Graz Center for Machine Learning

IRT Physics Networking Event 0.1:
Physics-Informed Machine Learning & Surrogate Modelling

Agenda & Abstracts

Organizer: S. Ranftl

Kindly register informally at ranftl@tugraz.at
or on-site for organization purposes - Thank you!

Overview & Schedule

Graz Center for Machine Learning
Interdisciplinary Research Topic: Physics-Informed Machine Learning

What: GraML Networking Event: Physics-informed Machine Learning and Surrogate Modeling v0.1
When: 12th July 2023
Where: HS BMT, BMTEG138, Stremayrgasse 16 EG, TU Graz

Schedule acc. to Central European Summer Time (UTC+2)
15 min per talk incl. discussion. Suggestion: 12 min talk + 3 min discussion

From	Till	
09:00	09:05	Welcome: Robert Legenstein & Sascha Ranftl
09:05	09:20	**Sascha Ranftl**, Inst. Theoretical Physics, TU Graz
		A connection between probability, physics and neural networks
09:20	09:35	**Franz Rohrhofer / Bernhard Geiger**, Know Center
		Training gives me PINNs and needles - on the complexity of training physics-informed neural networks
09:35	09:50	**Alexandra Serebrennikova / Karin Zojer**, Inst. Solid State Physics, TU Graz
		Applications of PINNs for real-world inverse problems on the example of transport
		of organic volatiles through paper
09:50	10:20	**COFFEE BREAK**
10:20	10:35	**Lukas Hörmann / Oliver Hofmann**, Inst. Solid State Physics, TU Graz
		Smart-Data Machine-Learning for Surface Structure Search
10:35	10:50	**Andreas Hauser**, Inst. Experimental Physics, TU Graz
		Improved GPR algorithms for energy predictions of molecules in porous structures
10:50	11:05	**Stefan Kowarik**, Inst. Chemistry, KFU Graz
		Machine Learning for Closed-Loop Experiment Control and Online Analysis
11:05	11:35	**COFFEE BREAK**
11:35	11:50	**Johannes Hoffer**, voestalpine aerospace
		Robust Bayesian Target Value Optimization
11:50	12:05	**Shaoheng Guan**, Inst. Theoretical Physics, TU Graz
		Advantages and challenges of neural networks for constitutive modeling
12:05	12:20	**Eniz Muselic / Alice Reinbacher-Köstinger**, Inst. of Fundamentals & Theory in Electrical Engineering, TU Graz
		Machine Learning and Topology Optimization
12:20	12:35	**Jan Hansen**, Institute for Electronics, TU Graz
		Using surrogates to improve the electromagnetic properties of electric vehicles
12:35	12:40	Closing

Abstracts

A Connection between Probability, Physics and Neural Networks

Sascha Ranftl

Institute of Theoretical Physics-Computational Physics, TU Graz

I illustrate an approach that can be exploited for constructing neural networks that a priori obey physical laws. We start with a simple single-layer neural network (NN) but refrain from choosing the activation functions yet. Under certain conditions and in the infinite-width limit, we may apply the central limit theorem, upon which the NN output becomes Gaussian. We may then investigate and manipulate the limit network by falling back on Gaussian process (GP) theory. It is observed that linear operators acting upon a GP again yield a GP. This also holds true for differential operators defining differential equations and describing physical laws. If we demand the GP, or equivalently the limit network, to obey the physical law, then this yields an equation for the covariance function or kernel of the GP, whose solution equivalently constrains the model to obey the physical law. The central limit theorem then suggests that NNs can be constructed to obey a physical law by choosing the activation functions such that they match a particular kernel in the infinite-width limit. The activation functions constructed in this way guarantee the NN to a priori obey the physics, up to the approximation error of non-infinite network width. Simple examples of the homogeneous 1D-Helmholtz equation are discussed and compared to naive kernels and activations.

Key Words: Bayes; probability; neural networks; Gaussian process; kernels; covariance functions; activation functions; physics-informed machine learning; differential equations; PDEs; ODEs; linear operators; linear constraints; inverse kernel trick

TRAINING GIVES ME PINNS AND NEEDLES – ON THE COMPLEXITY OF TRAINING PHYSICS-INFORMED NEURAL NETWORKS

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ABSTRACT

Physics-informed neural networks (PINNs) [1] have become increasingly popular in various disciplines such as engineering or biomedicine, and are capable of solving differential equations given only information about the initial and boundary conditions (IC/BCs). However, previous attempts have shown that training PINNs in this context is a difficult endeavour, often leading to incorrectly predicted system dynamics. Therefore, a larger part of the scientific literature on PINNs proposes remedies to these training difficulties, including changes to training objectives, novel ways how these objectives are evaluated [2], and approaches to better balance conflicting objectives inherent in PINNs [3].

