Solving Scheduling Problems with Quantum Computing: a Study on Flexible Open Shop

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ABSTRACT

Despite quantum computing is revealing an increasingly promising technology that has the potential to introduce a significant speed-up in many areas of computation, the number of problems that it can represent and solve is currently rather limited. Therefore, one of the current challenges faced by the quantum computing community is to broaden the class of problems that can be tackled. Among these problems, scheduling problems are a class of particularly interesting and hard combinatorial problems; in this paper, we present a novel solution for representing and solving the Flexible Open Shop Scheduling Problem (FOSSP) to optimality by minimizing the makespan. We firstly present a compact formulation of this problem as a Quadratic unconstrained binary optimization (QUBO), which can be used to solve this problem with a quantum annealer. Then, we proceed to the Quantum Approximate Optimization Algorithm (QAOA) problem formulation, thus producing both the cost and mix Hamiltonians related to the problem. From the Hamiltonians, we provide the complete description of the quantum circuit that can be used to tackle the FOSSP within the QAOA framework. This second approach can be used to solve the optimization problem with a general-purpose quantum gate-based hardware.

CCS CONCEPTS

• **Theory of computation → Quantum computation theory**; **Scheduling algorithms**; • **Computer systems organization → Quantum computing**.

KEYWORDS

quantum computing, scheduling, flexible open-shop, quadratic unconstrained binary optimization, QAOA, adiabatic quantum computing, quantum circuits

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1 INTRODUCTION

Quantum computing has emerged as a promising technology with the potential to revolutionize many areas of computation [17, 19], including optimization and scheduling problems. Scheduling problems are ubiquitous in various fields [18], ranging from transportation and logistics to manufacturing and healthcare. These problems entail the allocation of resources to a set of tasks subject to various constraints, and pursue various objectives, such as minimizing the total processing time or maximizing the utilization of resources. Due to their combinatorial nature, scheduling problems are typically NP-hard, which means that classical computers are unable to solve them efficiently for large problem sizes.

Quantum computing has recently emerged as a promising tool for tackling NP-hard optimization problems, including scheduling problems. The Ising model [15], which is a mathematical representation of interacting spins on a lattice, can be extracted from the Quadratic Unconstrained Binary Optimization (QUBO) formalism and can be used to represent scheduling problems. Quantum annealing [13] is a quantum computing approach that employs the Ising model to find the optimal solution for a given problem.

This paper considers a variant of the Flexible Open Shop Scheduling Problem (FOSSP) [3], an extension of the well-known Open Shop Scheduling Problem (OSSP) [1], which has applications in many areas including timetabling, satellite communication, health care management, transport and tourism. Starting from a quadratic unconstrained binary optimization (QUBO) representation of the FOSSP problem, subsequently translated in terms of the Ising mathematical model[15], the paper proposes a Quantum Approximate Optimization Algorithm (QAOA) formulation [8], thus producing both the cost and mix Hamiltonians related to the problem. In addition, the paper aims to explore the advantages and limitations of quantum annealing in comparison to the gate-model used in the QAOA approach [11].

The remainder of the paper is structured as follows: Section 2 provides a brief overview of quantum computing. Section 3 introduces the proposed scheduling problem, whereas Section 4 considers the application of the QUBO model. Section5 discusses the application of the QAOA model for solving the proposed scheduling problem. Finally, Section 6 concludes the paper with a summary of the findings and an outlook on the future work.

2 BACKGROUND

A *Quadratic Unconstrained Binary Optimization* problem (*QUBO*),[1] is a mathematical formulation that encompasses a wide range of critical *Combinatorial Optimization* problems. QUBO has been surveyed in [2, 14] and the first work on QUBO dates back to 1960 [12]. A solution for a QUBO problem corresponds to minimizing a quadratic function over binary variables (0/1), whose coefficients can be represented using a symmetric square matrix. QUBO problems are NP-Complete: therefore, a vast literature is dedicated to approximate solvers based on heuristics or meta-heuristics, such as *simulated annealing* (*SA*), *tabu-serch*, *genetic algorithms* or *evolutionary computing* [14]. The literature also presents some exact methods that are capable of solving QUBO problems with 100-500 variables [14]. Moerover, *quantum* annealers and Fujitsu's *digital annealers*[2] can be also used to find global minima by using quantum *fluctuations*. QUBO models are at the heart of experimentation with quantum computers built by D-Wave Systems[3]. QUBO has been intensively investigated and is used to characterize and solve a wide range of optimization problems, such as SAT Problems, Constraint Satisfaction Problems, Maximum Cut Problems, Graph Coloring Problems, Maximum Clique Problems, General 0/1 Programming Problems and many more [10], including scheduling problems [7]. In addition, there exist QUBO embeddings for Support Vector Machines, Clustering algorithms, Markov Random Fields [16], Probabilistic Reasoning [4], and Argumentation [5].

