An introduction to variational quantum algorithms on gate-based quantum computing for combinatorial optimization problems

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Abstract

Noisy intermediate-scale quantum computers (NISQ computers) are now readily available, motivating many researchers to experiment with Variational Quantum Algorithms (VQAs). Among them, the Quantum Approximate Optimization Algorithm (QAOA) is one of the most popular one studied by the combinatorial optimization community. In this tutorial, we provide a mathematical description of the class of Variational Quantum Algorithms, assuming no previous knowledge of quantum physics from the readers. We introduce precisely the key aspects of these hybrid algorithms on the quantum side (parametrized quantum circuit) and the classical side (guiding function, optimizer). We devote a particular attention to QAOA, detailing the quantum circuits involved in that algorithm, as well as the properties satisfied by its possible guiding functions. Finally, we discuss the recent literature on QAOA, highlighting several research trends.

keywords: Variational Quantum Algorithm, QAOA, Combinatorial Optimization, Metaheuristics

1 Introduction

This tutorial aims to provide the operational research community with some background knowledge of quantum computing and explore the particular branch of heuristic quantum algorithms for combinatorial optimization. Today, the quantum information theory community is excited by the emergence of quantum computers first theorized in the 1980s. Indeed, since then, some theoretical advantages of quantum algorithms compared with classical algorithms have been proved for several problems. For instance, the Quantum Phase Estimation [24], which is the subroutine of Shor's algorithm [41], enables the latter to solve the integer factorization problem efficiently. Moreover, Grover Search [15] finds an element in an unstructured base with a quadratic speedup compared with classical algorithms. This algorithm is also used as a subroutine in dynamic programming algorithms to improve their exponential complexity for problems such as the Travelling Salesman Problem and the Minimum Set Cover [1]. More recently, a polynomial speedup that relies on a Quantum Interior Point Method [22] applies to Linear Programming, Semi-Definite Programming, and Second-Order Cone Programming [23]. Furthermore, a quantum subroutine for the Simplex also provides a polynomial speedup [34].

These algorithms prove quantum advantages on numerous problems, but their implementations require a lot of quantum resources with high quality. Specifically, they need quantum computers

with many qubits that can interact two by two and quantum operations that can be applied in a row on qubits without generating noise, namely they can support deep-depth quantum circuits. Such quantum computers are believed to be built in the medium term but current devices are noisy intermediate-scale quantum computers, usually referred to as NISQ computers [38]. Therefore, NISQ computers cannot handle the implementations of such algorithms. These physical limitations encouraged quantum algorithm theory to look into *lighter* quantum algorithms to implement them on quantum computers today. It consists of hybrid algorithms that require both quantum and classical resources. Indeed, the classical part overcomes the limited and noisy quantum resources, whereas the quantum part still takes partial advantage of quantum information theory. This tutorial focuses on a particular type of hybrid algorithm, that is the class of Variational Quantum Algorithms (VQAs).

Variational Quantum Algorithms are heuristic algorithms that alternate between a quantum circuit and a classical optimizer. They tackle optimization problems of the form

$$\min_{x\in\{0,1\}^n} f(x)\,, \tag{1}$$

where f is any function defined on $\{0,1\}^n$. VQAs are of great interest to the quantum information theory community today because they have the convenient property of an adjustable quantum circuits' depth, making them implementable on the current NISQ computers. The variational approach of VQAs [5] consists of probing the initial search space $\{0,1\}^n$ with a relatively small set of parameters optimized classically. Specifically, these parameters describe a probability distribution over the search space. This description results from a sequence of quantum logic gates: this is a quantum circuit. VQAs take advantage of the quantum computing principle [35] that prepares a probability distribution over an exponential search space in a short sequence of quantum gates. The choice of the quantum circuit, and in particular the number of parameters, is a huge stake for VQAs [33]. On the one hand, the more parameters, the more precise the search space probing. On the other hand, too many parameters can harden the classical optimization part. The function that drives this optimization, which depends on the probability distribution and f, is also a non-trivial choice and worth investigating [2].

In this tutorial, we provide a mathematical description of Variational Quantum Algorithms and focus on one of them, specifically the Quantum Approximate Optimization Algorithm (QAOA) [9]. We shall also devote particular attention to problems in which f is a polynomial function. In Section 2, we give a brief introduction to the basics of quantum computing for combinatorial optimization. Notice that the model of quantum computation considered is the gate-based model, also called the circuit model. Then, in Section 3, we describe the general class of VQAs, starting by defining the different parts that constitute and define a VQA, namely the quantum circuit (also called *ansatz* in the literature), the classical optimizer, and the guiding function driving the classical optimization. Then, we characterize each part with properties that should be valid for potential theoretical guarantees. Eventually, in Section 4, we focus on a particular case of VQAs, the Quantum Approximate Optimization Algorithm. We describe the necessary reformulation of the initial problem (1) into a hermitian matrix (also called Hamiltonian in the literature) to be solved by QAOA and analyze this algorithm in light of the previous properties of Section 3. We also provide a universal decomposition of the QAOA quantum circuit for the general case where f is polynomial while, as far as we know, only the quadratic f case had been treated in the literature so far. Finally, we give a condensed overview of empirical trends and theoretical limitations of QAOA. We remind some helpful basic notions of linear algebra in Appendix A. Furthermore, the proofs of technical properties of the function optimized in VQAs and specific constructions

of the quantum circuit in QAOA are deferred to Appendices B.1 and B.2, respectively.

2 Basics of quantum computing for combinatorial optimization

This section aims to provide the basic notions of quantum computing necessary for the understanding of the quantum resolution of combinatorial problems.

2.1 Quantum bits

Let $|0\rangle$ and $|1\rangle$ denote the basic states of our quantum computer (the counterpart of states 0 and 1 in classical computers). The first building block of quantum algorithms is the quantum bit, also called qubit.

Definition 1 (Qubit)**.** *We define a qubit as*

$$|q\rangle = q_0 |0\rangle + q_1 |1\rangle \ , \tag{2}$$

where $(q_0, q_1) \in \mathbb{C}^2$ *is a pair of complex numbers that satisfies the normalizing condition*

$$|q_0|^2 + |q_1|^2 = 1 \, .$$

We say that q_0 *and* q_1 *are the* coordinates *of* $|q\rangle$ *in the basis* $(|0\rangle, |1\rangle)$*.*

It is often convenient to use the matrix representation of $|0\rangle$ and $|1\rangle$, namely

$$|0\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \text{ and } |1\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix} .$$

With this matrix representation, the qubit $|q\rangle$ defined in (2) is equal to

$$|q\rangle = \begin{pmatrix} q_0 \\ q_1 \end{pmatrix} .$$

Example 2. *Important examples of one-qubit states are* $\frac{|0\rangle+|1\rangle}{\sqrt{2}}$ *and* $\frac{|0\rangle-|1\rangle}{\sqrt{2}}$*. These are usually denoted as* $|+\rangle$ *and* $|-\rangle$*, respectively.*

The algorithms studied in this paper typically manipulate quantum states of larger dimension. Specifically, let n denote the number of qubits that our quantum computing device is able to manipulate simultaneously. An n-qubit state is defined by 2^n complex numbers that satisfy the normalizing condition and represent the normal decomposition on the canonical basis.

Definition 3 (Canonical basis)**.** *The canonical basis of an* n*-qubit state is the set*

$$\mathcal{CB}_n = \left(\bigotimes_{k=1}^{n} \left| i^{(k)} \right\rangle , (i^{(1)}, \ldots, i^{(n)}) \in \{0,1\}^n \right) ,$$

where $i^{(k)}$ *represents the state of the* k*-th qubit. The canonical basis is the set of all possible combinations of tensor products of* n *one-qubit basis states,* $|0\rangle$ *and* $|1\rangle$*. For more readability, we omit to write the tensor product between qubits, i.e. we refer to the canonical basis as*

$$\mathcal{CB}_n = (|i\rangle , i \in \{0,1\}^n) \, .$$

Definition 4 (n-qubit state)**.** *An n-qubit state $|\psi\rangle$ is a normalized linear combination of the basis states in $\mathcal{CB}_n$,*

$$|\psi\rangle = \sum_{i\in\{0,1\}^n} \psi_i \, |i\rangle \ ,$$

where $(\psi_i)_{i\in\{0,1\}^n} \in \mathbb{C}^{2^n}$ are its coordinates, which satisfy the normalizing condition

$$\langle\psi|\psi\rangle = \sum_{i\in\{0,1\}^n} |\psi_i|^2 = 1 \, . \tag{3}$$

For $n = 1$, we find the definition of a qubit (Definition 1), as expected.

Example 5. *For instance, $\frac{|00\rangle+|11\rangle}{\sqrt{2}}$, called $|\psi_+\rangle$, is a two-qubit state. Its matrix representation is :*

$$\begin{aligned}
|\psi_+\rangle &= \frac{|00\rangle + |11\rangle}{\sqrt{2}} \\
&= \frac{1}{\sqrt{2}} \left(\begin{pmatrix} 1 \\ 0 \end{pmatrix} \otimes \begin{pmatrix} 1 \\ 0 \end{pmatrix} + \begin{pmatrix} 0 \\ 1 \end{pmatrix} \otimes \begin{pmatrix} 0 \\ 1 \end{pmatrix} \right) \\
&= \frac{1}{\sqrt{2}} \left(\begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix} + \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix} \right) \\
&= \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 0 \\ 0 \\ 1 \end{pmatrix} .
\end{aligned}$$

Remark 6. *Our notation $(\psi_i)_{i\in\{0,1\}^n} \in \mathbb{C}^{2^n}$ for the coordinates of $|\psi\rangle$ in basis $\mathcal{CB}_n$ is used to simplify the presentation throughout. It is, however, uncommon in the quantum computing literature where different bases may be used.*

2.2 Quantum gates

In the model of gate-based quantum computation, qubits are manipulated with quantum gates. Mathematically speaking, these quantum gates are modeled by unitary matrices. More precisely, a quantum gate that manipulates n-qubit states is a matrix in $\mathcal{M}_{2^n}(\mathbb{C})$ that modifies the 2^n complex coefficients of a quantum state such that they still satisfy the normalizing condition (3).

Definition 7 (Unitary matrix)**.** *A matrix $U \in \mathcal{M}_{2^n}(\mathbb{C})$ is unitary if its inverse is equal to its conjugate transpose (denoted by the dagger symbol $\dagger$) :*

$$UU^\dagger = U^\dagger U = I \, .$$

Notice that the application of a quantum gate is logically reversible.

We easily see that a unitary matrix U preserves the normalizing condition since, denoting $|\psi'\rangle = U\,|\psi\rangle$, we have

$$\langle\psi'|\psi'\rangle = \langle\psi|\, U^\dagger U \,|\psi\rangle = \langle\psi|\psi\rangle \ .$$

As an illustration, we describe below all the possible one-qubit gates, i.e. all the unitary matrices in $\mathcal{M}_2(\mathbb{C})$.

Example 8 (Generic one-qubit gate)**.** *A generic one-qubit gate* $U = \begin{pmatrix} a & b \\ c & d \end{pmatrix} \in \mathcal{M}_2(\mathbb{C})$ *satisfies*

$$\begin{cases} |a|^2 + |b|^2 = 1 \\ a\bar{c} + b\bar{d} = 0 \\ \bar{a}c + \bar{b}d = 0 \\ |c|^2 + |d|^2 = 1 \end{cases}$$

Its application on a qubit $|q\rangle = q_0 |0\rangle + q_1 |1\rangle$ *is:*

$$U|q\rangle = \begin{pmatrix} a & b \\ c & d \end{pmatrix} \begin{pmatrix} q_0 \\ q_1 \end{pmatrix} = \begin{pmatrix} aq_0 + bq_1 \\ cq_0 + dq_1 \end{pmatrix} = (aq_0 + bq_1)|0\rangle + (cq_0 + dq_1)|1\rangle = |q'\rangle \tag{4}$$

We introduce next the circuit representation of a quantum gate, which is a useful formalism to represent unitary matrices. Specifically, Figure 1 represents the application of the quantum gate U to the one-qubit state $|q\rangle$, as in (4), by:

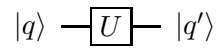

Figure 1: Circuit of gate U applying to $|q\rangle$.

This representation easily generalizes to n-qubit quantum gates, where each *horizontal line* is associated with a qubit.

2.3 Quantum circuits

We can manipulate quantum gates to build other quantum gates in two different ways. The first one is the *composition*, and the other one is the *tensor product*.

