Gradient flows: challenges and new directions

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Abstracts

Benamou, Jean-David

An entropy minimization approach to second-order variational mean-field games

We propose in [1] a new viewpoint on variational mean-field games with diffusion and quadratic Hamiltonian. We show the equivalence of such mean-field games with a relative entropy minimization at the level of probabilities on curves. We also address the time-discretization of such problems, establish Γ-convergence results as the time step vanishes and propose an efficient algorithm relying on this entropic interpretation as well as on the Sinkhorn scaling algorithm.

[1] Benamou, Jean-David and Carlier, Guillaume and Marino, Simone Di and Nenna, Luca, *An entropy minimization approach to second-order variational mean-field games*, preprint, hal-01848370, 2018 https://hal.archives-ouvertes.fr/hal-01848370

Brenier, Yann

The arctangential heat equation: geometry and numerics

We show the geometric origin of the nonlinear heat equation with arctangential nonlinearity:

$$\partial_t u = \Delta\big(\arctan(u)\big)$$

by deriving it, together and in duality with the mean-curvature flow equation, from the minimal surface equation in Minkowski space, through a suitable quadratic change of time. We discuss its interpretation á la Otto as a gradient flow with respect to the transport metric. We also show that, written in non-conservative form and properly discretized, this arctangential heat equation might be a useful tool for image processing and data analysis.

Bruna, Maria

Asymptotic gradient flows for interacting particle systems

In this talk we will introduce the concept of asymptotic gradient flows. These are a generalisation of gradient flows for nonlinear partial differential equations with asymptotically small terms. I will illustrate their properties with an example, namely a cross-diffusion model describing interactions between two distinct populations.

Budd, Chris

Modified error estimates for discrete variational derivative methods

Many PDEs (for example the Swift–Hohenberg equation and the the KdV equation) have a variational structure. As a direct consequence of this structure we can deduce the existence of properties such as dissipation and conservation laws, as well as the existence of (for example) soliton solutions. A discrete variational derivative method exploits this variational structure when discretising the PDE. In this talk I will use a modified equation analysis to show that the discrete solution of such a method can be considered to be samples of a function which also satisfies a modified variational principle. It is then possible to derive a series of novel conservation or dissipation laws for this new function which mimic those of the original. I will show how these new laws can be constructed and the various consequences of them. This will include the existence of discrete soliton solutions of the KdV equation

Cuturi, Marco

Regularization for optimal transport and Dynamic Time Warping

We present in this talk two regularization strategies to smooth two popular discrepancy functions in data-sciences, the Wasserstein distance and the Dynamic Time Warping score. We show how these two strategies are different yet related in the sense that they both exploit different ways to smooth a min function using the soft-minimum function. We show that these regularizations enable the use of automatic differentiation toolboxes and illustrate this with a few applications to imaging and machine learning.

Fonseca, Irene

Mathematical analysis of novel advanced materials: epitaxy and quantum dots

Quantum dots are man-made nanocrystals of semiconducting materials. Their formation and assembly patterns play a central role in nanotechnology, and in particular in the optoelectronic properties of semiconductors. Changing the dots' size and shape gives rise to many applications that permeate our daily lives, such as the new Samsung QLED TV monitor that uses quantum dots to turn "light into perfect color"!

Quantum dots are obtained via the deposition of a crystalline overlayer (epitaxial film) on a crystalline substrate. When the thickness of the film reaches a critical value, the profile of the film becomes corrugated and islands (quantum dots) form. As the creation of quantum dots evolves with time, materials defects appear. Their modelling is of great interest in materials science since material properties, including rigidity and conductivity, can be strongly influenced by the presence of defects such as dislocations.

In this talk we will use methods from the calculus of variations and partial differential equations to model and mathematically analyze the onset of quantum dots, the regularity and evolution of their shapes, and the nucleation and motion of dislocations.

