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

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Summary

Quantum hardware comes with a different computing paradigm and new ways to tackle applications. Much effort has to be put into understanding how to leverage this technology to give real-world advantages in areas of interest for industries such as combinatorial optimization or machine learning.

Variational quantum algorithms (VQAs) have been introduced as a way to work within the scope of reach of the current imperfect and unstable hardware. A VQA boils down to a parameterized quantum circuit, which is a quantum circuit with adjustable real-valued parameters. These parameters are generally tweaked by a classical optimization algorithm to optimize a quantity of interest.

As VQAs are most often used as heuristics, it is not clear whether they genuinely outperform current classical state-of-the-art algorithms in relevant domains of application. Plus, a VQA can come with many components (which can also be called hyperparameters) making it a (growing) complex system to analyze performances on many considered tasks. Consequently, we will face the issues of algorithm selection and configuration, which we tackle through this thesis on many examples relevant to industrial applications. In this thesis, VQAs for combinatorial optimization, chemistry/material science, and machine learning problems were considered.

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 demonstrate 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.

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, how to run successfully a VQA becomes even more relevant and more complicated. 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.