Definition 9 (Composition of quantum gates)**.** *The composition of gates only operates between gates acting on the same qubits. Let* k *be the number of involved qubits. The composition of* $U_1 \in \mathcal{M}_{2^k}(\mathbb{C})$ *and* $U_2 \in \mathcal{M}_{2^k}(\mathbb{C})$ *consists of the application of* U_1 *followed by the application of* U_2*. The matrix representation of this composition is the product* U_2U_1*. The circuit representation of this composition is illustrated on Figure 2 for* $k = 3$*.*

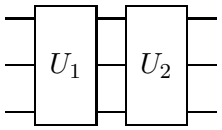

Figure 2: Composition of U_1 and U_2.

It can be seen as a series sequence of gates.

Notice that we read from right to left in the matrix representation, and from left to right in the circuit representation. Moreover, in the circuit representation, qubits are numbered in ascending order from top to bottom.

Definition 10 (Tensor product of quantum gates)**.** *The tensor product of gates only operates between gates acting on different qubits. Suppose* $U_1 \in \mathcal{M}_{2^k}(\mathbb{C})$ *applies on the first* k *qubits and*

$U_2 \in \mathcal{M}_{2^{k'}}(\mathbb{C})$ applies on the k' following ones. Their tensor product is the application of U_1 and U_2 on respective qubits in parallel. The matrix representation of this tensor product is $U_1 \otimes U_2$ (Definition 40). The circuit representation is depicted on Figure 3 for $k = 3$ and $k' = 2$.

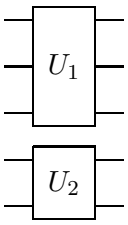

Figure 3: Tensor product of U_1 and U_2.

Notice that when we apply a quantum gate on k qubits of an n-qubit system, it supposes that we apply identity gate $I = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$ on the qubits not concerned. For instance, let us consider a 3-qubit system on which we apply $U \in \mathcal{M}_2(\mathbb{C})$ on qubit number 2. The matrix representation of the resulting 3-qubit gate is $I \otimes U \otimes I$, and its circuit representation is illustrated on Figure 4, where the application of I is usually replaced by a simple wire.

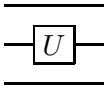

Figure 4: Application of U to qubit number 2.

One readily verifies that both composition and tensor product transform unitary matrices into a resulting unitary matrix.

Throughout, we consider that a quantum algorithm is a quantum circuit acting on n qubits, that is, a sequence of quantum gates' compositions and/or tensor products. These quantum gates can be k-qubit gates, for $k \in [n]$. However, quantum gates involving many qubits are typically not implementable natively on quantum computers and need to be decomposed into smaller and simpler gates. This set of small gates can be considered as the quantum counterpart of the elementary logic gates used in classical circuit computing to assess the circuit complexity of a classical algorithm. Thus, an n-qubit quantum algorithm is described by a unitary matrix in $\mathcal{M}_{2^n}(\mathbb{C})$, and we decompose it as a sequence of universal gates (Definition 11) to obtain the complexity of the quantum algorithm.

Definition 11 (Set of universal gates)**.** *A set of quantum gates PU is* universal *if we can decompose any n-qubit quantum gate through a circuit composed solely of the gates in PU.*

Fortunately, there exist different universal sets of quantum gates. We introduce below such a set formed of four types of gates. First, we consider three following families of one-qubit gates, each of which is parametrized by a real number $\theta \in \mathbb{R}$:

$$R_X(\theta) = \begin{pmatrix} \cos\frac{\theta}{2} & -i\sin\frac{\theta}{2} \\ -i\sin\frac{\theta}{2} & \cos\frac{\theta}{2} \end{pmatrix}, \tag{5}$$

$$R_Y(\theta) = \begin{pmatrix} \cos\frac{\theta}{2} & -\sin\frac{\theta}{2} \\ \sin\frac{\theta}{2} & \cos\frac{\theta}{2} \end{pmatrix}, \tag{6}$$

$$R_Z(\theta) = \begin{pmatrix} e^{-i\frac{\theta}{2}} & 0 \\ 0 & e^{i\frac{\theta}{2}} \end{pmatrix}. \tag{7}$$

Notice that these gates are often referred to as rotation gates because they correspond to rotations in a certain representation of qubits, known as the Bloch sphere [31]. Second, we consider the two-qubit gate CX:

$$CX = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix}. \tag{8}$$

CX applies gate $X = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$ on the second qubit if and only if the first qubit is in state $|1\rangle$.

Remark 12 (Notation on gates indexes)**.** *Henceforth, we use the notation $R_{X,i}$ for the application of R_X on qubit i (and the application of identity matrix on the remaining qubits). We do the same with $R_{Y,i}$ and $R_{Z,i}$. We note $CX_{i,j}$ the application of CX gate to qubits i and j : X is applied to qubit j if and only if qubit i is in state $|1\rangle$.*

Theorem 13 (Universal gates [35])**.** *The set of one-qubit gates and the CX gate* (8) *is universal. Thus, because any one-qubit gate is the composition of rotation gates* (5)–(7)*, the set $PU = \{R_X(\alpha), R_Y(\beta), R_Z(\gamma), CX : \alpha, \beta, \gamma \in \mathbb{R}\}$ is universal.*

In comparison, the sets of gates {NAND}, {NOR}, {NOT, AND} and {NOT, OR} are universal for classical computation. Indeed, we can compute any arbitrary classical function with them. In view of the above, we typically consider that the quantum counterpart of the classical number of elementary operations is the number of universal gates used to decompose the circuit. Of course, this decomposition depends on the set of universal gates PU considered, but the number of gates required is the same with any set, modulo a multiplicative constant [35]. Thereafter, we only consider the set PU defined in Theorem 13. This choice is motivated by the algorithms we study in this paper, as it will be convenient to express them with this set. Furthermore, if we consider the family of circuits $(\mathcal{C}_n)_{n\in\mathbb{N}}$ where $\mathcal{C}_n$ is a circuit on n qubits and is decomposed on $\mathcal{O}(poly(n))$ universal quantum gates, then this family is said *efficient*.

2.4 Non-classical behaviors

The quantum algorithms we present in this paper rely on three characteristics of quantum states with no classical equivalent: measurement, superposition, and entanglement. Let us present these notions through the bare minimum mathematical background.

2.4.1 Measurement

We need to measure a quantum state $|\psi\rangle$ to get information from it. Otherwise, no information is accessible. The peculiar property of measurement is that it only extracts partial information from the quantum state: the single measurement output of $|\psi\rangle$ is a bitstring.

Definition 14 (Measurement)**.** *In the gate-based quantum model, the measurement $\mathcal{M}$ of an n-qubit state $|\psi\rangle = \sum_{i\in\{0,1\}^n} \psi_i |i\rangle$ outputs the n-bitstring i with probability $|\psi_i|^2$. After having been measured, state $|\psi\rangle$ no longer exists: it has been replaced by the state $|i\rangle$.*

For example, measuring qubit $|q\rangle = q_0 |0\rangle + q_1 |1\rangle$ outputs 0 with probability $|q_0|^2$ and 1 with probability $|q_1|^2$, and changes the state $|q\rangle$ to $|0\rangle$ and $|1\rangle$, respectively. A measurement appears as a loss of information. Indeed, we describe an n-qubit state by 2^n normalized complex coefficients, but we only extract an n-bitstring after measuring it. The perfect knowledge of the probabilities representing a given quantum state $|\psi\rangle$, namely the square module of each of its coordinates $(|\psi_i|^2)_{i\in\{0,1\}^n} \in [0,1]^{2^n}$, can be obtained only if we measure $|\psi\rangle$ an infinite number of times. Notice that it requires resetting state $|\psi\rangle$ after each measurement.

Remark 15 (Sampling of quantum states)**.** *In reality we are limited to approximating a given quantum state through sampling. In particular, if $|\psi\rangle$ is the result of an algorithm, this means we have to repeat the same algorithm for every measurement of $|\psi\rangle$ we wish to perform.*

2.4.2 Superposition

Classically, the state of an n-bit computer is given by a bitstring in $\{0,1\}^n$. We have seen so far that the state of an n-qubit quantum computer is given by its coordinates $(\psi_i)_{i\in\{0,1\}^n} \in \mathbb{C}^{2^n}$, which satisfy $\sum_{i\in\{0,1\}^n} |\psi_i|^2 = 1$. In general, more than one of the coordinates are different from 0, meaning that measuring $|\psi\rangle$ may result in different bitstring $i \in \{0,1\}^n$.

Definition 16 (Superposition)**.** *A quantum state $|\psi\rangle$ is said in superposition if $|\psi\rangle = \sum_{i\in\{0,1\}^n} \psi_i |i\rangle$ where there are at least two terms with non-zero coefficients in the sum. A quantum state that is not a basis state is in superposition.*

The following Hadamard gate is the usual one-qubit gate that produces superposition starting from a canonical basis state.

Example 17 (Hadamard gate)**.** *The Hadamard gate $H = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}$ is essential in quantum computing because it creates superposition starting from a basis state. We obtain the state $|+\rangle$, respectively $|-\rangle$, of Example 2 by applying H on $|0\rangle$, respectively $|1\rangle$:*

$$H|0\rangle = \frac{|0\rangle + |1\rangle}{\sqrt{2}} = |+\rangle \ ,$$
$$H|1\rangle = \frac{|0\rangle - |1\rangle}{\sqrt{2}} = |-\rangle \ .$$

Example 18 (Uniform superposition)**.** *The two states $|+\rangle$ and $|-\rangle$ are in uniform superposition because both have the same probability of being measured as 0 or 1. In general, an n-qubit state uniformly superposed is equal to $\frac{1}{\sqrt{2^n}} \sum_{j\in\{0,1\}^n} e^{i\alpha_j} |j\rangle$, with $\alpha_j \in [0, 2\pi[$, $\forall j \in \{0,1\}^n$. In what follows, we shall often use the uniformly superposed n-qubit state $|+\rangle^{\otimes n} = \frac{1}{\sqrt{2^n}} \sum_{i\in\{0,1\}^n} |i\rangle$.*

Notice that applying an n-qubit quantum gate U to $|\psi\rangle$ possibly modifies the 2^n coordinates of $|\psi\rangle$ since

$$U|\psi\rangle = \sum_{i\in\{0,1\}^n} \psi'_i |i\rangle \ ,$$

where possibly each ψ_i' differs from ψ_i. This is the case, for instance, when applying the tensor product of n Hadamard gates, each applied to a qubit initially in state $|0\rangle$, specifically

$$H^{\otimes n}|0\rangle^{\otimes n} = \bigotimes_{i=1}^{n} H|0\rangle = \bigotimes_{i=1}^{n}\left(\frac{|0\rangle+|1\rangle}{\sqrt{2}}\right) = \frac{1}{\sqrt{2^n}}\sum_{i\in\{0,1\}^n}|i\rangle = |+\rangle^{\otimes n}\,. \tag{9}$$

Equation (9) illustrates the potential benefit of quantum circuits: applying $\mathcal{O}(n)$ universal one-qubit gates impacts the exponentially many coefficients of $|\psi\rangle$. Indeed, one readily verifies that $H = R_X(\pi)R_Y(\frac{\pi}{2})$ modulo a global phase[1], so $H^{\otimes n}$ amounts to applying $2n$ universal one-qubit gates.

2.4.3 Entanglement

Each quantum state is either a product state or an entangled state. Entanglement has the peculiar and helpful property that we can apply a circuit only on a part of the n-qubit system, and as a result, the whole system is affected.

Definition 19 (Product state)**.** *An n-qubit state is a product state if it is the tensor product of n one-qubit states. In other words, an n-qubit state $|\psi\rangle$ is a product state if it exists $2n$ complex coefficients $(q_0^{(j)}, q_1^{(j)})_{j\in[n]}$ such that*

$$|\psi\rangle = \bigotimes_{j=1}^{n}(q_0^{(j)}|0\rangle + q_1^{(j)}|1\rangle),\ \textit{with}\ |q_0^{(j)}|^2 + |q_1^{(j)}|^2 = 1, \forall j \in [n]\,.$$

Thus, each state of a qubit that composes $|\psi\rangle$ can be described independently of the states of the other.

If an n-qubit state is not a product state, it is an entangled state.

Definition 20 (Entangled state)**.** *An n-qubit state $|\psi\rangle = \sum_{i\in\{0,1\}^n}\psi_i|i\rangle$ is entangled if the numerical values of its coordinates $(\psi_i)_{i\in\{0,1\}^n} \in \mathbb{C}^{2^n}$ admit no solution $(q_0^{(j)}, q_1^{(j)})_{j\in[n]} \in \mathbb{C}^{2n}$ to the system*

$$\begin{cases} \displaystyle\sum_{i\in\{0,1\}^n}\psi_i|i\rangle = \bigotimes_{j=1}^{n}(q_0^{(j)}|0\rangle + q_1^{(j)}|1\rangle) \\ |q_0^{(j)}|^2 + |q_1^{(j)}|^2 = 1, \forall j \in [\![1, n]\!] \end{cases}$$

It means that operations performed on some coordinates of the entangled state can affect the other coordinates without direct operations on them.