Another approach used to solve combinatorial optimization problems with quantum machines is the Quantum Approximate Optimization Algorithm (QAOA) [8, 11], which has revealed to be very versatile for the resolution of a wide range of different problems [21, 21]. This algorithm is structured as a hybrid process, in which a classical computer optimizes a discrete function F by means of a quantum parameterized circuit $C(\beta_1, \gamma_1, \ldots, \beta_p, \gamma_p)$. The optimization process searches for the values of the parameters $\beta_1, \gamma_1, \ldots, \beta_p, \gamma_p$ such that C prepares a good quantum state $|\beta_1, \gamma_1, \ldots, \beta_p, \gamma_p\rangle$, i.e. measuring this state, very good solutions of F are extracted. Typically, the circuit has a small number of real-values parameters $\beta_1, \gamma_1, \ldots, \beta_p, \gamma_p$ which are optimized by a gradient-descent approach or with some derivative-free methods, like COBYLA or Nelder-Mead.

In general, these quantum circuits C are characterized by a high number of commuting quantum gates (i.e., gates among which no particular order is superimposed) that allow for great flexibility and parallelism in the quantum gates execution. The typical QAOA circuit C is divided in the following ordered phases: (i) *initial state preparation* (INIT block), (ii) *phase-shift* (P-S block), and (iii) *mixing* (MIX block). The blocks P-S and MIX are repeated for p times.

Specifically, the *initial state preparation* phase serves the purpose of initializing the quantum states to represent a *feasible* initial assignment, the *phase shift* (P-S) layer is composed of a series of phase-shift (R_Z and R_{ZZ}) gates realizing the *problem Hamiltonian* (H_g) whose state of lowest energy corresponds to the minimum of the objective function we are aiming at, and finally the *MIX* layer

[1]Different names and abbreviations may be found in the literature, as for example *Unconstrained Binary Quadratic Programming* (*UBPQ*) [14], or *Quadratic Pseudo-Boolean optimization* (*QPBO*) [2].
[2]Fujitsu's digital annealer: https://bit.ly/3ySnkrq.
[3]D-Wave webiste: https://www.dwavesys.com.

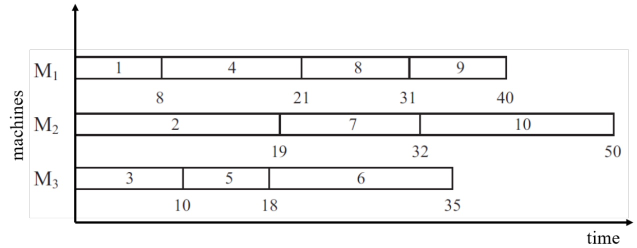

Figure 1: Example of Flexible Open Shop scheduling solution, composed 10 activities assigned to 3 machines. The makespan of the solution schedule is equal to 50.

serves the purpose of mixing the states that evolve from the PS, thus functioning as a driver to explore new regions of the solution space and allowing the algorithm to escape from local minima and converge towards the optimal solution.

QAOA has been successfully applied to many combinatorial optimization problems.

3 THE PROBLEM

In the Flexible Open Shop Scheduling problem we have n operations $o_1, \ldots, o_n$, each of them has to be performed on any of m machines $M_1, \ldots, M_m$ (see Figure 1 for a simple example that uses 3 machines and 10 operations). There are no precedence relation among the operations. The processing time of o_i on the machine M_j is p_{ij}. The problem is to assign each operation o_i to a machine $M(o_i)$ such that the largest end time of all the operations is minimized. It is easy that this problem corresponds to minimizing the makespan of all the machines.

In more details, let $C_j = \sum_{i\,:\,M(o_i)=M_j} p_{ij}$ be the processing time of all the operations assigned the machine M_j; then, the problem requires to minimize C_{max}, i.e. the time

$$C_{max} = \max\{C_1, \ldots C_m\}$$

This combinatorial optimization problem is NP-hard and there exist many approaches to solve it, ranging from exact algorithms to metaheuristics approaches.

4 FORMULATION AS QUBO

The formulation of this problem as a QUBO problem is performed in the following way. Let $\{x_{ij}\}$, for $i = 1, \ldots, n$ and $j = 1, \ldots, m$, be a set of mn binary variables which represent the *one-hot* encoding of the assignment operation-machine, i.e., $x_{ij} = 1$ if and only if o_i is assigned to M_j.

