Variational Quantum Linear Solver

Introduction to Quantum Computing

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GitHub Repository

https://github.com/kthod/VQLS_algorithm.git

Introduction

$$\boldsymbol{Ax} = \boldsymbol{b} \text{ where } \boldsymbol{A} \in R^{N\times N} \text{ and } \boldsymbol{x}, \boldsymbol{b} \in \boldsymbol{R^N}$$

Existing classical algorithms solves the problem with polynomial scaling in N

Introduction

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Exponential speedup can be achieved using the quantum algorithm **HHL** which:

- Determines a quantum state $|x\rangle$ that is proportional to $\boldsymbol{x}$: $|x\rangle \sim \boldsymbol{x}$
- Achieves polylogarithmic scaling in N

However

- Demanding implementation

Instead a Variational Hybrid Quantum Classical Algorithm can be used

The Variational Quantum Linear Solves (VQLS)

- Can be performed in NISQ quantum computers

Complexity of the VQLS algorithm

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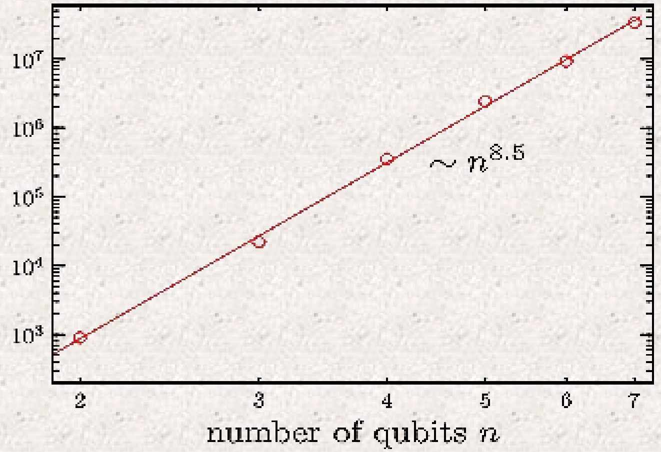
- The obtained relation for running time scaling with n is :

$$y \sim n^{8.5}$$

Since $N = 2^n \Leftrightarrow n = \log N$

$$y \sim (\log N)^{8.5}$$

Which is polylogarithmical in N



Time to solution scaling with n. Figure taken from original paper

Time to solution scaling with n. Measurements taken using our implementation of VQLS

Description of the algorithm

Input

- A matrix $\boldsymbol{A}$ that, must be given as a linear combination of L unitaries $A_1 ,A_2,\ldots,A_L$ such that

$$\boldsymbol{A} = \sum_{l=1}^{L} c_l A_l$$

 where c_l is a complex number

- An operator U that prepares a quantum state $|b\rangle$ that is proportional to the vector **b**, such that

$$U|0\rangle = |b\rangle$$

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Goal

Determine a state $|x\rangle$ such that $A|x\rangle$ is proportional to $|b\rangle$, or equivalently:

$$|\psi\rangle := \frac{\boldsymbol{A}|x\rangle}{\sqrt{\langle x|\boldsymbol{A}^\dagger \boldsymbol{A}|x\rangle}} \approx |b\rangle$$

Description of the algorithm

- $|x\rangle$ is approximated using a set of parameters $\boldsymbol{\alpha} = (\alpha_1, \alpha_2, \ldots)$ such that
    - $|x(\boldsymbol{\alpha})\rangle = V(\boldsymbol{\alpha})|\mathbf{0}\rangle$

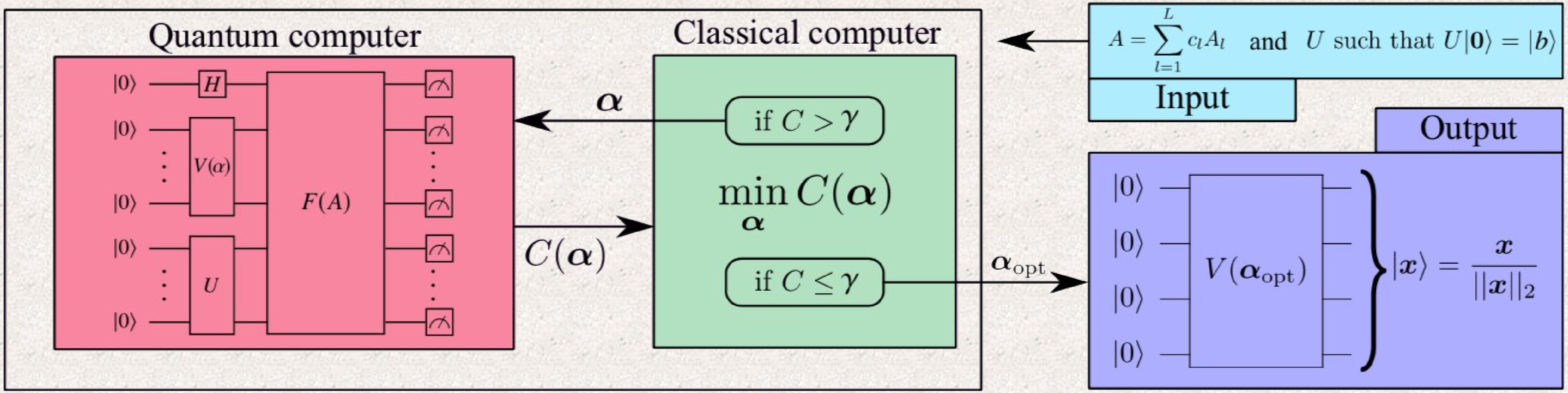
The operator $V(\boldsymbol{\alpha})$ is called **Ansatz** and is capable of generating any arbitrary state in Hilbert space

