Classically, a mountain-pass argument identifies the energy gap Δ between a minimum and another saddle point. Similar to the Arrhenius law for chemical reactions, the energy barrier Δ determines the metastable time scale of the N-particle system. Indeed, the seminal work [3] connects the free energy $\mathcal{F}_\kappa$ with the large deviation rate function for the N weakly interacting diffusions in (1) as $N \to \infty$.

A mountain-pass theorem in $\mathcal{P}(\mathbb{T}_L^d)$ equipped with the Wasserstein metric comes with two difficulties: Firstly, $\mathcal{P}(\mathbb{T}_L^d)$ is only a metric space for which the theory of mountain-pass theorems is not fully developed. Secondly, the free energy functional (3) is just lower semicontinuous in the weak topology for probability measures.

These difficulties are overcome in [5] by using the notion of the weak metric slope $|d\mathcal{F}_\kappa|$ introduced in [7]. The notion is applicable to lower semicontinuous functionals on $\mathcal{P}(\mathbb{T}_L^d)$ as long as they are λ-convex by working with the extension of the functional to its epigraph based on ideas in [4]. In fact for λ-convex functionals, the metric slope $|\partial\mathcal{F}_\kappa|$ can be identified with the weak one $|d\mathcal{F}_\kappa|$.

Theorem [5]**.** *If $\mathcal{F}_{\kappa_c}$ has two distinct minimizers $\varrho_\infty \equiv 1/L^d$ and $\varrho_{\kappa_c} \in \mathcal{P}(\mathbb{T}_L^d)$, then there exists $\varrho^* \in \mathcal{P}(\mathbb{T}_L^d)$ distinct from ϱ_∞ and ϱ_{κ_c} such that $|\partial\mathcal{F}_{\kappa_c}|(\varrho^*) = 0$. Moreover, the energy barrier satisfies*

$$\Delta = \mathcal{F}_{\kappa_c}(\varrho^*) - \mathcal{F}_{\kappa_c}(\varrho_\infty) = \inf_{\gamma\in\Gamma} \max_{t\in[0,T]} \mathcal{F}_\kappa(\gamma(t)) - \mathcal{F}_{\kappa_c}(\mu) > 0\,,$$

where $\Gamma = \{C([0,T];\mathcal{P}(\mathbb{T}_L^d)) : \gamma(0) = \varrho_\infty, \gamma(T) = \varrho_{\kappa_c}\}$.

Thanks to the result in [3], this identifies the metastable time scale of the N interacting diffusions as $e^{-N\Delta}$ for $N \to \infty$.

The numerical approximation of the above found critical points asks for a structure-preserving numerical scheme for the gradient flow (2) to capture equilibria and saddle points with high accuracy. In [9], a finite volume scheme is defined on a family of Voronoi tesselations $\mathcal{T}^h$ with $\sup_K \operatorname{diam} K \le h$ by the discrete continuity equation

$$|K|\frac{\rho_K^{n+1} - \rho_K^n}{\delta t} + \sum_{L\sim K} \frac{|K|L|}{d_{KL}} f_{KL}^{n+1} = 0 \tag{4}$$

together with normal interface flux f_{KL}^{n+1} following the Scharfetter–Gummel interpolation

$$f_{KL}^{n+1} = \theta_\sigma\big(\rho_K^{n+1}, \rho_L^{n+1}, q_{KL}^{n+1}\big) = q_{KL}^{n+1} \frac{\rho_K^{n+1} e^{\frac{q_{KL}^{n+1}}{2\sigma}} - \rho_L^{n+1} e^{-\frac{q_{KL}^{n+1}}{2\sigma}}}{e^{\frac{q_{KL}^{n+1}}{2\sigma}} - e^{-\frac{q_{KL}^{n+1}}{2\sigma}}} \tag{5}$$

and discrete potential gradient

$$q_{KL}^{n+1} = \sum_{J\in\mathcal{T}} |J|\ \frac{\rho_J^{n+1} + \rho_J^n}{2}\big(W(x_K - x_J) - W(x_L - x_J)\big). \tag{6}$$

Let us note, that $\theta_\sigma(a,b,v) \to a(v_+)^2 + b(v_-)^2$ for $\sigma \to 0$, which is exactly the upwind interpolation. The following statement hightlights the structure-preserving properties of the scheme and its convergence as $\delta t, h \to 0$.

