Methods of validation of modern quantum architectures

Summary of doctoral dissertation

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English abstract

In the last decade the idea of quantum computing has become a reality. Noisy Intermediate-Scale Quantum (NISQ) devices are storming the market, with a wide selection of devices based on different architectures and accompanying software solutions. Among hardware providers offering public access to their gate-based devices, one could mention Rigetti, IBM, IonQ or Xanadu. Other vendors offer devices operating in different paradigms. Especially, one could mention D-Wave and their quantum annealers. Most vendors provide their own software stack and application programming interface for accessing their devices. Nowadays, everyone can make simple computations on these devices.

It is well known that NISQ devices have limitations. For that, a natural question arises: what extent can those devices perform meaningful computations? To answer this question, one has to devise a methodology for validating them. As a validation of quantum architectures, we refer to testing the correctness of their functioning and ability to perform the tasks they were designed for. Due to the numerous errors, there is therefore a significant need to develop validation processes that allow for the best imaging of the accuracy and precision of the operation of computing platforms.

This dissertation aims to investigate new validation methods for modern gate model-inspired NISQ devices. In the work, we analyze both theoretical and engineering aspects. We focus on the construction of validation methods and their adaptation to available NISQ quantum architectures. We would like to show that the created theoretical models will also allow obtaining new concepts of benchmarking modern quantum systems.

Initially, we consider validation method based on the problem of learning von Neumann measurements known also as the storage and retrieval (SAR). In general approach of SAR, we want to approximate an unknown von Neumann measurement which we were able to perform N times experimentally. This strategy consists of preparing some initial state, applying the unknown measurement N times, and finally, a retrieval operation that returns an approximation of the unknown measurement. The scheme is optimal when it achieves the highest possible fidelity of the approximation. Our main goal is to estimate the asymptotic behaviour of the maximum value of the average fidelity function for SAR of von Neumann measurements and determine possibly the best approximation of the optimal scheme. The primary tools used in SAR are quantum combs. In addition to quantum combs, we will also use the quantum causal structures theory to show an advantage of this approach.

Next, we introduce a validation method based on the scheme of discrimination of von Neumann measurements. To illustrate the scheme of discrimination, let us consider an experiment in which we use an unknown measurement device. The only information we have is that it performs one of two measurements. Our goal is to indicate, with as high probability as possible, which of the measurements was used during the experiment. Next, we would like to construct an optimal discrimination strategy, for which we get the maximum probability of correct discrimination.

Finally, we consider the task of certification between von Neumann measurements. Here, we are interested in a binary certification scheme in which the null and alternative hypotheses are single-element sets. The goal of certification is to minimize the probability of the type II error given some fixed statistical significance. Next, similar to the problem of discrimination, we would like to construct an optimal certification strategy, which

minimizes such a probability.

As an engineering aspect of the dissertation, we introduce PyQBench – an innovative open-source framework for benchmarking gate-based quantum computers. PyQBench benchmarks NISQ devices by verifying their capability based on the discrimination and certification schemes. PyQBench offers a simplified, ready-to-use, command line interface (CLI) for running benchmarks using a predefined parametrized Fourier family of measurements. For more advanced scenarios, PyQBench offers a way of employing user-defined measurements instead of predefined ones. We will show that the proposed models and obtained results have led to a new aspect of benchmarking NISQ devices.

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

1. The usage of the quantum causal structure theory provides more efficient methods for the problem of learning von Neumann measurements.

2. The problem of distinguishing and certifying von Neumann measurements can be used to create a new aspect of benchmarking for modern gate model-inspired NISQ devices.

The work consists of nine chapters and three appendices. The first chapter presents an introduction to quantum information theory and the motivation for the research. The next two chapters recall the necessary mathematical framework and basic concepts used in quantum information theory. The rest of the dissertation was based on three published articles and one preprint.

