AKPIK 1: Theory of Machine Learning (joint session MP/AKPIK)

Time: Wednesday 13:45–14:45 Location: ZHG001

AKPIK 1.1 Wed 13:45 ZHG001

Time Series Analysis of machine learned Quantum Systems — •Kai-Hendrik Henk and Wolfgang Paul — Martin-Luther-Universität Halle-Wittenberg, Halle(Saale), Deutschland

The Rayleigh-Ritz variation principle is a proven way to find ground states and energies for bound quantum systems in the Schrödinger picture. Advances in machine learning and neural networks make it possible to extend it from an analytical search from a subspace of the complete Hilbert space to the a numerical search in the almost complete Hilbert space. Here, we extend the Rayleigh-Ritz principle to Nelson's stochastic mechanics formulation of non-relativistic quantum mechanics, and propose an algorithm to find the osmotic velocities $u(x)$, which contain the information of a quantum systems in this picture (*Phys. Rev. A 108, 062412*). Motivated by experiments by the Aspelmeyer group at the University of Vienna using quantum levitodynamics (see for example *Nature 595, 373-377 (2021)*), we apply the algorithm to the harmonic oscillator, the Gaussian and the Lorentzian potential and analyze them using methods from time series analysis and phase portraits.

References: *Henk, K.-H., and Paul, W. Machine learning quantum mechanical ground states based on stochastic mechanics. Phys. Rev. A 108 (Dec 2023), 062412*

AKPIK 1.2 Wed 14:05 ZHG001

Opening the Black Box: predicting the trainability of deep neural networks with reconstruction entropy — •Yanick Thurn[1], Ro Jefferson[2], and Johanna Erdmenger[1] — [1]Institute for Theoretical Physics and Astrophysics, Julius-Maximilians-University Wuerzburg — [2]Institute for Theoretical Physics, and Department of Information and Computing Sciences, Utrecht University

An important challenge in machine learning is to predict the initial conditions under which a given neural network will be trainable. We present a method for predicting the trainable regime in parameter space for deep feedforward neural networks (DNNs) based on reconstructing the input from subsequent activation layers via a cascade of single-layer auxiliary networks. We show that a single epoch of training of the shallow cascade networks is sufficient to predict the trainability of the deep feedforward network on a range of datasets (MNIST, CIFAR10, FashionMNIST, and white noise). Moreover, our approach illustrates the networks decision making process by displaying the changes performed on the input data at each layer, which we demonstrate for both a DNN trained on MNIST and the vgg16 CNN trained on the ImageNet dataset.

AKPIK 1.3 Wed 14:25 ZHG001

Analytic continuation of Greens functions with a neural network — •Martin Rackl, Yanick Thurn, Fakher Assaad, Anika Götz, René Meyer, and Johanna Erdmenger — Julius-Maximilians University Würzburg, Am Hubland, 97074 Würzburg, Germany

An important problem in many-body physics is to reconstruct the spectral density from the imaginary-time domain Greens function. Typically, this Greens function is generated by Monte Carlo methods. As the one-point fermionic kernel diverges for large frequencies, the numerical noise present generically causes instabilities. A standard method to tackle the reconstruction of the spectral density is the maximum entropy method (MaxEnt). In this paper, we follow a different approach and use a convolutional neural network for obtaining the spectral density for a given imaginary time Greens function. The network is very sensitive to the nature of the training data that we create using random Gaussians. Here we improve the training data set available by considering collision centres for Gaussians rather than uniformly distributed Gaussians. Our network is constructed in such a way that its output fulfils the positive semidefiniteness of the spectral density and is ppropriately normalized. We compare the results of this network with results of MaxEnt for the same problem. This comparison is performed for different cases: artificial test data, spin-charge separation in the 1d Hubbard model. Using the Wasserstein distance as metric, we find that the network performs in the same order of magnitude of accuracy as MaxEnt.