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Quantum Computing and Optimization: A Comparative Analysis of Classical and Quantum Algorithms

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ABSTRACT

Quantum computing is an emerging field that integrates principles of quantum mechanics with computer science, mathematics, and electrical engineering to address complex computational problems. This paper explores the potential of quantum computing in the realm of mathematical optimization, where classical algorithms have traditionally been employed. By examining both classical and quantum optimization algorithms, such as Quantum Annealing and the Quantum Approximate Optimization Algorithm (QAOA), we highlight the current advancements and challenges in achieving quantum speedup. Although no general quantum algorithm provides a speedup for global optimization problems, certain classes benefit from quantum approaches. This paper discusses the foundational principles, recent developments, and comparative performance of classical and quantum optimization techniques, emphasizing the transformative potential of quantum computing.

Keywords: Quantum Computing, Mathematical Optimization, Quantum Annealing, Quantum Approximate Optimization Algorithm (QAOA), Classical Algorithms, Global Optimization, Variation Algorithms, NISQ Computers

INTRODUCTION

Optimization is the process of finding the input that minimizes or maximizes a given mathematical function. This field has vast applications in commerce, industry, and science, where classical computers have traditionally been used to solve practical optimization problems [1, 2]. These classical solvers iteratively refine solutions until a satisfactory outcome is reached. Global optimization, a specific subset, involves finding the absolute best solution in the entire search space, often employing methods like backtracking search algorithms [3, 4]. Quantum computing, a field that merges quantum physics with computational techniques, holds promise for revolutionizing optimization. Quantum algorithms, such as Shor's algorithm, demonstrate potential exponential speedup over classical methods for certain problems [5]. This paper reviewed the principles of quantum mechanics that underpin quantum computing, explored classical and quantum optimization techniques, and evaluated their relative performance and applicability.

Quantum Computing

Given a mathematical function of one or more variables, optimization is the problem of finding the input that minimizes or maximizes the value of the function. Throughout history, numerous mathematical and computational techniques have been developed to attack these tasks and optimization has been observed in various forms in a large number of commercial/industrial applications as well as scientific studies [6, 7]. In solving practical optimization problems, classical computers are currently used. In general, these everyday classical optimization solvers work on the principle of iteratively refining a proposal solution until a 'trough' (or peak) is found that fulfills the desired quality constraints. It has been known for many years that some specific forms of optimization problems form a class called GLOBAL OPTIMIZATION; for example, it was shown that smooth unimodal functions can have only one global minimum and that a convergence to the global minimum can be found deterministically by using a backtracking search algorithm that refines a search 'trough' (proposal solution) based on local probe readings in the neighborhood [8, 9]. To date, there are no known quantum algorithms that provide speedup for problems in the general case of global optimization. However, at least for some particular classes of optimization problems, quantum algorithms can provide exponential speedup [10, 11]. Quantum computing is a flourishing field that merges the disciplines of quantum physics, mathematics, computer science, and electrical engineering to create a new technology for secure communication, improving machine learning algorithms from the classical point of view, better optimization algorithms, and improved planning or scheduling algorithms [12, 13]. Let's take an example of cryptography, a quantum computer can attack the current public key cryptosystems. Shor's algorithm for factoring is as of 2021, around 30 million times faster than currently best known classical algorithms. Quantum computers can solve particular optimization problems exponentially faster than classical computers [14, 15].

Basic Principles of Quantum Mechanics

Apart from these complex mathematical and analytical models, what is more, exciting in the field of quantum mechanics is that these complex models can also be presented very vividly in the form of a new approach to computing and that is Quantum Computing [16, 17]. Else it makes sense if we think of classical computing as the art of arranging 0s and 1s to manipulate and retrieve the desired output based on choices in the arrangement [18, 19]. So, this new computing made us think in the new realm of physics that is Quantum Physics. At this point, we start converging our views to more concrete mathematics and physics where we see the classical computers as a subset or reformulation of the quantum computing world. With this highly deterministic and predictable classical world we have, we find extremely unconventional gadgets and pieces of mathematics when we step into the world of quantum computing [20, 21]. Quantum mechanics is a theory that explains the behavior of fundamental particles and their interactions with other particles under different conditions. The central highlight of quantum mechanics is that it is probabilistic, meaning that we can predict the behavior of a system only statistically [22, 23]. With the Birth of quantum mechanics in the early 20th century, comes a lot of controversial aspects of nature, and it is the pioneers of this theory like Erwin Schrödinger, Max Born, and Werner Heisenberg who gave us a thorough understanding of the same. Due to these complex statistical predictions, many problems emerged in the mathematical model of these atomic systems [24, 25]. For example, there is no concept of $\lambda = pt$ in quantum mechanics and this is where we start to face issues of conservation of momentum and energy [26].

