論文の内容の要旨

Classification and Representation of Physical States by Neural Networks

(ニューラルネットワークによる物理状態の判定および表現)

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The revolutionary success of the artificial neural network boosted the advancement in various fields in computer science such as the image or speech recognition and machine translation. Although the theoretical understanding on the success of the neural networks has not been fully explored, it is not too bold to state that the practical factors are three-fold: the drastic improvement in the computational resource, the development of efficient optimization technique, and the increase in the number of variational parameters which enhances the representation power. While the technology itself was invented in the field of machine learning, the target problems can be ubiquitous; the methodology awaits further opportunity to exert its potential in other research fields. Numerous problems in condensed matter physics or statistical physics are excellent candidates, and indeed novel ideas and techniques have been developed rapidly through integration of knowledge. In the current thesis, we intensively focus on the classification and representation tasks that are expected to advance dramatically by interdisciplinary study.

The classification task aims to build a machine that assigns discrete labels for finite- or infinite-dimensional data. In automated tagging for digital images, for instance, the data representing the RGB values are processed by a "prediction machine" which calculates the labels based on image recognition techniques. The neural network is commonly used to perform such a complicated mapping from the RGB values to the label. The machine learning community has recognized the task of developing an efficient classification machine as one of the central problems for visionary, audible or market data. Recent findings show that the background of the data could be even more diverse; the neural network can handle data gathered via scientific experiments or numerical simulations that are intended to investigate natural phenomena.

Needless to say, the classification of phases is one of the fundamental tasks in physics as well. It is not difficult to imagine that the classification task in systems with local order parameter is in good connection with the ordinary image recognition technique. Even more intriguing direction is the classification of topological phases, which cannot be characterized by local order parameters. Since the discovery of the quantum Hall effect, physicists have been fascinated by the bizarre concept of classifying quantum states based on the band topology of wave functions. Considering the profoundness and abundance of its nature, it can be undoubtedly counted as one of the most significant and yet difficult classification tasks in condensed matter physics. In particular, the challenge lies in the disordered regime.

While the disorder and impurity are present in real materials, the commonly used formulae for topological invariants break down when the translation symmetry is absent. An image-classification-based approach offers a powerful method to compensate for this gap. In the Chapter 3 of this thesis, we discuss a method to predict the quantum phases under disorder based on a machine trained to classify phases in the clean limit.

Another valuable task with progressive results is the representation of physical states. In the present thesis, the representation is defined as the explicit expression of physical states including the ground-state wave function of isolated quantum systems, the Boltzmann weight of a state in the thermodynamic equilibrium, and the stationary-state density matrix of open quantum systems. For instance, an exactly soluble model can be rephrased as "a model with the exact representation of eigenstates available" and an attempt to calculate the ground state via variational optimization can be described as the "calculation of the approximate representation of the ground state."

It is notable that the approximate representation of classical data (or physical states in classical systems) has been studied intensively in the field of machine learning and statistics. An example is the inverse engineering of the model that reproduces the obtained dataset. Various approaches have been developed for parameter estimation including mean field theory, contrastive-divergence method, and the use of variational autoregressive model. While such approximate representations in condensed matter physics can also be used to accelerate the Monte Carlo simulations, the construction process requires some extra numerical cost. It is desirable to have a training-free algorithm that draws samples efficiently. As we discuss in Chapter 4, this strongly motivates us to construct an exact transformation of a model with difficulty in sampling into another equivalent one with different representation in which a fast sampling algorithm is applicable. In particular, we consider a mapping of a model with many-body interacting binary degrees of freedom into the Boltzmann machine, which consists of only two-spin interactions and local magnetic field. We demonstrate that such a representation is beneficial from the viewpoint of Monte Carlo simulations since the celebrated cluster update algorithm becomes applicable.

For quantum many-body systems, the search for approximate representations has been one of the most significant issues concerning the numerical investigation. The main objective is to alleviate the bottlenecks that arise in principle when one attempts to tackle a quantum many-body system on a classical computer, namely the exponential increase in the memory consumption and numerical cost. Unless a quantum simulator or universal quantum computer with sufficient fidelity is built, the growth of the computational cost severely limits the size of systems accessible via full-space approach such as the exact diagonalization. We instead aim to tackle with some variational function that accurately captures the property of the physical system with reduced number of parameters.