Theorem [9]**.** *Assume that $h|\partial K| \le C_{\text{iso}}|K|$ for all $K \in \mathcal{T}^h$, then $\exists!\{\rho^n\}_{n\in\mathbb{N}}$ solution of the scheme (4)–(6) and it holds*

- *Discrete free energy dissipation principle*

$$\frac{\mathcal{F}^h(\rho^{n+1}) - \mathcal{F}^h(\rho^n)}{\delta t} + \sigma\frac{\mathcal{H}(\rho^n \mid \rho^{n+1})}{\delta t} = -\mathcal{D}^h(\rho^{n+1});$$

- *Characterization of stationary states of scheme as critical point of $\mathcal{F}^h$ and vanishing dissipation $\mathcal{D}^h = 0$;*

- *Longtime behavior of scheme to discrete stationary states;*
- *convergence of scheme as* $\delta t, h \to 0$ *to solutions of* (2).

The scheme's numerical implementation can resolve the dynamic in the presence of a discontinuous phase transition and seems to be promising to approximate the saddle point by a suitable string method. Finally, we expect that the flux interpolation (5) can be brought into a generalized (non-symmetric, non-homogeneous) gradient structure following ideas developed in the works [1, 6, 8].

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Optimal Transport "Distances" in Quantum Mechanics

François Golse

(joint work with E. Caglioti, C. Mouhot, T. Paul)

Quantum mechanics is known to be well approximated by classical mechanics for particles with typical action $\gg \hbar$ (Planck's constant). This approximation involves high frequencies in the wave functions, and is formulated in terms of weak convergence. Wasserstein distances, on the other hand, are known to metrize the weak convergence of probability measures. Can one extend Wasserstein distances to compare quantum and classical densities (which are very different objects)?

The analogue of the set $\mathcal{P}(\mathbf{R}^d \times \mathbf{R}^d)$ of Borel probability measures on $\mathbf{R}^d \times \mathbf{R}^d$ is $\mathcal{D}(\mathfrak{H}) := \{T \in \mathcal{L}(\mathfrak{H}) \text{ s.t. } T = T^* \geq 0 \text{ and } \mathrm{tr}(T) = 1\}$, denoting $\mathfrak{H} = L^2(\mathbf{R}^d)$. Let $\mathcal{P}_2(\mathbf{R}^d \times \mathbf{R}^d)$ be the set of Borel probability measures on $\mathbf{R}^d \times \mathbf{R}^d$ with finite second moments, and $\mathcal{D}_2(\mathfrak{H}) := \{T \in \mathcal{D}(\mathfrak{H}) \text{ s.t. } \mathrm{tr}(T^{1/2}(|x|^2 - \Delta_x)T^{1/2}) < \infty\}$, which is its quantum analogue. We seek to extend the Wasserstein distance $\mathcal{W}_2$ with exponent 2 to $\mathfrak{D} := \mathcal{P}_2(\mathbf{R}^d \times \mathbf{R}^d) \cup \mathcal{D}_2(\mathfrak{H})$.

For $\mu, \nu \in \mathcal{P}(\mathbf{R}^d \times \mathbf{R}^d)$, denote by $\mathcal{C}(\mu, \nu)$ the set of couplings (transport plans) between μ and ν. Similarly, for $R, S \in \mathcal{D}(\mathfrak{H})$, the set of couplings of R and S is $\mathcal{C}(R, S) := \{T \in \mathcal{D}(\mathfrak{H} \otimes \mathfrak{H}) \text{ s.t. } \mathrm{tr}(T(A \otimes I + I \otimes B)) = \mathrm{tr}(RA + SB),\ A, B \in \mathcal{L}(\mathfrak{H})\}$. Likewise, a coupling of a probability density f on $\mathbf{R}^{2d}$ and of $R \in \mathcal{D}(\mathfrak{H})$ is an operator-valued map $Q : \mathbf{R}^{2d} \ni (x, \xi) \mapsto Q(x, \xi) \in \mathcal{L}(\mathfrak{H})$ such that

