Quantum Approximate Optimization Algorithm

Performance on Max-Cut using Heuristic Parameter determination

Joost Bus

Delft University of Technology, the Netherlands

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Supervisors
Matthias Möller
Carmina G. Almudever

Contact: `j.c.p.bus@student.tudelft.nl`

Overview

Why Quantum Computing?

- Medicine
- Chemistry
- Cryptography
- Optimization

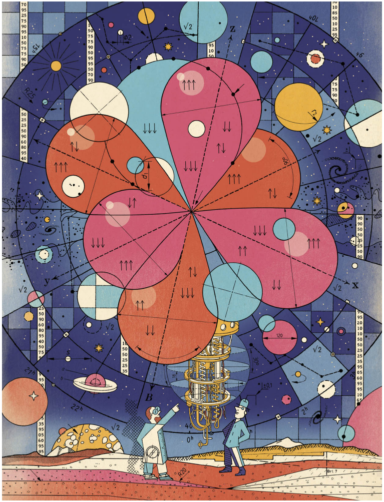

Illustration by Christian Gralingen

Are we there yet?

The current state of Quantum Computers

- $10 \sim 100$ qubits
- Limited connectivity
- Non-negligible error rates
- No error correction

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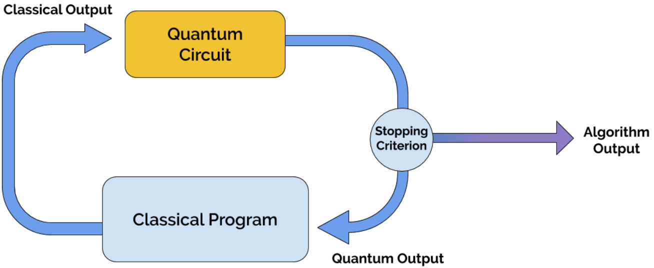

Figure from Entropica Labs

Quantum Computing - The basics

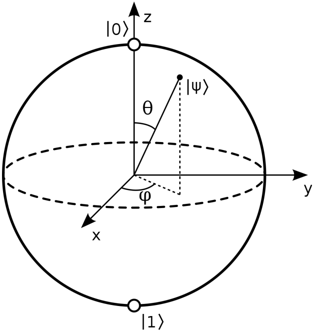

Figure from Wikipedia - Bloch sphere

Quantum Computing - The basics

One quantum bit or qubit can be described as a **superposition**, or (linear) combination of two states with corresponding **amplitudes**

$$|\psi\rangle = \alpha_1|0\rangle + \alpha_2|1\rangle \quad (1)$$

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Similarly, for a two qubit system we the system is described with four amplitudes.

$$\alpha_1|00\rangle + \alpha_2|01\rangle + \alpha_3|10\rangle + \alpha_4|11\rangle \tag{2}$$

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In general, we need 2^n amplitudes to describe an n qubit system and some say the system is in $\mathbf{2^n}$ **states** "at the same time". Hence the exponential power of the quantum computer.

$$\alpha_1|0\dots0\rangle + \dots + \alpha_{2^n}|1\dots1\rangle \tag{3}$$

Quantum Computing - The basics

However, we are not able to measure the amplitudes directly. Upon measurement, the system **collapses** into *one* classical state with probability related to the magnitude of the corresponding amplitude.

Quantum Computing - The basics

Example with 2 qubits

Given the following system

$$\alpha_1|00\rangle + \alpha_2|01\rangle + \alpha_3|10\rangle + \alpha_4|11\rangle \tag{4}$$

we find the following results with their corresponding probabilities

State	Amplitude	Probability
00	α_1	$\lvert\alpha_1\rvert^2$
01	α_2	$\lvert\alpha_2\rvert^2$
10	α_3	$\lvert\alpha_3\rvert^2$
11	α_4	$\lvert\alpha_4\rvert^2$

Quantum Computing - The basics

So the amplitudes have a special meaning: **the squared magnitude signifies the probability of a particular state.** We can change the amplitudes by applying **gates**, which are descibed by (unitary) matrices.

