Algorithm selection and configuration for Noisy Intermediate Scale Quantum methods for industrial applications

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Chapter 1

Introduction

1.1 Background

The field of quantum computing has gotten increased attention as a different paradigm than classical computing for solving complex problems [142]. Quantum computers are defined as computers relying on principles from quantum mechanics to perform computation, and many implementations are being proposed. However, currently available quantum computers are very unstable, noisy, and hard to scale up. Hence, quantum algorithms that could run on current noisy hardware, in the so-called noisy intermediate-scale quantum (NISQ) era [156], which are also relevant for industrial applications, are the subject of many research topics.

The quantum community has come up with a large number of proposals for how relevant problems could be tackled with such devices. One of the main directions is the usage of hybrid quantum-classical schemes [37, 55, 40, 18, 134, 57]. A part of the computation is then carried out on a quantum computer and the classical device handles the rest. Such hybrid algorithms are most often employed as *heuristics*, i.e. approaches to solving a problem of interest whose proposed solution is not guaranteed to be optimal. Thus it is not clear whether they genuinely outperform current classical state-of-the-art algorithms in relevant domains of application. Additionally, such hybrid algorithms come with many internal components (i.e. the classical optimization algorithm used, many hyperparameters of a quantum neural network, etc.) or can be extended with new ones, which can affect their performances. Hence, they should be chosen well for achieving optimal performance.

Consequently, we will face the issues of *algorithm selection and configuration* [89].

Given many instances of a problem, the algorithm selection problem concerns selecting the best-performing algorithm for a given instance. The configuration problem is about finding how to set well the internal component of an algorithm in general. For instance, finding the best-performing classical optimization algorithm for a hybrid quantum-classical algorithm is a configuration problem.

In this thesis, we tackle two main research questions related to *algorithm selection and configuration* for hybrid quantum-classical algorithms:

> **RQ1** The first one is about understanding when a hybrid quantum-classical algorithm can be used against a classical counterpart.
>
> **RQ2** The second research question is about identifying the key internal components of hybrid quantum-classical algorithms and how to set them well.

We perform many algorithm selection and configuration studies on several common NISQ algorithms that can be applied to industrial problems from different fields. We contribute to understanding and improving their performances, toward helping the design of better hybrid quantum-classical algorithms for practice. Our contributions are summarized in more detail in the next section.

1.2 Contributions

The work described in this thesis has been performed within a collaboration between Leiden University and TotalEnergies which funded this Ph.D. The Ph.D. started with the aim to study the application in relevant domains of a few hybrid quantum-classical algorithms commonly found in the quantum literature named *variational quantum algorithms* (VQAs) [40], which will be presented in the next chapter. VQAs have many possible applications, from the more natural application of simulating quantum systems [134, 166, 71] (primarily to chemistry use cases) to optimization use cases [57, 201, 79] and machine learning [18]. These applications are all relevant to industrial problems in the energy sector.

The new hybrid quantum-classical algorithms we study are evolving to improve their performances toward becoming more practical and competing with classical counterparts. Hence, to achieve these goals, they are going through empirical studies and domain-specific enhancements. As research questions, we are interested in developing new methods and identifying key components to improve the design of hybrid quantum-classical algorithms relevant to applications in the above-mentioned fields.

In this thesis, we study several common VQAs from the literature and contribute to the issues of *algorithm selection and configuration* VQAs face. We do so through many empirical studies and with the usage of many benchmarking techniques. The dissertation is outlined as follows:

- Chapter 2 introduces the basic concepts of quantum computing and VQAs. We also review different VQA workflows related to quantum applications with a focus on applications related to the energy sector. The applications which we are interested in belong to the fields of chemistry, combinatorial optimization, and machine learning.

- In Chapter 3, we introduce ideas from the algorithm selection domain to a quantum algorithm designed to tackle combinatorial optimization problems. The latter is called Quantum Approximate Optimization Algorithm (QAOA) and is benchmarked against a classical counterpart. The contents of this chapter are (partly) based on [135] (item 1 in the next list of the author's contribution).

- Chapter 4 demonstrates an example of algorithm configuration problem with the usage of unsupervised machine learning techniques to set the internal parameters of QAOA. The contents of this chapter are (partly) based on [138] (item 4 in the next list of the author's contribution).

- In Chapter 5, we present a hybrid quantum-classical algorithm combining QAOA and a classical heuristic named tabu search. Such a combination allows us to tackle larger problems than the number of qubits would allow running only a quantum algorithm. The contents of this chapter are (partly) based on [139] (item 3 in the next list of the author's contribution).

- For chemistry and material science applications, we identify the best-performing classical optimization algorithm for VQAs. A benchmarking of classical optimization algorithms is carried out in Chapter 6. The contents of this chapter are (partly) based on [24] (item 2 in the next list of the author's contribution).

- VQAs for machine learning have many hyperparameters and their importance is assessed in Chapter 7. We apply the functional ANOVA framework for hyperparameter importance on VQAs for machine learning, namely quantum neural networks. The contents of this chapter are (partly) based on [137] (item 5 in the next list of the author's contribution).

- Finally, Chapter 8 concludes with the design of a resource frugal optimizer for quantum machine learning tasks. Benchmarking of this optimizer against previous existing frugal methods is performed to demonstrate better performances for similar resource counts. The contents of this chapter are (partly) based on [136] (item 6 in the next list of the author's contribution).

1.3 Author's Contributions

Below we list publications the author has contributed to and presented in this thesis in chronological order:

1. Charles Moussa, Henri Calandra, and Vedran Dunjko. To quantum or not to quantum: towards algorithm selection in near-term quantum optimization. *Quantum Science and Technology*, 5(4):044009, 2020.

2. Xavier Bonet-Monroig, Hao Wang, Diederick Vermetten, Bruno Senjean, Charles Moussa, Thomas Bäck, Vedran Dunjko, and Thomas E. O'Brien. Performance comparison of optimization methods on variational quantum algorithms. *Phys. Rev. A*, 107:032407, Mar 20232023.

3. Charles Moussa, Hao Wang, Henri Calandra, Thomas Bäck, and Vedran Dunjko. Tabu-driven quantum neighborhood samplers. In Christine Zarges and Sébastien Verel, editors, *Evolutionary Computation in Combinatorial Optimization, Evocop 2021*, pages 100–119, Cham, 2021. Springer International Publishing.

4. Charles Moussa, Hao Wang, Thomas Bäck, and Vedran Dunjko. Unsupervised strategies for identifying optimal parameters in quantum approximate optimization algorithm. *EPJ Quantum Technology*, 9(1), 2022.

5. Charles Moussa, Jan N. van Rijn, Thomas Bäck, and Vedran Dunjko. Hyperparameter importance of quantum neural networks across small datasets. In Poncelet Pascal and Dino Ienco, editors, *Discovery Science*, pages 32–46, Cham, 2022. Springer Nature Switzerland.

6. Charles Moussa, Max Hunter Gordon, Michal Baczyk, M. Cerezo, Lukasz Cincio, and Patrick J. Coles. Resource frugal optimizer for quantum machine learning. *arXiv:2211.04965*, 2022 (submitted to journal Quantum Science and Technology).