The first paper, described in Chapter 4, concerns the von Neumann measurement learning scheme. Next, in Chapter 5, we explore the possibility of using the quantum causal structure theory in the task of von Neumann measurement learning. In Chapter 6, we present the problem of distinguishing von Neumann measurements, whereas in Chapter 7 we introduce PyQBench, an innovative open-source framework for benchmarking gate-based quantum computers based on the scheme of discrimination. In Chapter 8, focus on a validation scheme by certifying two von Neumann measurements and next we extend PyQBench to benchmarking using this approach. Finally, Chapter 9 contains the conclusions of the dissertation and summarizes the results of the presented research.

1 List of publications

Publications relevant to the dissertation are highlighted bold.

Published work

1. Przemysław Sadowski, Łukasz Pawela, Paulina Lewandowska, and Ryszard Kukulski *Quantum walks on hypergraphs*, International Journal of Theoretical Physics, vol. 58, (2019). arXiv: `https://arxiv.org/abs/1809.04521`

2. Paulina Lewandowska, Ryszard Kukulski, and Łukasz Pawela, *Optimal representation of quantum channels*, Computational Science - ICCS 2020, (2020). arXiv: `https://arxiv.org/abs/2002.05507`

3. Ryszard Kukulski, Paulina Lewandowska, and Łukasz Pawela, *Perturbation of the numerical range of unitary matrices*, Computational Science - ICCS 2020, (2020). arXiv: `https://arxiv.org/abs/2002.05553`

4. **Paulina Lewandowska, Aleksandra Krawiec, Ryszard Kukulski, Łukasz Pawela, and Zbigniew Puchała, *On the optimal certification of von Neumann measurements*, Scientific Reports, vol. 11, (2021). arXiv:** `https://arxiv.org/abs/2009.06776`

5. **Paulina Lewandowska, Ryszard Kukulski, Łukasz Pawela, and Zbigniew Puchała, *Storage and retrieval of von Neumann measurements*, Physical Review A, vol. 106, issue 5, (2022). arXiv:** `https://arxiv.org/abs/2204.03029`

6. Paulina Lewandowska, Łukasz Pawela, and Zbigniew Puchała, *Strategies for single-shot discrimination of process matrices*, Scientific Reports, vol. 13, (2023). arXiv: `https://arxiv.org/abs/2210.14575`

Preprints

1. **Konrad Jałowiecki, Paulina Lewandowska and Łukasz Pawela, *PyQBench: a Python library for benchmarking gate-based quantum computers*, (2023). arXiv:** `https://arxiv.org/abs/2304.00045`

2 Extended summary

In the last decade the idea of quantum computing has become a reality. Noisy Intermediate-Scale Quantum (NISQ) [1] devices are storming the market with a wide selection of devices based on different architectures and accompanying software solutions. Among hardware providers offering public access to their gate-based devices, one could mention IBM [2], Rigetti [3], Oxford Quantum Group [4], IonQ [5], or Xanadu [6]. Other vendors offer devices operating in different paradigms. Notably, one could mention D-Wave [7] and their quantum annealers, or QuEra devices [8] based on neural atoms. Most vendors provide their own software stack and application programming interface for accessing their devices. To name a few, Rigetti's computers are available through their Forest SDK [9] and PyQuil library [10] and IBM Q [2] computers can be accessed through Qiskit [11] or IBM Quantum Experience web interface [12]. Some cloud services, like Amazon Braket [13], offer access to several quantum devices under an unified API. On top of that, several libraries and frameworks can integrate with different hardware vendors. Examples of such frameworks include IBM Q's Qiskit or Zapata Computing's Orquestra [14]. Nowadays, everyone can make simple computations on these devices.

It is well known that NISQ devices have limitations [15]. For that, a natural question arises: what extent can those devices perform meaningful computations? To answer this question, one has to devise a methodology for validating them. As a validation of quantum architectures, we refer to testing the correctness of their functioning and ability to perform the tasks they were designed for. The validation task has been highlighted as a significant challenge to scalable quantum computing technology. Due to the numerous errors, there is therefore a significant need to develop validation processes that allow for the best imaging of the accuracy and precision of the operation of computing platforms. The search for practical and reliable tools for the validation of quantum architecture has attracted a lot of attention in recent years [16–20].