Notice that when an n-qubit system is entangled, it makes no sense to speak about qubit number $k \in [n]$ because isolated qubits are not defined. Notice also that there is a difference between superposition and entanglement. A state is in superposition if at least two non-zero coefficients are in its basis decomposition. A state is entangled if it cannot be written as a tensor product of independent qubits, implying that it is in superposition.

To illustrate the notion of entanglement, we consider the following quantum circuit on Figure 5. Starting from a two-qubit product state $|00\rangle$, it results an entangled state.

[1]Two quantum states $|\psi\rangle$ and $|\psi'\rangle = e^{i\alpha}|\psi\rangle$, with $\alpha \in [0, 2\pi[$, that only differ by a global phase are indiscernible by measurement. Thus, we do not consider global phase of quantum states nor quantum gates.

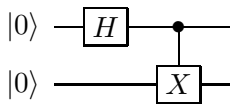

Figure 5: Entangling circuit.

This circuit is the application of Hadamard gate on qubit 1, followed by $CX_{1,2}$. The quantum state that results is $|\Phi^+\rangle$ of Example 5:

$$\begin{aligned} CX_{1,2}(H \otimes I)\,|00\rangle &= CX_{1,2}\left(\frac{1}{\sqrt{2}}(|00\rangle + |10\rangle)\right) \\ &= \frac{1}{\sqrt{2}}\left(CX_{1,2}\,|00\rangle + CX_{1,2}\,|10\rangle\right) \\ &= \frac{1}{\sqrt{2}}(|00\rangle + |11\rangle) \\ &= \left|\Phi^+\right\rangle . \end{aligned}$$

We prove now by contradiction that $|\Phi^+\rangle$ is entangled. Suppose that $|\Phi^+\rangle$ is a product state. Thus, there exists $(q_0^{(0)}, q_1^{(0)}) \in \mathbb{C}^2$ such as $|q_0^{(0)}|^2 + |q_1^{(0)}|^2 = 1$ and $(q_0^{(1)}, q_1^{(1)}) \in \mathbb{C}^2$ such as $|q_0^{(1)}|^2 + |q_1^{(1)}|^2 = 1$, satisfying:

$$\begin{aligned} \left|\Phi^+\right\rangle &= (q_0^{(0)}\,|0\rangle + q_1^{(0)}\,|1\rangle) \otimes (q_0^{(1)}\,|0\rangle + q_1^{(1)}\,|1\rangle) \\ &= q_0^{(0)}q_0^{(1)}\,|00\rangle + q_0^{(0)}q_1^{(1)}\,|01\rangle + q_1^{(0)}q_0^{(1)}\,|10\rangle + q_1^{(0)}q_1^{(1)}\,|11\rangle . \end{aligned}$$

Because the decomposition of a quantum state's coordinates is unique in the canonical basis, it follows by identification:

$$\begin{cases} q_0^{(0)}q_0^{(1)} &= \frac{1}{\sqrt{2}} \\ q_0^{(0)}q_1^{(1)} &= 0 \\ q_1^{(0)}q_0^{(1)} &= 0 \\ q_1^{(0)}q_1^{(1)} &= \frac{1}{\sqrt{2}} \end{cases}$$

This equation system admits no solution. We deduce that $|\Phi^+\rangle = \frac{|00\rangle + |11\rangle}{\sqrt{2}}$ is not a product state, it is entangled.

3 Variational Quantum Algorithms for optimization

Some of the quantum algorithms that tackle combinatorial optimization problems are Variational Quantum Algorithms (VQAs) [5]. They are hybrid algorithms because they require both quantum and classical computations. VQAs are studied today because they represent an alternative approach that reduces the quality and quantity of the quantum resources needed [37]. Specifically, they are designed to run on the NISQ era [38] where quantum computers are noisy with few qubits: for instance, they harness low-depth quantum circuits.

In this section, we consider optimization problems of the form

$$\min_{x \in \{0,1\}^n} f(x)\,, \tag{1}$$

where f is any function defined on $\{0,1\}^n$. We note $\mathcal{F}$ the set of optimal solutions.

3.1 General description

Variational Quantum Algorithms are hybrid algorithms that, given an input $|0\rangle^{\otimes n}$, alternate between a quantum part and a classical part. Henceforth, we note $|0_n\rangle$ the state $|0\rangle^{\otimes n}$ to ease the reading.

The quantum part applies a quantum circuit on the n-qubit system that constitutes the quantum computer. Importantly, *variational* in VQAs stands for the parametrization of the quantum circuit. Let $d \in \mathbb{N}$ be the number of parameters.

Definition 21. *A parametrized quantum circuit is a continuous function $U : \mathbb{R}^d \to \mathcal{M}_{2^n}(\mathbb{C})$ mapping any $\theta \in \mathbb{R}^d$ to unitary matrix $U(\theta)$.*

As defined in Subsection 2.3, a quantum circuit is a sequence of universal quantum gates' compositions and/or tensor products. Thus, each coefficients of matrix $U(\theta)$ are continuous functions on $\mathbb{R}^d$.

Example 22. *A simple example of a parametrized quantum circuit for $n = 3$ and $d = 3$ is depicted in Figure 6.*

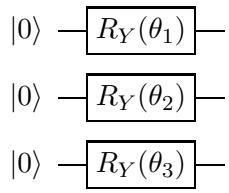

Figure 6: Quantum circuit parametrized by $(\theta_1, \theta_2, \theta_3) \in \mathbb{R}^3$.

The expression of $U(\theta)$ for this circuit is as follows: $\forall \theta = (\theta_1, \theta_2, \theta_3) \in \mathbb{R}^3$,

$$
\begin{aligned}
U(\theta) &= R_Y(\theta_1) \otimes R_Y(\theta_2) \otimes R_Y(\theta_3) \\
&= \begin{pmatrix} \cos\frac{\theta_1}{2} & -\sin\frac{\theta_1}{2} \\ \sin\frac{\theta_1}{2} & \cos\frac{\theta_1}{2} \end{pmatrix} \otimes \begin{pmatrix} \cos\frac{\theta_2}{2} & -\sin\frac{\theta_2}{2} \\ \sin\frac{\theta_2}{2} & \cos\frac{\theta_2}{2} \end{pmatrix} \otimes \begin{pmatrix} \cos\frac{\theta_3}{2} & -\sin\frac{\theta_3}{2} \\ \sin\frac{\theta_3}{2} & \cos\frac{\theta_3}{2} \end{pmatrix} \\
&= \begin{pmatrix}
c_1c_2c_3 & -c_1c_2s_3 & -c_1s_2c_3 & c_1s_2s_3 & -s_1c_2c_3 & s_1c_2s_3 & s_1s_2c_3 & -s_1s_2s_3 \\
c_1c_2s_3 & c_1c_2c_3 & -c_1s_2s_3 & -c_1s_2c_3 & -s_1c_2s_3 & -s_1c_2c_3 & s_1s_2s_3 & s_1s_2c_3 \\
c_1s_2c_3 & -c_1s_2s_3 & c_1c_2c_3 & -c_1c_2s_3 & -s_1s_2c_3 & s_1s_2s_3 & -s_1c_2c_3 & s_1c_2s_3 \\
c_1s_2s_3 & c_1s_2c_3 & c_1c_2s_3 & c_1c_2c_3 & -s_1s_2s_3 & -s_1s_2c_3 & -s_1c_2s_3 & -s_1c_2c_3 \\
s_1c_2c_3 & -s_1c_2s_3 & -s_1s_2c_3 & s_1s_2s_3 & c_1c_2c_3 & -c_1c_2s_3 & -c_1s_2c_3 & c_1s_2s_3 \\
s_1c_2s_3 & s_1c_2c_3 & -s_1s_2s_3 & -s_1s_2c_3 & c_1c_2s_3 & c_1c_2c_3 & -c_1s_2s_3 & -c_1s_2c_3 \\
s_1s_2c_3 & -s_1s_2s_3 & s_1c_2c_3 & -s_1c_2s_3 & c_1s_2c_3 & -c_1s_2s_3 & c_1c_2c_3 & -c_1c_2s_3 \\
s_1s_2s_3 & s_1s_2c_3 & s_1c_2s_3 & s_1c_2c_3 & c_1s_2s_3 & c_1s_2c_3 & c_1c_2s_3 & c_1c_2c_3
\end{pmatrix},
\end{aligned}
$$

where $c_i = \cos\frac{\theta_i}{2}$ and $s_i = \sin\frac{\theta_i}{2}$ for $i \in [3]$.

Remark 23. *The use of the generalized circuit to n qubits $\bigotimes_{i=1}^{n} R_{Y,i}(\theta_i)$ amounts to a continuous relaxation of the $\{0,1\}$-problem (1), where each decision variable $x_i \in [0,1]$ is represented by a rotation angle $\theta_i \in [0, 2\pi]$ as follows:*

$$x_i = \left(\cos\frac{\theta_i}{2}\right)^2.$$

The classical part consists of a classical optimization over the parameters $\theta \in \mathbb{R}^d$. The classical optimizer essentially aims at finding the optimal parameters θ^* that lead to optimal solutions with high probability, specifically, such that

$$\sum_{s\in\mathcal{F}} |\langle s| U(\theta^*) |0_n\rangle|^2 \geq 1-\epsilon\,, \tag{10}$$

for small $\epsilon > 0$. Henceforth, we use notation $|x\rangle$ instead of $|i\rangle$ to efficiently recall that we deal with solutions of optimization problems.

3.2 Classical part

The classical part of VQAs is characterized by two aspects: the function that guides the optimization and the optimizer itself.

3.2.1 Guiding function

Let $g : \mathbb{R}^d \to \mathbb{R}$ be the guiding function, formally defined in Definition 24 below, that the classical optimizer minimizes. The function g acts as a link between the quantum and classical parts. For a given $\theta \in \mathbb{R}^d$, it evaluates $U(\theta)|0_n\rangle$ *according to* f as we will exemplify below. Notice that f and g are distinct since g is defined on $\mathbb{R}^d$ and outputs a quality measure of an n-qubit quantum state whereas f is defined on $\{0,1\}^n$. Let us denote $\mathcal{F}_{\text{quant}} = \left\{\sum_{s\in\mathcal{F}} \psi_s |s\rangle : \sum_{s\in\mathcal{F}} |\psi_s|^2 = 1\right\}$ as the set of quantum states that are superpositions of optimal solutions of problem (1). Naturally, we would like to define g such that minimizing g tends to minimize f.

Definition 24 (Guiding function)**.** *Let $g : \mathbb{R}^d \to \mathbb{R}$ be a function and $\mathcal{G}$ be its set of minimizers. We call g a guiding function for f with respect to U if g is continuous and*

$$\{U(\theta)|0_n\rangle : \theta \in \mathcal{G}\} \subseteq \mathcal{F}_{quant}\,. \tag{11}$$

In other words, optima of a guiding function g must lead to optima of f or superpositions of optima of f. Thus, minimizing g amounts to minimizing f. Without any information on $\mathcal{F}$, we need to choose a quantum circuit U such that any optimal solution $s \in \mathcal{F}$ is reachable, specifically,

$$\{U(\theta)|0_n\rangle : \theta \in \mathbb{R}^d\} \supseteq \mathcal{CB}_n\,. \tag{12}$$

Notice that this condition is weak and easily satisfied. Indeed, the circuit depicted in Figure 6 satisfies this condition. If ever one is interested in finding all optimal solutions of problem (1), the circuit and the guiding function should satisfy instead the stronger condition

$$\{U(\theta)|0_n\rangle : \theta \in \mathcal{G}\} = \mathcal{F}_{\text{quant}}\,. \tag{13}$$

In that case, U satisfying (12) is not enough. We need to choose U that can reach any n-qubit quantum states, specifically,

$$\{U(\theta)|0_n\rangle : \theta \in \mathbb{R}^d\} = \left\{\sum_{x\in\{0,1\}^n} \psi_x |x\rangle : \sum_{x\in\{0,1\}^n} |\psi_x|^2 = 1\right\}.$$

A popular choice for the guiding function in the literature is the mean function

$$g_{\text{mean}}(\theta) = \sum_{x \in \{0,1\}^n} p_\theta(x) f(x)\,, \tag{14}$$

where $p_\theta(x) = |\langle x| U(\theta) |0_n\rangle|^2$ is the probability of finding x when $U(\theta)|0_n\rangle$ is measured. We show next that g_{mean} is indeed a guiding function according to Definition 24, see Appendix B.1.1 for a proof.

