



Miniworkshop

Differential equations and machine learning

9 April 2021 – virtual workshop

9:00 - 9:15	Welcome	P. Spichtinger
9:15 - 10:00	Introduction to Machine Learning	M. Wand
10:00 - 10:45	Machine learning and differential equations	A. Hildebrandt
10:45 - 11:15	BREAK	
11:15 - 12:00	Universal approximators in modeling, system inference, and identification	J. Martensen
12:00 - 13:00	LUNCHBREAK	
13:00 - 13:45	Applications of ML and ODEs	A. Hildebrandt
13:45 - 14:30	From Monte-Carlo simulations of cloud particle ensembles to ODEs with help of machine learning	A. Seifert
14:30 - 14:45	BREAK	
14:45 - 15:45	Discussion	all
15:45 - 16:00	Closing remarks & Farewell	P. Spichtinger

Abstracts

Introduction to Machine Learning

M. Wand, JGU Mainz

to be determined

Machine learning and differential equations

A. Hildebrandt, JGU Mainz

to be determined

Universal approximators in modeling, system inference, and identification

J. Martensen, Otto-von-Guericke-Universität Magdeburg

The use of neural networks within the modeling of dynamic systems has gained a lot of momentum over the past decade. Recent approaches include Lagrangian and Hamiltonian Networks to discover processes governed by conservation laws, autoencoder to find a set of coordinates for a canonical representation or a transformed system representation.

Especially in the case of scientific machine learning, this prior knowledge about the processes at hand is of utmost importance, given sparse measurement data and the need to comply with known physical laws. In this talk, we briefly discuss the history, applications, current developments, and possible future of hybrid dynamical systems for the inference of missing interactions for ordinary and partial differential equations and show some recent examples from the field of biology and pharmacy.

Applications of ML and ODEs

A. Hildebrandt, JGU Mainz

to be determined

From Monte-Carlo simulations of cloud particle ensembles to ODEs with help of machine learning

Axel Seifert, DWD Offenbach

Formulating ODEs that describe the time evolution of an ensemble of cloud particles is a classic problem in cloud physics. Usually this is approached by methods borrowed from statistical mechanics, but other methods like regression

models or even look-up tables derived from numerical solutions have been used throughout the last decades. More recently, two developments have the potential to change the way how we model and simulate clouds. Firstly, Monte-Carlo methods to explicitly simulate the evolution of the particle ensemble have gained renewed attention due to the availability of more efficient algorithms, like the super-droplet method, and the increase in computing power. Such Lagrangian particle methods are exceptionally attractive for particles that cannot be described by a single property, like mass or size, but have a more complicated internal composition or structure that needs to be evolved in time and through the particle ensemble. Secondly, machine learning (ML) methods offer the promise to speed up the formulation of bulk models in form of ODE systems from such detailed benchmark simulations. Using ML makes it possible to aim for more complicated ODE systems and, hence, a more complete description of the physical system than classic methods would usually allow. Knowing that cloud uncertainties are at the heart of many challenges in atmospheric science, this might be a route that is worth exploring. I will present some first and rather naive attempts to apply machine learning to this problem. Interestingly, ML not only provides a semi-automatic workflow to derive the sought-after ODEs, but it can also foster a deeper understanding of the challenges and caveats involved.