DynaLearn Project (2020-2023): Final report

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Abstract

DynaLearn: When neural nets meet Physics: Neural networks are powerful objects used in machine learning, but poorly understood from a theoretical point of view. A recent line of research consist in studying the flow of information through or in these networks through the lens of dynamical systems and their associated Physics. The **Dynalearn project** aims at contributing on those aspects in a two-fold way:

- By exploring how dynamical formulation of learning process can help in understanding better learning deep neural architectures, as well as proposing new learning paradigms based on the regularization of the flows of information;

- By leveraging on novel neural architectures and available data to devise new data-driven dynamical simulation models, with applications in Earth Observation and Medical Imaging.

Keywords: machine learning ; deep learning ; dynamical systems ; optimal transport ; diffeomorphic flows ; fluids dynamics

1. Initial motivations

The dynamical system-based approach makes it possible to formalize the evolution of the flow in deep architectures, and to precisely define the evolution equation and associated properties. The considered theoretical background of the Dynalearn project builds upon the relationship between fluid dynamics, information geometry and machine learning. Broadly speaking, geodesic flows can be regarded as solutions of Euler equations in fluid dynamics. As such, deep learning architectures can be viewed as numerical schemes for geodesic flow estimation. ResNet architectures are a typical example, which relates to ODE solvers [Rousseau2019]. This also bridges to the optimal transport problem, which amounts to geodesic flows under volume-preserving constraints [Brenier1989]. In this context, we aim to develop a unifying mathematical framework for a rigorous and computationally-efficient design, implementation and study of learning processes, including deep networks. Through the development of flow-based approaches, we expect major breakthroughs in the characterization, specification and application of these learning processes from theoretical consideration on mapping estimation, stability, diffeomorphism and optimal control. To reach this goal, we will tackle the following questions:

- How can a learning system be expressed as a dynamical system, where the flow of information operates inside a neural network architecture?
- How can machine and deep learning helps in simulating complex dynamic systems by providing means of representing the associated flows?
- How can deep learning systems use OR improve simulation techniques of stochastic dynamical systems to handle uncertainty?

In this project, we plan to examine those questions through the prism of optimal transport, which is a powerful theory to model those flows. We start by reviewing in very general terms the main features of this theory, and we then describe how we can apply it for the considered two tasks of this project.

2. Contributions

2.1. Optimal Transport and flows in probability space. In the context of this project, we are interested in understanding the flows of information in machine learning methods such as deep learning. We started by examining and studying methods such as normalizing flows, that allow to transport an unknown probability distribution onto a a simpler, parametric one, such as a Gaussian, with a tractable likelihood. We then naturally extend this study to optimal transport, which provides a natural framework for expressing such operations. As one of our goal was to consider transfer between incomparable spaces, we first examined Gromov-Wasserstein distances, for which we designed efficient computation algorithm based on subspace projections (detours) (Bonet et al., 2021a). We then switched to gradient flows in probability spaces, where we designed a fast solver based on sliced version of the optimal transport (Wasserstein) distance (Bonet et al., 2022).

2.2. Distances in non-Euclidean probability spaces. While many Machine Learning methods were developed or transposed on Riemannian manifolds to tackle data with known non Euclidean geometry, Optimal Transport (OT) methods on such spaces have not received much attention. The main OT tool on these spaces is the Wasserstein distance which suffers from a heavy computational burden. On Euclidean spaces, a popular alternative is the Sliced-Wasserstein distance, which leverages a closed-form solution of the Wasserstein distance in one dimension, but which is not readily available on manifolds. In the context of the PhD of **Clément Bonet** (Bonet, 2023), we derive general constructions of Sliced-Wasserstein distances on Non-Euclidean spaces. We first started to study how to transpose Sliced-Wasserstein distances to the case of positively curved space, such as the Sphere (Bonet et al., 2023a), with applications to analysis of geophysical data on the surface of Earth, and self-supervised representation learning in more abstract spaces. We then derive general constructions of Sliced-Wasserstein distances on Cartan-Hadamard manifolds (Bonet et al., 2023b,c), Riemannian manifolds with non-positive curvature, which include among others Hyperbolic spaces or the space of Symmetric Positive Definite matrices. We then studied different applications, ranging from Brain-Computer interface signals . Additionally, we derive non-parametric schemes to minimize these new distances by approximating their Wasserstein gradient flows. This works had a recent application in computer graphics, where it was used to design an efficient method for blue noise sampling of general meshes (Genest et al., 2024). This last work won the **best paper prize** of the Eurographics conference.