Lamacz, Agnes

Overdamped limit of the Vlasov–Fokker–Planck equation: a variational approach

Coarse-graining is the procedure of approximating a complex system by a simpler or lower-dimensional one, often in some limiting regime. Rigorous proofs of such limits typically hinge on exploiting certain structural features of the equations such as variational-evolution structures, which, for instance, are present in gradient flows. In this talk we introduce and discuss such a variational structure arising from the theory of large deviations for stochastic processes. We show how in systems, which are characterized by a large deviation rate functional, passing to a limit is facilitated by the dual formulation of the rate functional, in a way that interacts particularly well with coarse-graining. Being closely related to classical variational methods for gradient flows, our approach is also applicable to systems with non-dissipative effects. As an example we use the technique to derive the large friction (overdamped) limit of the Vlasov–Fokker–Planck equation. The talk is based on a joint work with M. Hong Duong, Mark A. Peletier and Upanshu Sharma.

Maas, Jan

Gromov–Hausdorff convergence of discrete optimal transport

For a natural class of discretisations of a convex domain in R^n, we consider the dynamical optimal transport metric for probability measures on the discrete mesh. Although the associated discrete heat flow converges to the continuous heat flow, we show that the transport metric may fail to converge to the 2-Kantorovich metric. Under an additional symmetry assumption on the mesh, we show that Gromov-Hausdorff convergence to the 2-Kantorovich metric holds. This is joint work with Peter Gladbach and Eva Kopfer.

Matthes, Daniel

A semi-implicit time discretization for fourth order diffusion equations with nonlinear mobility

For approximate solution of nonlinear diffusion equations of the form

$$\partial_t \rho = \mathrm{div}\big(m(\rho)\nabla E'(\rho)\big)$$

with a Dirichlet-type energy E and a nonlinear mobility m, a time-discrete JKO scheme

$$\rho_\tau^n = \mathrm{argmin}_\rho [W_m^2(\rho, \rho_\tau^{n-1}) + E(\rho)]$$

appears to be a reasonable option: if it works, it preserves mass and positivity of ρ, dissipates E, and the like. However, the definition of the mobility-adapted transportation metric W_m via Benamou–Brenier is not straight-forward unless m is a concave function. We present a modified semi-discrete approach that guarantees convergence of the ρ_τ^n to a weak solution ρ even for a class of non-concave m's. We shall also briefly discuss applications to coupled systems of diffusion equations.

Mielke, Alexander

On notions of evolutionary Gamma convergence for gradient systems

Considering a family of gradient systems depending on a small parameter, it is natural to ask for the limiting (also called effective) gradient system if the parameter tends to 0. We propose some ideas towards the derivation of the effective gradient structure that are based on De Giorgi's Energy-Dissipation Principle (EDP). We discuss several versions of EDP convergence and show by examples that the theory is flexible enough to allow for situations where starting from quadratic dissipation potentials we arrive at effective dissipation potentials that are no longer quadratic.

Otto, Felix

The thresholding scheme for mean curvature flow and De Giorgi's ideas for minimizing movements

We consider the thresholding scheme, a practically relevant time discretization for mean curvature flow (MCF) introduced by Bence–Merriman–Osher; and prove a (conditional) convergence result in the multi-phase case. The proof is based on the interpretation of the thresholding scheme as a minimizing movement scheme, which means that the thresholding scheme preserves the structure of (multi-phase) mean curvature flow as a gradient flow with respect to the total interfacial energy (joint work with Selim Esedoglu). We use ideas of De Giorgi to show that the limit satisfies Brakke's inequality, a way to encode MCF as a gradient flow. Indeed, his abstract notions of metric slope and of variational interpolation for minimizing movements, as formulated by Ambrosio–Gigli–Savare, are tailor-made for this limit. This is joint work with Tim Laux.

Peyré, Gabriel

Computational optimal transport for data sciences

Optimal transport (OT) has become a fundamental mathematical tool at the interface between calculus of variations, partial differential equations and probability. It took however much more time for this notion to become mainstream in numerical applications. This situation is in large part due to the high computational cost of the underlying optimization problems. There is a recent wave of activity on the use of OT-related methods in fields as diverse as computer vision, computer graphics, statistical inference, machine learning and image processing. In this talk, I will review an emerging class of numerical approaches for the approximate resolution of OT-based optimization problems. This offers a new perspective for the application of OT in imaging sciences (to perform color transfer or shape and texture morphing) and machine learning (to perform clustering, classification and generative models in deep learning). More information and references can be found on the website of our book "Computational Optimal Transport" https://optimaltransport.github.io/"

Poon, Clarice

On the total variation Wasserstein gradient flow and the TV-JKO scheme

I will present a study of the JKO scheme for the total variation functional. In particular, I will discuss a characterisation of the optimisers, some of their qualitative properties (e.g. a sort of maximum principle) and finally, in dimension one, the convergence as the time step goes to zero to a solution of a fourth-order nonlinear evolution equation. This is joint work with Guillaume Carlier.