- The configuration of the parameters $\boldsymbol{\alpha}$ is happening through a classical optimizer that aims to minimize a **cost function** $C(\boldsymbol{\alpha})$

- A quantum circuit evaluates the cost function $C(\boldsymbol{\alpha})$

Description of the algorithm

Interaction between the Quantum circuit and the classical optimizer



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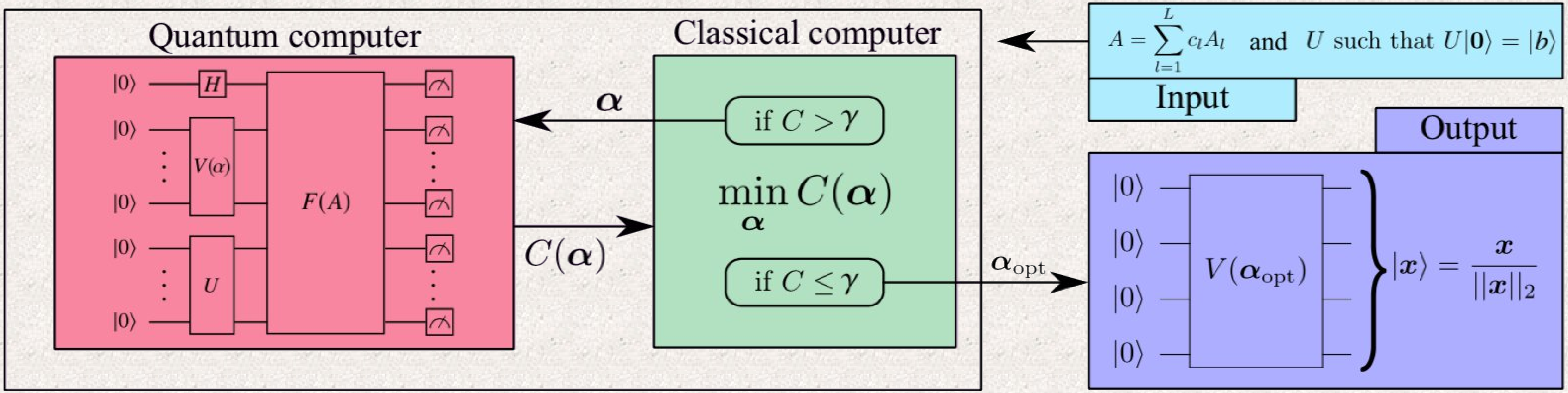
Interaction between the Quantum circuit and the classical optimizer

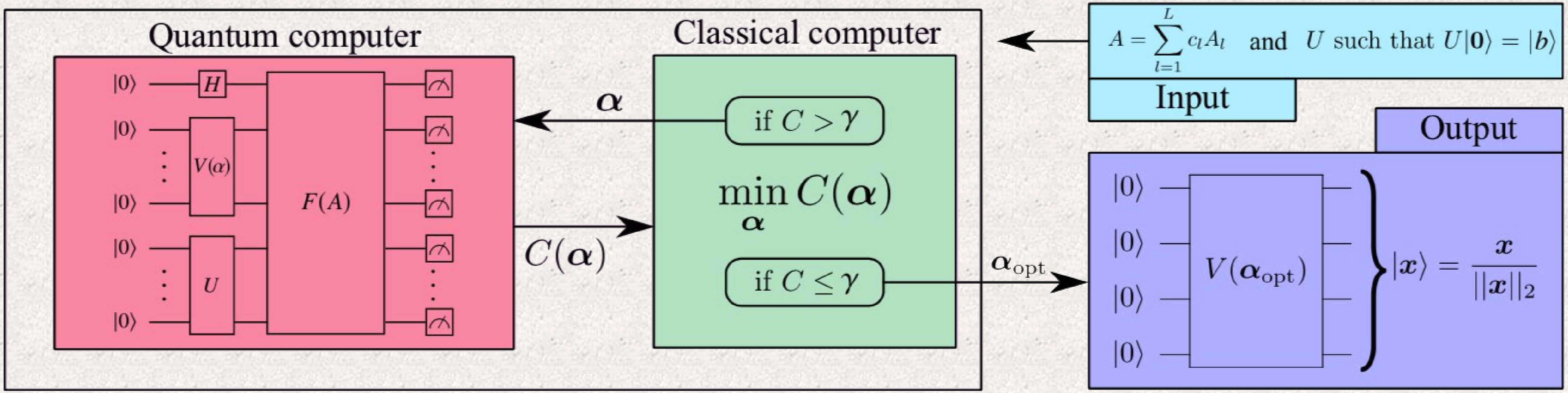
- The quantum circuit receives as input the parameters $\boldsymbol{\alpha}$ and evaluates the cost function on this point $C(\boldsymbol{\alpha})$



Description of the algorithm

<u>Interaction between the Quantum circuit and the classical optimizer</u>

- The quantum circuit receives as input the parameters $\boldsymbol{\alpha}$ and evaluates the cost function on this point $C(\boldsymbol{\alpha})$
- The classical optimizer, uses the output value $C(\boldsymbol{\alpha})$, to determine a new set of parameters $\boldsymbol{\alpha}'$ such that, $C(\boldsymbol{\alpha}') < C(\boldsymbol{\alpha})$



