universität wien

FAKULTÄT FÜR MATHEMATIK
Dekan Univ.-Prof. Dr. Radu Ioan Boţ

Einladung zur öffentlichen Defensio

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Thema der Dissertation

Transferable Neural Network Wavefunctions

Abstract:
Solutions to the Schrödinger Equation, referred to as wave functions, allow in principle to predict any property of any molecule or material. Finding solutions efficiently is therefore crucial to computational discovery and understanding of new materials such as drugs, catalysts or superconductors. However due to the large dimensionality of the problem and the high accuracy required for practical applications, designing efficient methods to find approximate solutions is challenging. One recently proposed method is to combine Variational Monte Carlo (VMC) with neural network wavefunctions: This method represents the wavefunction as a neural network, estimates the corresponding energy of the ansatz via Monte Carlo integration, and minimizes this energy via gradient based optimization. Due to the high expressivity of neural networks this ansatz achieves exceptionally high accuracy with moderate scaling of computational costs.

However for practical applications, which often require solutions for many different molecules or geometries, this approach often proves unfeasible since it necessitates an expensive optimization for every new system. This work introduces transferable neural network wavefunctions, capable of simultaneously representing wavefunctions for many distinct molecules. Transferable neural network wavefunctions yield solutions to the Schrödinger Equation for many systems in parallel and even allow to use wavefunctions optimized on a set of training molecules to be applied to new, previously unseen systems. This thesis provides a brief introduction to the field of neural network wavefunction VMC and contains several related publications. These successively builds towards a transferable neural network wavefunction - starting from the single molecule case, via distinct geometries of a single molecule, towards a fully end-to-end machine learned neural network wavefunction applied to a diverse dataset of organic molecules.

Prüfungssenat

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Zeit und Ort

Freitag, 27. September 2024, 14:00 Uhr

Online:

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