Application of machine learning in quantum computer science

Summary of doctoral dissertation

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Abstract in English

The presented dissertation is focused on the selection of the parameters characterising the evolution of quantum dynamics to obtain a given operation. We consider two aspects of quantum computing engineering. The first aspect concerns the problem of the quantum control, i.e. finding a sequence of control pulses, which will steer the basic quantum operations to obtain other, more complex operations. Particularly, in this thesis we propose the utilisation of machine learning techniques for finding such control pulses. The second aspect concerns the computation on the Noisy Intermediate Scale Quantum (NISQ) devices. In this dissertation, we analyse the classical-quantum hybrid algorithm – Variational Quantum Eigensolver, which is aimed at finding such parameters of a quantum circuit that will return the desired state. This optimisation algorithm can provide computational benefits, for example, in quantum chemistry.

The results presented in this dissertation can be summarized by two hypotheses.

1. Machine learning techniques can provide robust methods for generating quantum control pulses for arbitrary unitary operations.

2. Periodic structure of the optimisation landscape can be utilised to accelerate the optimisation procedure in variational quantum eigensolver approach.

The thesis consists of six chapters. The first chapter provides an introduction and motivation of this dissertation. In the second chapter, basic concepts of quantum information theory and machine learning methods utilised in the thesis are introduced.

In the third chapter, we study the functional relationship between quantum control pulses in the idealised case and the pulses in the presence of an undesired drift. We show that a class of artificial neural networks called LSTM is capable of modelling this functional relationship with high efficiency. Hence, such networks can provide the correction scheme required to counterbalance the effect of the drift. Our solution can be used to study the mapping from quantum control pulses to system dynamics and analysing its behaviour with respect to the local variations in the control profile.

In chapter 4, we extend the results related to the application of LSTM network. To achieve this, we analyse the properties of the network constructing such approximation. Our main goal is to study the flexibility of the data representation in the context of the selected quantum control task. We consider two alternative machine learning methods based on a geometrical and time-series character of data, respectively. We demonstrate that the utilisation of the geometrical

structure of control pulses is sufficient for achieving high-fidelity of the implemented evolution. We also demonstrate that recurrent neural networks, unlike geometrical methods, can be used to generate control pulses for the systems with variable strength of the disturbance. The presented results suggest that there are some types of non-trivial quantum control tasks for which simple geometrical data representation and processing is competitive to more sophisticated methods.

In chapter 5, we analyse the properties of the cost function of the VQE problem and utilise that knowledge for the construction of a new, faster algorithm. Next, we propose an efficient method for simultaneously learning both the structure and parameter values of quantum circuits with only a small computational overhead. Shallow circuits trained using structure learning perform significantly better than the circuits trained using parameter updates alone, making this method particularly suitable for use in noisy intermediate-scale quantum computers. We demonstrate a method for training a variational quantum eigensolver, which is suitable for applications in quantum chemistry. In particular, we use our methods for finding the ground states of lithium hydride and the Heisenberg model in simulation, and for finding the ground state of hydrogen gas in the IBM Melbourne quantum computer.

Chapter 6 contains the conclusions of the dissertation and summarises the results of the presented research. The, consideration of LSTM as an approximation of correction of control pulses and the proposition of new algorithms outperforming optimisation of VQE problems both support the presented hypotheses.

Streszczenie w języku polskim

Niniejsza rozprawa skupia się na doborze parametrów charakteryzujących ewolucję dynamiki kwantowej do uzyskania zadanej operacji. Rozważamy dwa aspekty inżynierii obliczeń kwantowych. Pierwszy aspekt dotyczy problemu kontroli kwantowej, tj. znalezienia sekwencji impulsów kontrolnych, które sterują podstawowymi operacjami kwantowymi w celu uzyskania innych, bardziej złożonych operacji. W szczególności w tej pracy proponujemy wykorzystanie technik uczenia maszynowego do znajdowania takich impulsów kontrolnych. Drugi aspekt dotyczy obliczeń na urządzeniach kwantowych Noisy Intermediate Scale (NISQ). W niniejszej rozprawie analizujemy hybrydowy klasyczno-kwantowy algorytm – Variational Quantum Eigensolver (VQE) – który ma na celu znalezienie takich parametrów obwodu kwantowego, które zwrócą żądany stan. Pokazujemy, że zaproponowany algorytm optymalizacji może zapewnić korzyści obliczeniowe, na przykład w chemii kwantowej. Wyniki przedstawione w tej rozprawie można streścić w dwóch hipotezach.

