UNIKASSEL VERSITÄT

Physikalisches Kolloquium

Thursday, 25.04.2019, 16:15, HS 100
Reception with coffee & cookies 15:45
(For university staff: please bring your own cup for sustainability reasons)

Prof. Roman Krems, University of British Columbia, Vancouver/Canada:

Bayesian Machine Learning for Quantum Molecular Dynamics

Abstract
I will discuss our recent work on applications of Bayesian machine learning for quantum molecular dynamics. To take advantage of machine learning, it is useful to approach quantum molecular dynamics in somewhat unconventional ways. I will advocate a particular formulation of quantum dynamics in the form of a machine learning simulator of the Schrodinger equation. If combined with the Bayesian statistics, such a simulator allows one to obtain not only the quantum predictions but also the error bars of the dynamical results associated with uncertainties of inputs (such as the potential energy surface or non-adiabatic couplings) into the nuclear Schrodinger equation. Instead of viewing atoms as undergoing dynamics on a given potential energy surface, Bayesian machine learning allows one to formulate the problem as the Schrodinger equation with a non-parametric distribution of potential energy surfaces that becomes conditioned by the desired dynamical properties (such as the experimental measurements). I will discuss the application of such machine learning models for the design of efficient quantum dynamics calculations.
I will also show how machine learning models can be used to correlate rigorous results with approximate calculations, providing accurate interpolation of exact results. Finally, I will present evidence that it is possible to build Bayesian machine learning models capable of physically extrapolating the solutions of the Schrodinger equation. This is particularly valuable as such models could complement common discovery tools to explore physical properties of complex systems at Hamiltonian parameters not accessible by rigorous quantum calculations or experiments.
To set the ground for the above, I will begin by a general discussion of the Bayesian approach to machine learning, the connection between neural networks and Gaussian processes and a description of Bayesian optimization.

All of you interested in physics are cordially invited!

Contact: Prof. Dr. Christiane Koch, Theoretical Physics III, More Information: uni-kassel.de/go/physikalisches_kolloquium