DEVELOPMENT OF HEURISTIC METHODS ON REVERSIBLE AND QUANTUM COMPUTERS

Teză de doctorat – Rezumat

pentru obținerea titlului științific de doctor la
Universitatea Politehnica Timișoara
în domeniul de doctorat Calculatoare și Tehnologia Informației

autor ing. Sebastian Mihai ARDELEAN
conducător științific Prof.univ.dr.ing. Mihai UDRESCU-MILOSAV
luna septembrie anul 2024

This Ph.D. thesis addresses the development and optimization of heuristic algorithms on quantum computers, with a focus on true quantum genetic algorithms. The novelty of the thesis is represented by the instantiation of the Reduced Quantum Genetic Algorithm (RQGA) [1] framework for solving NP-hard problems and by the introduction of a novel hybrid algorithm that combines a classical genetic algorithm with RQGA--referred to as Hybrid Quantum Algorithm with Genetic Optimization (HQAGO).

In the first chapter I present the motivation and the thesis goals. Heuristic methods, particularly Genetic Algorithms (GA), have received significant research attention and are widely acknowledged as one of the most commonly used forms of evolutionary computation [2]. Genetic Algorithms (GA) represent computational methodologies inspired by natural selection, utilized to optimize problems [3] [2] [4]. On the other hand, quantum computation is very powerful in solving diverse problems owing to its distinctive properties and phenomena such as entanglement, interference, and exponential parallelism [2] [5]. As sustaining Moore's law becomes more challenging, the search for alternative solutions to meet power and performance demands has intensified [6]. Quantum computing has emerged as one of the most promising options. Thus, a merge between genetic algorithms and quantum computing appears to be beneficial [1]. By simulating quantum circuits implementing GA across various highly customizable noise models and executing Genetic Algorithms on real quantum computers, we can analyze this category of heuristic techniques within the quantum domain for NP-hard problems [5] [7].

Chapter 2, *Background*, is divided into two parts: *Quantum Computation* and *Genetic Algorithms*. Related to the quantum computation and quantum information, the literature provides numerous relevant references from which we pinpoint [5], [8], and [7], used in laying the foundation of the Section *Quantum Computation*. Quantum computing has the potential for significant speedups over conventional computing systems in a wide range of practical applications, from commerce [9], industry [10], and finance [11] to chemistry [12], biology [13], medicine [14], climate modeling [15], and even artificial intelligence [16].

In the domain of genetic algorithms, we mention [2]and [17]as notable references, which provide inspiration for shaping Section *Genetic Algorithms*.

Chapter 3 is dedicated to the state-of-the-art quantum genetic algorithms. The Reduced Quantum Genetic Algorithm (RQGA) [1] framework is introduced, as well as existing research on the use of quantum computing to solve the graph coloring problem [18].

Chapter 4 defines a new quantum simulation library that uses behavioral modeling of quantum circuits, allowing the possibility of simulating complex circuits with a low memory footprint compared to other simulators based on structural modeling. In addition, this chapter presents the architectural view of this library.

Chapter 5 is dedicated to the applications of Reduced Quantum Genetic Algorithm (RQGA) and the experimental results. The framework is implemented and tested by solving two NP-complete problems, the knapsack and graph coloring problems, and the results are compared to other quantum solutions that solve the above-mentioned problems. Consequently, we introduce an instantiation of Reduced Quantum Genetic Algorithm (RQGA) capable of solving NP-hard graph coloring in $\mathcal{O}\left(\sqrt{\mathrm{N}}\right)$. This proposed implementation handles both vertex and edge coloring and can ascertain the chromatic number (i.e., the minimum number of colors required to color a graph). We assess the outcomes, analyze algorithm's convergence, and measure the performance utilizing the Qiskit simulation framework. Our Reduced Quantum Genetic Algorithm (RQGA) circuit implementation and graph coloring outcomes show that quantum heuristics can address complex computational problems more efficiently compared to the conventional methods. Additionally, we instantiate the RQGA framework for resolving the knapsack problem, analyzing circuit complexity regarding the required number of qubits and the number of utilized quantum gates.