$$Q(x,\xi) = Q(x,\xi)^* \geq 0\,, \quad \mathrm{tr}_{\mathfrak{H}}(Q(x,\xi)) = f(x,\xi) \text{ a.e. and } \int_{\mathbf{R}^{2d}} Q(x,\xi)dxd\xi = R.$$

The set of couplings of f and R is denoted $\mathcal{C}(f, R)$.

Next we define the classical-to-quantum transport cost as the differential operator $c_\hbar(x, \xi)$ in the variable y parametrized by (x, ξ)

$$c_\hbar(x,\xi) := |x - y|^2 + |\xi + i\hbar\nabla_y|^2 \geq d\hbar I_{\mathfrak{H}}\,.$$

Likewise, we define the quantum-to-quantum transport cost as the differential operator $C_\hbar$ in the variable x, y

$$C_\hbar := |x - y|^2 - \hbar^2|\nabla_x - \nabla_y|^2 \geq 2d\hbar I_{\mathfrak{H}\otimes\mathfrak{H}}\,.$$

(The lower bounds on the self-adjoint operators $c_\hbar(x, \xi)$ and $C_\hbar$ are consequences of the Heisenberg uncertainty inequality.)

With these notions we define an extension $\mathfrak{d}$ of the Wasserstein distance $\mathcal{W}_2$ to $\mathfrak{D} \times \mathfrak{D}$ as follows: for $\mu, \nu \in \mathcal{P}_2(\mathbf{R}^d \times \mathbf{R}^d)$, set $\mathfrak{d}(\mu, \nu) = \mathcal{W}_2(\mu, \nu)$. For all $R, S \in \mathcal{D}_2(\mathfrak{H})$, set

$$\mathfrak{d}(R,S) = \inf_{T\in\mathcal{C}(R,S)} \mathrm{tr}_{\mathfrak{H}\otimes\mathfrak{H}}(T^{1/2}CT^{1/2})^{1/2} \geq \sqrt{2d\hbar}\,,$$

and, for each probability density f on $\mathbf{R}^{2d}$ with finite second moments, set

$$\mathfrak{d}(f,R) = \inf_{Q\in\mathcal{C}(f,R)} \left(\int_{\mathbf{R}^{2d}} \mathrm{tr}_{\mathfrak{H}}(Q(x,\xi)^{1/2}c_\hbar(x,\xi)Q(x,\xi)^{1/2})dxd\xi\right)^{1/2} \geq \sqrt{d\hbar}\,.$$

(In particular $\mathfrak{d}(R, R) > 0$, so that $\mathfrak{d}$ is not a bona fide metric on $\mathfrak{D}$.)

Next we explain how to compute or estimate $\mathfrak{d}(R, S)$ or $\mathfrak{d}(f, R)$ for some examples of density probabilities f on $\mathbf{R}^{2d}$, or of quantum densities $R, S \in \mathcal{D}(\mathfrak{H})$. First we recall the notion of Gaussian coherent state denoted

$$|q,p\rangle(x) := (\pi\hbar)^{-d/4}\exp(-|x-q|^2/2\hbar)\exp(ip\cdot x/\hbar)$$

For $\mu \in \mathcal{P}(\mathbf{R}^{2d})$, the Töplitz transform of μ is the operator

$$\mathcal{T}[\mu] := \int_{\mathbf{R}^{2d}} |q,p\rangle\langle q,p|\mu(dqdp)$$

(with Dirac's notation $|\psi\rangle\langle\psi|$ designating the orthogonal projection on $\mathbf{C}\psi$). For $R \in \mathcal{D}(\mathfrak{H})$, the Husimi transform of R is the probability density

$$\mathcal{H}[R](q,p) := \tfrac{1}{(2\pi)^d}\langle q,p|R|q,p\rangle = \tfrac{1}{(2\pi)^d}\mathrm{tr}(R|q,p\rangle\langle q,p|)\,.$$