Description of the algorithm

<u>Interaction between the Quantum circuit and the classical optimizer</u>

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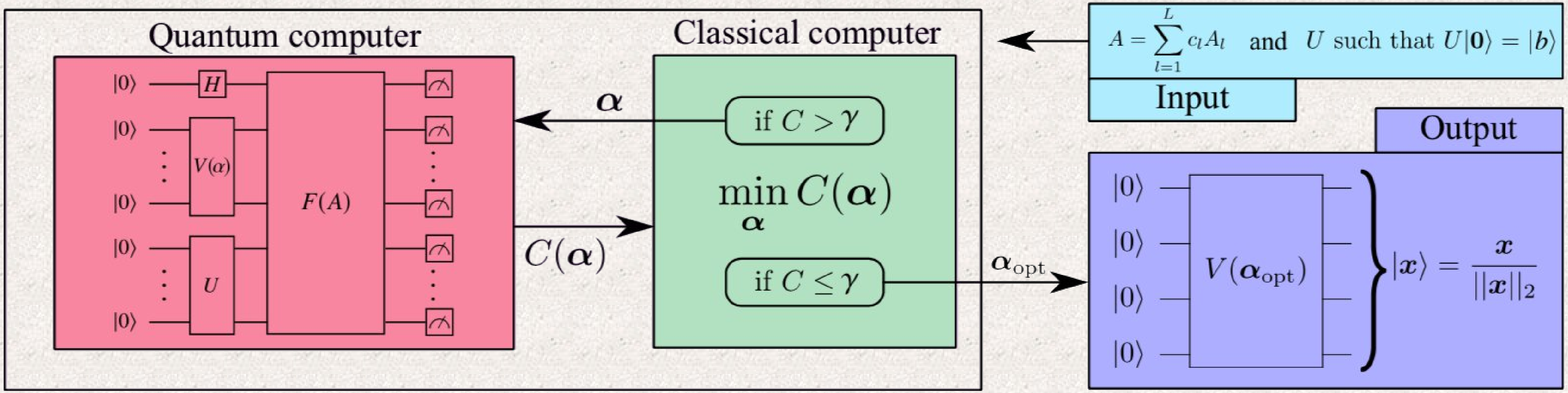
- The classical optimizer, uses the output value $C(\boldsymbol{\alpha})$, to determine a new set of parameters $\boldsymbol{\alpha}'$ such that, $C(\boldsymbol{\alpha}') < C(\boldsymbol{\alpha})$
- The quantum circuit is fed with the new set of parameters $\boldsymbol{\alpha}'$ and the process repeats itself until the cost function reaches its global minimum : $C(\boldsymbol{\alpha}_{opt}) = 0 \rightarrow |x(\boldsymbol{\alpha}_{opt})\rangle = |x\rangle$



The Ansatz

Capable of generating any arbitrary state on Hilbert space, including the entangled ones

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<u>Consists of :</u>

- Rotation single-qubit gates R_X, R_Y, R_Z for “exploring” the space. Each one of the rotation gates should correspond to one of the parameters $\boldsymbol{\alpha} = (\alpha_1, \alpha_2, \ldots)$

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Distinguishing two types of Ansatzes:

- The Fixed-Structure Anstatz

- The Variable-Structure Ansatz

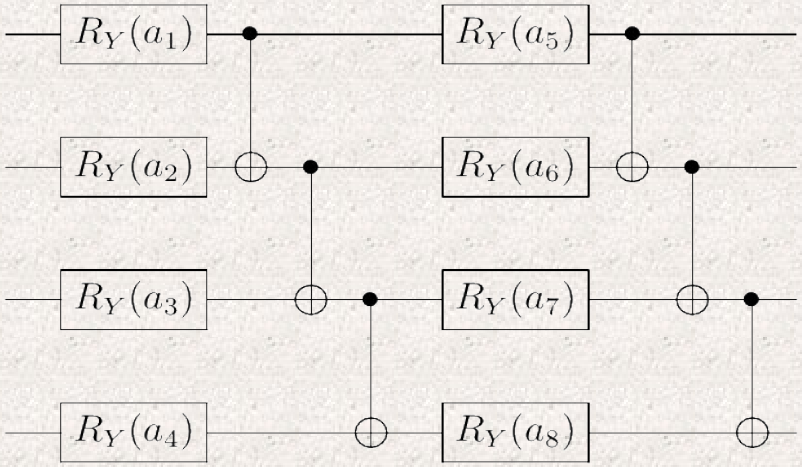
We are only concerned with Fixed-Structure Anstatz

The Ansatz

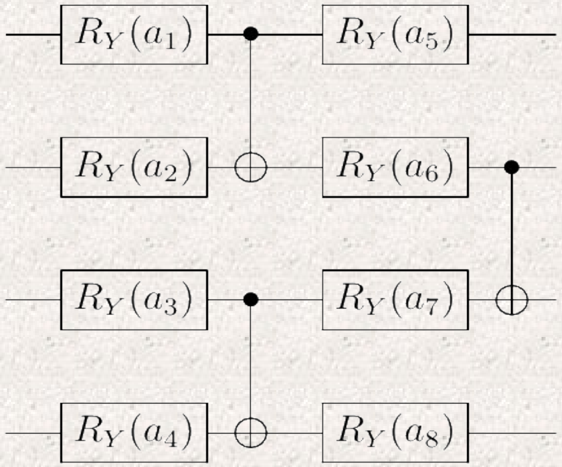
<u>Fixed-Structure Anstaz</u>

Placement of the gates remains the same throughout the execution of the algorithm

Two examples are the following:



linear entanglement



alternating entanglement

Ansatz with alternating entanglement is more efficient in terms of effective parameters per two-qubit gate

The Cost Function

Define $|\psi\rangle \;=\; |\psi(\boldsymbol{\alpha})\rangle \;:=\; \boldsymbol{A}\,|x(\boldsymbol{\alpha})\rangle$

We construct a cost function which takes its minimum value C=0 when $|\psi\rangle$ and $|b\rangle$ have the maximum overlap

The general form of a cost function in VQA is $C_G = \langle \psi | H_G | \psi \rangle$