1. Techniki uczenia maszynowego mogą zapewnić wydajne metody generowania kwantowych impulsów kontrolnych dla dowolnych operacji unitarnych.

2. Okresowa struktura funkcji celu optymalizacji może być wykorzystana do przyspieszenia procedury optymalizacji w algorytmie VQE.

Praca składa się z sześciu rozdziałów. Pierwszy rozdział zawiera wprowadzenie i motywację dla prowadzonych badań. W drugim rozdziale przedstawiono podstawowe pojęcia teorii informacji kwantowej oraz metod uczenia maszynowego, które są wykorzystane w dalszych rozdziałach dysertacji.

W trzecim rozdziale badamy związek między impulsami kontroli kwantowej w przypadku idealnym a pulsami w obecności niepożądanego dryftu. Pokazujemy, że rekurencyjne sieci neuronowe, a konkretnie klasa sieci Long Short-Term Memory (LSTM), jest w stanie modelować funkcję opisująca ten związek z wysoką wydajnością. Dlatego takie sieci mogą zapewniać schemat korekcji wymagany do zrównoważenia efektu niepożądanego dryftu. Nasze rozwiązanie może być wykorzystane do badania mapowania kwantowych impulsów kontrolnych w dynamikę systemu i analizy jego zachowania w odniesieniu do lokalnych zmian profilu kontroli.

W rozdziale 4 rozszerzamy wyniki związane z zastosowaniem sieci LSTM. Aby to osiągnąć, analizujemy właściwości sieci konstruującej przybliżenie odwzorowania między impulsami kontroli. Naszym głównym celem jest zbadanie elastyczności reprezentacji danych w kontekście wybranych

zadań kontroli kwantowej. Rozważamy dwie alternatywne metody uczenia maszynowego oparte odpowiednio na danych geometrycznych i szeregach czasowych. Pokazujemy, że wykorzystanie struktury geometrycznej impulsów sterujących jest wystarczające do osiągnięcia wysokiej wierności zaimplementowanej ewolucji. Wykazujemy również, że rekurencyjne sieci neuronowe, w przeciwieństwie do metod geometrycznych, mogą być wykorzystywane do generowania impulsów sterujących dla układów o zmiennej sile zakłócenia. Przedstawione wyniki sugerują, że istnieją pewne rodzaje nietrywialnych zadań kontroli kwantowej, dla których proste reprezentowanie i przetwarzanie danych geometrycznych jest konkurencyjne w stosunku do bardziej wyrafinowanych metod.

W rozdziale 5 analizujemy właściwości funkcji kosztu problemu VQE i wykorzystujemy tę wiedzę do budowy nowego, szybszego algorytmu optymalizacji. Następnie proponujemy wydajną metodę jednoczesnego uczenia się zarówno struktury, jak i wartości parametrów obwodów kwantowych przy niewielkim obciążeniu obliczeniowym. Płytkie obwody wyćwiczone przy użyciu uczenia struktury działają znacznie lepiej niż obwody wyuczone przy użyciu samych aktualizacji parametrów. Dzięki temu ta metoda jest szczególnie odpowiednia do stosowania w zaszumionych komputerach kwantowych. Pokazujemy,że zaproponowana metoda optymalizacji algorytmu VQE, jest odpowiedni do zastosowań w chemii kwantowej. W szczególności używamy naszych metod do znajdowania stanów podstawowych wodorku litu i modelu Heisenberga w symulacji oraz do znajdowania stanu podstawowego gazu wodorowego na komputerze kwantowym IBM Melbourne.