Proposition 25. *Function g_{mean} is a guiding function.*

Example 26. *We illustrate the mean function on the 3-qubit quantum circuit $U(\theta)$ depicted in Figure 6. The generalization of its computation for n qubits is trivial since it needs to replace 3 by n. The single application of rotation gate R_Y (6) of angle θ_i on a qubit initially on state $|0\rangle$ is*

$$\begin{aligned} R_Y(\theta_i)|0\rangle &= \cos\frac{\theta_i}{2}|0\rangle + \sin\frac{\theta_i}{2}|1\rangle \\ &= \sum_{j\in\{0,1\}} \cos\frac{\theta_i - j\pi}{2}|j\rangle\,, \end{aligned}$$

since $\sin(\phi) = \cos\left(\phi - \frac{\pi}{2}\right)$ for $\phi \in \mathbb{R}$. Eventually, the quantum state resulting from $U(\theta)$ is

$$\begin{aligned} U(\theta)|0_n\rangle &= \bigotimes_{i=1}^{3} R_{Y,i}(\theta_i)|0\rangle \\ &= \sum_{j_1,j_2,j_3\in\{0,1\}} \left(\prod_{i=1}^{3} \cos\frac{\theta_i - j_i\pi}{2}\right)|j_1 j_2 j_3\rangle\,. \end{aligned}$$

Thus, the probability to measure $x = x_1x_2x_3 \in \{0,1\}^3$ is

$$p_\theta(x) = \left(\prod_{i=1}^{3} \cos\frac{\theta_i - x_i\pi}{2}\right)^2\,, \tag{15}$$

and the expression of g_{mean} of equation (14) directly results from it.

Other functions are compatible with Definition 24. One of these functions encountered in the literature is the Gibbs function [26] which stems from statistical mechanics. Let $\eta > 0$ be a parameter to be set. The Gibbs function is defined as

$$g_{G,\eta}(\theta) = -\ln\left(\sum_{x\in\{0,1\}^n} p_\theta(x) e^{-\eta f(x)}\right)\,. \tag{16}$$

The choice of this function is motivated by the exponential shape that highly rewards the increase of probabilities of low-cost states. Notice that for small η, minimizing the Gibbs function is essentially equivalent to minimizing the mean function in the sense that the Taylor series of $g_{G,\eta}$ at first order in $\eta = 0$ gives $g_{G,\eta} = \eta g_{\text{mean}}$. We show next that $g_{G,\eta}$ is indeed a guiding function according to Definition 24, see Appendix B.1.2 for a proof.

Proposition 27. *Let $\eta > 0$. Function $g_{G,\eta}$ is a guiding function.*

One might suggest other guiding functions, such as the minimum function

$$g_{\min}(\theta) = \min_{x\,:\,p_\theta(x)>0} f(x)\,. \tag{17}$$

However, $g_{\min}$ does not verify (11), and is not even continuous, hardening its optimization and excluding its choice for the guiding function.

Example 28. *Let us illustrate that g_{min} is not a guiding function. For that, we consider the circuit of Figure 6 and the following function $f : \{0,1\}^3 \mapsto \mathbb{R}$ to optimize,*

$$\begin{cases} f(0,0,0) & = 1 \\ f(x) & = 0\,, \quad \forall x \neq (0,0,0) \end{cases}$$

where $f^* = 0$ is the optimal value. Function g_{min} reaches its optimal value $g^*_{min} = 0$ on the set of its optimizers

$$\mathcal{G} = \mathbb{R}^3 \setminus \{(2k\pi, 2k\pi, 2k\pi) : k \in \mathbb{Z}\}\,.$$

However,

$$\forall \theta \in \mathcal{G} \setminus \{((2k+1)\pi, (2k+1)\pi, (2k+1)\pi) : k \in \mathbb{Z}\}\,, U(\theta)\,|0_n\rangle \notin \mathcal{F}_{quant}\,,$$

because there is a non-zero probability of sampling $(0,0,0)$. Thus, g_{min} violates (11). Moreover, g_{min} is not continuous. Indeed, $g_{min}(0,0,0) = 1$, whereas $\forall \epsilon > 0\,, g_{min}(\epsilon,0,0) = 0$.

The above observation motivated [2] to suggest another function, the CVaR (Conditional Value-at-Risk) function. The CVaR function is the average on the lower α-tail of values of f encountered, where $\alpha \in]0,1]$ is a parameter to be set. Let $(x_1, \ldots, x_{2^n})$ be the n-bitstrings sorted in non decreasing order, namely $f(x_i) \leq f(x_{i+1})$ for any $i \in [2^n - 1]$. Let N_α be the index that delimits the α-tail elements of the distribution, specifically,

$$N_\alpha = \min\left\{ N \geq 1 : \sum_{i=1}^{N} p_\theta(x_i) \geq \alpha \right\}\,.$$

Then, the CVaR function is

$$g_{C,\alpha}(\theta) = \frac{1}{\sum_{i=1}^{N_\alpha} p_\theta(x_i)} \sum_{i=1}^{N_\alpha} p_\theta(x_i) f(x_i)\,. \tag{18}$$

The special case $\alpha = 1$ implies $g_\alpha = g_{\text{mean}}$, whereas when α approaches zero, we find $g_{\min}$.

The CVaR function is an alternative to the non-smooth minimum function. While CVaR does not verify (11) either, it keeps continuity and still focuses on the best solutions that appear on the probability distribution.

Example 29. *Let us illustrate the violation of* (11) *by the* CVaR *function, for any $\alpha \in]0,1[$. For that, we consider function f of Example 28 with the same quantum circuit of Figure 6. Let $\alpha \in]0,1[$. Let us find $\theta \in \mathcal{G}$ such that $U(\theta)\,|0_n\rangle \notin \mathcal{F}_{quant}$. In other words, we search $\theta \in \mathbb{R}^3$ such that*

$$g_{C,\alpha}(\theta) = 0 \;\; \textit{and} \;\; p_\theta(0,0,0) > 0\,.$$

Let us look at $\theta = (\pi - \epsilon, 0, 0)$, where $\epsilon \in]0,\pi[$. According to (15)*, we have*

$$p_\theta(0,0,0) = \cos^2\left(\frac{\pi - \epsilon}{2}\right) > 0\,.$$

It remains to choose ϵ to ensure $g_{C,\alpha}(\theta) = 0$. Namely, we want ϵ such that

$$\sum_{x \neq (0,0,0)} p_\theta(x) \geq \alpha \,,$$

meaning

$$1 - \cos^2\left(\frac{\pi - \epsilon}{2}\right) \geq \alpha \,.$$

This holds for any $\epsilon \leq \pi - 2\arccos\left(\sqrt{1-\alpha}\right)$.

Even if CVaR does not verify (11), it can be seen as a pseudo-guiding function, defined just below. Notice that in practice, using the CVaR function seems appropriate because it accepts a probability of measuring optimal solutions after optimizing to be lower than one, such as expressed in (10).

Definition 30 (Pseudo-guiding function)**.** *Let $g : \mathbb{R}^d \to \mathbb{R}$ be a function and $\mathcal{G}$ be its set of minimizers. We call g a pseudo-guiding function for f with respect to U if g is continuous and if there exists $\alpha \in]0,1[$ such that optima of g can lead to non-optimal solutions of f with a probability strictly lower than $1-\alpha$. Specifically, let $\theta \in \mathcal{G}$. Thus, either $U(\theta)\left|0_n\right\rangle \in \mathcal{F}_{quant}$ or $\sum_{x \notin \mathcal{F}} |\left\langle x\right| U(\theta)\left|0_n\right\rangle|^2 < 1-\alpha$.*

We show next that $g_{C,\alpha}$ is indeed a pseudo-guiding function according to Definition 30, see Appendix B.1.3 for a proof.

Proposition 31. *Let $\alpha \in]0,1[$. Function $g_{C,\alpha}$ is a pseudo-guiding function.*

3.2.2 Classical optimizer

The role of the classical optimizer is to minimize the guiding function. The function g is continuous and is usually differentiable but not convex. Any unconstrained optimization algorithm can be used to minimize g, such as local search or descent gradient method.

To speak in terms of stochastic optimization, the classical optimizer aims to solve the stochastic programming model under endogenous uncertainty

$$\min_\theta \{g(\theta) = \mathbb{E}[G(\theta, \xi_\theta)]\} \,, \tag{19}$$

where the definition of G depends on the choice of a specific guiding function, and ξ_θ is an endogenous vector that depends on θ. Specifically, ξ_θ is a discrete random variable, with the set of possible outcomes $\{0,1\}^n$ and the following distribution probability:

$$\mathbb{P}(\xi_\theta = x) = p_\theta(x), \quad \forall x \in \{0,1\}^n \,.$$

Thus, this problem falls into the class of stochastic dependent-decision probabilities problems [19]. In practice, the classical optimizer approximates the function by a Monte Carlo estimation as follows:

$$\hat{g}_N(\theta) = \frac{1}{N}\sum_{j=1}^{N} G(\theta, \xi_\theta^j) \,,$$

where $\{\xi_\theta^j\}_{j\in[N]}$ is a sample of size N from the distribution of ξ_θ. Notice that for a given θ, the quantity $\hat{g}_N(\theta)$ itself is a random variable since its value depends on the sample that has

been generated, which is random. In contrast, the value of $g(\theta)$ is deterministic. In practice, the classical optimizer iterates the loop that consists of, given a sampling distribution of size N of the quantum state $U(\theta)\,|0_n\rangle$ (Remark 15), outputs a θ'. This θ' is then transmitted to the quantum part. Eventually, the aim is to output θ^* such that $U(\theta)\,|0_n\rangle \subseteq \mathcal{F}_{\text{quant}}$. In each iteration, the value of $\hat{g}_N(\theta)$ is computed. Notice that according to the Law of Large Numbers [40], $\hat{g}_N(\theta)$ converges with probability one to $g(\theta)$ as $N \to \infty$.

For instance, for the case of $g = g_{\text{mean}}$, we have

$$G(\theta, \xi_\theta) = f(\xi_\theta)\,.$$

Hence, for each $\xi_\theta^j \in \{0,1\}^n$ sampled, either we compute classically $f(\xi_\theta^j)$ and store it if not already computed, or we get its value. Thus, we can compute $\hat{g}_N(\theta)$. Notice that for the CVaR function, we compute the empirical mean only on the best $\lceil \alpha N \rceil$ values $f(\xi_\theta)$ found by sampling.

The solution returned by the VQA is the minimum value of f encountered while the algorithm runs.

4 Quantum Approximate Optimization Algorithm

We assume throughout this section that the function f to be minimized is polynomial. First, we reformulate problem (1) to a more suitable form for quantum optimization. This reformulation is motivated by the quantum adiabatic evolution [10] that, for a given hermitian matrix[2], approximates the eigenvector with the lowest eigenvalue under certain conditions. For that, we interpret the objective function of problem (1) as an hermitian matrix H_f such that each eigenvector $|u_x\rangle$ is matching a classical solution $x \in \{0,1\}^n$ with an eigenvalue equal to $f(x)$, specifically,

$$H_f\,|u_x\rangle = f(x)\,|u_x\rangle\ .$$

Thus, the solutions of problem (1) are the solutions corresponding to the lowest eigenvalues of H_f. The Quantum Approximate Optimization Algorithm (QAOA) [9] presented in this section aims to find the lowest eigenvalue of H_f.

4.1 Problem reformulation

The construction of H_f is as follows. First, we transform the $\{0,1\}$-problem (1) into a $\{-1,1\}$-problem. For that, we apply the following linear transformation: for $x = (x_1, \ldots, x_n) \in \{0,1\}^n$, we define $z = (z_1, \ldots, z_n) \in \{-1,1\}^n$ where

$$z_i = 1 - 2x_i\,, \forall i \in [n]\,. \tag{20}$$

This leads to the problem

$$\min_{z \in \{-1,1\}^n} f_{\pm 1}(z) = \sum_{\alpha=(\alpha_1,\ldots\alpha_n)\in\{0,1\}^n} h_\alpha \prod_{i=1}^{n} z_i^{\alpha_i}\,,$$

where $h_\alpha \in \mathbb{R}, \forall \alpha \in \{0,1\}^n$. Second, we define H_f as

$$H_f = \sum_{\alpha=(\alpha_1,\ldots\alpha_n)\in\{0,1\}^n} h_\alpha \bigotimes_{i=1}^{n} Z_i^{\alpha_i}\,,$$

[2] A complex square matrix is hermitian if it is equal to its conjugate transpose.

where $Z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$, $Z^0 = I$ and $Z^1 = Z$. We note Z_i the application of Z to qubit i. Notice that Z is equal to the universal gate $R_Z(\pi)$ modulo a global phase (see (7)). This construction of H_f leads to the following property.

