Quantum Computing and Quantum Machine Learning

Master of Science Thesis Project

Dec 1, 2022

Quantum Computing and Machine Learning

Quantum Computing and Machine Learning are two of the most promising approaches for studying complex physical systems where several length and energy scales are involved. Traditional many-particle methods, either quantum mechanical or classical ones, face huge dimensionality problems when applied to studies of systems with many interacting particles. To be able to define properly effective potentials for realistic molecular dynamics simulations of billions or more particles, requires both precise quantum mechanical studies as well as algorithms that allow for parametrizations and simplifications of quantum mechanical results. Quantum Computing offers now an interesting avenue, together with traditional algorithms, for studying complex quantum mechanical systems. Machine Learning on the other hand allows us to parametrize these results in terms of classical interactions. These interactions are in turn suitable for large scale molecular dynamics simulations of complicated systems spanning from subatomic physics to materials science and life science.

Possible Projects

Boltzmann machines, from classical ones to quantum Boltzmann machines (Classical and Quantum Machine Learning). Boltzmann Machines (BMs) offer a powerful framework for modeling probability distributions. These types of neural networks use an undirected graph-structure to encode relevant information. More precisely, the respective information is stored in bias coefficients and connection weights of network nodes, which are typically related to binary spin-systems and grouped into those that determine the output, the visible nodes, and those that act as latent variables, the hidden nodes.

Furthermore, the network structure is linked to an energy function which facilitates the definition of a probability distribution over the possible node configurations by using a concept from statistical mechanics, i.e., Gibbs states. The aim of BM training is to learn a set of weights such that the resulting model approximates a target probability distribution which is implicitly given by training data. This setting can be formulated as discriminative as well as generative learning task. Applications have been studied in a large variety of domains such as the analysis of quantum many-body systems, statistics, biochemistry, social networks, signal processing and finance

BMs are complicated to train in practice because the loss function's derivative requires the evaluation of a normalization factor, the partition function, that is generally difficult to compute. Usually, it is approximated using Markov Chain Monte Carlo methods which may require long runtimes until convergence

Quantum Boltzmann Machines (QBMs) are a natural adaption of BMs to the quantum computing framework. Instead of an energy function with nodes being represented by binary spin values, QBMs define the underlying network using a Hermitian operator, normally a parameterized Hamiltonian, see references [1,2] below.

Here we will focus on classification problems such as the famous MNIST data set which contains handwritten numbers from 0 to 9. This can serve as a starting point. More data sets can be included at a later stage. The next project parallels this but replaces Boltzmann machines with Autoencoders.

Literature:

1. Amin et al., **Quantum Boltzmann Machines**, Physical Review X **8**, 021050 (2018).

2. Zoufal et al., **Variational Quantum Boltzmann Machines**, ArXiv:2006.06004.

3. Maria Schuld and Francesco Petruccione, **Supervised Learning with Quantum Computers**, Springer, 2018.

From Classical Autoenconders to Quantum Autoenconders and classification problems (Classical and Quantum Machine Learning). Classical autoencoders are neural networks that can learn efficient low dimensional representations of data in higher dimensional space. The task of an autoencoder is, given an input x, is to map x to a lower dimensional point y such that x can likely be recovered from y. The structure of the underlying autoencoder network can be chosen to represent the data on a smaller dimension, effectively compressing the input.

Inspired by this idea, we would like to, following references [1,2] below, to introduce Quantum Autoencoders to compress a particular dataset like the famous MNIST data set which contains handwritten numbers from 0 to 9.

Literature:

1. Carlos Bravo-Prieto, **Quantum autoencoders with enhanced data encoding**, see `https://arxiv.org/pdf/2010.06599.pdf`

2. Jonathan Romero et al, **Quantum autoencoders for efficient compression of quantum data**, see `https://arxiv.org/pdf/1612.02806.pdf`

3. Maria Schuld and Francesco Petruccione, **Supervised Learning with Quantum Computers**, Springer, 2018. See `https://www.springer.com/gp/book/9783319964232`

Bayesian phase difference estimation (Quantum-mechanical many-body Physics). Quantum computers can perform full configuration interaction (full-CI) calculations by utilising the quantum phase estimation (QPE) algorithms including Bayesian phase estimation (BPE) and iterative quantum phase estimation (IQPE). In these quantum algorithms, the time evolution of wave functions for atoms and molecules is simulated conditionally with an ancillary qubit as the control, which make implementation to real quantum devices difficult. Also, most of the problems in many-body physics discuss energy differences between two states rather than total energies themselves, and thus direct calculations of energy gaps in for example atoms and molecules are promising for future applications of quantum computers to real quantum mechanical many-body problems. In the race of finding efficient quantum algorithms to solve quantum chemistry problems, we would like to study a Bayesian phase difference estimation (BPDE) algorithm, which is a general algorithm to calculate the difference of two eigenphases of unitary operators in the several cases of the direct calculations of energy gaps between selected many-body states states on quantum computers.

Variational Quantum Eigensolvers (Quantum-mechanical many-body Physics). The specific task here is to implenent and study Quantum Computing algorithms like the Quantum-Phase Estimation algorithm and Variational Quantum Eigensolvers for solving quantum mechanical many-particle problems. Recent scientific articles have shown the reliability of these methods on existing and real quantum computers, see for example references [1-5] below.

Here the focus is first on tailoring a Hamiltonian like the pairing Hamiltonian and/or Anderson Hamiltonian in terms of quantum gates, as done in references [3-5].

Reproducing these results will be the first step of this thesis project. The next step includes adding more complicated terms to the Hamiltonian, like a particle-hole interaction as done in the work of Hjorth-Jensen et al.

The final step is to implement the action of these Hamiltonians on existing quantum computers like Rigetti's Quantum Computer.

The projects can easily be split into several parts and form the basis for collaborations among several students.

Literature:

1. Dumitrescu et al, see `https://arxiv.org/abs/1801.03897`
2. Yuan et al., **Theory of Variational Quantum Simulations**, see `https://arxiv.org/abs/1812.08767`
3. Ovrum and Hjorth-Jensen, see `https://arxiv.org/abs/0705.1928`

4. Stian Bilek, Master of Science Thesis, University of Oslo, 2020, see https://www.duo.uio.no/handle/10852/82489

5. Heine Åbø Olsson, Master of Science Thesis, University of Oslo, 2020, see https://www.duo.uio.no/handle/10852/81259

Analysis of entanglement in quantum computers. The aim of this project is to study various ways of analyzing entanglement theoretically by computing for example the von Neumann entropy of a quantum mechanical many-body system. The systems we are aiming at here are so-called quantum dots systems which are candidates from making quantum gates and circuits. The theoretical results are planned to be linked with experimental interpretations via Quantum state tomography, which is the standard technique for estimating the quantum state of small systems. If possible, this project could be linked with studies of quantum tomography from the SpinQ quantum computer at OsloMet.

Literature:

1. B. P. Lanyon et al, **Efficient tomography of a quantum many-body system**, Nature Physics **13**, 1158 (2017), see https://www.nature.com/articles/nphys4244