Internship: Deep Learning and Differential Equations for simulating Physical Phenomena

Informations

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Duration : 6 month in 2021

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Candidate profile: Master or engineering degree in computer science or applied mathematics. The topic is at the crossroad of machine learning and numerical analysis. The candidate should have a strong scientific background with good technical skills in programming.

Gratification : classical French internship gratification around 550 E/ mois

Context

Differential equations (DEs) play a prominent role for modeling complex system dynamics in applied mathematics, physics and other disciplines. They are usually derived from physical laws. However, in many situations the governing equations of the underlying system are not fully known. Huge quantities of data characterizing complex phenomena are today available through observations or simulation. This opens opportunities for considering combining physical and statistical machine learning (ML) models. From a Deep Neural Networks (DNN) perspective, despite their success for many applications, training DNNs is still a complex task, heavily relying on heuristics and DNNs remain analytically unexplained. Recently a new formulation of DNNs has started to spread: the DNN is considered as the discretization of a continuous flow satisfying some ordinary differential equation (ODE). This promising new research trend is aimed at analyzing and controlling DNNs by taking advantage of the rich background of numerical analysis. These two observations are incentives to develop research at the interplay of DNNs and DEs. This research direction has recently emerged. The first workshop on this topic was held at the ICLR 2020 conference (a major machine learning conference) under the name "Integration of Deep Neural Models and Differential Equations".

Objective

Differential equations form one of the bedrocks of scientific computing, while neural networks have emerged as the preferred tool of modern machine learning. They offer complementary strengths: the modelling power and interpretability of differential equations, and the approximation and generalization power of deep neural networks. The objective of the internship is to develop links between DNNs and DEs in order to start answering central questions like: how could DNNs be used to solve DEs, how the concepts of numerical analysis could be adapted to DNNs, how to develop hybrid models incorporating both NN modules and ODE/PDE solvers? Two directions will be explored. su

Hybrid systems - Interfacing DNNs and ODE/PDE

The key issue addressed here is how to combine prior information expressed as PDEs and information extracted from data. There are several instances for which this is a sensible approach. ML comes as a complement to numerical models by allowing to take into account information not present in the model or to integrate information provided by observation data. From a DNN perspective, physical background constitutes prior knowledge that guides and constrains the learning process. For example, we have shown how to learn the motion field characterizing an advection-diffusion system (de Bezenac et al. 2018). Here we will consider a general process where there is a source of physical knowledge in the form of PDEs that represents partial information about the underlying process, and we will analyze different schemes to complement this information with DNNs. This raises several open questions such as the characterization of the solutions of such systems and their coherence, the derivation of a learning framework allowing us to combine differentiable solvers and DNN modules, and the development of corresponding algorithms. Experimentally, we will examine different problem cases where a partially known physical model is complemented by ML modules. The starting point for this research will be the recent publication (Le Guen et al. 2021).

Extrapolation / Robustness

Depending on the progress on the first topic, one will consider the issue of generalization of hybrid models. Explicit physical models come with certain guarantees and can be used in any context where the model is valid. This is not the case for DNNs, and we have no guarantee that they can be extrapolated to unknown situations or initial conditions. Generalization has been at the heart of ML for several years. We propose here to tackle the problem by drawing inspiration from recent ML frameworks such as (Arjovski et al 2020).

Position w.r.t. State of the Art

Solving DEs with DNNs dates back to the 90es (Lagaris et al. 1998), but it is only very recently (2017-2018) that this research topic fully emerged. This rapidly growing field motivates the interest of several communities. Two main directions are currently investigated. One is how to use DNNs for solving and identifying PDEs (Rudy et al. 2017, Raissi 2018, Long et al. 2018, Sirignano and Spiliopoulos 2018). The other direction comes from the interpretation of successful DNNs like ResNET as ODE discretization schemes [Ruthotto and Haber 2018, Lu et al. 2018]. This motivates the development of new DNN architectures. The issues of stability and robustness for different schemes is currently being investigated (Haber et al. 2019, Chang et al. 2018). (Chen et al. 2018) uses ODE solvers for supervised learning problems. Learning dynamics from incomplete information is addressed in (Ayed et al. 2020), insertion of physical priors in DNNs in (de Bezenac et al. 2018), and more general hybridization schemes in (Le Guen et al. 2021)

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