Theorem 1. [7, 8] For f probability density on $\mathbf{R}^{2d}$ with finite second moments and $\mu, \nu \in \mathcal{P}_2(\mathbf{R}^d \times \mathbf{R}^d)$, one has

$$\mathfrak{d}(\mathcal{T}[\mu], \mathcal{T}[\nu])^2 \leq \mathcal{W}_2(\mu, \nu)^2 + 2d\hbar\,, \qquad \mathfrak{d}(\mathcal{T}[\mu], \mathcal{T}[\mu])^2 = 2d\hbar\,,$$
$$\mathfrak{d}(f, \mathcal{T}[\nu])^2 \leq \mathcal{W}_2(f, \nu)^2 + d\hbar\,, \qquad \mathfrak{d}(f, \mathcal{T}[f])^2 = d\hbar\,.$$

For $R, S \in \mathcal{D}_2(\mathfrak{H})$

$$\mathcal{W}_2(\mathcal{H}[R], \mathcal{H}[S])^2 \leq \mathfrak{d}(R, S)^2 + 2d\hbar\,,$$
$$\mathcal{W}_2(f, \mathcal{H}[R])^2 \leq \mathfrak{d}(f, R)^2 + d\hbar\,.$$

Moreover, if $\mathrm{rank}(R) = 1$, then

$$\mathfrak{d}(f, R) = \left(\int_{\mathbf{R}^{2d}} \mathrm{tr}_{\mathfrak{H}}(R^{1/2} c_\hbar(x, \xi) R^{1/2}) f(x, \xi) dx d\xi \right)^{1/2},$$
$$\mathfrak{d}(R, S) = \mathrm{tr}_{\mathfrak{H} \otimes \mathfrak{H}}((R \otimes S)^{1/2} C (R \otimes S)^{1/2})^{1/2}\,.$$

It may happen that the first inequality in Theorem 1 is an equality: this is the case for instance if μ and ν are Dirac measures (see [9]). Another example, for $d = 1$ and $0 < a < b$, is the case where

$$\mu = \tfrac{1}{2}(\delta_{(+a,0)} + \delta_{(-a,0)})\,, \quad \nu = \tfrac{1}{2}(\delta_{(+b,0)} + \delta_{(-b,0)})\,,$$
$$\text{so that } \mathfrak{d}(\mathcal{T}[\mu], \mathcal{T}[\nu])^2 = \mathcal{W}_2(\mu, \nu)^2 + 2d\hbar\,.$$

The first inequality in Theorem 1 is an equality if and only if an optimal coupling of $\mathcal{T}[\mu]$ and $\mathcal{T}[\nu]$ is $\mathcal{T}[\Pi]$, where Π is an optimal coupling of μ and ν. However, it may happen that the first inequality in Theorem 1 is strict: for instance, setting

$$\rho = \tfrac{1+\epsilon}{2}\delta_{(+a,0)} + \tfrac{1-\epsilon}{2}\delta_{(-a,0)} \text{ implies that } \mathfrak{d}(\mathcal{T}[\mu], \mathcal{T}[\rho])^2 < \mathcal{W}_2(\mu, \rho)^2 + 2d\hbar$$

for $0 < \epsilon \ll 1$. In this case, denoting $|k, l\rangle := |ka, 0\rangle \otimes |la, 0\rangle$, one finds that optimal couplings of $\mathcal{T}[\mu]$ and $\mathcal{T}[\rho]$ are of the form

$$T = \sum_{k,l \in \{\pm\}} \tau_{klkl} |k, l\rangle\langle k, l| + \sum_{\substack{k,l,m,n \in \{\pm\} \\ (k,l) \neq (m,n)}} \tau_{klmn} |k, l\rangle\langle m, n| =: T_1 + T_2$$

where T_1 is a Töplitz coupling of $\mathcal{T}[\mu]$ and $\mathcal{T}[\rho]$, while T_2 is a purely quantum correction which has no classical interpretation. See [2] for these examples.