Rozdział 6 zawiera wnioski z rozprawy i podsumowuje wyniki przedstawionych badań. Rozważenie LSTM jako aproksymacji korekcji impulsów sterujących oraz propozycja nowych algorytmów przewyższających optymalizację problemów VQE popierają przedstawione hipotezy.

List of publications

Published work

1. Mateusz Ostaszewski, Przemysław Sadowski, and Piotr Gawron. *Quantum image classification using principal component analysis*, Theoretical and Applied Informatics 27.1 (2015): 1–12. arXiv:1504.00580

2. Przemysław Sadowski, Jarosław Adam Miszczak, and Mateusz Ostaszewski. *Lively quantum walks on cycles*, Journal of Physics A: Mathematical and Theoretical 49.37 (2016): 375302. arXiv:1512.02802

3. Krzysztof Domino, Adam Glos, and Mateusz Ostaszewski. *Superdiffusive quantum stochastic walk definable on arbitrary directed graph*, Quantum Information & Computation 17, 11–12 (2017): 973-986. arXiv:1701.04624

4. Adam Glos, Jarosław Adam Miszczak, and Mateusz Ostaszewski. *Limiting properties of stochastic quantum walks on directed graphs*, Journal of Physics A: Mathematical and Theoretical 51.3 (2017): 035304. arXiv:1703.01792

5. Krzysztof Domino, Adam Glos, Mateusz Ostaszewski, Łukasz Pawela, and Przemysław Sadowski, *Properties of quantum walks from the asymptotic scaling exponent*, Quantum Info. Comput. 18, 3–4 (2018), 181–197. arXiv:1611.01349

6. Adam Glos, Jarosław Adam Miszczak, and Mateusz Ostaszewski. *QSWalk.jl: Julia package for quantum stochastic walks analysis*, Computer Physics Communications 235 (2019): 414–421. arXiv:1801.01294

7. **Mateusz Ostaszewski, Jarosław Adam Miszczak, Leonardo Banchi, and Przemysław Sadowski, *Approximation of quantum control correction scheme using deep neural networks*, Quantum Information Processing, 18(5), (2019) 126. arXiv:1803.05193**

8. Edward Grant, Leonard Wossnig, Mateusz Ostaszewski, and Marcello Benedetti, *An*

initialization strategy for addressing barren plateaus in parametrized quantum circuits, Quantum, 3, (2019) 214. arXiv:1903.05076

Preprints

1. **Mateusz Ostaszewski, Edward Grant, and Marcello Benedetti. *Quantum circuit structure learning*, (2019). arXiv:1905.09692**

2. **Mateusz Ostaszewski, Jarosław Adam Miszczak, and Przemysław Sadowski. *Geometrical versus time-series representation of data in learning quantum control*, (2018). arXiv:1803.05169**

3. Wojciech Masarczyk, Przemysław Głomb, Bartosz Grabowski, Mateusz Ostaszewski, *Effective transfer learning for hyperspectral image classification with deep convolutional neural networks*, (2019). arXiv:1909.05507

Publications related to the dissertation are highlighted in **bold font**.

Extended summary

In the recent decade the idea of quantum computing becomes reality. Companies like IBM[1], Rigetti[2], and D-Wave[3] have their own quantum computers, which are available for general access. Nowadays, everyone is able to make simple computations on these devices. Therefore, there is a significant need for the development of the algorithmic solutions which can enable the best utilization of provided computational platforms.

The potential resulting from quantum technology has been noticed by the European Union, which announce a Quantum Technologies Flagship programme focused on the utilization of this potential [1, 2, 3]. The fact that this technology has not only a scientific potential but also a commercial aptitude can be concluded from the significant interest of software industry. This includes numerous arising start-ups oriented on this technology, like Xandau[4], Rahko[5], and Cambridge Quantum Computing[6], as well as the established players, including Microsoft, Amazon and Google.

