Quantum Computing and Quantum Machine Learning
Boltzmann Machines and AutoEncoders

Master of Science thesis project

December 1, 2022

Introduction and overview

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.

Specific tasks and milestones

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. Alternatively, one can study autoencoders only. It is possible to collaborate with other students on the code developments.

From Classical Autoenconders to Quantum Autoenconders and classification problems (Classical and Quantum Machine Learning).

As an alternative to Boltzmann machines, one can implement and study quantum Autoencoders. 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 can alternatively, following references [4-6] below, introduce Quantum Autoencoders to compress a particular dataset like the famous MNIST data set which contains handwritten numbers from 0 to 9.

The specific task here

1. Spring 2023: Start writing a code for classical Boltzmann machines (alternatively autoencoders) and apply these to a classification problem like the MNIST data set. Finalize courses
2. Fall 2023: Extend the program from spring 2023 to quantum Boltzmann machines and/or Quantum variational autoencoders.
3. Spring 2024: Perform studies of various datasets and start wirting and finalizing thesis.

The thesis is expected to be handed in May/June 2024

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.
4. Carlos Bravo-Prieto, **Quantum autoencoders with enhanced data encoding**, see https://arxiv.org/pdf/2010.06599.pdf
5. Khoshaman et al., **Quantum Variational autoencoders**, ArXiv:1802.05779.
6. Jonathan Romero et al, **Quantum autoencoders for efficient compression of quantum data**, see https://arxiv.org/pdf/1612.02806.pdf