Data and Dynamical Systems
Données et systèmes dynamiques
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JAHRUL ALAM, Memorial University of Newfoundland
Dictionary-based operator learning for nonlinear partial differential equations

The study of turbulent flows is computationally intensive due to the intrinsic multi-scale behavior of their nonlinear dynamics. Thus, it requires relatively high-resolution grids to capture their complexity fully. For instance, imagine the range of length and time scales in the numerical study of a hurricane passing over a city. The field of fluid mechanics traditionally deals with massive amounts of data. However, methods to precisely quantify complex and multi-scale phenomena of fluid flows remain unresolved to a large extent. More specifically, turbulent fluid data require algorithms capable of addressing nonlinearities and multi-scale phenomena that may not be available in classical machine learning methods. This talk presents a dictionary-based operator learning method as a reduced-order data-driven model of the chaotic behavior of turbulent flows. First, I will outline the convergence criteria for extracting the governing operator from noisy measurements underlying a nonlinear dynamical system. I will then show numerical results comparing dictionary-based and neural network-based methods. Finally, I will discuss the dictionary-based reduced-order representation of the Naiver-Stokes operator. The current findings indicate the potential extension of wavelet methods in dictionary-based operator learning for chaotic systems.

ALEX BIHLO, Memorial University of Newfoundland
A multi-model physics-informed neural network approach for solving the shallow-water equations on the sphere

We propose the use of physics-informed neural networks for solving the shallow-water equations on the sphere in the meteorological context. Physics-informed neural networks are trained to satisfy the differential equations along with the prescribed initial and boundary data, and thus can be seen as an alternative approach to solving differential equations compared to traditional numerical approaches such as finite difference, finite volume or spectral methods. We discuss the training difficulties of physics-informed neural networks for the shallow-water equations on the sphere and propose a simple multi-model approach to tackle test cases of comparatively long time intervals. Here we train a sequence of neural networks instead of a single neural network for the entire integration interval. We also avoid the use of a boundary value loss by encoding the boundary conditions in a custom neural network layer. We illustrate the abilities of the method by solving the most prominent test cases proposed by Williamson et al. [J. Comput. Phys. 102 (1992), 211-224]. This is joint work with Roman O. Popovych.

MONICA COJOCARU, University of Guelph
Reclustering populations based on mobility driven well-mixing using reinforcement learning - disease spread insights

In this talk we present an algorithm designed to recast a population (here that of the US) through the lens of county population's mobility patterns. The result is a reclustering of the US population in regions that are not geographically distinct, but instead have low inter-region travelling. Such subpopulations are now well-mixed from the perspective of a ODE model of SEIR-type, hence in-depth analyses of infection spread are much better supported. We highlight differences and similarities in the epidemic evolution of Covid-19 in 2020 in the US, following the population reclustering, and the interplay between population socio-demographic factors, NPI compliance (i.e., masks) and sizes of the initial local reproduction numbers, R0, and time delays between local peaks and sizes of reported incidence throughout 2020. Further, we look at ways to use the current Covid-19 based modelling to derive insights on the impact of different pathogen scenarios such as flu.

MARICELA BEST MCKAY, University of British Columbia
Approximation rates and training dynamics for Physics-informed Neural Networks

Physics-informed Neural Networks (PINNs) are an alternative to traditional numerical methods for approximating solutions to systems of Partial Differential Equations. They are especially promising for applications where it is desirable to include real-world data into a numerical model. However, PINNs can be particularly challenging to train. PINNs may fail to train altogether for multi-scale problems, or problems containing multiple frequencies. The gradient flow for PINN loss functions often exhibits characteristics of stiffness and instability. Even when PINNs are able to train, they are unable to achieve the high-order accuracy of traditional methods. Recently, theoretical guarantees for the approximation rates of continuous functions by ReLU networks have been proposed. These rates rely on the existence of an optimal network, which may or may not be findable during training. While ReLU is not a suitable choice for most PINNs, we demonstrate that ReLU like activation functions can improve PINN training dynamics. We illustrate how challenges in PINN training dynamics impact numerical error rates and explore the gaps between theory and practice for the PINN setting.

FLORIAN PUCHHAMMER, University of Waterloo
Simulating Chemical Reaction Networks with Randomized Quasi-Monte Carlo

The τ-leap algorithm by Gillespie is used to simulate chemical reaction networks as a discrete time Markov chain, as an alternative to solving the typically high-dimensional chemical master equation. The objective is to estimate the expectation of a function of the molecule numbers at a given future time. We combine this approach with a powerful randomized quasi-Monte Carlo (RQMC) technique, Array-RQMC, which has been proven to outperform Monte Carlo and conventional RQMC in many applications. For chemical reaction networks, this combination can reduce the variance by factors in the thousands, compared to Monte Carlo. Even more than it was observed for ordinary RQMC by Beentjes and Baker (2018).

Array-RQMC efficiently simulates an array of realizations of the Markov chain in parallel, but requires to sort the chains at each step by their (multi-dimensional) states. In our simulations, Array-RQMC always performed better than ordinary MC, regardless of the sort. Yet, the choice of the sorting function can have a significant impact on both variance reduction and simulation speed. We demonstrate how different sorting algorithms can increase the efficiency of the method and discuss how they can be customized for specific applications and for different performance measures.

GIANG TRAN, University of Waterloo
Epidemiological Predictive Modelling using Delayed Time Embedding

In this talk, we will present a new method to predict the infectious using sparse random feature models. The model is motivated by Taken's delay embedding theorem and the theoretical guarantee of sparse random features. The proposed model outperforms the benchmark on various real datasets, including COVID19, Ebola, and Flu datasets.