The core motivation behind the development of the theory, as well as the hardware, required for computation, is to perform algorithms. In the case of quantum computation, the algorithms are expressed in the form of a quantum evolution. Therefore, in order to execute quantum algorithms on quantum hardware, one needs to tailor the form of the evolution. The general idea of this dissertation is to focus on the selection of the parameters describing the quantum evolution. For this purpose, we will consider two aspects of the creation of quantum operations – quantum control and quantum circuits.

The main goal of quantum informatics is the utilization of a system working according to the rules of quantum mechanics for computation. Achieving this aim requires mastering the

[1] `https://www.ibm.com/quantum-computing/`
[2] `https://www.rigetti.com/`
[3] `https://www.dwavesys.com/`
[4] `https://www.xanadu.ai/`
[5] `https://rahko.ai/`
[6] `https://cambridgequantum.com/`

methods of quantum control [4]. The purpose of this area of quantum engineering is to find such sequences of control pulses that will control the quantum apparatus, and enable the realization of a given state transformation. Research in this field is crucial for many components of quantum technologies, such as high fidelity gates for universal quantum computation or quantum metrology.

Recently, significant research effort has been invested in the application of machine learning methods in quantum information processing [5, 6]. In particular, the optimisation techniques borrowed from machine learning have been used to optimise the dynamics of quantum systems [7], either for quantum control [8, 9] and simulation [10], or for implementing quantum gates with suitable time-independent Hamiltonians [11]. These techniques also include quantum control techniques from dynamic optimization [12] and reinforcement learning [13, 14]. In the presence of noise, neural networks offer tools for optimising dynamical decoupling which can be seen as a quantum control correction scheme as considered by us, in a special case of the target operation being identity [15]. On the level of gate decomposition, neural networks have also been applied to the problem of decomposing arbitrary operations as a sequence of elementary gate sets [16, 17].

In this thesis, we analyse a method, based on an artificial neural network (ANN) to study the correction scheme between control pulses obtained in the ideal case and those obtained when the system is subjected to undesired dynamics. We demonstrate that the utilised network has high efficiency and can be used to the analysis of the properties of the model. Moreover, we scrutinise this approach in the context of classical machine learning methods.

The ideas introduced above will be focused around the **Hypothesis 1**

> *Machine learning techniques can provide robust methods for generating quantum control pulses for arbitrary unitary operations.*

Another aspect of quantum computation considered in this hypothesis will focus on the Noisy Intermediate Scale Quantum (NISQ) technology. To put it briefly, this term, introduced by the physicist John Preskill in late 2017, concerns the utilization of quantum devices which are available right now, provided among others, by the companies mentioned at the beginning of this chapter. The accuracy of the computations preformed on these machines is not perfect. This is due to the fact that each operation is fraught with noise. However, the number of available qubits is increasing, and according to the latest developments [18], right now it is sufficient to reveal the superiority of quantum devices over classical ones in some computational aspects.

This supremacy is often connected with a fact that a quantum operation, which can be executed naturally on a quantum device, is challenging to perform on a classical computer. The

Variational Quantum Eigensolver (VQE) algorithm is a good example. It is a classical/quantum hybrid algorithm which can be used to find the minimal eigenvalue of some large hermitian matrix M. The core idea is to use some parametrization of vector $|\psi(\boldsymbol{\theta})\rangle$, where $\boldsymbol{\theta}$ are the parameters, and change these parameters to minimize the objective expressed as overlap $\langle\psi(\boldsymbol{\theta})|M|\psi(\boldsymbol{\theta})\rangle$. The preparation of such vector, and obtaining this overlap, can be naturally performed on a quantum device. The classical part of this algorithm is based on tuning the parameters $\boldsymbol{\theta}$, which are applied on a quantum computer.