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A suitable Hamiltonian H_G to take advantage of the overlap is

$$H_G = \mathrm{I} - |b\rangle\langle b|.$$

Hence the cost function is

$$\hat{C}_G = \langle\psi|(\mathbb{I} - |b\rangle\langle b|)|\psi\rangle = \langle\psi|\psi\rangle - |\langle b|\psi\rangle|^2$$

with $0 \leq \hat{C}_G \leq \langle\psi|\psi\rangle$

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A potential small $\langle\psi|\psi\rangle$ would be problematic, so we use instead a normalized version of the cost function

$$C_G = \frac{\hat{C}_G}{\langle\psi|\psi\rangle} = 1 - \frac{|\langle b|\psi\rangle|^2}{\langle\psi|\psi\rangle}$$

The Cost Function

Using that $|b\rangle = U|\mathbf{0}\rangle$ and $|\psi\rangle = A|x(\boldsymbol{\alpha})\rangle = \sum_{l=1}^{L} c_l A_l V(\boldsymbol{\alpha})|\mathbf{0}\rangle$

$$C_G = 1 - \frac{\langle\psi|b\rangle\langle b|\psi\rangle}{\langle\psi|\psi\rangle} = 1 - \frac{\left(\sum_{l=1}^{L} c_l^* \langle\mathbf{0}|V^\dagger(\boldsymbol{\alpha})A_l^\dagger U|\mathbf{0}\rangle\right)\left(\sum_{l=1}^{L} c_l \langle\mathbf{0}|U^\dagger A_l V(\boldsymbol{\alpha})|\mathbf{0}\rangle\right)}{\left(\sum_{l=1}^{L} c_l^* \langle\mathbf{0}|V^\dagger(\boldsymbol{\alpha})A_l^\dagger\right)\left(\sum_{l=1}^{L} c_l A_l V(\boldsymbol{\alpha})|\mathbf{0}\rangle\right)} =$$

$$= 1 - \frac{\sum_{l=1}^{L}\sum_{l'=1}^{L} c_{l'} c_l^* \langle\mathbf{0}|V^\dagger(\boldsymbol{\alpha})A_l^\dagger U|\mathbf{0}\rangle\langle\mathbf{0}|U^\dagger A_{l'} V(\boldsymbol{\alpha})|\mathbf{0}\rangle}{\sum_{l=1}^{L}\sum_{l'=1}^{L} c_{l'} c_l^* \langle\mathbf{0}|V^\dagger(\boldsymbol{\alpha})A_l^\dagger A_{l'} V(\boldsymbol{\alpha})|\mathbf{0}\rangle}$$

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$$= 1 - \frac{\sum_{l=1}^{L}\sum_{l'=1}^{L} c_{l'} c_l^* \langle\mathbf{0}| V^\dagger(\boldsymbol{\alpha}) A_l^\dagger U |\mathbf{0}\rangle \langle\mathbf{0}| U^\dagger A_{l'} V(\boldsymbol{\alpha}) |\mathbf{0}\rangle}{\sum_{l=1}^{L}\sum_{l'=1}^{L} c_{l'} c_l^* \langle\mathbf{0}| V^\dagger(\boldsymbol{\alpha}) A_l^\dagger A_{l'} V(\boldsymbol{\alpha}) |\mathbf{0}\rangle}$$

The above is called **Global Cost Function**

- Can exhibit barren plateaus for a large number of qubits

The Cost Function

To tackle this problem we divide the problem up into multiple single-qubit terms by replacing the term $|\mathbf{0}\rangle\langle\mathbf{0}|$ with $\frac{1}{n}\sum_{j=0}^{n-1}(|0_j\rangle\langle 0_j| \otimes \mathbb{I}_{\bar{j}})$.

The produced cost is function is called **Local Cost Function** $H_L = \mathbb{I} - \frac{1}{n}\sum_{j=1}^{n}|0_j\rangle\langle 0_j| \otimes \mathbb{I}_{\bar{j}}$

$$C_L = 1 - \frac{\sum_{l=1}^{L}\sum_{l'=1}^{L} c_{l'}c_l^* \langle\mathbf{0}| V^\dagger(\boldsymbol{\alpha})A_l^\dagger U\left(\frac{1}{n}\sum_{j=0}^{n-1}(|0_j\rangle\langle 0_j| \otimes \mathbb{I}_{\bar{j}})\right)U^\dagger A_{l'}V(\boldsymbol{\alpha})|\mathbf{0}\rangle}{\sum_{l=1}^{L}\sum_{l'=1}^{L} c_{l'}c_l^* \langle\mathbf{0}| V^\dagger(\boldsymbol{\alpha})A_l^\dagger A_{l'}V(\boldsymbol{\alpha})|\mathbf{0}\rangle} =$$

$$= 1 - \frac{1}{n}\frac{\sum_{l=1}^{L}\sum_{l'=1}^{L}\sum_{j=0}^{n-1} c_{l'}c_l^* \langle\mathbf{0}| V^\dagger(\boldsymbol{\alpha})A_l^\dagger U(|0_j\rangle\langle 0_j| \otimes \mathbb{I}_{\bar{j}})U^\dagger A_{l'}V(\boldsymbol{\alpha})|\mathbf{0}\rangle}{\sum_{l=1}^{L}\sum_{l'=1}^{L} c_{l'}c_l^* \langle\mathbf{0}| V^\dagger(\boldsymbol{\alpha})A_l^\dagger A_{l'}V(\boldsymbol{\alpha})|\mathbf{0}\rangle}$$

