INSTITUT DES SYSTEMES INTELLIGENTS ET DE ROBOTIQUE
THESIS OFFER

Subject

Subject: Physics-Aware Deep Learning for Modeling Spatio-Temporal Dynamics.

Supervisor: Patrick Gallinari

Collaboration within the framework of the thesis: INRIA team Ange, Paris; Inria team Epione, Sophia; Institut d'Alembert, Sorbonne University.

Host laboratory: ISIR (Institut des Systèmes Intelligents et de Robotique), Campus Pierre et Marie Curie, 4 place Jussieu, 75005 Paris.

Start date: October/November 2023
Note: The research topic is open and depending on the candidate profile could be oriented more on the theory or on the application side

Keywords: deep learning, physics-aware deep learning, climate data, fluid dynamics, earth science

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Application deadline: 15/12/2023

Description

Context:

Physics-aware deep learning is an emerging research field aiming at investigating the potential of AI methods to advance scientific research for the modeling of complex natural phenomena. This research topic investigates how to leverage prior knowledge of first principles (physics) together with the ability of machine learning at extracting information from data. This is a fast-growing field with the potential to boost scientific progress and to change the way we develop research in a whole range of scientific domains. An area where this idea raises high hopes is the modeling of complex dynamics characterizing natural phenomena occurring in domains as diverse as climate science, earth science, biology, fluid dynamics, etc. This will be the focus of the PhD project.

Research Directions:

The direct application of state-of-the-art deep learning (DL) methods for modeling and solving physical dynamics occurring in nature is limited by the complexity of the underlying phenomena, the need for large amounts of data and their inability to learn physically consistent laws. This has motivated the recent exploration of physics-aware methods incorporating prior knowledge, by researchers from different communities (Willard et al. 2020, Thuerey et al. 2021). Although promising and rapidly developing, this research field faces several challenges. For this PhD project we will address two main challenges, namely the construction of hybrid models for integrating physics with DL and generalization issues which condition the usability of DL for physics.

- Integrating DL and physics for spatio-temporal dynamics forecasting and solving PDEs
In physics and many related fields, partial differential equations (PDEs) are the main tool for modeling and characterizing the dynamics underlying complex phenomena. Combining PDE models with ML is then a natural idea when building physics-aware DL models and it is one of the key challenges in the field. For now, this has been explored for two main directions: (i) augmenting low resolution solvers with ML in order to reach the accuracy of high-fidelity models at a reduced computational cost (Belbute-Perez et al. 2020, Kochkov et al. 2021, Um et al. 2020), and (ii) complementing incomplete physical models with ML by integrating observation data through machine learning (Yin et al. 2021a, Dona et al. 2022). The former topic is crucial for the entire field of numerical simulation while the latter allows for explorations beyond the current limits of numerical models. Simultaneously, the recent advances in neural operators (Li et al. 2021, Lu et al. 2021, Li et al. 2022, Yin et al. 2023) offer new methods for learning and modeling dynamics at different resolutions in space and time, providing the possibility of combining and learning multiple spatio-temporal scales within a unified formalism, a challenge in ML. A first direction of the PhD will then be to investigate physics-aware ML models by exploring the potential developments of hybrid models together with neural operators.

- Domain generalization for deep learning based dynamical models
Explicit physical models come with guarantees and can be used in any context (also called domain or environment) where the model is valid. These models reflect explicit causality relations between the different variables involved in the model. This is not the case for DL: statistical models learn correlations from sample observations, their validity is usually limited to the context of the training domain, and we have no guarantee that they extrapolate to new physical environments. This is a critical issue for the adoption of ML for modeling the physical world. Models of real-world dynamics should account for a wide range of contexts resulting from different forces, different initial and boundary conditions or different prior parameters conditioning the phenomenon. Ensuring generalization to these different contexts and environments is critical for real world applications. Surprisingly, only a few works have explored this challenging direction. In relation with the construction of hybrid models as described above, one will investigate this issue along two main directions. The first one exploits ideas from learning from multiple environments through task decomposition as in (Yin et al. 2021b, Kirchmeyer et al. 2022). This is a purely data-based approach. The second one, takes a dual perspective, relying on prior physical knowledge of the system equations and directly targets the problem of solving parametric PDEs (Huang 2022), exploiting ideas from meta-learning (Finn 2016).

Required Profile:

Master degree in computer science or applied mathematics, Engineering school. Background and experience in machine learning. Good technical skills in programming.

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