In our own work, we have investigated the underlying reasons for training difficulties in PINNs with a particular focus on the mathematics of physical and dynamical systems, such as for fluid flow or pendulum dynamics. We have shown that several "nonphysical" solutions are represented by minima in the optimization landscape of the PINN training, and slow down or even prevent convergence to the correct system dynamics. More specifically, we have shown that fixed points of dynamical systems, which appear as constant solutions in ordinary differentiation equation (ODEs) or steady-state solutions in partial differential equations (PDEs), are attractive for PINN training [4] (see Fig. 1). What is more, we have observed that the physics training loss is affected by the complexity of the solution, as measured by the energy of its high-frequency components. This is connected to the so-called spectral bias of network training [5], which leads to low-frequency components of the target function being learned easier and faster than its high-frequency components. This spectral bias has interesting consequences in vanilla PINNs, in which the IC/BCs are enforced via a separate loss term. In such a setting, the PINN can trade between accurately learning the IC/BCs and learning a solution that satisfies the given system of differential equations. If a small shift in initial conditions thus leads to significantly simpler, i.e., smoother, system dynamics (as is common in chaotic systems), then the PINN will shift the initial condition accordingly [6]. The result is a physically correct solution for a wrong initial condition. The relative weights assigned to fitting the IC/BCs and to satisfying the governing differential equations, respectively, influence the capability of the PINN to make such a trade-off and determine the position on the observable Pareto front to which the PINN converges after training.

Both effects – convergence to nonphysical solutions affected by fixed points, and to physical solutions for wrong initial conditions – are strongly affected by parameters of the system of differential equations and the size of the computational domain. Indeed, the observable Pareto front for a PINN trained with gradient methods changes substantially with the system parameters, even when feature scaling is applied. This makes choosing the corresponding loss weights difficult [7]. Our results further consistently showed that smaller

Applications of PINNs for real-world inverse problems on the example of transport of organic volatiles through paper

Alexandra Serebrennikova, Karin Zojer

Institute for Solid State Physics, TU Graz

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This talk will explore the application of Physics-Informed Neural Networks (PINNs) to solve real-world inverse problems, focusing on the transport of organic volatiles through paper. PINNs integrate physics-based knowledge into neural networks, enabling efficient and accurate solutions. By incorporating governing physical laws and constraints, PINNs reduce the need for extensive data when solving inverse problems.

Using organic volatile transport in paper as an example, we demonstrate how PINNs can reconstruct diffusion and sorption processes with limited data. We discuss the formulation, training, and interpretation of results, highlighting the knowledge on some useful insights and tricks gained through our research process in the past two years.
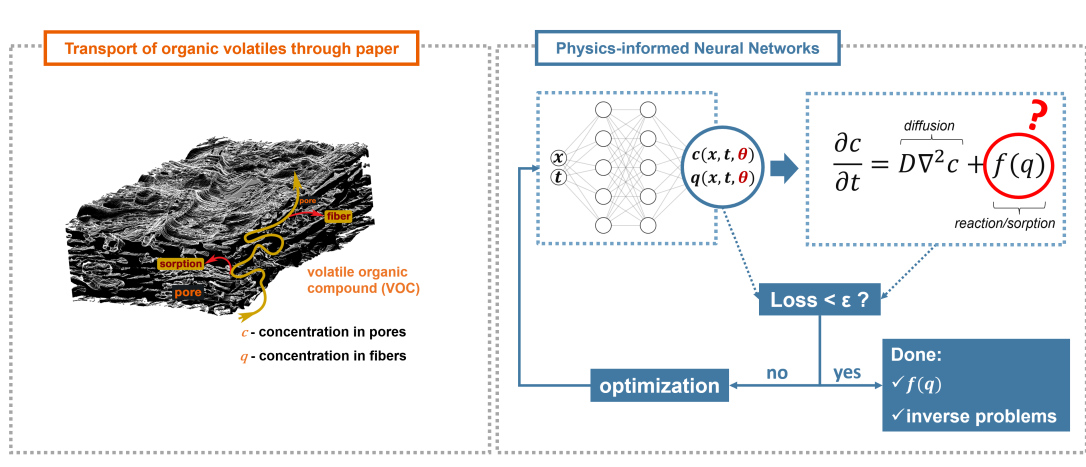

Figure 1: PINNs in real-world applications

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Smart-Data Machine-Learning for Surface Structure Search

Lukas Hörmann, Oliver Hofmann

Institute of Solid State Physics, TU Graz

The key challenge for surface structure search is the enormous number of possible polymorphs. Finding the lowest energy polymorph with conventional stochastic algorithms would require an insurmountable computational effort. We overcome this using the quasi-deterministic SAMPLE approach, which is based on smart-data machine-learning and experimental design theory. A few hundred DFT calculations suffice to exhaustively predict the local minima of the potential energy surface. To gain maximal insight from a limited amount of data, we employ an energy model based on molecule-substrate and molecule-molecule interactions. Using Bayesian linear regression, it extracts them directly from formation energies of polymorphs. SAMPLE assigns each interaction a feature based on atom distances. The features differentiate between atom species, allowing to separate contributions of various molecule-fragments to the formation energy, yielding knowledge about why a particular polymorph forms.