To prove that the local cost function suits our problem we use that

$$C_L \le C_G \le nC_L$$

Which implies that $C_G \to 0 \Leftrightarrow C_L \to 0$

The Cost Function

Evaluation of the cost function using quantum circuit

- For Global Cost Function we have to evaluate the terms:

$$\beta_{ll'} = \langle \mathbf{0} | V^\dagger(\boldsymbol{\alpha}) A_l^\dagger A_{l'} V(\boldsymbol{\alpha}) | \mathbf{0} \rangle$$

and

$$\gamma_{ll'} = \langle \mathbf{0} | V^\dagger(\boldsymbol{\alpha}) A_l^\dagger U | \mathbf{0} \rangle \langle \mathbf{0} | U^\dagger A_{l'} V(\boldsymbol{\alpha}) | \mathbf{0} \rangle$$

- For Local Cost Function we have to evaluate the terms:

$$\beta_{ll'} = \langle \mathbf{0} | V^\dagger(\boldsymbol{\alpha}) A_l^\dagger A_{l'} V(\boldsymbol{\alpha}) | \mathbf{0} \rangle$$

and

$$\delta_{ll'}^{(j)} = \langle \mathbf{0} | V^\dagger(\boldsymbol{\alpha}) A_l^\dagger U (|0_j\rangle \langle 0_j| \otimes \mathbb{I}_{\bar{j}}) U^\dagger A_{l'} V(\boldsymbol{\alpha}) | \mathbf{0} \rangle$$

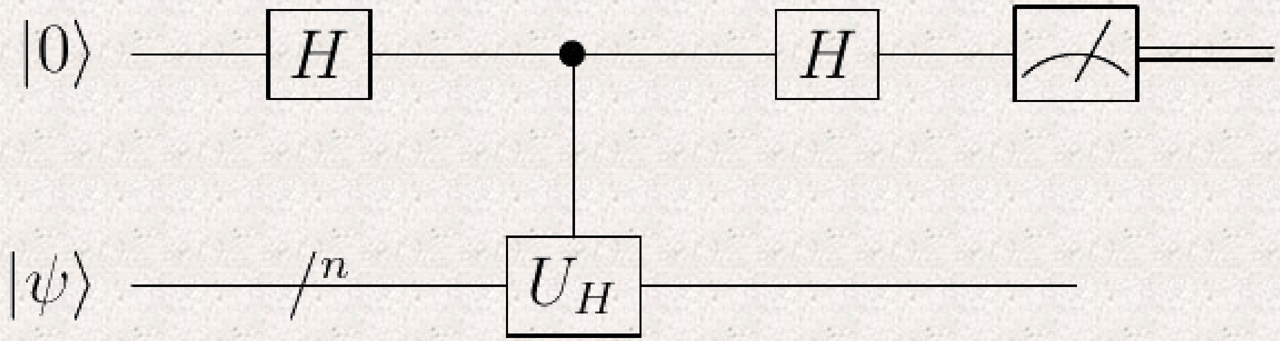
Using that $|0_j\rangle\langle 0_j| = \frac{1}{2}\left(I_j + Z_j\right)$, the last one can be rewritten as

$$\delta_{ll'}^{(j)} = \beta_{ll'} + \langle \mathbf{0} | V^\dagger(\boldsymbol{\alpha}) A_l^\dagger U (Z_j \otimes \mathbb{I}_{\bar{j}}) U^\dagger A_{l'} V(\boldsymbol{\alpha}) | \mathbf{0} \rangle$$

The Cost Function

How can we evaluate the previous terms?

We employ a quantum circuit called **The Hadamard Test**



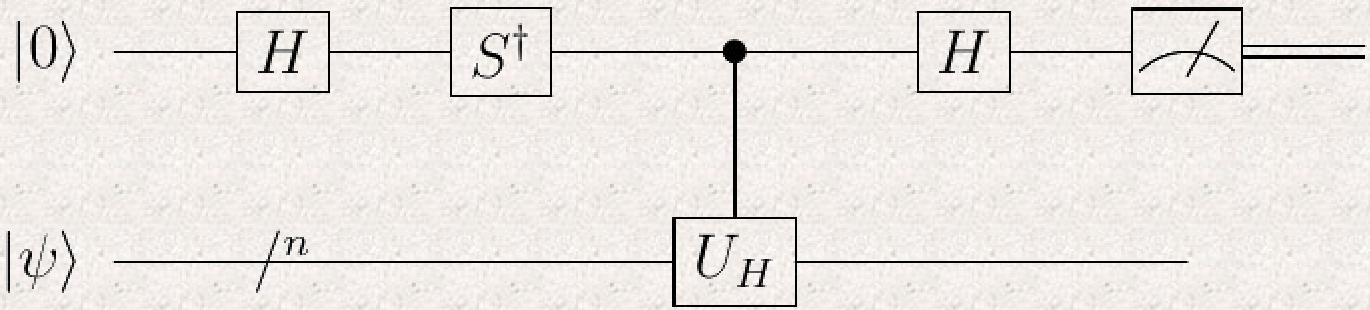
The circuit above can calculate the term $Re\left[\langle\psi|U_H|\psi\rangle\right]$

- The probability of measuring the first qubit (**ancilla**) to be 0 is $P(0) \;=\; \frac{1}{2}\left(1 + Re\left[\langle\psi|U_H|\psi\rangle\right]\right)$
- The probability of measuring the ancilla qubit to be 1 is $P(1) \;=\; \frac{1}{2}\left(1 - Re\left[\langle\psi|U_H|\psi\rangle\right]\right)$

Hence $P(0) - P(1) = Re\left[\langle\psi|U_H|\psi\rangle\right]$

The Cost Function

For the Imaginary part we simple add a $S^{\dagger}$ gate after the first Hadamard on the ancilla qubit



The circuit above can calculate the term $Im\left[\langle\psi|U_H|\psi\rangle\right]$