Next we check whether $\mathfrak{d}$ satisfies the triangle inequality.

Theorem 2. [10] For all $\rho_1, \rho_2, \rho_3 \in \mathfrak{D}$, one has

$$\mathfrak{d}(\rho_1, \rho_3) < \mathfrak{d}(\rho_1, \rho_2) + \mathfrak{d}(\rho_2, \rho_3) + \sqrt{d\hbar}\,.$$

If $\rho_2 \in \mathcal{P}_2(\mathbf{R}^d \times \mathbf{R}^d)$, then

$$\mathfrak{d}(\rho_1, \rho_3) \leq \mathfrak{d}(\rho_1, \rho_2) + \mathfrak{d}(\rho_2, \rho_3)\,.$$

Theorem 2 allows defining $\mathfrak{d}(\mu, R)$ for all $\mu \in \mathcal{P}_2(\mathbf{R}^d \times \mathbf{R}^d)$ and $R \in \mathcal{D}_2(\mathfrak{H})$ by a density argument. With the material introduced above, one easily arrives at the following picture: the set of phase space densities $\mathcal{P}_2(\mathbf{R}^d \times \mathbf{R}^d)$ with the Wasserstein metric $\mathcal{W}_2$ is the classical ($\hbar \to 0^+$) limit in $\mathfrak{D}$ of the set of quantum density operators $\mathcal{D}_2(\mathfrak{H})$ equipped with the "pseudometric" $\mathfrak{d}$.

Theorem 3. [11] Let $R_\hbar, S_\hbar \in \mathcal{D}_2(\mathfrak{H})$ and $\mu, \nu \in \mathcal{P}_2(\mathbf{R}^d \times \mathbf{R}^d)$; then

$$\mathfrak{d}(\mu, R_\hbar) + \mathfrak{d}(\nu, S_\hbar) \to 0 \implies \mathfrak{d}(R_\hbar, S_\hbar) \to \mathcal{W}_2(\mu, \nu) \text{ as } \hbar \to 0^+ .$$

Finally, we discuss some applications of the "pseudometric" $\mathfrak{d}$. The first one is the simultaneous mean-field and classical limit for N-particle quantum dynamics. Consider the N-particle quantum Hamiltonian

$$\mathbf{H}_N = \sum_{k=1}^{N} -\tfrac{1}{2}\hbar^2 \Delta_{x_k} + \frac{1}{N} \sum_{1 \le k < l \le N} V(x_k - x_l) \quad \text{ on } \mathfrak{H}^{\otimes N}$$

and let $f \in C(\mathbf{R}_+; (\mathcal{P}_2(\mathbf{R}^d_x \times \mathbf{R}^d_\xi), \mathcal{W}_2))$ be a weak solution of the Vlasov equation

$$(\partial_t + \xi \cdot \nabla_x) f = \nabla_x (V \star_{x,\xi} f) \cdot \nabla_\xi f \,, \quad f\Big|_{t=0} = f^{in} .$$

Theorem 4 [7]**.** Let $V \in C^{1,1}(\mathbf{R}^d)$ be even, and set $L := 2 + \max(4\mathrm{Lip}(\nabla V)^2, 1)$. Then, for all $t \ge 0$, one has

$$\frac{\mathfrak{d}(f(t)^{\otimes N}, e^{-it\mathbf{H}_N/\hbar} \mathcal{T}[(f^{in})^{\otimes N}] e^{+it\mathbf{H}_N/\hbar})^2}{N} \le d\hbar e^{Lt} + \frac{4\|\nabla V\|_{L^\infty}}{N-1} \frac{e^{Lt} - 1}{L} .$$

Other applications include the convergence of time splitting schemes for quantum dynamics [6], the controllability of quantum dynamics [11]...

There have been other attempts at generalizing Wasserstein distances to the quantum setting: [4], §7.7 of [1] and [3, 5].

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