Mathematical Optimization

To solve optimization problems, classical information processing uses algorithms. Examples of classical optimization algorithms include the Nelder-Mead simplex search algorithm, which is very effective in an arbitrary number of dimensions when derivatives are not known or convexity and boundedness are uncertain. Other examples include coordinate search methods, which perform an exhaustive line search in each direction and use its results to determine the subsequent line searches and limits on the search step size to mitigate divergence [27-29]. Simulated annealing uses the Metropolis algorithm or other statistical mechanics techniques to solve large, multivariate problems. Certain algorithms like the Matt-ball method rely on a likelihood ratio and are therefore not efficient when the distribution is exponentially hard to sample from once a set of variables is fixed. Optimization problems are everywhere. They arise in transporting goods, resource management, and scheduling production. Some common optimization tasks include finding the shortest route for moving information or material, designing electronics for performance and cost, and maximizing returns on an investment portfolio [30-32]. Familiar optimization problems include finding the most likely source of a signal "originating" from many sources (Gaussian Maximum Likelihood Estimation), clustering data into as few sets as possible (k-Means), and picking fewer variables than an infinite list that on average models the data just a little bit worse (Stepwise). Finding the best path through a graph is of widespread interest in computer algorithms because the task appears in many important settings like routing network traffic and identifying software viruses/bots [33-35]. Mathematical optimization is a subfield of mathematics and computer science concerned with finding the "best" solution to a problem out of all of the possible solutions. That is, mathematical optimization seeks the maximum or minimum of a quantity of interest, subject to some constraints. Optimization problems take many forms and can be categorized in terms of the number of free variables, linearity, convexity, and structure. Algorithms for optimization tasks are foundational in computer science and used in nearly all areas of engineering and computational science, including machine learning, statistics, data modeling, and quantum information science [36-38].

Fundamental Concepts and Problem Formulations

Quantum optimization centers mainly on classical combinatorial optimization mathematical problems, which specifically belong to non-convex problems. Quantum optimization methods for continuous problems are classically obtained as a result of the exploitation of the Continuous Variable Quantum Computing (CVQC) protocol in the quantum algorithm design, and the problem setup differs between the single objective and multi-objective mathematical problem formulations. Two basic approaches design the quantum optimization methods: quantum-based meta-heuristic mathematical methods and quantum non-meta-heuristic search methods. Quantum-based meta-heuristic methods transform the quantum meta-heuristic algorithms applied to the large-scale combinatorial problem of size n and the quantum ANN meta-heuristic algorithm [39, 40]. Quantum non-meta-heuristic search methods include the Variational Quantum Eigensolver (VQE), Quantum Approximate Optimization Algorithm (QAOA), Quantum Adiabatic Algorithm (QAAQ), Quantum Amplitude Estimation (QAE) and the Harrow-Hassidim- Lloyd (HHL) algorithm. The QEO design can belong to quantum combinatorial optimization problems, quantum continuous optimization problems, or hybrid-discrete-continuous mathematical problem formulations, and the hybrid D/Q optimization problem is defined [41, 42]. Quantum computing is a paradigm of computation that uses quantum mechanical phenomena, such as superposition and entanglement to process information. It can be devised as a mathematics framework and exploited to solve problems that belong to emerging fields of quantum computing algorithms, quantum machine learning, and quantum supremacy. Mathematics optimization aims to find the best solution, the global minimum, of a given problem under some conditions [43, 44]. Let us assume to have a smoothly-real function f(x) of n-real variables, such that we want to solve minf(x) with subject to x = (x1, . . . , xn)∈AN, with AN ⊂ Rn. The solution to the mathematical optimization presented in the previous description is formally written as the following: x∗ = argmin{ f(x) | f(x) ≤ f(x∗0), x ∈ AN } with f(x∗) = min{ f(x) | x ∈ AN } and x∗0 optimization starting point (or initial/guess solution) of the optimization problem. In the context of optimization, SOTA classical methods can be classified into local and global optimization methods and machine-learning supported mathematical optimization strategies [45, 46].

