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

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Chapter 9

Conclusions and outlook

In this chapter, we conclude the work done in this thesis, by presenting the research direction, and our results related to this direction on VQAs. We also discuss future research opportunities.

As we have seen throughout the previous chapters in this thesis, VQAs are evolving hybrid quantum-classical algorithms most often used as heuristics and designed to tackle relevant applications for industries in the NISQ era. Such hybrid algorithms can be complex with many components or hyperparameters to work with. They will also have to be compared with classical counterparts. Hence, they will face the problems of *algorithm selection and configuration*, and they will go through empirical studies and domain-specific enhancements. In this thesis, we demonstrated these problems on VQAs for combinatorial optimization, chemistry, and machine learning applications. We demonstrated many benchmarking techniques useful for the design of VQAs and their usage. Next, we will refer back to our research questions and restate the results obtained in this thesis.

1. Our first research question **RQ1** is about understanding when a hybrid quantum-classical algorithm can be used against a classical counterpart. In Chapter 3, we introduce the principle of algorithm selection to quantum optimization algorithms. The algorithm selection problem boils down to the design of a classification algorithm, which can efficiently detect whether a given problem instance satisfies one criterion or many criteria to be used against other algorithms. We demonstrated a case of algorithm selection with QAOA against a classical counterpart and proved the decision to be NP-hard. The algorithm selection methodology can be extended to many other settings where a quantum algorithm will

be considered against a classical counterpart.

2. Our second research question **RQ2** is about identifying the key internal components of hybrid quantum-classical algorithms and how to set them well. In chapters 4, 6 and 8, we addressed the problem of algorithm configuration, specifically to the parameter-setting algorithms (such as classical optimizers), key components of VQAs as they affect greatly their results. To determine the well-performing ones, we use benchmarking methodologies. In each chapter, we tackled this problem in a different context. In Chapter 6, existing optimizers, SPSA and CMA-ES, were studied for VQE settings on several chemistry and material science problems. We obtained comparable performances between them, although CMA-ES obtains better results on the more challenging and interesting systems. On the contrary, a new optimizer was designed in Chapter 8 in the context of QML applications. Its design was guided by using many theoretical concepts to obtain practical improvements over other previous state-of-art QML optimizers. In Chapter 4, we benchmarked unsupervised techniques for setting the parameters of QAOA circuits relying on the concentration property as an argument to save numerous quantum circuit calls that would be used by a classical optimizer. We empirically showed that using instance encodings (by computing features or computing them with a model) for angle-setting strategies yields better results than using angle values only.

3. The principles of algorithm selection and configuration were also demonstrated with a new hybrid algorithm that can help solve problems considering (some of the) limitations of real devices. In Chapter 5, we demonstrated a combination of tabu search with QAOA used as a neighborhood sampler and our results demonstrate potential in solving large problems with limited quantum resources. This also opens up the topics of sampling and multiobjective aspects of quantum algorithms that allow balancing between exploration and exploitation, a very important concept in search algorithms. We believe our approach combined with benchmarking analyses will provide new promising ways to maximize the use of limited near-term quantum computing architectures for real-world and industrial optimization problems.

4. VQAs may come with many possible hyperparameters (such as the number of layers, the circuit architecture, and the used optimizer), adding complexity to their usage in practice. Analyzing which ones matter or not for a given domain can help reduce the usage of (potentially expensive) quantum resources. This

research question, as a part of **RQ2**, was discussed in Chapter 7 through a study done on quantum neural networks and classical datasets. Using functional ANOVA, a hyperparameter importance framework, we distinguished three main levels of importance. On the one hand, Adam's learning rate, depth, and data encoding strategy are deemed very important, as we expected. On the other hand, the less considered hyperparameters such as the particular choice of the entangling gate and using 3 rotation types in the variational layer are in the least important group. We envision such studies with techniques such as functional ANOVA to be employed in future works related to quantum machine learning and understanding how to apply quantum models in practice.

The methodologies used in our studies are agnostic to the considered VQA and the settings upon which a VQA is run. Our goal during research was to show by examples the benefits of such methodologies for algorithm selection and configuration in the context of NISQ algorithms and for designing hybrid quantum-classical algorithms on many domains of applications relevant to industries. The methodologies can be extended to noisy settings, with other noise-mitigation techniques to run VQAs better and faster on real quantum devices. New VQA algorithms that will be designed in the future will also benefit from such benchmarking studies. As quantum hardware keeps improving, with hybrid clusters of many types of hardware, and of course, many possibilities to run VQAs with many targeted applications, the algorithm selection and configuration problems become even more relevant. We hope the work reported in this thesis will help in applying standard and normalized practices for designing better hybrid quantum-classical workflows tailored to many potential applications of quantum computing. In particular, the applications of VQAs related to the energy sector will benefit from such studies as demonstrated for combinatorial optimization, chemistry, and machine learning. Indeed, tailoring and extending these algorithms and studies for other problems and data from the energy sector will be a logical next step for future research to continue exploring the potential value of quantum algorithms in this sector.