Rossi, Riccarda

On the Weighted Energy-Dissipation principle for gradient flows in metric spaces

We discuss a variational approach to the analysis of gradient flows in metric spaces, based on the minimization of the associated Weighted Energy-Dissipation (WED) functional. The latter is a parameter-dependent global-in-time functional of trajectories featuring the weighted sum of energetic and dissipative terms. As the parameter tends to zero, its minimizers are shown to converge, up to subsequences, to curves of maximal slope with respect to the energy functional driving the gradient flow. The WED approach thus provides a new and general variational approximation procedure, hence a new existence proof, for metric gradient flows.

Savare, Giuseppe

Singular perturbation of gradient flows

We study the limit of gradient flows generated by time-dependent non convex functionals when the quadratic dissipation vanishes. The limit evolution is driven by the critical point of the functional and raises challenging mathematical questions, due to the lack of compactness (BV estimates are not available in general) and to the possible occurrence of oscillations, bifurcations and jumps. We will discuss a variational approach to these problems and propose a suitable notion of evolution. (In collaboration with Virginia Agostiniani and Riccarda Rossi)

Schmitzer, Bernhard

Numerical approximation of optimal transport type gradient flows

The gradient flow of a functional with respect to the Wasserstein-2 metric is defined as the limit of a time-discrete implicit Euler scheme. Similarly, one can study Euler steps of more general optimal transport type distances such as the 'unbalanced' Hellinger–Kantorovich distance or the adapted Benamou–Brenier formula for discrete Markov kernels introduced by Maas. Numerical approximations of these schemes are challenging due to the computational complexity of transport distances and the additional optimization over the 'free marginal'. We present two numerical approaches and corresponding convergence results; one based on entropy regularization and generalized Sinkhorn algorithms for standard optimal transport and the Hellinger–Kantorovich distance; and a proximal splitting method for the distance introduced by Maas.

Wirth, Benedikt

The spline energy on Riemannian manifolds

Variational spline curves (that is, minimizers of the spline energy, the average squared acceleration) represent a simple and efficient tool for data interpolation in Euclidean space. However, several applications from computer vision require interpolation of manifold-valued data. It turns out that well-posedness of splines is much more intricate on nonlinear and high-dimensional spaces and requires quite strong conditions on the metric of the underlying manifold. This may also have implications on the use of the linearized spline energy as a metric for gradient flows of curves in the manifold. We will analyse and discuss splines as well as their discrete counterparts on Riemannian manifolds.

Yarman, Evren

In search for an efficient multivariate data decomposition

I will be sharing some lessons we learned and challenges we encountered while developing some variational methods for multivariate data decomposition.

Zimmer, Johannes

From fluctuations in particle systems to gradient flows

Fluctuations of particle systems encode information about the macroscopic evolution; fluctuation-dissipation theorems are a classic example. There are different descriptions of such fluctuations, among them variational formulations related to Onsager–Machlup theory, and via infinite-dimensional fluctuation-dissipation theorems. In this talk, it will be shown how the many-particle evolution of gradient flows can be extracted from such formulations. This is joint work with P. Embacher, N. Dirr, X. Li and C. Reina.

Zygalakis, Konstantinos

Explicit stabilised Runge–Kutta methods for optimization

Explicit stabilized Runge–Kutta (RK) methods are explicit one-step methods with extended stability domains along the negative real axis. These methods are intended for large systems of ordinary differential equations originating mainly from semidiscretization in space of parabolic or hyperbolic-parabolic equations. In this talk we will explore their applicability to optimization of strongly convex functions. In particular, for quadratic problems it is possible to show rigorously that for suitable choice of algorithmic parameters the convergence rate matches the one of the conjugate gradient. In the general case, numerical investigations indicate that the convergence rate remains the same and the corresponding algorithm is able to outperform state of the art optimization algorithms such as the Nesterov's accelerated method.