Condensed Matter Theory Center



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"Machine Learning the Many-Body Problem"

Abstract: Condensed matter physics is the study of the collective behavior of infinitely complex assemblies of electrons, nuclei, magnetic moments, atoms or qubits. This complexity is reminiscent of the "curse of dimensionality" commonly encountered in machine learning. Despite this curse, the machine learning community has developed techniques with remarkable abilities to classify, characterize and interpret complex sets of data, such as images and natural language recordings. Here, we show that modern architectures for supervised learning, such as fully-connected and convolutional neural networks, can identify phases and phase transitions in a variety of condensed matter Hamiltonians. Readily programmable through open-source software libraries, neural networks can be trained to detect multiple types of order parameter, as well as highly non-trivial states with no conventional order, directly from raw state configurations sampled with standard Monte Carlo. Further, Monte Carlo configurations can be used to train a stochastic variant of a neural network, called a Restricted Boltzmann Machine (RBM), for use in unsupervised learning applications. We show how RBMs, once trained, can be sampled much like a physical Hamiltonian to produce configurations useful for estimating physical observables. Finally, we explore the representational power of RBMs, their role in deep learning, and its possible relationship to the renormalization group.

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