Classical Simulation of Quantum Circuits with Restricted Boltzman Machines

Master's Thesis Proposal
by Jannes Stubbeman

Arbeitsgruppe
Quanteninformatik

1 Introduction

Quantum computers have the potential to solve certain computational task exponentially faster than classical computers [11, 17]. Demonstrating *quantum supremacy* [16], that is the moment a physical quantum computer outperforms classical computers on a given task for the first time, is a major step into the direction of realizing large scale quantum computers and currently a very active field of research [3, 14, 2, 5, 1, 4].

Last year, a team of researchers from Google claimed to have reached quantum supremacy with a 53 qubit quantum processor [3]. However, as also quantum processors are not perfect but suffer from decoherent noise, the question persists if classical approximations of quantum computing can still challenge those results [18].

Recently, neural networks have been successfully applied to the classical approximate simulation of quantum systems and quantum computing [7, 13]. Applying them to quantum supremacy experiments therefore might give new insights about the limits of classical simulations of quantum computing and the state of quantum supremacy.

2 Current state of research

Exact classical simulations of quantum systems require up to exponential computational resources [11]. Harnessing the characteristics of quantum physics for computation therefore opens the possibility to build quantum computers which can outperform classical computers on certain computational tasks [17]. The moment when a physical quantum computer outperforms any classical computer on a well defined task for the first time has been coined *quantum supremacy* by John Preskill in 2012 and is currently a very active field of research.

Different proposals for quantum supremacy experiments like Boson Sampling [1], Fourier Transform [10] and Random Circuit Sampling (RCS) [4] have been given and theoretically analyzed. With recent progress in building quantum computers based on superconducting qubits, Random Circuit Sampling became the most promising to be physically realized in the near future [5].

The proposal for RCS is based on the fact that the output distributions of random circuits of specific structures will approximate the Porter-Thomson distribution and are prone to single gate errors. By that they are not only hard to simulate classically but the cross entropy fidelity of the classical simulation and the output of a quantum processor also acts as a benchmark for the fidelity of the quantum device [4]. Complexity theoretic evidence for a worst to average case reduction completes the theory of RCS as a well defined quantum supremacy experiment [5].

Recently, a research team from Google performed RCS on a 53 qubits superconducting quantum processor and claimed to have demonstrated quantum supremacy [3]. Nevertheless, a team from IBM claimed that the classical exact simulations of the random circuits could run within four days rather than the reported 10,000 years by the Google team thus questioning the claim [15].

As quantum processors will not be perfect but suffer from decoherent noise, perfect simulations of the quantum circuits are not even necessary to challenge the quantum supremacy claims. As long as physical quantum computers can not outperform classical approximate simulations in terms of noise, quantum supremacy has not been reached [4]. Indeed, Tensor Network states produce a similar fidelity to the one from Google's quantum processor on the RCS task with overhead only polynomial in the circuits size and depths, thus questioning the claim for quantum supremacy even further [10].

While Tensor Network states are a known classical approximation technique for quantum systems for some time, recently neural networks gained popularity as a new Ansatz for the classical simulation of quantum physics. Carleo applied Restricted Boltzmann Machines (RBM) to learn the wavefunctions of many body quantum systems [7]. Afterwards, Gao could give theoretic proof that while General Boltzmann machines are able to represent quantum states exactly but make the sampling process P# hard, RBMs can approximate any quantum system with a worst case exponential number of hidden units while keeping the sampling runtime efficient [12].

In 2018, Jónsso applied RBMs to the classical simulation of quantum circuits with a gate fidelity of 10^{-3} [13]. This opens the question of which cross entropy fidelities on the RCS experiments can be reached by RBMs and thus how they compare to Tensor Network states and Google's quantum processor.

3 Goals of the thesis

The thesis should study how well the RBM Ansatz from [13] performs on the random circuit sampling experiments. It should give the reader an introduction to quantum computing and Restricted Boltzmann machines including their applications to quantum circuits.

The Random Circuit Sampling task will be justified as suited for quantum supremacy experiments and Google's results should be presented. Own experiments should be conducted for circuit sizes which can still be verified using the Noctua cluster from the University of Paderborn [9].

If feasible, larger supercomputing facilities should be contacted to run experiments on more qubits than possible on the Nocuta cluster.

Additionaly, the netket library [6] should be adapted to include RBM simulations of quantum circuits and be made available to the public as an open source project as part of the thesis.

4 Preliminary outline of the thesis

1. Introduction
2. Definitions and notation
3. Quantum Computing
    a) Qubits
    b) Gates
    c) Quantum Circuits
4. Boltzmann machines
    a) Overview
    b) Supervised Learning
    c) Application to Quantum Comupting
5. Quantum Supremacy
    a) Definition
    b) Random Circuit Sampling
        i. Porter-Thomas distribution
        ii. Cross entropy fidelity
        iii. Average to Worst case reduction
    c) Google's Quantum Supremacy Experiment
    d) Tensor Network States for RCS
6. Experiments
7. Evaluation
8. Outlook

5 Work plan

The following aspects of the thesis have been identified and define the working packages of the thesis.

5.1 Research and Theory

As a preparation of the thesis and a feasibility study, state of the art work has already been studied and understood on a good level of detail. Over the first 1.5 months (considering restricions mentioned below), further details will be clarified, including the proof of worst to average case reduction of random circuits, tensor network states and the fidelity results of the later and Google's quantum processor. New research in the field should be studied and included if applicable and feasible when it becomes published.

5.2 Implementation

In a prestudy, the adaption of the netket library has already been started and prepared to run circuits with the gate set of X, Y, Z, H, $RZ(\theta)$ and $Z(\theta)$ on circuits defined in the QASM language [8]. For the RCS experiments, $sqrtX$ and $sqrtY$ which work similar to the Hadamard gate are still needed. The implementation of these gates including a testing phase is expected to take one more week and should be done next.

5.3 Experiments

First experimets for random ciruit sampling have already been setup and run on noctua to verify the feasibility of the setup. When the implementation of the RBM Ansatz is finished, new experiments should be started, adapet and be run in the background while further undertanding the theoretic backgrounds mentioned above. Running the experiments is expected to take 1.5 months with little manual work. The maintenance of noctua in mid of March has to be considered and will extend the pure time allocated for the experiments by two weeks.

Another two weeks are reserved for the evaluation and discussion of the results with my supervisors.

5.4 Writing

The introductary chapters of the thesis will be written either when time is left during the phase of further understanding of the theoretic background or afterwards. When the experiments finished, the results should be written down. Thus the main writing phase of the thesis should start in 2 months and be finished after another 2 months.

The last weeks shold be reserved for proof reading and fine tuning of the thesis.

5.5 Defense

The defense of the thesis should either happen in the planned seminar of thesis students in the quantum computer science departement either at the end or as soon as the results are available. The latter option will allow to include results of potential discussions into the thesis' evaluation sections.

Another alternative to the students seminar will be the inderdisciplinary quantum networks seminar if free slots are available. The preperation of the defense is considered to take up to one week of work. This buffer is included in the research and proof reading phases.

5.6 Summary

So in summary, the timeline for the thesis will bee:

1. Finish Implementation (1 week)
2. Experiments setup (1 week)
3. *Running Experiments (8 weeks in the background)*
4. Further research and Theory (6 weeks)
5. Evaluation (3 weeks)
6. Writing (6 weeks)
7. Defense (1 week)
8. Proof reading and finishing up (2 weeks)

Date:

Jun. Prof. Dr. Sevag Gharibian	Jannes Stubbeman

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