Classical Algorithms for Mathematical Optimization

There are also specifically tailored algorithms to solve convex optimization problems, but the current interest in quantum algorithms is mostly focused on non-convex problems. The state-of-the-art quantum algorithms for non-convex mathematical optimization can be grouped into quantum annealing and Quantum Approximate Optimization Algorithms (QAOA). Classical algorithms include evolutionary algorithms, greedy methods, linear and non-linear programming, and penalty and barrier methods as well as algorithms dealing with other reformulations of the original problem [47, 48]. Although all the classical methods offer both convergence and termination, a critique of the classical algorithms is that they are only locally convergent [49, 50]. Typically, their progress terminates when having reached sufficient precision or when a certain number of iterations have been passed. Since large-scale optimization problems are usually non-convex, the chance of finding the global minimum a priori is negligible in classical methods. Classic heuristics often achieve super-linear or even exponential convergence rates but sacrifice the guarantee to obtain a global solution [51, 52]. The domain of mathematical optimization is vast and of paramount importance in many applicable fields. It can be categorized into continuous, discrete, and combinatorial optimization problems, further compounded by the multiplicity of objective functions and constraint types. Classical algorithms for mathematical optimization are highly effective and an overwhelming amount of literature has been dedicated to the subject [53, 54].

Quantum Computing for Optimization Problems

The quantum approximate optimization algorithm (QAOA) is a hardware-efficient variational algorithm particularly designed for near-term quantum computers, and it has been widely adopted and studied as a framework to address the problem of combinatorial optimization. When addressing the scheduling problem, QAOA reports reasonable outcomes. However, the requirements for the quantum resources necessary for QAOA optimization limited the scale of the scheduling challenge and may lead to suboptimal answers. Nevertheless, the main advantages of utilizing QAOA compared to classical algorithms lie in its potential for faster runtime as well as its capacity to seek the optimal answers simultaneously [55-57]. Discrete/continuous optimization typically emerges in a wide range of practical optimization problems, such as constrained optimization, mixed-integer linear programming, and global optimization. Classical solution strategies include gradient-based continuous optimization solvers and exact/computational combinatorial optimization solution solvers including branch and bound and branch and cut [58, 59]. The hybrid discrete/continuous class of optimization problems is NP-hard, and exact methods are quite limited because many of them are contingent on highly efficient QUBO convertors. There exists a need for novel and robust solution strategies for large-scale hybrid optimization problems to serve as the basis for cross-layer and end-to-end accommodations for network resources in integrated fronthaul/backhaul/cloud segments, network slicing, and reconfiguration. Key enabling technologies include quantum computing, quantum computation, quantum annealing, and quantum adiabatic optimization [60, 61]. The famous computer scientist Ronald Rivest once referred to optimization as the "science of better", This science usually requires the discovery of a configuration or decision choice that is best among a set of different alternatives. For a classical computer, this is challenging, but for a quantum computer, it's possible to solve them faster than any other computer, specifically in terms of the number of computational steps or algorithms that the computer employs. Quantum computing provides two primary algorithms for optimization problems in two main models. The first is the Quantum Adiabatic Algorithm (QAOA), which is designed for solving combinatorial optimization tasks such as Max-Cut and Traveling Salesman, and the second is Grover's search algorithm, which is attributed as the most frequently referenced optimization algorithm utilized by the quantum computer [62, 63]. In the presence of imperfections in quantum computers, physical qubits in a quantum computer are susceptible to disturbances and noise, considered the main barriers that limit the potential of the quantum computer to approach its idealized strategy for quantum computation. However, algorithm developers are designing algorithm architectures that function effectively despite these limitations, frequently referred to as "quantum optimizers" [64, 65].

Quantum Annealing

Quantum Annealing Optimization applications are useful for commercial, governmental, and scientific activities such as supply chain logistics, robotics, quantum machine learning, and deep neuroscience. Quantum annealing is a successful quantum approach, especially for optimization. Currently, the biggest challenge of quantum annealing is how to have a full quantum implementation. Further, quantum annealing becomes part of a NISQ quantum computational approach for an enhanced rather than complete quantum implementation [66, 67]. Selecting highly programmable and leak-resistant qubits to be the main qubits in implementation and setting less leakage-resistant qubits to be the ancillary qubits can improve the performance of quantum annealing. Quantum annealing algorithm encodes optimization problems into quantum Hamiltonians (H(t)) and then adiabatically (i.e., slowly with time) evolves this Hamiltonian into an annealing final Hamiltonian which adiabatically also transforms back to standard optimization cost functions to be measured. The important characteristic of natural quantum annealing is that it halves hardware demands in doing optimization due to quantum parallelism [68, 69]. Algorithms are a key part of any quantum computing framework, and mathematical optimization is one of the main problems in the field of computer science. Quantum annealing, a prominent quantum optimization algorithm, is on pace for near-term implementation on existing quantum hardware [70, 71]. Quantum annealing is based on adiabatic quantum computation and can be performed on superconducting qubits, ions trapped in electromagnetic fields, or other quantum hardware. Some notable quantum annealers include the D-Wave 2X, 2000Q, and Advantage, and the upcoming Bo Eun, Clare, and Anneata machines [72, 73].