Proposition 32. *The eigenvectors of H_f are the canonical basis $|x\rangle \in \mathcal{CB}_n$ with eigenvalues that are the cost of the solutions $f(x)$, specifically,*

$$\forall |x\rangle \in \mathcal{CB}_n, \;\; H_f |x\rangle = f(x) |x\rangle \; . \tag{21}$$

Proof. First, the eigenvectors of H_f are the canonical basis states. Indeed, each term of the sum that constitutes H_f is a tensor product of n matrices I or Z, both diagonal. Thus, H_f is a 2^n diagonal matrix. Second, let us find the eigenvalues associated with the eigenvectors. Let $|x = x_1, \ldots, x_n\rangle$ be in $\mathcal{CB}_n$. Let $z = (z_1, \ldots, z_n)$ be the result of transformation (20). Thus, $Z |x_i\rangle = z_i |x_i\rangle \; , \forall i \in [n]$ and

$$\begin{aligned}
H_f |x\rangle &= \sum_{\alpha=(\alpha_1,\ldots,\alpha_n)\in\{0,1\}^n} h_\alpha \bigotimes_{i=1}^{n} Z_i^{\alpha_i} |x_i\rangle \\
&= \sum_{\alpha=(\alpha_1,\ldots,\alpha_n)\in\{0,1\}^n} h_\alpha \bigotimes_{i=1}^{n} z_i^{\alpha_i} |x_i\rangle \\
&= \left(\sum_{\alpha=(\alpha_1,\ldots,\alpha_n)\in\{0,1\}^n} h_\alpha \prod_{i=1}^{n} z_i^{\alpha_i} \right) |x\rangle \\
&= f_{\pm}(z) |x\rangle \\
&= f(x) |x\rangle \; .
\end{aligned}$$

□

Example 33. *We illustrate this transformation on a small example with $n = 2$. Let us consider the problem*

$$\min_{x\in\{0,1\}^2} f(x) = x_1 + 2x_2 - 3x_1x_2 \, .$$

The equivalent $\{-1, 1\}$-problem is

$$\min_{z\in\{-1,1\}^2} f_{\pm 1}(z) = \frac{1}{4}z_1 - \frac{1}{4}z_2 - \frac{3}{4}z_1z_2 + \frac{3}{4} \, .$$

Thus, the hermitian matrix associated with the problem is

$$H_f = \frac{1}{4}Z \otimes I - \frac{1}{4}I \otimes Z - \frac{3}{4}Z \otimes Z + \frac{3}{4}I \otimes I \, .$$

To illustrate (21)*, we compute the eigenvalue of the canonical basis state $|10\rangle$.*

$$\begin{aligned}
H_f |10\rangle &= \frac{1}{4}(Z \otimes I) |10\rangle - \frac{1}{4}(I \otimes Z) |10\rangle - \frac{3}{4}(Z \otimes Z) |10\rangle + \frac{3}{4}(I \otimes I) |10\rangle \\
&= -\frac{1}{4} |10\rangle - \frac{1}{4} |10\rangle + \frac{3}{4} |10\rangle + \frac{3}{4} |10\rangle \\
&= |10\rangle \\
&= f(10) |10\rangle \; ,
\end{aligned}$$

because $f(10) = 1$.

Notice that most of the problems solved with QAOA in the literature are QUBO (Quadratic Unconstrained Binary Optimization) problems. Thus, H_f has the specific form

$$H_f = \sum_i h_{ii} Z_i + \sum_{i<j} h_{ij} Z_i \otimes Z_j \,,$$

where $h_{ij} \in \mathbb{R}$, $\forall i \leq j$. It is justified by the fact that solving QUBO problems to optimality is *already* NP-hard, and the quantum gates of the circuit are easier to implement on hardware in that case.

4.2 Quantum part

QAOA is a Variational Quantum Algorithm where the quantum part derives from the Hamiltonian H_f. This quantum part consists of a quantum circuit with $2p$ parameters $(\boldsymbol{\gamma}, \boldsymbol{\beta}) = (\gamma_1, \ldots, \gamma_p, \beta_1, \ldots, \beta_p) \in \mathbb{R}^{2p}$, where p is called *depth*. The quantum circuit $U(\boldsymbol{\gamma}, \boldsymbol{\beta})$ is the sequence of p layers of two blocs, initially applied to the uniform superposition $|+\rangle^{\otimes n}$ (see Example 18). The first bloc is of the form $\mathrm{Exp}(H_f, \gamma)$, for $\gamma \in \mathbb{R}$, which is the unitary operator (see Definition 43) associated with the Hamiltonian H_f. The second bloc is of the form $\mathrm{Exp}(H_B, \beta)$, for $\beta \in \mathbb{R}$, which is the unitary operator associated with the Hamiltonian $H_B = \sum_{i=1}^{n} R_{X,i}(\pi)$. Thus, the quantum circuit is

$$U(\boldsymbol{\gamma}, \boldsymbol{\beta}) = \mathrm{Exp}(H_B, \beta_p)\mathrm{Exp}(H_f, \gamma_p) \ldots \mathrm{Exp}(H_B, \beta_1)\mathrm{Exp}(H_f, \gamma_1) \, |+\rangle^{\otimes n} \,. \tag{22}$$

The three propositions that follow express the quantum circuit of QAOA with the set of universal gates (see Theorem 13). We give first the general decomposition of the QAOA quantum circuit defined in (22), see Appendix B.2.1 for a proof.

Proposition 34. *The first bloc* $\mathrm{Exp}(H_f, \gamma)$ *parametrized by* $\gamma \in \mathbb{R}$ *is*

$$\mathrm{Exp}(H_f, \gamma) = \prod_{\alpha \in \{0,1\}^n} \mathrm{Exp}(\bigotimes_{i=1}^{n} Z_i^{\alpha_i}, h_\alpha \gamma) \,.$$

The second bloc $\mathrm{Exp}(H_B, \beta)$ *parametrized by* $\beta \in \mathbb{R}$ *is*

$$\mathrm{Exp}(H_B, \beta) = \bigotimes_{i=1}^{n} R_{X,i}(2\beta) \,.$$

The particular case of QUBO is mainly considered in the literature. Thus, we propose next a decomposition of the QAOA quantum circuit for this specific case, see Appendix B.2.2 for a proof.

Proposition 35. *For the case of QUBO, the expression of* $\mathrm{Exp}(H_f, \gamma)$ *simplifies in*

$$\mathrm{Exp}(H_f, \gamma) = \left(\bigotimes_{i=1}^{n} R_{Z,i}(2h_{ii}\gamma) \right) \prod_{i<j} CX_{i,j} R_{Z,j}(2h_{i,j}\gamma) CX_{i,j} \,,$$

and is rather easily implemented with universal quantum gates.

The decomposition in universal quantum gates of the term $\mathrm{Exp}(Z_i \otimes Z_j, t)$ for the specific case of QUBO (see Proposition 35) is mainly used in the literature. We propose in Proposition 37 a generalization of such a decomposition for the term $\mathrm{Exp}(\bigotimes_{i=1}^{n} Z^{\alpha_i}, t)$, where the number of Z gates in effect can be bigger than two, namely, $|\{\alpha_i,\, i \in [n] : \alpha_i = 1\}| \geq 2$. This proposition enables us to overtake the QUBO problems, namely, to deal with a polynomial function f with a degree strictly larger than two. We introduce next a technical result that will be necessary to derive the subsequent proposition, see Appendix B.2.3 for a proof.

Lemma 36. $\forall n \in \mathbb{N}^*$,

$$(I^{\otimes n-1} \otimes X) e^{-itZ^{\otimes n}} (I^{\otimes n-1} \otimes X) = e^{itZ^{\otimes n}} .$$

The proposition that follows enables a decomposition in universal quantum gates of any quantum circuit of QAOA, see Appendix B.2.4 for a proof.

Proposition 37. *Let us consider the subsystem composed of the N qubits to which the Z gate is applied. Specifically, $N = |\{\alpha_i\, i \in [n] : \alpha_i = 1\}|$, and we renumber the qubits in question in $[N]$. Thus, for $N \geq 2$, the term $\mathrm{Exp}(\bigotimes_{i=1}^{n} Z^{\alpha_i}, t)$ on this subsystem simplifies in*

$$\mathrm{Exp}(Z^{\otimes N}, t) = \prod_{j=0}^{N-2} CX_{1,N-j} R_{Z,N}(2t) \prod_{j=0}^{N-2} CX_{1,N-j} .$$

We represent this decomposition on Figure 7.

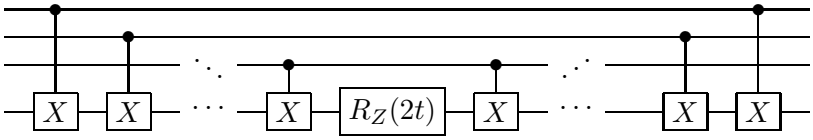

Figure 7: Decomposition of $\mathrm{Exp}(Z^{\otimes N}, t)$ on the N-qubit subsystem.

Example 38. *We illustrate the construction of the quantum circuit with the problem of Example 33 where $n = 2$, for the case $p = 1$. Thus,*

$$U(\gamma, \beta) = \mathrm{Exp}(H_B, \beta)\mathrm{Exp}(H_f, \gamma) \left|+\right\rangle^{\otimes 2}, \quad \forall \gamma, \beta \in \mathbb{R} .$$

The circuit is detailed in Figure 8.

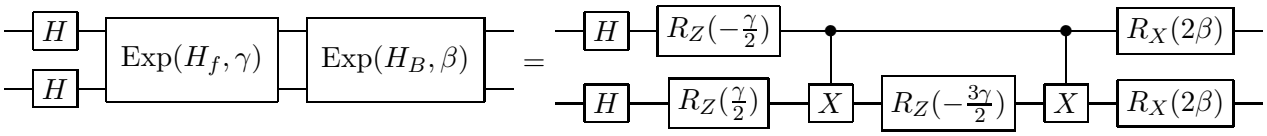

Figure 8: QAOA circuit of Example 33 for $p = 1$.

Notice that we do not take into account the term $\frac{3}{4} I \otimes I$ of H_f in this circuit. More generally, the term $h_{0\ldots0} I^{\otimes n}$ of H_f never appears on the quantum circuit because it represents a constant term and does not influence the optimization.

Notice that the choice of QAOA circuit does not ensure (12). For example, one can show that the probability of measuring 00 at the end of the circuit depicted in Figure 8 never reaches 1. Specifically,

$$p_{(\gamma,\beta)}(00) = |\langle 00| \operatorname{Exp}(H_B,\beta)\operatorname{Exp}(H_f,\gamma)|+\rangle^{\otimes 2}|^2 < \frac{1}{2}, \quad \forall \gamma,\beta \in \mathbb{R}\,.$$

However, QAOA satisfies another important property: it uses entangling gates. Each gate $\operatorname{Exp}(Z_i \otimes Z_j, t)$, for $t \in \mathbb{R} \setminus \{k\pi : k \in \mathbb{Z}\}$, entangles the qubits i and j. Indeed, $\operatorname{Exp}(Z_i \otimes Z_j, t) = CX_{i,j}R_{Z,j}(2t)CX_{i,j}$, and unless $R_{Z,j}(2t) = I$, namely $t \in \{k\pi : k \in \mathbb{Z}\}$, the CNOT gate operates[3] and creates entanglement as mentioned in Subsection 2.4.3. The other gates, which are one-qubit gates, do not have this power. Entanglement is not necessary to (12). However, Remark 23 can justify the use of entanglement gate. Indeed, without it, it seems unlikely to achieve better results than pure classical optimization because the optimizer essentially solves a classical continuous relaxation.

In fact, the popularity of QAOA originates essentially from the fact that it mimics the adiabatic schedule [43]. The n-qubit system verifies the adiabatic condition when $p \to \infty$ and ensures that for a particular set of parameters, the quantum circuit gives the exact solution. However, quantum computers' quality today makes implementations on large instances impossible. But because the number of gates of the quantum circuit is $\mathcal{O}(pn^2)$, for small depth d, QAOA, and more generally VQAs, can still be implemented on current NISQ computers.

5 Literature review for QAOA

Many papers have recently addressed the empirical evaluation of QAOA, some also comparing it with specific implementations of VQA. We present below a non-exhaustive list of these trends, we mention several theoretical limitations for specific cases known up to now and we end with the different leverages that are at stake to improve QAOA performances.

5.1 Empirical and theoretical trends on QAOA

Let us begin with the numerical trends of QAOA performances. All the empirical experiments are presented on small instances because quantum computers' quality today makes implementations on large instances impossible, leading to difficult conclusions. Thus, many experiments are done on classical simulators of quantum computers. Most of the empirical results of QAOA apply to the MAX-CUT problem because it was initially the first application of QAOA [9].

