Abstract

Machine learning, which has been developing rapidly in recent years, has had a significant impact on the field of physics. It is performed on a large amount of data using algorithms such as neural networks, which enable appropriate inferences about unknown data. Before the development of machine learning, humans adjusted detailed algorithms and made inferences based on the results of the analysis. However, by using machine learning, it has become possible to leave the detailed processing to the learning algorithm without human intervention and to achieve higher accuracy than ever before.

An application in physics is found in the problem of obtaining the wave function of quantum many-body systems, whose Hilbert space increases exponentially with the system size. In conventional methods, human intuitions or empirical rules are often used to prepare variational wave functions, but tremendous efforts are required to achieve high accuracy. To solve this difficulty, machine learning has been successfully applied in recent years. However, especially for fermionic systems, an efficient method remains elusive due to the negative sign problem associated with particle exchanges.

Another important application is found in the inverse problem — designing a physical system from desired physical properties. In materials science, conventional theoretical studies often search for the optimal Hamiltonian by constructing a candidate Hamiltonian based on first principles, experience, or intuition, and then calculating the desired physical quantity while varying the parameters in the Hamiltonian. However, such approaches are not only computationally expensive and less versatile, but also difficult to explore qualitatively new physics. To overcome this, the inverse approach to construct the Hamiltonian from the desired physical properties has been studied using, such as the Bayesian optimization, generative models, and the perturbation theory. However, many challenges still remain, including the computational cost, the generalization performance, and the applicable range.

In this thesis, we develop new methods to solve these problems and demonstrated their efficiencies. The key technique in these methods is automatic differentiation, which can efficiently optimize a large number of parameters. For the problem of the quantum many-body wave functions, we develop new frameworks for fermionic systems. Meanwhile, for the

problem of the inverse approach, we develop a versatile framework to construct a Hamiltonian that exhibits the desired physical properties.

For the problem with the quantum many-body wave functions in fermionic systems, many previous studies have employed the Slater determinant to represent the sign change of the wave function associated with the anticommutation relation for fermions. However, the calculation of the Slater determinant requires a computational cost of $O(N^3)$ when the number of particles is N, which is a bottleneck in these calculation schemes. To circumvent the difficulty, we develop a variational method using neural networks that do not use the Slater determinant. In this method, the sign change associated with the anticommutation relation is explicitly represented by defining the order of the configuration of particles in real space, while the other part of the wave function is approximated by a feed-forward neural network. This enables us to reduce the computational cost to $O(N)$ at the best. Furthermore, we improve the accuracy by using, such as the symmetry of the system, the representative states, and data preprocessing. By applying this method to the Hubbard model on a two-dimensional square lattice, we show that it can achieve higher accuracy than the many-variable variational Monte Carlo method, which is known to be one of the most accurate methods.

We also develop an alternative method for fermionic systems. In this case, we compute the wave function by taking the Slater determinant after deforming the one-body part of the wave function using a neural network. We adopt two types of neural networks: feed-forward and convolutional neural networks. Applying this method to the Hubbard model, we achieve higher accuracy compared to the simple Slater determinant and pair product states.

For the inverse problem, we propose a new framework to automatically construct a Hamiltonian that satisfies desired physical properties. In this framework, a large number of parameters in a Hamiltonian are optimized using automatic differentiation to minimize the objective function. The advantage lies in the use of analytical derivatives derived by automatic differentiation in the optimization, which circumvents training with data and generalization problems associated with, for instance, neural networks. We demonstrate the efficiency of this framework for two properties: the anomalous Hall effect and the photovoltaic effect. We first show that our method can automatically rediscover the Haldane model exhibiting the spontaneous quantum anomalous Hall effect by considering a tight-binding model on a honeycomb lattice. Then, we show the discovery of a new Hamiltonian on a triangular lattice with an anomalous Hall conductivity six times larger than that of the Haldane model. For the photovoltaic effect, we are able to automatically generate a spin-charge coupled Hamiltonian that can produce a photocurrent of about 900 A/m^2. The framework proposed here is applicable to a wide range of systems and physical properties, including first-principles Hamiltonians, strongly correlated electron systems, and interacting bosonic systems.

Throughout this thesis, by applying neural networks and automatic differentiation, we develop new variational methods that provide both high computational accuracy and low computational cost for fermionic systems, and a new framework that automatically designs Hamiltonians exhibiting the physical properties of interest. Since our methods are versatile, they will stimulate further studies in a wide range of applications.