The constraints on x_{ij} are

$$\sum_{j=1}^{m} x_{ij} = 1 \qquad (1)$$

for $i = 1, \ldots, n$. These constraints enforce that each operation is assigned exactly to one machine.

Let l be the number of bits required to represent the quantity

$$\max\{\sum_{i=1}^{n} p_{ij} \ : \ j = 1, \ldots, m\},$$

i.e., all the possible values for the makespan. Let $\{z_0, \ldots, z_{l-1}\}$ be a set of l binary variables, and let $z = \sum_{h=0}^{l-1} 2^h z_h$ be the value corresponding to C_{max}, which is to be minimized.

Let $\sum_{i=1}^{n} x_{ij} p_{ij}$ be the sum of all the durations of the operations assigned to the j-th machine M_j, and let $\{\tau_{jh}\}$, for $j = 1, \ldots, m$ and $h = 0, \ldots, l-1$, be a set of ml binary variables, which are used to encode each inequality $C_j \leq z$, for each M_j, by means of the linear constraint

$$\sum_{i=1}^{n} x_{ij} p_{ij} + \sum_{h=0}^{l-1} 2^h \tau_{jh} = z \tag{2}$$

where the number $\sum_{h=0}^{l-1} 2^h \tau_{jh}$ serves as a slack term which transforms the inequality $\sum_{i=1}^{n} x_{ij} p_{ij} \leq z$ to the equality relation (2). Hence the objective function to be minimized is

$$f(x, z, \tau) = \sum_{h=0}^{l-1} 2^h z_h + K_1 \sum_{i=1}^{n} \left(\sum_{j=1}^{m} x_{ij} - 1 \right)^2 + K_2 \sum_{j=1}^{m} \left(\sum_{i=1}^{n} x_{ij} p_{ij} + \sum_{h=0}^{l-1} 2^h (\tau_{jh} - z_h) \right)^2 \tag{3}$$

where the first term corresponds to z and K_1 and K_2 are two constants large enough to enforce the constraints among the variables.

The number of binary variables present in f is $mn + l + ml = mn + (m+1)l$, which is polynomial in m, n and l. In particular, it is worth noticing that the number l grows logarithmically with respect to the processing times p_{ij}. This formulation of the FOSSP as a QUBO problem enables to use Quantum and Digital Annealers for its resolution.

5 FORMULATION FOR QAOA

As opposed to the QUBO formulation, in the QAOA formulation of the FOSSP it is possible to exploit the fact that the variables x_{ij} are mutually exclusive and exhaustive. In fact, it is possible to start with an initial state which is a superposition of all the legal operation-machine assignments (i.e., that satisfy the equation 1) and to use the MIX_{XY} gates as mixing blocks for qubits associated to x_{ij} because they do not produce any illegal state. The details are described later in this section.

Hence, the objective function is reduced to

$$g(x, z, \tau) = \sum_{h=0}^{l-1} 2^h z_h + K_2 \sum_{j=1}^{m} \left(\sum_{i=1}^{n} x_{ij} p_{ij} + \sum_{h=0}^{l-1} 2^h (\tau_{jh} - z_h) \right)^2 \tag{4}$$

The circuit needs $mn+(m+1)l$ qubits, which are divided in n registers of size m $R_1, \ldots, R_n$ and $m+1$ registers $S_0, S_1, \ldots, S_m$ of size l. For each $i = 1, \ldots, n$, the register R_i corresponds to the binary variables $x_{i1}, \ldots, x_{im}$. The register S_0 encodes the bits $z_0, \ldots, z_{l-1}$, while each registers S_j, with $j = 1, \ldots, m$ encodes the bits $\tau_{j0}, \ldots, \tau_{j,l-1}$.

The Hamiltonian associated to g is

$$H_g = H_z + K_2 \sum_{j=1}^{m} H_{C_j}$$

where H_z is the Hamiltonian related to the term $\sum_{h=0}^{l-1} 2^h z_h$, while H_{C_j} is the Hamiltonian related to the term

$$\left(\sum_{i=1}^{n} x_{ij} p_{ij} + \sum_{h=0}^{l-1} 2^h (\tau_{jh} - z_h)\right)^2,$$

for each $j = 1, \ldots, m$.

The analytical form of H_z is

$$H_z = \frac{1}{2}(2^l - 1)I - \frac{1}{2} \sum_{h=0}^{l-1} 2^h Z_h^{(0)} \tag{5}$$

where $Z_h^{(0)}$ is the gate Z applied to the h-th qubit of the register S_0.