The recent findings for the ability of the neural network as a representation machine have attracted intensive attention. Carleo and Troyer [Science **355**, 602 (2017)] showed that the restricted Boltzmann machine (RBM), a representation machine with auxiliary degrees of freedom that interact with the whole system, can be optimized via the variational Monte Carlo method to accurately express the ground states of quantum spin models. Since then, there has been continuous effort to extend the variational method to the excited states, imaginary time evolution toward the ground state, the finite temperature state etc. Although the applicability has been largely expanded, the approximate representation by the neural network has yet to be applied to one of the most challenging problems in modern condensed matter physics – the open quantum many-body systems. It is notoriously difficult to solve the fundamental equation of motions for such systems, which is often well captured by the time-homogeneous quantum master equation. Motivated by such situations, in Chapter 5, we develop a new algorithm to construct the approximate representation of the nonequilibrium stationary state of open quantum many-body systems. The variational optimization of an ansatz based on the complex-valued restricted Boltzmann machine is shown to efficiently simulate the stationary states of quantum dynamics obeying the time-homogeneous quantum master equations.

The organization of the present thesis is given as follows. In Chapter 1, we first introduce the notions in machine learning to see that problems in physics can be reformulated from the perspective of algorithm design. Then we overview the application of machine learning techniques to the classification and representation tasks in physics. We also provide the outline of the thesis.

In Chapter 2, we introduce the machines that are used for the classification and representation tasks. In particular, we focus on the simplest and most versatile machines applied to the classification and representation tasks. As the classification machine, we introduce the multilayer perceptron and the convolutional neural network. Either is a non-linear function consisting of huge number of parameters such that arbitrary function can be expressed by increasing the degrees of freedom. As the representation machine, we introduce the Boltzmann machine. Furthermore, models with restrictions on the connectivity between the physical and auxiliary spins are given to define the restricted and deep Boltzmann machines. We also discuss the complex-valued Boltzmann machine as well.

In Chapter 3, we develop a new scheme to classify the quantum phases of free-fermion systems under disorder. Given the disorder that keeps the discrete symmetries of the ensemble as a whole, we argue that translational symmetry, which is broken in the individual quasiparticle distribution, is recovered statistically by taking the ensemble average. This enables one to classify the quantum phases in the disordered regime using a neural network trained in the clean limit. We demonstrate our method by applying it to a two-dimensional system in the class DIII by showing that the result obtained from the machine is totally consistent with the calculation by other independent methods.

In Chapter 4, we find an exact representation of the generalized Ising models using the Boltzmann machine. We show that the appropriate combination of the algebraic transformations, namely the star-triangle and decoration-iteration transformations, allows one to express the many-spin interaction in terms of fewer-spin interactions at the expense of the degrees of freedom. Furthermore, we find that the application of such a representation is beneficial from the viewpoint of Monte Carlo simulations since the celebrated cluster update algorithm becomes applicable. We demonstrate this point by applying the cluster-update algorithm by Swendsen and Wang, and find that the critical slowing down is drastically reduced in a model with two- and three-spin interactions on the Kagomé lattice.

In Chapter 5, we develop a numerical algorithm that builds the approximate representation of stationary states in open quantum many-body systems. Our algorithm, dubbed as the neural stationary state algorithm, performs a variational optimization of an ansatz based on the complex-valued restricted Boltzmann machine to compute the stationary states of quantum dynamics obeying the time-homogeneous quantum master equations. This is enabled by considering a mapping of the stationary-state search problem into finding a zero-energy ground state of an appropriate Hermitian operator. Our method is demonstrated to simulate various dissipative spin systems efficiently, i.e., the transverse-field Ising models in both one and two dimensions and the XYZ model in one dimension that are subject to damping effect.

Chapter 6 is devoted to the Summary of this thesis. Some supplemental materials are provided in Appendices.