In Chapter 6 the Hybrid Quantum Algorithm with Genetic Optimization (HQAGO) is introduced as an optimization of RQGA. The novel algorithm uses the genetic algorithm as a classical optimization of a fully quantum algorithm. Classical genetic algorithms are employed to fix specific qubits to a value, thus reducing the search space for the fully quantum algorithm. The new algorithm and the classical optimization are detailed in this chapter. In addition, we introduce the theoretical analysis of space and time complexities and the experimental results that confirm our assessments.

Quantum Genetic Algorithms (QGAs) integrate genetic programming and quantum computing to address search and optimization problems. Most QGA approaches add quantum features to operators of genetic algorithms, such as selection, crossover, or mutation [3]. In contrast, Reduced Quantum Genetic Algorithm (RQGA) differs as a fully quantum algorithm [1] [3], encoding the entire search space (population) as a superposition of all potential solutions (chromosomes) using the individuals' quantum register. The fitness function operates on the individuals' quantum register to derive corresponding fitness values within the superposition of chromosomes. RQGA employs Grover's algorithm to find the best fitness value and its corresponding chromosome (i.e., the solution or one of the solutions). Grover's algorithm [19] exhibits a complexity of $\mathcal{O}\left(\sqrt{\mathrm{N}}\right)$, where N represents the number of superposed individual chromosomes. However, RQGA operates within an exponentially large search space ($\mathrm{N} = 2^{\mathrm{n}}$, with n as the number of qubits in the individuals' quantum register), resulting in an exponential runtime of $\mathcal{O}\left(2^{\mathrm{n}/2}\right)$. Therefore, we propose an optimization solution for RQGA to control algorithm's complexity by selecting a limited number of qubits in the individuals' register and fixing the remaining ones as classical values ('0' and '1') using a genetic algorithm. Additionally, we enhance RQGA's performance by eliminating unfit solutions and constraining the search to the valid individuals' area. Combining these approaches, we introduce a novel quantum genetic algorithm, Hybrid Quantum Algorithm with Genetic Optimization (HQAGO), capable of solving search problems in $\mathcal{O}\left(2^{(\mathrm{n}-\mathrm{k})/2}\right)$ oracle queries, where k denotes the number of fixed classical bits in the individuals' register.

Chapter 7 elaborates on methods for using quantum computing and quantum algorithms for applications in Big Data. The chapter is divided into two sections. Section *Quantum random number generator* introduces a framework that interacts with the IDQ's Quantis Appliance network-attached device [20] and is easy to introduce in research and embedded projects. The framework consists of a library implemented in the C programming language, Python bindings through a C extension interface, a Python module for creating pools of true random numbers, and a command-line application for immediate requests of random numbers. The second section, *Analyzing drug datasets using quantum technologies*, is dedicated to the analysis of drug complex networks built with information from the DrugBank database [21].

Chapter 8 is dedicated to conclusions, stating contributions to state-of-the-art research, and envisioning future work. I outline the implementation of the Reduced Quantum Genetic Algorithm (RQGA) to tackle the graph coloring problem using the Qiskit toolchain [22] [23]. In doing so, I present a purely quantum heuristic approach that solves the problem in $\mathcal{O}\left(\sqrt{\frac{2^n}{M}}\right)$ Grover oracle queries. Additionally, we offer innovative and efficient solutions for the graph node coloring problem, the edge coloring problem, and determining the chromatic number of a graph. Additionally, I instantiate the framework for addressing the knapsack problem and examine the circuit complexity concerning the required number of qubits and quantum gates utilized.

I introduce an innovative quantum genetic algorithm, based on RQGA, that controls the complexity of the quantum algorithm by reducing its search space. Consequently, the proposed Hybrid Quantum Algorithm with Genetic Optimization (HQAGO) solves NP-hard problems in $\mathcal{O}\left(\sqrt{2^{n-k}}\right)$ oracle queries. Therefore, the algorithm enables the solution of complex problems using fewer qubits at the cost of adding additional circuitry to instantiate conventional Genetic Algorithm (GA). I implement a framework for interacting with IDQ's Quantis Appliance network-attached device for requesting quantum random numbers and tackle the optimization of Big Data processing with quantum technologies. Possible research paths emerged for the use of our new hybrid algorithm, HQAGO, in molecular docking to predict the conformations bound of flexible ligands to macromolecular targets and to tune the structure and parameters of neural networks. Another possible research path that is of great interest involves tackling the domain of evolvable quantum circuits and reconfigurable quantum networks.