The real application of the problem which can be solved by VQE arises from quantum chemistry [19, 20], where hermitian matrix M represents the Hamiltonian of chemical particles. Moreover, the VQE procedure has a lot in common with a more general the concept of Quantum Neural Networks (QNN) [21, 22]. Without going into details, we would like to notice that the optimization methods developed for VQE can be applied, or at least can be useful for the optimization methods in QNN. The context of research will be focused on the **Hypothesis 2**

> *Periodic structure of the optimization landscape can be utilized to accelerate the optimization procedure in the variational quantum eigensolver approach.*

We will analyse the behaviour of the objective function $\langle\psi(\boldsymbol{\theta})|M|\psi(\boldsymbol{\theta})\rangle$ with respect to some class of parametrization of the vector $|\psi(\boldsymbol{\theta})\rangle$, and prove its periodical behaviour relative to individual parameters $\theta \in \boldsymbol{\theta}$. Based on this knowledge, we will propose two algorithms, based on the coordinate minimisation procedure [23]. Finally, we will report the efficiency of these algorithms in comparison to other optimisation algorithms and show the results of the experiments performed on the IBM Melbourne quantum computer for quantum chemistry problem of hydrogen gas.

The remaining part of this dissertation consists of five chapters. The second chapter includes mathematical introduction to quantum information theory and an overview of machine learning concepts. We introduced formalism of quantum mechanics, elements of quantum computation, and quantum control. Concerning machine learning we discuss clusterization and classification based on geometrical representation of the data, and artificial neural network concept and the LSTM architecture.

The third and fourth chapters are focused on Hypothesis 1. In the third chapter, we consider the scheme of correction of idealised quantum control pulses into the pulses steering the quantum system with undesired drift acting with force γ. As idealised control pulses, we will understand the pulses which steer the system without any undesired dynamics. In Chapter 3, we propose the utilisation of recurrent neural networks – LSTM [24] – as an approximation of such a correction

scheme. As a part of analysing this idea, we examine the performance of such an approximation, and demonstrate the utilisation of this approximation. The results of Chapter 3 are based on the article:

- Ostaszewski, M., J.A. Miszczak, L. Banchi, P. Sadowski, *Approximation of quantum control correction scheme using deep neural networks*, Quantum Information Processing, 18(5), (2019) 126.

In Chapter 4, we extend the idea of the previous chapter, and compare the utilisation of LSTM networks with the utilisation of standard geometrical algorithms – kNN and k-means algorithms. One of the differences between these two approaches is a treatment of the data. The LSTM takes into account the time-series character of the data. On the other hand, geometrical methods treat data as points in space without giving any meaning to the dimensions of the space. These two methods will be compared in two aspects, the efficiency of correction, and the ability of generalisation with respect to new values of undesired drift powers γ. The efficiency will be measured by examining how accurately corrected control pulses are steering a quantum system. The generalisation will be examined in the following scenario: We train the considered approaches in the cases where the undesired drift power will be from some fixed set $\gamma \in A$. The test procedure includes the cases where the quantum system has an undesired drift with new values $\gamma' \notin A$. The results of Chapter 4 are based on the article:

- M. Ostaszewski, J.A. Miszczak, P. Sadowski, *Geometrical versus time-series representation of data in learning quantum control*, (2018). arXiv:1803.05169

In Chapter 5, we will consider Hypothesis 2. We will formulate the optimisation problem of Variational Quantum Eigensolver (VQE). Next, we will demonstrate the theoretical considerations about the periodical behaviour of the objective function. Based on this observation, we will propose two algorithms `Rotosolve` and `Rotoselect`. To put if briefly, the difference between these algorithms is that the `Rotosolve` is just an optimisation algorithm that efficiently minimises the objective function, while the `Rotoselect` expands the range of action of the `Rotosolve`, and also changes the structure of the parametrisation template. Therefore, this second algorithm is adjusting the parametrisation to the objective function. The results of Chapter 5 are based on the article:

- M. Ostaszewski, E. Grant, M. Benedetti, *Quantum circuit structure learning*, (2019). arXiv:1905.09692

The last chapter concludes the presented results of this dissertation. We sum up the results obtained in the previous Sections. Moreover, we indicate the connections between the introduced hypotheses and the performed experiments and the conclusions resulting from them.

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