- The probability of measuring the ancilla qubit to be 0 is $P(0) \;=\; \frac{1}{2}\left(1 + Im\left[\langle\psi|U_H|\psi\rangle\right]\right)$
- The probability of measuring the ancilla qubit to be 1 is $P(1) \;=\; \frac{1}{2}\left(1 - Im\left[\langle\psi|U_H|\psi\rangle\right]\right)$

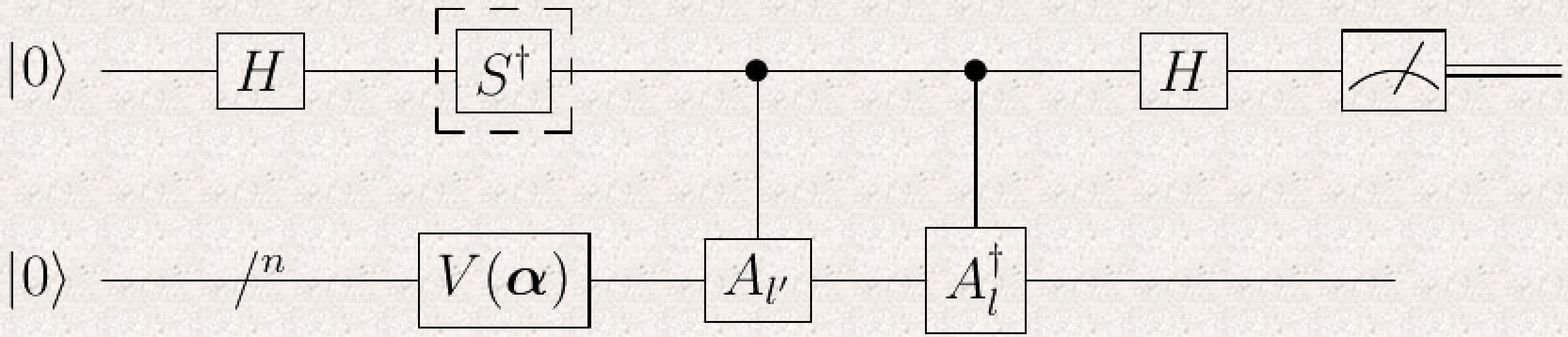
Hence $P(0) - P(1) = Im\left[\langle\psi|U_H|\psi\rangle\right]$

The Cost Function

How can we apply the hadamard test for our purpose?

To calculate the terms $\beta_{ll'} = \langle \mathbf{0} | V^\dagger(\boldsymbol{\alpha}) A_l^\dagger A_{l'} V(\boldsymbol{\alpha}) | \mathbf{0} \rangle$ we set:

$|\psi\rangle = V(\boldsymbol{\alpha}) |\mathbf{0}\rangle$ and $U_H = A_l^\dagger A_{l'}$

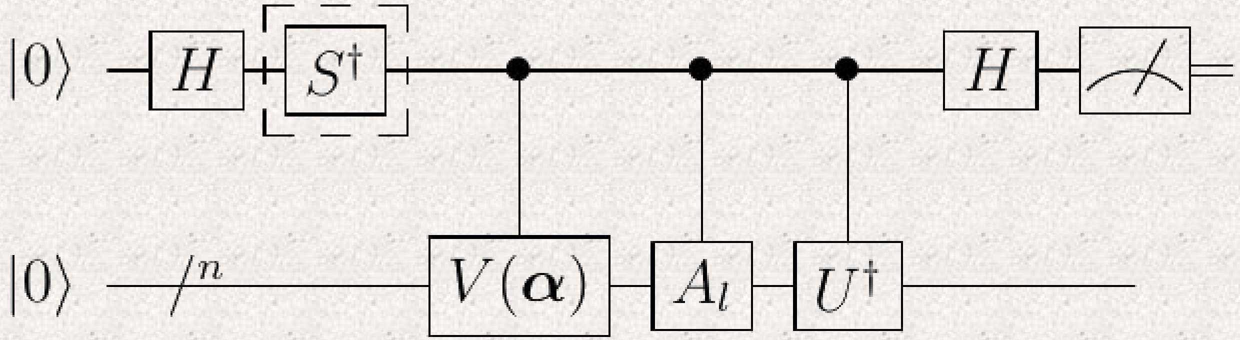


The Cost Function

To calculate the terms $\gamma_{ll'} = \langle \mathbf{0}| V^\dagger(\boldsymbol{\alpha}) A_l^\dagger U |\mathbf{0}\rangle \langle \mathbf{0}| U^\dagger A_{l'} V(\boldsymbol{\alpha}) |\mathbf{0}\rangle$:

$$\langle \mathbf{0}| V^\dagger(\boldsymbol{\alpha}) A_l^\dagger U |\mathbf{0}\rangle = (\langle \mathbf{0}| U^\dagger A_l V(\boldsymbol{\alpha}) |\mathbf{0}\rangle)^\dagger = (\langle \mathbf{0}| U^\dagger A_l V(\boldsymbol{\alpha}) |\mathbf{0}\rangle)^*$$

Thus by setting $|\psi\rangle = |\mathbf{0}\rangle$ and $U_H = U^\dagger A_l V(\boldsymbol{\alpha})$ we can calculate $\gamma_{ll'}$ by using the following circuit twice