Improved GPR algorithms for energy predictions of molecules in porous structures

Johannes K. Krondorfer, Christian W. Binder, and Andreas W. Hauser

Institute of Experimental Physics, TU Graz

The simulation of gas adsorption, storage, separation and diffusion processes in porous materials requires detailed knowledge of the corresponding potential energy surfaces. In this talk, a new algorithm is presented, specifically developed for situations where a single molecule or 'mobile phase' is embedded in a highly symmetric molecular environment. Our approach is based on a symmetry-enhanced version of Gaussian process regression with embedded gradient information and uses an active learning strategy to keep the number of single point evaluations to a minimum. We test the performance of our algorithm for a selection of molecular sieving problems, i.e. the separation of gas molecules via effectively two-dimensional membranes.

Machine Learning for Closed-Loop Experiment Control and Online Analysis

Stefan Kowarik

Institute of Chemistry, Karl-Franzens-Universität Graz

This talk presents the application of machine learning (ML) in closed-loop experiment control and online analysis, specifically focusing on X-ray scattering. We utilize dense and convolutional neural networks to extract sample parameters from X-ray scattering data, demonstrating that neural networks yield less scatter and greater precision in analyzing X-ray reflectivity (XRR) curves compared to traditional fit algorithms. Expanding beyond static sample analysis, we employ a convolutional neural network approach to analyze time-dependent XRR curves acquired during thin film deposition. Our approach leverages a physics model of thin film deposition for parameter reduction and data regularization. This enables high-fidelity analysis of noisy or sparsely sampled XRR data. We further discuss the integration of ML into a closed-loop workflow for X-ray reflectometry, using organic thin film growth as an example. The accuracy and robustness of ML methods are demonstrated for XRR curve analysis and Bragg reflections, enabling autonomous control over vacuum deposition setups. This work will impact research with large or rapidly generated datasets as are common at large scale X-ray facilities among others.

Robust Bayesian Target Value Optimization

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We consider the problem of finding an input to a stochastic black box function such that the scalar output of the black box function is as close as possible to a target value in the sense of the expected squared error. While the optimization of stochastic black boxes is classic in (robust) Bayesian optimization, the current approaches based on Gaussian processes predominantly focus either on (i) maximization/minimization rather than target value optimization or (ii) on the expectation, but not the variance of the output, ignoring output variations due to stochasticity in uncontrollable environmental variables. In this work, we fill this gap and derive acquisition functions for common criteria such as the expected improvement, the probability of improvement, and the lower confidence bound, assuming that aleatoric effects are Gaussian with known variance. Our experiments illustrate that this setting is compatible with certain extensions of Gaussian processes, and show that the thus derived acquisition functions can outperform classical Bayesian optimization even if the latter assumptions are violated. An industrial use case in billet forging is presented

Advantages and challenges of neural networks for the constitutive modelling

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Dated: June 26, 2023

Abstract

Neural networks serve as surrogate models that effectively expedite multi-scale computations. However, when employing this black box approach in practical engineering calculations, two significant challenges arise: ensuring accuracy and achieving generalization. Can neural networks be effectively employed to replicate the constitutive responses of materials in boundary value problem (BVP) calculations, and how well do they perform?

Recent studies have demonstrated the capability of recurrent neural networks in reproducing the history-dependent intrinsic response of granular materials [4]. By integrating the trained neural network into a finite element solver, the computational cost of multi-scale calculations can be significantly reduced [2, 5]. However, subsequent research has revealed that the network-based model exhibits a high degree of reliance on the available data [1]. The neural network model gradually accumulates prediction errors over iterations, leading to overall prediction instability when the input values exceed the range covered by the training data. Since the training sample space is limited while the potential strain paths in BVP calculations are infinite, the generalisation capability of the network becomes crucial in accurately predicting stresses for unseen strain paths. To address this issue, a machine-learning material cell has been proposed by introducing physical constraints [3]. These physical constraints serve a dual purpose: firstly, they assist the material cell in identifying patterns within the data, and secondly, they aid the model in inferring stresses for strain paths that were not part of the training data. The material cell exhibits the potential to combine the flexibility of a data-driven approach with the stability typically associated with classic constitutive models.

When it comes to artificial intelligence chat, autonomous driving, or data-driven mechanics-based calculations, one crucial aspect is to perform an uncertainty analysis that corresponds to the decision results obtained from black box models. It is only when we can estimate the probability of error and accept it that this data-driven approach can effectively guide engineering practice. However, conducting an analysis of error rates poses a new challenge in itself.

References

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Machine Learning and Topology Optimization

Eniz Museljic, Alice Reinbacher-Köstinger

Institut für Grundlagen und Theorie der Elektrotechnik, TU Graz

Due to developments in additive manufacturing it is possible to produce more complex geometries. Topology optimization offers a concrete way of utilizing these technologies to create better structures and devices. We show an overview of the approaches on how machine learning methods can be utilized in topology optimization procedures.

Using surrogates to improve the electromagnetic properties of electric vehicles

Jan Hansen

Institut für Elektronik, TU Graz

With increasing sophistication of electric vehicle design, the optimization of the vehicles' electromagnetic properties becomes increasingly important. The numerical solution poses several problems, ranging from long computation times over model accuracy, multi-objective optimization up to risk analysis. Surrogate models may help to solve these problems, but there still is a long route ahead. This talk sketches the state-of-the-art and (many) open problems in this field.