There are many approaches to testing NISQ devices. The method of choice may depend on, for example, the amount and type of information we have or want to obtain, the system size or structure, the computational resources, or obtained noise. Many times, the complexity of a protocol can be traded for the amount of information about the validated device.

The most powerful but at the same time most resources demanded validating techniques are the full quantum tomography [21, 22] and the gateset tomography [23, 24]. The first idea is to obtain knowledge of the entire quantum state or transformation by performing sufficiently many measurements. The second one, whereas, instead of focusing on a single component of the experiment, characterizes an entire set of quantum gates used during the experiment. However, the tomography process is excessively costly in the size of the quantum system. Fortunately, many quantum states and operations used in realistic experiments have strict structures. For example, quantum states are often close to being pure or having a fixed low rank. For such cases, one may use compressed sensing tomography [25]. Another approach is tensor network tomography which gives excellent approximation under the assumption reconstructing of a quantum state by product operators [26, 27].

In contrast to the methods mentioned above, fidelity estimation aims merely at determining the distance between the actual quantum state or operation and the theoretical one. While fidelity estimation yields much less information than full tomography, one saves tremendously in measurement, sample complexity and resources. The initial research estimated the fidelity of an imperfect preparation of certain pure quantum states [28]. This protocol is extended to optimally estimating the fidelity of quantum channels [29] and, as we see in the dissertation, von Neumann measurements [30].

Another quantity used for validating NISQ devices is certification of quantum operations [31,32], which can be viewed as the extension of quantum hypotheses testing. The standard certification scheme assumes that we have two hypotheses – the null and the alternative and there is possibly one of two outcomes: either we accept or reject the null hypothesis. Like in classical hypothesis testing, here, we also have two possible types of errors. The type I error happens if we reject the null hypothesis when it is actually true, whereas the type II error happens if we accept the null hypothesis when we should have rejected it. The main aim of certification is finding the optimal strategy that minimizes one type of error when the other is fixed.

Certification of quantum objects is closely related to the other well-known method of validation, which is the problem of discrimination of those objects [33]. Intuitively, in the discrimination problem we are given one of two quantum objects sampled according to a given a priori probability distribution. Hence, the probability of making an error in the discrimination task is equal to the average of the type I and type II errors over the assumed probability distribution. Therefore, the discrimination problem can be seen as symmetric distinguishability instead of certification, which is asymmetric. In other words, the main difference between both approaches is that the main task of discrimination is the minimization over the average of both types of possible errors, while the certification concerns the minimization over one type of error when the bound of the other one is assumed. Both symmetric and asymmetric discrimination schemes have been developed for quantum states [34], unitary channels [32, 34] and general quantum channels [35], SIC POVM [36], or unknown quantum measurements [37]. This dissertation will extend these issues to the discrimination task of the von Neumann measurements [38, 39].

A still weaker method merely aims at the concept of randomized benchmarking [40]. In this approach, one sample circuits to be run from some predefined set of gates (e.g. from the Clifford group [41], or the random unitary gates [42]) and tests how much the output distribution obtained from the device running these circuits differs from the ideal one. It is also common to concatenate randomly chosen circuits with their inverses, which should yield the identity circuit, and run those concatenated circuits on the device.

It is also worth mention about validation methods characterizing an arbitrary quantum system based only on its classical input-output correlations. Examples include the cross-entropy benchmarking [43], or self-testing [44]. Building upon such notions of fidelities, specific quality measures have been introduced in different contexts. Examples include the cross-entropy function [45] strictly related to the maximum likelihood. Nevertheless, the work [46] has given birth to the field of self-testing. This work set the terminology and formalism which was adopted by later works. In particular, a self-testing protocol can be seen as a device-independent validation of a quantum system, assuming that the system can be prepared many times in an independent, identically distributed manner.

In the scope of the dissertation, we aim to investigate new validation methods for modern gate model-inspired NISQ devices. In the work, we analyze both theoretical and engineering aspects. We would like to show that the created theoretical models will also allow obtaining new concepts of benchmarking modern quantum systems. For this purpose, initially, we will focus on constraining validation methods. Secondly, we will implement the algorithms on current available NISQ devices.