Definition 39 (MAX-CUT problem)**.** *Let $G = (V, E)$ be a undirected graph. A cut in G is a subset $S \subseteq V$. We define its* cost *as the number of edges with one node in S and one node in $V \setminus S$. The MAX-CUT problem aims at finding a cut with maximum* cost*. A version with weighted edges can also be defined.*

Notice that for the MAX-CUT problem, with the notations of Section 4, the objective function is

$$f(x) = -\sum_{(i,j)\in E} x_i(1-x_j) + x_j(1-x_i)\,,$$

[3]For $t \in \{k\pi : k \in \mathbb{Z}\}$, $R_{Z,j}(2t) = I$. Thus, $CX_{i,j}R_{Z,j}(2t)CX_{i,j} = CX_{i,j}CX_{i,j} = I$ because CNOT is its own inverse.

where x_i is 1 if node i is in the cut, 0 otherwise. The hermitian matrix that corresponds to this problem is

$$H_f = -\frac{1}{2} \sum_{(i,j)\in E} 1 - Z_i Z_j \,.$$

The approximation ratio r mainly quantifies the performance of QAOA as follows:

$$r = \frac{f^{\mathrm{QAOA}}}{f^*} \,,$$

where f^{QAOA} is the value returned by QAOA, and f^* is the optimal value. Papers often compare this ratio with the best-known guaranteed ratio of Goemans-Williamson algorithm [14], specifically, $r = 0.87856$. The seminal paper of QAOA [9] provides a lower bound of r for the specific class of 3-regular graphs for $p = 1$ that is $r = 0.6924$. More precise analytical expressions of the lower bound of the ratio for $p = 1$ and for some other typical cases are given in [42].

Several empirical results on MAX-CUT spotlight patterns of optimal parameters and enable QAOA to exceed Goemans-Williamson bound for some specific instances. Some classes of MAX-CUT instances studied reveal patterns of optimal parameters. Thus, it seems to offer efficient heuristics for parameter selection and initialization. For example, the authors of [6] look at the class of Erdös-Rényi graphs (random graphs where an edge appears between two nodes with probability 0.5) of size up to 17 nodes, where the classical optimizer is an automatic differentiation with stochastic gradient descent. The authors of [27] examine the exhaustive set of graphs with $n \leq 9$ nodes, with the gradient-based search BFGS (Broyden-Fletcher-Goldfarb-Shanno algorithm [12]) for the classical optimizer. Both exhibit instances that exceed the bound of Goemans-Williamson for small depth, $p \leq 8$ and $p \leq 3$, respectively. The sets of unweighted and weighted 3-regular graphs also lead to patterns in [45] for graphs of a maximum size of 22 nodes. But even if the performance of QAOA sometimes exceeds the Goemans-Williamson bound for the low-depth circuits, it is believed that p must grow with the instance size to have a chance to outperform the best classical algorithms.

Indeed, some theoretical limits of QAOA are displayed, where the shape of the quantum state produced by the quantum circuit is at stake. The authors of [3] point out that the symmetry and locality of this resulting variational state fundamentally limit the performances of QAOA. Indeed, it shows that Goemans-Williamson outperforms QAOA for several instances of the MAX-CUT problem for any fixed depth p. Consequently, this paper suggests a non-local version of QAOA to overcome these limitations. The limits of the locality also appear when solving the problem of the Maximum Independent Set (MIS). In [8], MIS instances are random graphs of n vertices, with a fixed average degree $\bar{d}$. Thus, it proves that for depth $p \leq C \log(n)$, where C a constant depending of $\bar{d}$, QAOA cannot return an independent set better than 0.854 times the optimal for $\bar{d}$ large. Due to this locality issue, the author of [18] compares QAOA with *local* classical algorithms which also have this locality notion: at each step, the value of a variable is updated depending on the values of its *neighbors*, i.e. the variables that share the same term within the objective function. Namely, after t steps, the value of a variable depends on all information gathered in its *t-neighborhood*. Yet, these classical algorithms still outperform QAOA. A single step of these algorithms outperforms, resp. achieves the same performance as, a single step of QAOA ($p = 1$) for MAX-CUT instances, resp. MAX-3-LIN-2 instances. Notice that given binary variables and a set of linear equations modulo 2 with exactly three variables, the MAX-3-LIN-2 problem aims to find a variable value assignment that maximizes the number of satisfied equations.

5.2 Improvements and adaptations of QAOA

Despite the theoretical limitations displayed above, QAOA has leverages (guiding function, quantum circuit, classical optimizer, etc.) that are still of interest in the literature. We display some of these studies on different choices of leverages that empirically improve QAOA performances.

First, the guiding function is mainly the mean function (14) as in the seminal paper of QAOA. However, both the CVaR function (18) and the Gibbs function (16) give an alternative to the mean function and show empirical improvements. For the former, several optimization problems, such as MAX-CUT, Maximum Stable Set, MAX-3SAT, etc., are solved with QAOA in [2] and show better results with faster convergence. For the latter, the authors of [26] display better results solving MAX-CUT with this guiding function. Notice that comparing these improvements is hard because they use different classical optimizers.

Second, the choice of the quantum circuit is challenged in the literature. The underlying question is whether the quantum circuit of QAOA (see Subsection 4.2) is a good choice for finite depth p. Several papers suggest better circuits based on empirical results for small depth and small instances. For example, VQA with the circuit proposed in [2] has better performances than QAOA, or with the *Bang-Bang* circuit described in [44]. The benefit of entanglement gates in the circuit is also discussed in [33] without giving a clear advantage. Notice that the authors of [7] suggest to warm-start QAOA with either a continuous relaxation or a randomized rounding. This consists of initializing the quantum circuit with a solution of a continuous relaxation (Quadratic Programming or Semi Definite Programming), resp. with a randomly rounded solution of a continuous relaxation, instead of the state $|+\rangle^{\otimes n}$. In both cases, QAOA performances for small p are better with a warm-start.

The choice of the classical optimizer represents another leverage. The authors of [33] advise the choice of a global optimizer rather than a local optimizer to avoid numerous local optima. The expression of the quantum circuit can also produce barren plateaus, hardening the optimization [30, 21]. We do not list all the possible choices of VQA leverages. The survey [5] proposes other possibilities.

In parallel, several algorithms derived from QAOA are appearing in the literature. An adaptation of QAOA is the Recursive-QAOA [4], also called RQAOA. It applies first several times QAOA to the problem in order to reduce its size, namely the number of variables, according to the correlation that appears between some variables. Then, it solves with classical brute force the resulting smaller problem. This algorithm seems to be competitive compared to QAOA for problems such as MAX-k-CUT. The authors of [46] propose another algorithm, the Adapative-QAOA, that converges faster than QAOA on some instances of MAX-CUT. It consists of applying recursively QAOA, increasing step by step the depth of the quantum circuit.

Eventually, there is ongoing work on the formulation and implementation of the QAOA circuit to ease and lighten QAOA implementation. For instance, the authors of [20] expose a *global variable substitution method* that, given an initial linear formulation of a 3-SAT problem, exploits the advantage of product representation in QAOA and, thus, minimizes the circuit depth[4]. The shallower depth, the more efficient the implementation of the quantum circuit for NISQ computers. A different approach is proposed in [32], that is, given a quantum circuit, minimizes the circuit depth by solving a Mixed-Integer Program, with an optimality guarantee on the quantum circuit produced (it can find up to 57% reduction of the number of gates). It applies to any gate-based quantum algorithm and thus, can be applied to QAOA and, more generally, to VQAs.

[4]Notice that here we talk about the general depth, not p, which is the longest path in the circuit, namely the maximum number of gates executed on a qubit.

Notice that solving combinatorial optimization problems using QAOA involves first formulating them into unconstrained problems, and more precisely into QUBO for easier circuits. There are essentially two types of formulation. The first and most common one is to integrate constraints as suitable penalty terms into the objective function. For instance, in [28] we find formulations of Karp's 21 NP-complete problems, and the authors of [36] tackle the k-coloring graph problem with the same method. The tutorial [13] addresses more general cases for this formulation problem methodology. The second type of formulation is to change the expression of the *mixing* Hamiltonian (referred to as H_B in Section 4). Initially presented in [17], the main idea is to make this Hamiltonian varying the quantum state only in the feasible search space. Some problems have been specifically studied with this method, such as the traveling salesman problem [39].

6 Conclusion

In this tutorial, we have provided a mathematical description of VQAs and how they are translated into quantum algorithms. There has been a growing interest in VQAs, and more particularly QAOA, mostly because of their compatibility with NISQ computers. We have described how VQAs raise interesting questions regarding the choice of guiding functions and quantum circuits, among others. They also raise many technical questions that we did not address in this work, such as the noise at the implementation level [25].

Since its inception, researchers have argued about the potential advantages of QAOA over classical optimization algorithms [11, 27, 29]. This research seems to indicate that there is currently no scientific evidence that QAOA will soon beat classical heuristics. The available results even suggest the opposite, such as [18] showing that local search algorithms can do better at low depth. Moreover, the current numerical results are hard to assess because they are run on small instances for which optimal or near-optimal solutions can be obtained easily with classical algorithms. Hopefully, the quickly growing capabilities of quantum computers will soon lead to a better understanding of the numerical efficiency of such algorithms [16].

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A Basics of linear algebra

This section provides some basic notions of linear algebra used throughout the tutorial. Notice that some specific definitions, such as unitary and hermitian matrices, are introduced together with their use in quantum computing.

Definition 40 (Tensor product)**.** *Let* $A = \begin{pmatrix} a_{11} & \dots & a_{1m} \\ \vdots & \ddots & \vdots \\ a_{n1} & \dots & a_{nm} \end{pmatrix} \in \mathcal{M}_{n,m}(\mathbb{C})$ *and* $B = \begin{pmatrix} b_{11} & \dots & b_{1q} \\ \vdots & \ddots & \vdots \\ b_{p1} & \dots & b_{pq} \end{pmatrix} \in \mathcal{M}_{p,q}(\mathbb{C})$ *be two complex matrices. Then, we define their tensor product, bilinear operation, as*

$$A \otimes B = \begin{pmatrix} a_{11}B & \dots & a_{1m}B \\ \vdots & \ddots & \vdots \\ a_{n1}B & \dots & a_{nm}B \end{pmatrix} \in \mathcal{M}_{np,mq}(\mathbb{C})\,.$$

where $a_{ij}B = \begin{pmatrix} a_{ij}b_{11} & \dots & a_{ij}b_{1q} \\ \vdots & \ddots & \vdots \\ a_{ij}b_{p1} & \dots & a_{ij}b_{pq} \end{pmatrix} \in \mathcal{M}_{p,q}(\mathbb{C})$.

Proposition 41 (Tensor product properties)**.** *We draw attention to some useful properties of the tensor product :*

- $A \otimes B \neq B \otimes A$
- $(A \otimes B) \otimes C = A \otimes (B \otimes C) = A \otimes B \otimes C$
- $A \otimes (cB) = (cA) \otimes B = c(A \otimes B)$, *for* $c \in \mathbb{C}$

Definition 42 (Braket notation)**.** *We also introduce the* braket *notation used in quantum computing. Let* $\psi = \begin{pmatrix} \psi_1 \\ \vdots \\ \psi_{2^n} \end{pmatrix} \in \mathbb{C}^{2^n}$ *be a column vector. We note* $|\psi\rangle$*, said* ket ψ*, the vector* ψ *itself. Thus, we define* $\langle\psi|$*, said* bra ψ*, the conjugate transpose of* $|\psi\rangle$*. Specifically,*

$$|\psi\rangle = \psi = \begin{pmatrix} \psi_1 \\ \vdots \\ \psi_{2^n} \end{pmatrix},$$
$$\langle\psi| = \bar{\psi}^T = \begin{pmatrix} \bar{\psi_1} & \dots & \bar{\psi_{2^n}} \end{pmatrix}.$$

Thus, ket *vectors are always column vectors whereas* bra *vectors are row vectors. With this notation, the norm of the vector* ψ *is*

$$\langle\psi|\psi\rangle = \sum_{i=1}^{2^n} |\psi_i|^2 .$$

We also consider the complex inner product

$$\psi, \phi \mapsto \langle\psi|\phi\rangle ,$$

where we use the notation $\langle\psi| \cdot |\phi\rangle = \langle\psi|\phi\rangle$*. Notice that it is not commutative. Indeed, for* $\psi = \begin{pmatrix} \psi_1 \\ \vdots \\ \psi_{2^n} \end{pmatrix} \in \mathbb{C}^{2^n}$ *and* $\phi = \begin{pmatrix} \phi_1 \\ \vdots \\ \phi_{2^n} \end{pmatrix} \in \mathbb{C}^{2^n}$*, we have :*

$$\begin{aligned} \langle\phi|\psi\rangle &= \begin{pmatrix} \bar{\phi_1} & \dots & \bar{\phi_{2^n}} \end{pmatrix} \begin{pmatrix} \psi_1 \\ \vdots \\ \psi_{2^n} \end{pmatrix} \\ &= \sum_{i=1}^{2^n} \bar{\phi_i}\psi_i \\ &\neq \sum_{i=1}^{2^n} \phi_i\bar{\psi_i} = \langle\psi|\phi\rangle . \end{aligned}$$

Definition 43 (Unitary operator associated with hermitian matrix)**.** *Given a hermitian matrix A, we define its associated quantum gate* $\mathrm{Exp}(A,t)$ *parametrized by the parameter* $t \in \mathbb{R}$ *as :*

$$\begin{aligned}\mathrm{Exp}(A,t) &= e^{-iAt} \\ &= \sum_{k=0}^{\infty} \frac{1}{k!}(-i)^k t^k A^k \,.\end{aligned}$$

Because A is hermitian, $\mathrm{Exp}(A,t)$ *is a unitary matrix.*

B Omitted proofs

B.1 Guiding function properties

B.1.1 Proof of Proposition 25

Proposition 25. *Function g_{mean} is a guiding function.*

Proof. Let us prove that g_{mean} is continuous. Let $x \in \{0,1\}^n$. The function $\theta \mapsto p_\theta(x) = |\langle x| U(\theta) |0_n\rangle|^2$ is continuous, because each coefficient of $U(\theta)$ is continuous. Thus, because multiplication and addition preserve continuity, g_{mean} is continuous.