The analytical form of each Hamiltonian H_{C_j} is quite complex and involves the operators $Z_{i,j}^{\tau}$, which are the gates Z applied to the qubit j of the register S_i, the operators $Z_{i,j}^{x}$, which are the gates Z applied to the qubit j of the register R_i. and also the gates Z_h^0. H_{C_j} is composed as a quadratic polynomial of the operators mentioned above, i.e., it is a summation of a constant term (which can be neglected) and $\frac{(1+n+2l)(n+2l)}{2}$ terms, where each term is a monomial composed of a coefficient and a single operator, or a product of two operators.

The initialization phase is performed with two different methods. Each register R_i is initialized with the operator W_N, described in [9], and it will assume the state

$$\sqrt{\frac{1}{m}} \left(|100\ldots0\rangle + |010\ldots0\rangle + \cdots + |000\ldots1\rangle \right). \tag{6}$$

The other registers are initialized with the Hadamard gates H^l and they will assume the initial state

$$\sqrt{\frac{1}{2^l}} \sum_{h=0}^{2^l-1} |h\rangle . \tag{7}$$

The p-th phase shifting layer is composed by the rotation gates $R_Z(k\gamma_p)$, for each linear term appearing in the Hamiltonian H_g, and by the rotation gates $R_{ZZ}(k\gamma_p)$ for each nonlinear term of H_g (where k is the coefficient of term). Since all these gates commute with each other, any order of application can be used.

The p-th mixing layer, analogously as in the initialization phase, is divided in two parts. The mixing gates for the qubits of all the registers S_i are just the rotation gate $R_X(\beta_p)$. For the qubits of the registers R_i, we employ the strategy "Parity single-qudit ring mixer" as described in [11], to overcome the problem of non commutativity.

Specifically, the unitary transformation

$$U_j(\beta_p) = U_{j,\text{last}}(\beta_p) U_{j,\text{even}}(\beta_p) U_{j,\text{odd}}(\beta_p)$$

is applied to each register R_j. The transformation $U_{j,\text{even}}(\beta_p)$ is defined as

$$U_{j,\text{even}}(\beta_p) = \prod_{a \text{ even}} \exp\left(-i\beta_p (X_{j,a} X_{j,a+1} + Y_{j,a} Y_{j,a+1})\right)$$

where $X_{j,a}$ and $Y_{j,a}$ are the gates X and Y applied to a–th qubit of R_j, respectively. The unitary transformation $U_{j,\text{odd}}$ is analogously defined, while $U_{j,\text{last}}$ is $\exp\left(-i\beta_p (X_{j,m} X_{j,1} + Y_{j,m} Y_{j,1})\right)$, for m odd, otherwise it is the identity operator. The graphical representation

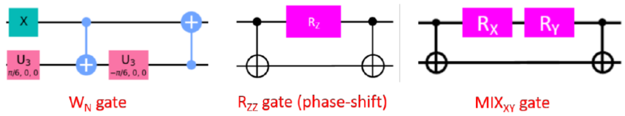

Figure 2: Graphical representation of the binary gates of the resulting quantum citcuit: the W_N gate used in the initialization of the R_i registers, the R_{ZZ} gate used in the construction of the nonlinear terms of H_g, and the MIX_{XY} used in the mixing Hamiltonian.

of all the binary gates that are present in the final circuit is shown in Figure 2.

The final step of the circuit comprises the measurement of the registers R_j, from which it is possible to extract a solution of the FOSSP instance.

6 CONCLUSIONS AND FUTURE WORK

In this paper we have proposed a novel formalization of the Flexible Open Shop Scheduling Problem for quantum computing resolution. We have firstly provided a compact formulation in the Quadratic Unconstrained Binary Optimization (QUBO) formalism, apt to be used with quantum annealers. Subsequently, we have provided a precise description of the resulting quantum circuit that represents the quantum segment of a Quantum Approximate Optimization Algorithm (QAOA). The presented circuit comprises the quantum gates that realize the initialization phase, the quantum gates that realize the cost Hamiltonian, and finally the gates that compose the mixing Hamiltonian.

As future work, we intend to test the proposed representations on Open Job Shop instances of size compatible with the currently available quantum architectures and/or their simulated counterparts.

Experimenting our approach on real quantum annealers requires to adapt the QUBO formulation, described in Section 4, to the topology of the architecture and to find the suitable values of the coefficients K_1 and K_2.

On the other hand, it is also possible to use the circuit, described in Section 5, within the QAOA framework either on a simulated or a real quantum backend. To this purpose, it will be necessary to tackle a number of further issues such as finding high-quality parameters to drive the quantum optimization process [20]. Given that the QAOA is a hybrid approach that is composed of a quantum processing component and a classical optimization component, another important aspect to take into account is the selection of a classic optimizer that is mostly effective for the problem at hand [6, 22]. Another possible future work is to generalize our approach to different scheduling problems, besides the FOSSP.

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