The first method concerns the quantum learning of von Neumann measurements. This approach is also known in the literature as storage and retrieval (SAR). In the general approach of SAR, we want to approximate an unknown von Neumann measurement which we were able to perform N times experimentally. This strategy is usually divided into two parts. The first one consists of preparing some initial quantum state and applying the unknown measurement N times, which allows us to store this operation for later use. The second one, whereas, consists a retrieval operation that returns an approximation of the unknown measurement. The scheme is optimal when it achieves the highest possible fidelity of the approximation. Our main goal is to estimate the asymptotic behaviour of the maximum value of the average fidelity function for SAR of von Neumann measurements and determine possibly the best approximation of the optimal scheme.

The main tools used in the dissertation are quantum networks, also known as quantum combs. Moreover, we will also use the quantum causal structures theory – a completely new approach in quantum information theory. We explore the possibility of using the quantum causal structure theory in the task of storage and retrieval of von Neumann measurements. For this purpose, we describe the part responsible for storing the quantum operation with a process matrix and then calculate the value of the fidelity function. This idea will be focused around **Hypothesis 1**.

The usage of quantum causal structure theory improves the value of fidelity function, providing a more efficient method of the storage and retrieval of von Neumann *measurements.*

Next, we introduce a validation method based on the scheme of discrimination of von Neumann measurements. We have calculated the maximum value of the probability of correct discrimination between the parameterized family of qubit measurements in the Fourier basis and computational basis. Moreover, we construct the optimal strategy, which maximizes the probability for this case. Next, we consider the certification task between two von Neumann measurements. Here, we are interested in a two-point (binary) certification scheme in which the null and alternative hypotheses are single-element sets. The goal is to minimize the probability of the type II error given some fixed statistical significance. Again, for the parameterized family of qubit measurements in the Fourier basis we calculate the exact value of the probability of the type II error and we create the optimal certification scheme.

As an engineering aspect of the dissertation, we introduce PyQBench – an innovative open-source framework for benchmarking gate-based quantum computers. PyQBench benchmarks NISQ devices by verifying their capability based on the discrimination and certification schemes. PyQBench offers a simplified, ready-to-use, command line interface (CLI) for running benchmarks using a predefined parametrized Fourier family of measurements. For more advanced scenarios, PyQBench offers a way of employing user-defined measurements instead of predefined ones. We will show that the proposed models and obtained results have led to a new aspect of benchmarking NISQ devices. Due to that, we formulate the second **Hypothesis 2**.

Validating techniques based on discrimination and certification of von Neumann measurements provide efficient methods for benchmarking current gate model-inspired NISQ devices.

The work consists of nine chapters and three appendices. The first Chapter presents an introduction to quantum information theory and the motivation for the research. Chapter 2 presents necessary mathematical framework. Chapter 3 devotes the basic concepts used in quantum information theory. The rest of the dissertation was based on three published articles and one preprint.

The first paper [30], described in Chapter 4, concerns the storage and retrieval of von Neumann measurements. In Chapter 5, we explore the possibility of using the quantum causal structure theory in the task of von Neumann measurement learning. In Chapter 6, we focus on the problem of discrimination von Neumann measurements. Chapter 7 introduces PyQBench [47], an innovative open-source framework for benchmarking gate-based quantum computers based on the discrimination scheme. Next, the work [48], presented in Chapter 8 focuses on another validation scheme based on the certification of von Neumann measurements. Due to obtained results, we furthermore extend PyQBench to benchmarks using certification scheme. Chapter 9 contains the conclusions of the dissertation and summarizes the results of the presented research.

In conclusion, three main topics have been explored in this dissertation: learning, discrimination and certification of von Neumann measurements. Results presented in Chapters 4-9 show that proper selection and adaptation of validating models allow for the practical engineering of current gate model-inspired NISQ devices which support the presented hypotheses.

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