We prove by contradiction that (11) holds. Let $\theta \in \mathcal{G}$ and let us consider the quantum state $|\psi(\theta)\rangle = U(\theta)|0_n\rangle$. Its decomposition in the canonical basis is $|\psi(\theta)\rangle = \sum_{x\in\{0,1\}^n} \psi_x |x\rangle$.

Assume that $|\psi(\theta)\rangle \notin \mathcal{F}_{\mathrm{quant}}$. By definition, there exists $x_0 \in \{0,1\}^n$ such that $x_0 \notin \mathcal{F}$ and $|\psi_{x_0}| \neq 0$. Thus,

$$\begin{aligned}g_{\mathrm{mean}}(\theta) &= \sum_{x\in\{0,1\}^n} |\psi_x|^2 f(x) \\ &= \sum_{x\in\mathcal{F}} |\psi_x|^2 f(x) + \sum_{x\notin\mathcal{F}} |\psi_x|^2 f(x) \\ &= \left(\sum_{x\in\mathcal{F}} |\psi_x|^2\right) f^* + \sum_{x\notin\mathcal{F}} |\psi_x|^2 f(x)\,,\end{aligned}$$

where f^* is the optimal value of f, reached on $\mathcal{F}$. By definition, $f(x) > f^*, \forall x \notin \mathcal{F}$, and because we assume that $|\psi_{x_0}| \neq 0$, thus the second term of the sum is bounded below as follows: $\sum_{x\notin\mathcal{F}} |\psi_x|^2 f(x) > \left(\sum_{x\notin\mathcal{F}} |\psi_x|^2\right) f^*$, where $\sum_{x\notin\mathcal{F}} |\psi_x|^2 \geq |\psi_{x_0}|^2 > 0$. Thus,

$$g_{\mathrm{mean}}(\theta) > \left(\sum_{x\in\mathcal{F}} |\psi_x|^2\right) f^* + \left(\sum_{x\notin\mathcal{F}} |\psi_x|^2\right) f^* = f^*\,.$$

This contradicts the previous statement that $\theta \in \mathcal{G}$, as one readily verifies that the minimum of g_{mean} is $g^*_{\mathrm{mean}} = f^*$. □

B.1.2 Proof of Proposition 27

Proposition 27. *Let $\eta > 0$. Function $g_{G,\eta}$ is a guiding function.*

Proof. Let us prove that $g_{G,\eta}$ is continuous. Let $x \in \{0,1\}^n$. The function $\theta \mapsto p_\theta(x) = |\langle x| U(\theta) |0_n\rangle|^2$ is continuous, because each coefficient of $U(\theta)$ is continuous. Thus, because multiplication, addition, and composition preserve continuity, $g_{G,\eta}$ is continuous.

Let $\eta > 0$. Let us prove by contradiction that (11) holds. As before, let $\theta \in \mathcal{G}$ and let us consider the quantum state $|\psi(\theta)\rangle = U(\theta)\,|0_n\rangle$. Its decomposition in the canonical basis is $|\psi(\theta)\rangle = \sum_{x\in\{0,1\}^n} \psi_x\,|x\rangle$. Assume that $|\psi(\theta)\rangle \notin \mathcal{F}_{\text{quant}}$. Thus, there exists $x_0 \in \{0,1\}^n$ such that $x_0 \notin \mathcal{F}$ and $|\psi_{x_0}| \neq 0$. Thus,

$$\begin{aligned} g_{G,\eta}(\theta) &= -\ln\left(\sum_{x\in\{0,1\}^n} |\psi_x|^2 e^{-\eta f(x)}\right) \\ &= -\ln\left(\sum_{x\in\mathcal{F}} |\psi_x|^2 e^{-\eta f(x)} + \sum_{x\notin\mathcal{F}} |\psi_x|^2 e^{-\eta f(x)}\right) \\ &= -\ln\left(\left(\sum_{x\in\mathcal{F}} |\psi_x|^2\right) e^{-\eta f^*} + \sum_{x\notin\mathcal{F}} |\psi_x|^2 e^{-\eta f(x)}\right), \end{aligned}$$

where f^* is the optimal value of f, reached on $\mathcal{F}$. By definition, $f(x) > f^*, \forall x \notin \mathcal{F}$, and because $\eta > 0$, we have $e^{-\eta f(x)} < e^{-\eta f^*}$. Moreover, we assume that $|\psi_{x_0}| \neq 0$, thus the second term of the sum in the logarithm is bounded above as follows: $\sum_{x\notin\mathcal{F}} |\psi_x|^2 e^{-\eta f(x)} < \left(\sum_{x\notin\mathcal{F}} |\psi_x|^2\right) e^{-\eta f^*}$, where $\sum_{x\notin\mathcal{F}} |\psi_x|^2 \geq |\psi_{x_0}|^2 > 0$. Thus, because $y \mapsto -\ln(y)$ is a decreasing function,

$$g_{G,\eta}(\theta) > -\ln\left(\left(\sum_{x\in\mathcal{F}} |\psi_x|^2\right) e^{-\eta f^*} + \left(\sum_{x\notin\mathcal{F}} |\psi_x|^2\right) e^{-\eta f^*}\right) = \eta f^*.$$

This contradicts the previous statement that $\theta \in \mathcal{G}$. Indeed, we can easily verify that the minimum of $g_{G,\eta}$ is $g^*_{G,\eta} = \eta f^*$. □

B.1.3 Proof of Proposition 31

Proposition 31. *Let $\alpha \in]0,1[$. Function $g_{C,\alpha}$ is a pseudo-guiding function.*

Proof. For the same reason as for g_{mean}, $g_{C,\alpha}$ is continuous.

Let $\alpha \in]0,1[\,, \theta \in \mathcal{G}$ and let us consider the quantum state $|\psi(\theta)\rangle = U(\theta)\,|0_n\rangle$. Its decomposition in the canonical basis is $|\psi(\theta)\rangle = \sum_{x\in\{0,1\}^n} \psi_x\,|x\rangle$.

Let us prove that either $|\psi(\theta)\rangle \in \mathcal{F}_{\text{quant}}$ or that $\sum_{x\notin\mathcal{F}} |\psi_x|^2 = \sum_{x=N_\mathcal{F}+1}^{2^n} |\psi_{x_i}|^2 < 1-\alpha$, where $N_\mathcal{F}$ is the index that delimits $\mathcal{F}$, specifically,

$$\mathcal{F} = \{x_i, i \in [N_\mathcal{F}]\}.$$

There are two cases for N_α (we recall that N_α depends on θ):

- If $N_\alpha \leq N_\mathcal{F}$, thus

$$\begin{aligned} g_{C,\alpha}(\theta) &= \frac{1}{\sum_{i\in[N_\alpha]\subseteq[N_\mathcal{F}]} |\psi_{x_i}|^2} \sum_{i\in[N_\alpha]\subseteq[N_\mathcal{F}]} |\psi_{x_i}|^2 f(x_i) \\ &= f^*, \end{aligned}$$

  where f^* is the optimal value of f, reached on $\mathcal{F}$. This contradicts (11) but the probability of sampling non-optimal solutions when measuring $|\psi(\theta)\rangle$ is strictly lower than $1-\alpha$. Indeed,

by definition of N_α,

$$\sum_{i=1}^{N_\mathcal{F}} |\psi_{x_i}|^2 \geq \sum_{i=1}^{N_\alpha} |\psi_{x_i}|^2 \geq \alpha\,.$$

- Otherwise, $N_\alpha > N_\mathcal{F}$. Let us prove by contradiction that $|\psi(\theta)\rangle \in \mathcal{F}_{\text{quant}}$. Assume that $|\psi(\theta)\rangle \notin \mathcal{F}_{\text{quant}}$. Thus, there exists $k > N_\mathcal{F}$ such that $|\psi_k| \neq 0$. We can show that $g_{C,\alpha}(\theta) > f^*$ using essentially the same proof as that of Proposition 25 for $x_0 = \min\{k > N_\mathcal{F} : |\psi_k| \neq 0\}$. This contradicts the statement that $\theta \in \mathcal{G}$, because the minimum of $g_{C,\alpha}$ is $g^*_{C,\alpha} = f^*$.

□

B.2 Quantum circuit of QAOA

B.2.1 Proof of Proposition 34

Proposition 34. *The first bloc* $\text{Exp}(H_f, \gamma)$ *parametrized by* $\gamma \in \mathbb{R}$ *is*

$$\text{Exp}(H_f, \gamma) = \prod_{\alpha \in \{0,1\}^n} \text{Exp}(\bigotimes_{i=1}^n Z_i^{\alpha_i}, h_\alpha \gamma)\,.$$

The second bloc $\text{Exp}(H_B, \beta)$ *parametrized by* $\beta \in \mathbb{R}$ *is*

$$\text{Exp}(H_B, \beta) = \bigotimes_{i=1}^n R_{X,i}(2\beta)\,.$$

Proof. Let $\gamma \in \mathbb{R}$ and let us consider the first bloc $\text{Exp}(H_f, \gamma)$. By Definition 43, and because each pair of matrices of the family $\{\bigotimes_{i=1}^n Z_i^{\alpha_i} : \alpha = (\alpha_1, \ldots, \alpha_n) \in \{0,1\}^n\}$ commutes two by two,

$$\begin{aligned}
\text{Exp}(H_f, \gamma) &= e^{-i(\sum_{\alpha=(\alpha_1,\ldots,\alpha_n)\in\{0,1\}^n} h_\alpha \bigotimes_{i=1}^n Z_i^{\alpha_i})\gamma} && (23)\\
&= \prod_{\alpha=(\alpha_1,\ldots,\alpha_n)\in\{0,1\}^n} e^{-ih_\alpha \bigotimes_{i=1}^n Z_i^{\alpha_i}\gamma} && (24)\\
&= \prod_{\alpha=(\alpha_1,\ldots,\alpha_n)\in\{0,1\}^n} \text{Exp}(\bigotimes_{i=1}^n Z_i^{\alpha_i}, h_\alpha\gamma)\,. && (25)
\end{aligned}$$

Let $\beta \in \mathbb{R}$ and let us consider the second bloc $\text{Exp}(H_B, \beta)$. For more readability, we write $X_i = R_{X,i}(\pi)$ the application of matrix $X = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$ on qubit i. With the same development as above, and because each pair of matrices of the family $\{X_i : i \in [n]\}$ commutes two by two,

$$\text{Exp}(H_B, \beta) = \prod_{i=1}^n \text{Exp}(X_i, \beta)\,.$$

Let $i \in [n]$. Thus,

$$\text{Exp}(X_i, \beta) = \sum_{k=0}^{\infty} \frac{1}{k!}(-i)^k \beta^k X_i^k \qquad (26)$$

$$= \sum_{k=0}^{\infty} \frac{1}{(2k)!}(-i)^{2k}\beta^{2k}X_i^{2k} + \sum_{k=0}^{\infty} \frac{1}{(2k+1)!}(-i)^{(2k+1)}\beta^{(2k+1)}X_i^{(2k+1)} \tag{27}$$

$$= \sum_{k=0}^{\infty} \frac{1}{(2k)!}(-i)^{2k}\beta^{2k}I + \sum_{k=0}^{\infty} \frac{1}{(2k+1)!}(-i)^{(2k+1)}\beta^{(2k+1)}X_i \tag{28}$$

$$= \sum_{k=0}^{\infty} \frac{1}{(2k)!}(-1)^{k}\beta^{2k}I - i\sum_{k=0}^{\infty} \frac{1}{(2k+1)!}(-1)^{k}\beta^{(2k+1)}X_i \tag{29}$$

$$= \cos(t)I - i\sin(t)X_i \tag{30}$$

$$= R_{X,i}(2\beta)\,, \tag{31}$$

where line (28) exploits the fact that $X^2 = I$, implying $X^{2k} = I$ and $X^{2k+1} = X$. Moreover, line (29) applies the definition of the complex number i, and one can recognize the power series of cosinus and sinus functions. □

B.2.2 Proof of Proposition 35

Proposition 35. *For the case of QUBO, the expression of* $\mathrm{Exp}(H_f, \gamma)$ *simplifies in*

$$\mathrm{Exp}(H_f, \gamma) = \left(\bigotimes_{i=1}^{n} R_{Z,i}(2h_{ii}\gamma)\right) \prod_{i<j} CX_{i,j}R_{Z,j}(2h_{i,j}\gamma)CX_{i,j}\,,$$

and is rather easily implemented with universal quantum gates.