Quantum Approximate Optimization Algorithm (QAOA)

In recent months, we have also been witnessing the implementation of quantum versions of the already mentioned approximate classical optimization algorithms for practical problems with large and non-trivial structures, and also for geometric optimization problems that are not directly based on combinatorial ones, such as continuous variants of graph semidefinite programming formulations, etc. Some works explored in depth some of the optimization problems for which it seems infeasible to obtain classic lower bounds [74, 75]. Concerning the applicability of QAOA, we also have to understand that its usage is not trivial, and also not immune to the effects of the enormous resource limitations of NISQ computers. Moreover, the quantum and mixed nature of the constraints give origin and introduce the necessity of using ancillae to enforce them, and also make the Pavage problem considered a non-trivial problem in that respect. Even though demonstrations of QAOA's potential to solve combinatorial optimization problems in proof-of-principle experiments with real NISQ hardware are increasing, there is an evident potential to extend current benchmarking efforts [76, 77]. The Quantum Approximate Optimization Algorithm (QAOA) is a variational quantum algorithm, which is among the leading candidates for achieving quantum advantage in the context of combinatorial optimization problems. In its most direct application, QAOA treats an optimization problem increasingly as a problem of finding the ground eigenstate of a certain Hamiltonian ω(Hp + Hm) through an initial-state preparation as a superposition of unstructured computational basis states, called a reference, followed by an iterative, adaptative rotation between those states, alternately under the Hamiltonians Hp and Hm, with the presence of more involved, ancilla-based circuits when found necessary for a more efficient standard cost function evaluation (the direct approach to problems involving such ancilla-based circuits is, for example, to interpret the property to be enforced as a quantum-constrained optimization problem, on which we nevertheless can still employ QAOA) [78, 79].

Comparative Analysis of Quantum and Classical Optimization Algorithms

Benchmarking is significantly important, the experimental results also show that the quantum optimization experiments using the same quantum annealer are deceptive because the optimization problems found in each trial run are different. Interestingly, hybrid algorithms obtain the quantum advantage and we simply conclude that the iterative-repeated classical optimization steps before and/or between the subroutines encoded by our quantum circuits could help attain the quantum advantage. Such diversity provides the penalty of its increased number of iterations, as well as both of our hybrid optimizers' robustness against noise. It ensures that a quantum speed-up will be achieved in individual trials even in highly diverse landscapes similar to those discovered here [80, 81]. Various factors play a role in accelerating the performance of the purely optimized algorithms and QAOA. The promised quantum advantage is subjected to many parameters, such as the structure of the input problem instance and allowable error rates. So, it is very important to benchmark the quantum algorithms repeatedly and abstractly (i.e., statistically average it) on massively repeated runs. We observe that the major deterministic algorithms with complex polynomial time in a noisy environment (i.e., NISQ era quantum computer) are supposed to perform better as variational algorithms because variational algorithms are exponentially large in the number of gates, improving the practical error rates [82, 83]. Quantum computing and its anticipated superiority over the traditional digital computer has the outstanding potential to address exponential-time-hard optimization problems with a polynomial-time complexity [84, 85]. Complexity classically increases with problem size, but quantumly, it remains in polynomial time, as in our experience with chemistry calculations. As we straightforwardly assess the speed-ups achieved through quantum algorithms (exponential, quadratic, polynomial, logarithmic, and constant), most of the pure optimization algorithms do not promise an exponential or quadratic advantage, however, the QAOA has the expected speedup [86, 87].

CONCLUSION

Quantum computing represents a significant leap forward in computational capabilities, particularly for optimization problems. While classical algorithms remain effective for many applications, quantum approaches like Quantum Annealing and QAOA offer potential speedup and improved efficiency for specific problem classes. Despite challenges, such as resource limitations and noise in NISQ computers, ongoing advancements in quantum algorithms and hardware suggest a promising future for quantum optimization. This comparative analysis underscores the transformative impact quantum computing could have on optimization, paving the way for new scientific and industrial applications.

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