Master Thesis: Data-Driven Machine Learning of Turbulence Models

Ludger Pähler

February 20, 2018

Abstract

In this project the student will implement her/his own version of a learning machine, leveraging the underlying laws of physics to then extract high-dimensional data patterns from Computational Fluid Dynamics simulations to for a data-driven discovery of the partial differential equations. This learning machine will then subsequently be extended to handle turbulence models, hence expanding on the current state of the art in research. Afterwards we will carry out a quantification of the uncertainties introduced by the Neural Network/ Deep Network utilizing techniques from Computer Vision and Bayesian Deep Learning.

1 Introduction

In the modern world input data from sensors is ubiquitous. Bringing structure in that data is hence paramount. An emerging research focus in that field is hence the effort to learn the underlying partial differential equations (PDEs) from that data. There exist two approaches to said input-output problem. We are thinking of the PDE as an abstract input-output map one are data-driven solutions to PDEs [5] and the other is the data-driven discovery of PDEs [6]; we will consider the latter. Both lean heavily on machine learning methodologies, as well as frameworks, developed over the past decade. While this approach exudes a certain sense of elegance it introduces a new set of problems to the discovery process. Neural Networks (NN) and especially Deep Neural Networks (DNN) introduce uncertainties into our problem the quantification of which is another active area of research [1]. There exist multiple possible expansions to said approaches such as the use of Deep Networks [4], placing a larger focus on the time evolution of the system such as in [7] or rather generalizing the approach by building on the method developed by Rudy where we train the state-vector of the PDE with a sparse matrix to return the PDE without the requirement of the learning machine having any prior knowledge about the structure of the underlying PDE [8].

2 Outline

2.1 Tasks

Learning Machine Code up a learning machine in Pytorch (or Tensorflow) with a clean documentation of your code and strict adherence to PEP8.

Testing on CFD Models Validating the implemented learning machine against results in the literature using the models implemented in the in-house C++ CFD code Alpaca.

Extension to Turbulence Models Extending the learning machine to be able to handle Turbulence models such as Shocktubes and Shock-Bubble Interactions.

Uncertainty Quantification of the NN and DNN Quantifying the uncertainty introduced to the problem by the used Neural Networks and/or Deep Neural Networks.

Literature Review Reading up on current research looking for possible extensions to the method which could improve upon the currently used method.

2.2 Requirements

- Good knowledge of Pytorch or Tensorflow and especially Python.
- High degree of self-motivation.
- Working knowledge of Bayesian Statistics.

2.3 Learning Goals

- Insight into state of the art Fluid Dynamics Research
- Introduction to the Quantification of Uncertainty in Complex Systems
- Limits of current Machine Learning based approaches in the Engineering Sciences

3 Contact

Ludger Pähler
Room: MW1610
E-Mail: ludger.paehler@tum.de
Phone: +49-89-289-16154

References

[1] Yarin Gal. *Uncertainty in Deep Learning*. PhD thesis, University of Cambridge, 2016.

[2] Yarin Gal and Zoubin Ghahramani. On modern deep learning and variational inference. In *Advances in Approximate Bayesian Inference workshop, NIPS*, volume 2, 2015.

[3] Alex Kendall and Yarin Gal. What uncertainties do we need in bayesian deep learning for computer vision? In *Advances in Neural Information Processing Systems*, pages 5580–5590, 2017.

[4] Maziar Raissi. Deep hidden physics models: Deep learning of nonlinear partial differential equations. *arXiv preprint arXiv:1801.06637*, 2018.

[5] Maziar Raissi, Paris Perdikaris, and George Em Karniadakis. Physics informed deep learning (part i): Data-driven solutions of nonlinear partial differential equations. *arXiv preprint arXiv:1711.10561*, 2017.

[6] Maziar Raissi, Paris Perdikaris, and George Em Karniadakis. Physics informed deep learning (part ii): Data-driven discovery of nonlinear partial differential equations. *arXiv preprint arXiv:1711.10566*, 2017.

[7] Maziar Raissi, Paris Perdikaris, and George Em Karniadakis. Multistep neural networks for data-driven discovery of nonlinear dynamical systems. *arXiv preprint arXiv:1801.01236*, 2018.

[8] Samuel H Rudy, Steven L Brunton, Joshua L Proctor, and J Nathan Kutz. Data-driven discovery fo partial differential equations. *Science Advances*, 3(4):e1602614, 2017.