Proof. Let $\gamma \in \mathbb{R}$. The application of (23)–(25) to the case of QUBO gives

$$\begin{aligned}
\mathrm{Exp}(H_f, \gamma) &= e^{-i(\sum_{i=1}^{n} h_{ii}Z_i + \sum_{i<j} h_{ij}Z_i\otimes Z_j)\gamma} \\
&= \prod_{i=1}^{n} e^{-iZ_i h_{ii}\gamma} \prod_{i<j} e^{-iZ_i\otimes Z_j h_{ij}\gamma} \\
&= \prod_{i=1}^{n} \mathrm{Exp}(Z_i, h_{ii}\gamma) \prod_{i<j} \mathrm{Exp}(Z_i \otimes Z_j, h_{ij}\gamma)\,.
\end{aligned}$$

Then, let us prove that, for $i \in [n]$ and $t \in \mathbb{R}$, $\mathrm{Exp}(Z_i, t) = R_{Z,i}(2t)$. The same development as above (28)–(30), replacing X by Z that have the same property $Z^2 = I$, gives

$$\mathrm{Exp}(Z_i, t) = \cos(t)I - i\sin(t)Z_i \tag{32}$$

$$= R_{Z,i}(2t)\,. \tag{33}$$

Eventually, line (32) is the application of the gate $\begin{pmatrix} e^{-it} & 0 \\ 0 & e^{it} \end{pmatrix} = R_Z(2t)$ on qubit i, and the identity on the others.

It remains to prove that, for $i < j \in [n]$ and $t \in \mathbb{R}$, $\mathrm{Exp}(Z_i \otimes Z_j, t) = CX_{i,j}R_{Z,j}(2t)CX_{i,j}$. Following the same developments as above, we have

$$\mathrm{Exp}(Z_i \otimes Z_j, t) = \cos(t)I - i\sin(t)Z_i \otimes Z_j\,. \tag{34}$$

We consider the two-qubit system that corresponds to the qubit i as the first qubit and the qubit j as the second qubit (the others are unchanged by the transformation). Thus, it remains to

prove the equality of the two circuits depicted on Figure 9.

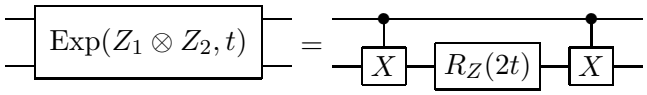

Figure 9: Decomposition of $\mathrm{Exp}(Z_1 \otimes Z_2, t)$ into universal gates.

On the one hand, (34) is the application of the gate $= \begin{pmatrix} R_Z(2t) & 0 \\ 0 & R_Z(-2t) \end{pmatrix}$ to this system. Indeed,

$$\begin{aligned}
\cos(t)I - i\sin(t)Z_1 \otimes Z_2 &= \cos(t)\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} - i\sin(t)\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \\
&= \begin{pmatrix} e^{-it} & 0 & 0 & 0 \\ 0 & e^{it} & 0 & 0 \\ 0 & 0 & e^{it} & 0 \\ 0 & 0 & 0 & e^{-it} \end{pmatrix} \\
&= \begin{pmatrix} R_Z(2t) & 0 \\ 0 & R_Z(-2t) \end{pmatrix}.
\end{aligned}$$

On the other hand, the composition of gates $CX_{1,2}R_{Z,2}(2t)CX_{1,2}$ on this system amounts to

$$\begin{aligned}
CX_{1,2}R_{Z,2}(2t)CX_{1,2} &= \begin{pmatrix} I & 0 \\ 0 & X \end{pmatrix}\begin{pmatrix} R_Z(2t) & 0 \\ 0 & R_Z(2t) \end{pmatrix}\begin{pmatrix} I & 0 \\ 0 & X \end{pmatrix} \\
&= \begin{pmatrix} R_Z(2t) & 0 \\ 0 & XR_Z(2t)X \end{pmatrix} \\
&= \begin{pmatrix} R_Z(2t) & 0 \\ 0 & R_Z(-2t) \end{pmatrix}.
\end{aligned}$$

Thus, the proof results from replacing t by appropriate values $h_{ii}\gamma$ for $i \in [n]$ and $h_{ij}\gamma$ for $i < j$. □

B.2.3 Proof of Lemma 36

Lemma 36. *$\forall n \in \mathbb{N}^*$,*

$$(I^{\otimes n-1} \otimes X)e^{-itZ^{\otimes n}}(I^{\otimes n-1} \otimes X) = e^{itZ^{\otimes n}}.$$

Proof. Let P_n be the statement

$$(I^{\otimes n-1} \otimes X)e^{-itZ^{\otimes n}}(I^{\otimes n-1} \otimes X) = e^{itZ^{\otimes n}}.$$

Let us prove by induction that P_n holds for all integer $n \in \mathbb{N}^*$.
Base case: Let us prove P_1. According to (33), $e^{-itZ} = R_Z(2t)$, thus,

$$Xe^{-itZ}X = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}\begin{pmatrix} e^{-it} & 0 \\ 0 & e^{it} \end{pmatrix}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

$$= \begin{pmatrix} e^{it} & 0 \\ 0 & e^{-it} \end{pmatrix}$$
$$= e^{itZ} .$$

Induction step: Let $n \geq 1$ be given and suppose P_n. Let us prove P_{n+1}. According to (35), we have $e^{-itZ^{\otimes n+1}} = \begin{pmatrix} e^{-itZ^{\otimes n}} & 0 \\ 0 & e^{itZ^{\otimes n}} \end{pmatrix}$. Thus,

$$\begin{aligned}(I^{\otimes n} \otimes X)e^{-itZ^{\otimes n+1}}(I^{\otimes n} \otimes X) &= (I \otimes I^{\otimes n-1} \otimes X)e^{-itZ^{\otimes n+1}}(I \otimes I^{\otimes n-1} \otimes X) \\ &= \begin{pmatrix} I^{\otimes n-1} \otimes X & 0 \\ 0 & I^{\otimes n-1} \otimes X \end{pmatrix} \begin{pmatrix} e^{-itZ^{\otimes n}} & 0 \\ 0 & e^{itZ^{\otimes n}} \end{pmatrix} \begin{pmatrix} I^{\otimes n-1} \otimes X & 0 \\ 0 & I^{\otimes n-1} \otimes X \end{pmatrix} \\ &= \begin{pmatrix} (I^{\otimes n-1} \otimes X)e^{-itZ^{\otimes n}}(I^{\otimes n-1} \otimes X) & 0 \\ 0 & (I^{\otimes n-1} \otimes X)e^{itZ^{\otimes n}}(I^{\otimes n-1} \otimes X) \end{pmatrix} .\end{aligned}$$

By induction hypothesis P_n,

$$\begin{aligned}(I^{\otimes n} \otimes X)e^{-itZ^{\otimes n+1}}(I^{\otimes n} \otimes X) &= \begin{pmatrix} e^{itZ^{\otimes n}} & 0 \\ 0 & e^{-itZ^{\otimes n}} \end{pmatrix} \\ &= e^{itZ^{\otimes n+1}} .\end{aligned}$$

□

B.2.4 Proof of Proposition 37

Proposition 37. *Let us consider the subsystem composed of the N qubits to which the Z gate is applied. Specifically, $N = |\{\alpha_i \, i \in [n] : \alpha_i = 1\}|$, and we renumber the qubits in question in $[N]$. Thus, for $N \geq 2$, the term $\mathrm{Exp}(\bigotimes_{i=1}^{n} Z^{\alpha_i}, t)$ on this subsystem simplifies in*

$$\mathrm{Exp}(Z^{\otimes N}, t) = \prod_{j=0}^{N-2} CX_{1,N-j} R_{Z,N}(2t) \prod_{j=0}^{N-2} CX_{1,N-j} .$$

We represent this decomposition on Figure 7.

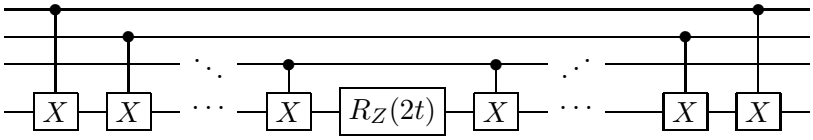

Figure 10: Decomposition of $\mathrm{Exp}(Z^{\otimes N}, t)$ on the N-qubit subsystem.

Proof. Let P_n be the statement

$$\mathrm{Exp}(Z^{\otimes n}, t) = \prod_{j=0}^{n-2} CX_{1,n-j} R_{Z,n}(2t) \prod_{j=0}^{n-2} CX_{1,n-j} .$$

Let us prove by induction that P_n holds for all integer $n \geq 2$.

Base case: Proposition 35 proves P_2.
Induction step: Let $n \geq 2$ be given and suppose P_n. Let us prove P_{n+1}.
On the one hand,

$$\mathrm{Exp}(Z^{\otimes n+1}, t) = e^{-itZ^{\otimes n+1}} = e^{-itZ \otimes Z^{\otimes n}}$$

where $Z \otimes Z^{\otimes n} = \begin{pmatrix} Z^{\otimes n} & 0 \\ 0 & -Z^{\otimes n} \end{pmatrix}$. This latter matrix is diagonal, thus,

$$\mathrm{Exp}(Z^{\otimes n+1}, t) = \begin{pmatrix} e^{-itZ^{\otimes n}} & 0 \\ 0 & e^{itZ^{\otimes n}} \end{pmatrix}. \tag{35}$$

On the other hand, we compute the term

$$\prod_{j=0}^{n-1} CX_{1,n+1-j} R_{Z,n+1}(2t) \prod_{j=0}^{n-1} CX_{1,n+1-j} = CX_{1,n+1} \left(\prod_{j=1}^{n-2} CX_{1,n+1-j} R_{Z,n+1}(2t) \prod_{j=1}^{n-2} CX_{1,n+1-j} \right) CX_{1,n+1}$$

that is represented on Figure 11, where $e^{-itZ^{\otimes n}}$ applies on the qubits 2 to n by induction hypothesis.

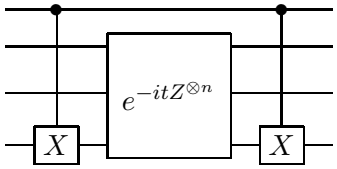

Figure 11: Circuit representation of $\prod_{j=0}^{n-1} CX_{1,n+1-j} R_{Z,n+1}(2t) \prod_{j=0}^{n-1} CX_{1,n+1-j}$.

Thus,

$$\begin{aligned}
\prod_{j=0}^{n-1} CX_{1,n+1-j} R_{Z,n+1}(2t) \prod_{j=0}^{n-1} CX_{1,n+1-j} &= CX_{1,n+1}(I \otimes e^{-itZ^{\otimes n}}) CX_{1,n+1} \\
&= \begin{pmatrix} I^{\otimes n} & 0 \\ 0 & I^{\otimes n-1} \otimes X \end{pmatrix} \begin{pmatrix} e^{-itZ^{\otimes n}} & 0 \\ 0 & e^{-itZ^{\otimes n}} \end{pmatrix} \begin{pmatrix} I^{\otimes n} & 0 \\ 0 & I^{\otimes n-1} \otimes X \end{pmatrix} \\
&= \begin{pmatrix} e^{-itZ^{\otimes n}} & 0 \\ 0 & (I^{\otimes n-1} \otimes X) e^{-itZ^{\otimes n}} (I^{\otimes n-1} \otimes X) \end{pmatrix} \\
&= \begin{pmatrix} e^{-itZ^{\otimes n}} & 0 \\ 0 & e^{itZ^{\otimes n}} \end{pmatrix},
\end{aligned}$$

where the last line comes from the application of Lemma 36. Thus,

$$\mathrm{Exp}(Z^{\otimes n+1}, t) = \prod_{j=0}^{n-1} CX_{1,n+1-j} R_{Z,n+1}(2t) \prod_{j=0}^{n-1} CX_{1,n+1-j},$$

proving P_{n+1}. □