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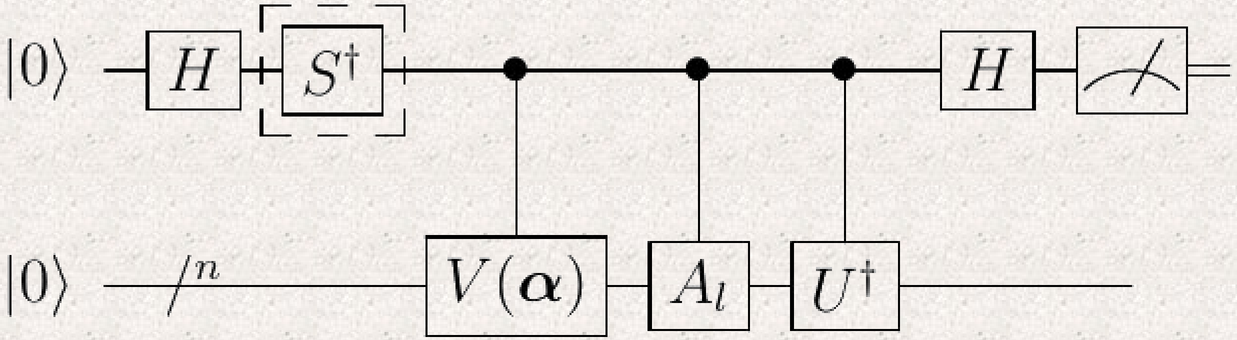
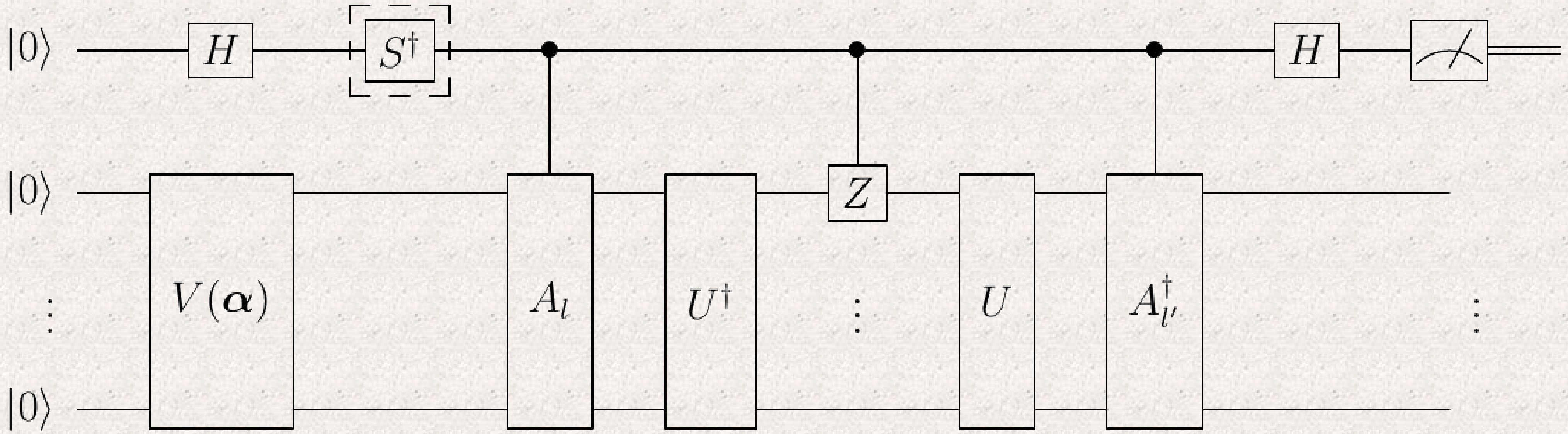


- An alternative way to calculate these term is by using an different subroutine called **The Hadamard-Overlap Test**

The Cost Function

To calculate the terms $\delta_{ll'}^{(j)} = \beta_{ll'} + \langle \mathbf{0} | V^\dagger(\boldsymbol{\alpha}) A_l^\dagger U (Z_j \otimes \mathbb{I}_{\bar{j}}) U^\dagger A_{l'} V(\boldsymbol{\alpha}) | \mathbf{0} \rangle$

We set $|\psi\rangle = V(\boldsymbol{\alpha}) |\mathbf{0}\rangle$ and $U_H = A_l^\dagger U (Z_j \otimes \mathbb{I}_{\bar{j}}) U^\dagger A_{l'}$



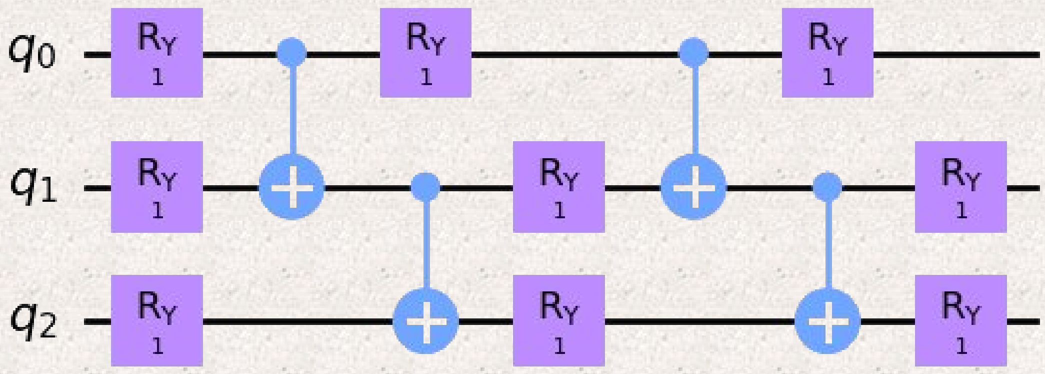
Qiskit Implementation

Using Qiskit we attempt to implement the VQLS algorithm and solve an example of a 3-qubits linear equations system $\boldsymbol{Ax} = \boldsymbol{b}$ with

$$\mathbf{A} = 0.4H_2 + 0.3Z_1 + 0.3X_3 \quad \text{and} \quad |b\rangle = H_1 \otimes H_2 \otimes H_3 \, |\mathbf{0}\rangle$$