Bibliography

[1] M. Udrescu, L. Prodan and M. Vlăduţiu, "Implementing quantum genetic algorithms: a solution based on Grover's algorithm," in *ConferenceProceedings of the 3rd Conference on Computing Frontiers*, 2006.

[2] L. Spector, Automatic Quantum Computer Programming: a genetic programming approach, vol. 7, Springer Science & Business Media, 2004.

[3] R. Lahoz-Beltra, "Quantum genetic algorithms for computer scientists," vol. 5, no. 4, p. 24, 2016.

[4] R. Matoušek, "Genetic algorithm and advanced tournament selection concept," pp. 189-196, 2009.

[5] M. A. Nielsen and I. Chuang, *Quantum computation and quantum information,* American Association of Physics Teachers, 2002.

[6] T. Häner, D. S. Steiger, M. Smelyanskiy and M. Troyer, "High performance emulation of quantum circuits," in *SC'16: ConferenceProceedings of the International Conference for High Performance Computing, Networking, Storage and Analysis*, 2016.

[7] N. S. Yanofsky and M. A. Mannucci, Quantum computing for computer scientists, Cambridge University Press, 2008.

[8] J. D. Hidary, Quantum computing: an applied approach, vol. 1, Springer, 2019.

[9] F. Bova, A. Goldfarb and R. G. Melko, "Commercial applications of quantum computing," vol. 8, no. 1, p. 2, 2021.

[10] A. Bayerstadler, G. Becquin, J. Binder, T. Botter, H. Ehm, T. Ehmer, M. Erdmann, N. Gaus, P. Harbach, M. Hess and others, "Industry quantum computing applications," vol. 8, no. 1, p. 25, 2021.

[11] R. Orús, S. Mugel and E. Lizaso, "Quantum computing for finance: Overview and prospects," vol. 4, p. 100028, 2019.

[12] P. J. Ollitrault, A. Miessen and I. Tavernelli, "Molecular quantum dynamics: A quantum computing perspective," vol. 54, no. 23, pp. 4229-4238, 2021.

[13] L. Marchetti, R. Nifosì, P. L. Martelli, E. Da Pozzo, V. Cappello, F. Banterle, M. L. Trincavelli, C. Martini and M. D'Elia, "Quantum computing algorithms: getting closer to critical problems in computational biology," vol. 23, no. 6, p. bbac437, 2022.

[14] J. Davids, N. Lidströmer and H. Ashrafian, "Artificial Intelligence in Medicine Using Quantum Computing in the Future of Healthcare," Springer, 2022, pp. 423-446.

[15] F. Tennie and T. N. Palmer, "Quantum Computers for Weather and Climate Prediction: The Good, the Bad, and the Noisy," vol. 104, no. 2, pp. E488-E500, 2023.

[16] V. Dunjko and H. J. Briegel, "Machine learning & artificial intelligence in the quantum domain: a review of recent progress," vol. 81, no. 7, p. 074001, 2018.

[17] M. Melanie, *An introduction to genetic algorithms. A Bradford book,* The MIT Press Cambridge, MA, 1999.

[18] S. Mahmoudi and S. Lotfi, "Modified cuckoo optimization algorithm (MCOA) to solve graph coloring problem," vol. 33, pp. 48-64, 2015.

[19] L. K. Grover, "A fast quantum mechanical algorithm for database search," in *ConferenceProceedings of the twenty-eighth annual ACM symposium on Theory of computing*, 1996.

[20] *Quantis Appliance 2.0.*

[21] D. S. Wishart, Y. D. Feunang, A. C. Guo, E. J. Lo, A. Marcu, J. R. Grant, T. Sajed, D. Johnson, C. Li, Z. Sayeeda and others, "DrugBank 5.0: a major update to the DrugBank database for 2018," vol. 46, no. D1, pp. D1074-D1082, 2018.

[22] M. S. ANIS, H. Abraham and et al., *Qiskit: An Open-source Framework for Quantum Computing,* 2021.

[23] R. Wille, R. Van Meter and Y. Naveh, "IBM's Qiskit Tool Chain: Working with and Developing for Real Quantum Computers," in *2019 Design, Automation & Test in Europe Conference & Exhibition (DATE)*, 2019.