Quantum Machine Learning

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.

Quantum computing is an emerging area of computer science that leverages the principles of quantum mechanics to perform computations beyond the capabilities of classical computers. Unlike classical computers, which use bits to represent data as 0s or 1s, quantum computers use quantum bits, or qubits. Qubits can exist in multiple states simultaneously (superposition) and can be entangled with one another, allowing quantum computers to process vast amounts of information in parallel.

These unique properties enable quantum computers to tackle problems that are currently intractable for classical systems, such as complex simulations in chemistry and physics, optimization problems, and large-scale data analysis.

Quantum machine learning (QML) is an interdisciplinary field that combines quantum computing with machine learning techniques. The goal is to enhance the performance of machine learning algorithms by utilizing quantum computing's capabilities.

In QML, quantum algorithms are developed to process and analyze data more efficiently than classical algorithms. This includes tasks like classification, regression, clustering, and dimensionality reduction. By exploiting quantum phenomena, QML has the potential to accelerate machine learning processes and handle larger datasets more effectively.

Quantum computing and QML hold promise for various applications, including:

1. Drug Discovery: Simulating molecular structures to expedite the development of new medications.

2. Financial Modeling: Optimizing portfolios and detecting fraudulent activities through complex data analysis.

3. Artificial Intelligence: Enhancing machine learning algorithms for faster and more accurate predictions.

As quantum hardware continues to advance, the integration of quantum computing into practical applications is becoming increasingly feasible, opening up for a new era of computational possibilities.

This thesis project deals with the study and implementation of quantum machine learning methods applied to classical machine learning data for supervised learning. The methods we will focus on are

1. Support vector machines and quantum support vector machines
2. Neural networks and quantum neural networks and possibly (if time allows)
3. Classical and quantum Boltzmann machines

The data sets will span both regression and classification problems, with an emphasis on simulating time series of relevance for financial problems. The thesis will be done in close collaboration with Norges Bank Invenstment Management, Simula Research laboratory and the University of Oslo.

Support vector machines

A central model in classical supervised learning is the support vector machine (SVM), which is a max-margin classifier. SVMs are widely used for binary classification and have extensions to regression problems as well. They build on statistical learning theory and are known for finding decision boundaries with maximal margin. In particular, SVMs can perform non-linear classification by employing the kernel trick, which implicitly maps data into a high-dimensional feature space via a kernel function.

A Quantum Support Vector Machine (QSVM) replaces the classical kernel or feature map with a quantum procedure. In QSVM, classical data points $\boldsymbol{x}$ are encoded into quantum states $|\phi(\boldsymbol{x})\rangle$ via a quantum feature map (a parameterized quantum circuit). The inner product (overlap) between two such states serves as a quantum kernel, measuring data similarity in a high-dimensional Hilbert space.

Quantum Neural Networks and Variational Circuits

The Variational Quantum Algorithm (VQA) is a Variational Quantum Circuit (VQC), that is a quantum circuit with tunable parameters and which is trained using a classical optimizer. In practice, a VQC (also called a Parameterized Quantum Circuit (PQC)) is used as a Quantum Neural Network (QNN): data are encoded into quantum states, a parameterized circuit is applied, and measurements yield outputs. For example, it has been shown recently that certain QNNs can exhibit higher effective dimension (and thus capacity to generalize) than comparable classical networks , suggesting a potential quantum advantage.

Boltzmann machines

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

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 reference [1] below.

Specific tasks and milestones. The aim of this thesis is to study the implementation and development of codes for several quantum machine learning methods, including quantum support vector machines, quantum neural networks and possibly Boltzmann machines, and possibly other classical machine learning algorithms, on a quantum computer. The thesis consists of three basic steps:

1. Develop a classical machine code for studies of classification and regression problems.

2. Compare the results from the classical Boltzmann machine with other deep learning methods.

3. Develop an implementation of a quantum Boltzmann machine code to be run on existing quantum computers and classical computers. Compare the performance of the quantum Boltzmann machines with exisiting classical deep learning methods.

The milestones are:

1. Spring 2025: Develop a code for classical Boltzmann machines to be applied to both classification and regression problems. In particular, the latter type of problem can be tailored to solving classical spin problems like the Ising model or quantum mechanical problems.

2. Fall 2025: Develop a code for variational Quantum Boltzmann machines following reference [2] here. Make comparisons with classical deep learning algorithms on selected classification and regression problems.

3. Spring 2026: The final part is to use the variational Quantum Boltzmann machines to study quantum mechanical systems. Finalize thesis.

The thesis is expected to be handed in May/June 2026.

Literature.

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

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

3. Claudio Conti, Quantum Machine Learning (Springer), sections 1.5-1.12 and chapter 2, see `https://link.springer.com/book/10.1007/978-3-031-44226-1`.