Qiskit Implementation

Linear entanglement ansatz was used with 9 rotation gates R_Y (therefore 9 parameters) and 4 *CNOTs gates*

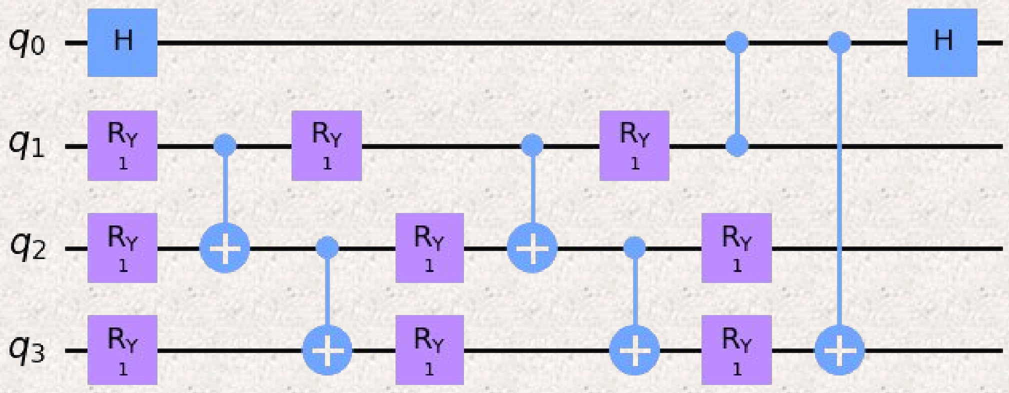


Since $\boldsymbol{A}$ and $|b\rangle$ are real, only rotation around the y-axis is required

Qiskit Implementation

Global cost function was used:

The Hadamard Test for evaluatind the terms $\beta_{ll'} = \langle \mathbf{0} | V^\dagger(\boldsymbol{\alpha}) A_l^\dagger A_{l'} V(\boldsymbol{\alpha}) | \mathbf{0} \rangle$



With $A_l = Z_1$ and $A_{l'} = X_3$

Qiskit Implementation

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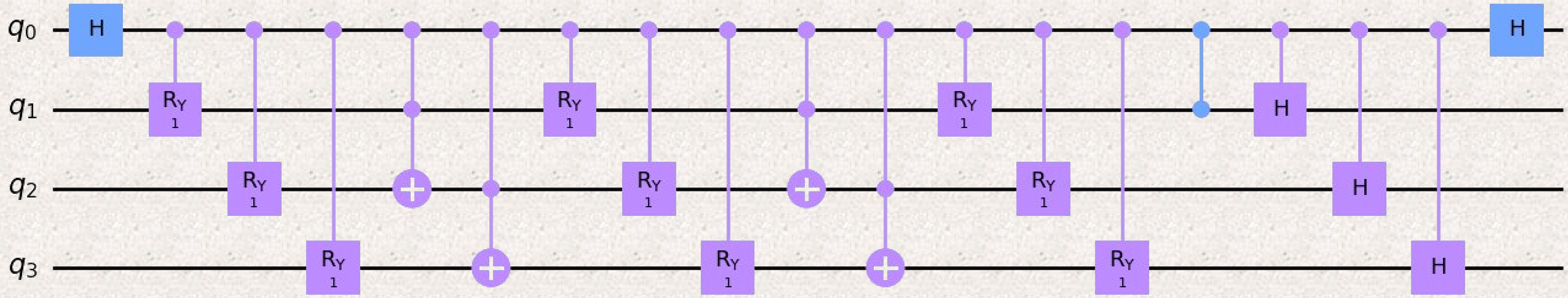

With $A_l = Z_1$

Qiskit Implementation

Our cost function is :

$$C_G = 1 - \frac{\sum_{l=1}^{L} \sum_{l'=1}^{L} c_{l'} c_l^* \gamma_{ll'}}{\sum_{l=1}^{L} \sum_{l'=1}^{L} c_{l'} c_l^* \beta_{ll'}}$$

We minize it using preferably a gradient free optimizer, like COBYLA, that is less vulnerable to barren plateaus

Qiskit Implementation

The output of the algorithm is:

```
    fun: 0.00012637933571213456
  maxcv: 0.0
message: 'Maximum number of function evaluations has been exceeded.'
   nfev: 200
 status: 2
success: False
      x: array([ 3.31224364,  1.54576436,  4.69185342, -0.94657516,  1.98048994,
        0.04202637,  0.11539815,  2.38380735,  3.18573665])
```

- *fun* is the final value of the cost function which is close to 0, as desired
- x is optimal point $\boldsymbol{\alpha}_{opt}$ which corresponds to the solution $|x\rangle = V(\boldsymbol{\alpha}_{opt})\,|\mathbf{0}\rangle$

Qiskit Implementation

To confirm that the obtained solution is correct we calculate the inner product

$$\langle x\boldsymbol{A}|b\rangle$$

with the expectation of being close to 1. The output is:

Qiskit Implementation

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$$\langle x\boldsymbol{A}|b\rangle$$

with the expectation of being close to 1. The output is:

```
<xA|b> = (0.9998736206641057-0j)
```

. . . It works !!!

Referances

VQLS ALgorithm

https://arxiv.org/pdf/1909.05820.pdf

https://qiskit.org/textbook/ch-paper-implementations/vqls.html

https://pennylane.ai/qml/demos/tutorial_vqls.html

Anstaz

https://arxiv.org/pdf/2111.13730.pdf

Cost Function

https://qiskit.org/textbook/ch-paper-implementations/vqls.html