Quantum Boltzmann Machines

Master of Science thesis project

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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.

Thesis Project

Boltzmann Machines (BMs) offer a powerful framework for modelling 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

However, 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, a parameterized Hamiltonian

$$H_\theta = \sum_{i=0}^{p-1} \theta_i h_i,$$

with $\theta \in \mathbb{R}^p$ and $h_i = \bigotimes_{j=0}^{n-1} \sigma_{j,i}$ for $\sigma_{j,i} \in I, X, Y, Z$ acting on the j^{th} qubit. The network nodes are hereby characterized by the Pauli matrices $\sigma_{j,i}$.

Specific tasks and milestones. The aim of this thesis is to study the implementation of

The thesis is expected to be handed in May/June 2022.

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