2.3. Super-resolution in Physical Imaging. This part tackles the challenge of **efficiently deriving high-resolution velocity fields from sparse, off-grid observations**. This task is of prime importance in fields like experimental fluid dynamics, computer vision, remote sensing, and medical imaging. Unlike traditional methods that rely on intensive numerical simulations or purely data-driven models, we focused here *physics-informed neural networks* (PINNs) and *neural field* (NF) neural models. These models' parameters are optimized by minimizing loss functions comprising data-fit terms and *PDE residuals* calculated via automatic differentiation. Both models employ coordinate-based neural networks that, in their vanilla formulation, suffer from the so-called spectral bias; that is, their solutions are biased toward the smooth representation of the data. In this project, we applied PINNs and NFs to spatially resolve the instantaneous measurements of isolated micro-particles exposed to airflow acceleration leveraging the 2D incompressible turbulent flow model, described by the Navier-Stokes (NS) equation. The approach we developed introduced physics-based *hard constraints* to inherently satisfy PDE terms and a *soft constraint* utilizing a *surrogate model* for regularizing unobserved scales. Specifically, our approach ensures **divergence-free** results and applies **statistical structure functions**, significantly enhancing the accuracy of super-resolved velocity fields in turbulent flows and reducing the computational complexity of computing PDEs directly. Recent advancements in back-end coding frameworks have made high-order derivative computations feasible. However, new challenges arose in training several objective functions at once, referred to as *multi-task learning*, and defining *stopping criteria*. Our work focused on using surrogate models in a pre-training phase, enabling more effective parameter initialization in deep learning models. We proposed new surrogate models and researched advanced methods to overcome the neural networks' spectral biases. Our key contribution was the application of statistical structure functions derived from Kolmogorov's turbulence theory and a computation of the resolved flow's energy spectrum as differentiable surrogate models for the NS PDE to regularize the unresolved scales (surrogate models). Moreover, we studied how wavelet and *Gabor filters* can be employed to replace the neural network's activation functions in order to extend the neural network bandwidth (spectral bias) and satisfy PDE by construction. This has been published in Di Carlo et al. (2022).

2.4. Euler equations and learning. We have also worked on the incorporation of some physical constraints directly in machine learning (ML) algorithms. In particular we have focused our attention on the Euler's equations which are widely used in fluid dynamics. From a non physical perspective, the solutions to the Euler's equation are geodesics in the space of volume preserving diffeomorphisms [Arnold 66]. The computation of geodesics are of particular interest in ML applications. They can be interpreted as the shortest path between the initial state and the output of the network allowing theoretical guarantees and a better understanding of the architecture. In practice, we have investigated the interpretation of ML algorithms as dynamical systems satisfying the Euler's equations. As part of Guillaume Morel's post-doctoral work, we proposed a method based on Brenier's polar factorization theorem to transform any trained normalizing flow into a more OT-efficient version without changing the final density. The Gaussian preserving transformation is implemented with the construction of high dimensional divergence free functions and the path leading to the estimated Monge map is further constrained to lie on a geodesic in the space of volume-preserving diffeomorphisms thanks to Euler's equations (Morel et al., 2023).

3. Summary and perspectives

During the project, the field has moved fast and attracted considerable attention in the machine and deep learning communities. Physics-Informed Neural Networks (PINN) are now state-of-the-art in numerous tasks involving predictions over physical systems. In the context of generative AI, diffusion models, based on a time-continuous PDE modeling of the generation process from a Gaussian noise to a learning distribution of objects of interest, is now the most competitive method in terms of image generation and empowers most of the commercial methods such as DALL-E or Midjourney. Following the intuitions of the project, this diffusion process gathers much ressemblance to the Schrödinger Bridge which is an entropic optimal transport problem.

The DynaLearn project's contributions belong to this line of work. Extending to Non-Euclidean spaces have opened the way for numerous perspectives where learning on data which can not be represented in vectors spaces revealed to be a rich and complex topic at the intersection of differential geometry, probability and machine learning. We have identified this topic as a meaningful scientific perspective, and some of the group researchers are involved in a PhD project (that should start in September, 2024) on this subject. Modelling using dynamical systems (divergence free fields) has also made it possible to explore new avenues of research into robustness to adversarial attacks through the work of a current PhD thesis. Additionally, we are also starting a PhD on the topic of optimal transport based diffusion models for image super-resolution in a context of Earth Observation. All of these topics perfectly fit with the upcoming SequoIA cluster in Artificial Intelligence, expected to start in 2024.

Publications during the project

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