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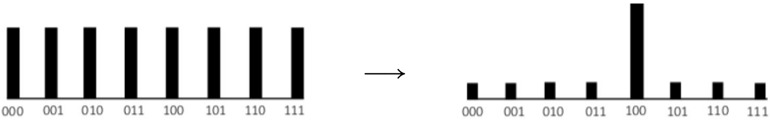

The Max-Cut problem

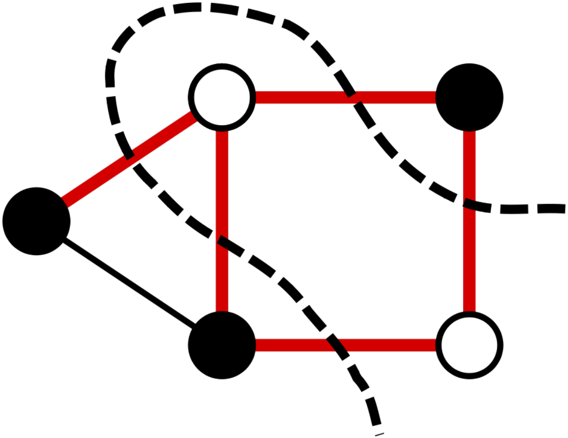

Figure from Wikipedia - Maximum cut

We would like to find a **bipartition** that maximizes the following **cost function**

$$C = \sum_{i \in S, j \in \bar{S}} w_{i,j} \tag{5}$$

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Equivalently, we can use a **binary string** to represent the bipartition

$$C = \sum_{\{i,j\}} \frac{w_{i,j}}{2}(1 - z_i z_j) \tag{6}$$

where $\boldsymbol{z} \in \{-1, 1\}^n$ and $z_i = \begin{cases} 1, & \text{if} \quad i \in S \\ -1, & \text{if} \quad i \in \bar{S} \end{cases}$

The Quantum Approximate Optimization Algorithm

The Quantum Approximate Optimization Algorithm is designed to tackle combinatorial optimization problems. In general, these can be specified with n bits and m clauses. The aim is to satisfy as many clauses as possible

$$C = \sum_{\alpha=1}^{m} C_\alpha \tag{7}$$

where $C_\alpha = \begin{cases} 1, & \text{if clause } C_\alpha \text{ is satisfied} \\ 0, & \text{if clause } C_\alpha \text{ is } \textit{not} \text{ satisfied} \end{cases}$

Schematic of the QAOA circuit

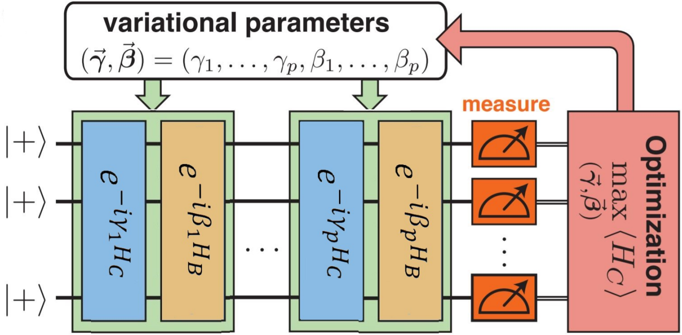
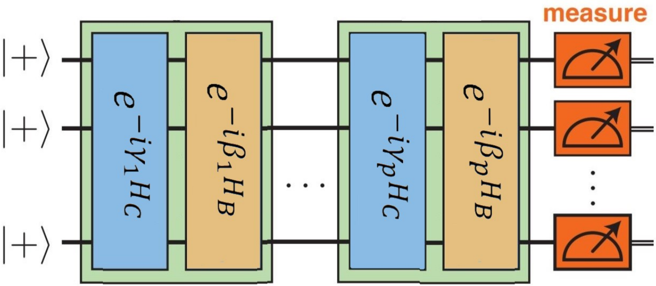


Figure adapted from Zhou et al. Quantum Approximate Optimization Algorithm: Performance, Mechanism, and Implementation on Near-Term Devices (2018)

The Quantum Part



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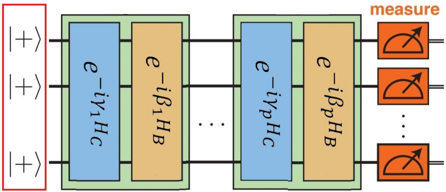
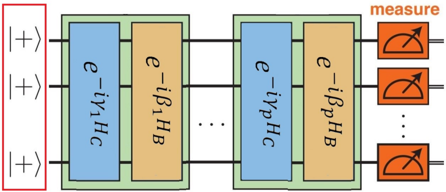


We start from $|+\rangle^{\otimes n}$ which is the **equal superposition** over all 2^n bit strings (or equivalently bipartitions)

$$|+\rangle^{\otimes n} = \frac{1}{\sqrt{2^n}} \sum_{\boldsymbol{x} \in \{0,1\}^n} |\boldsymbol{x}\rangle \tag{8}$$



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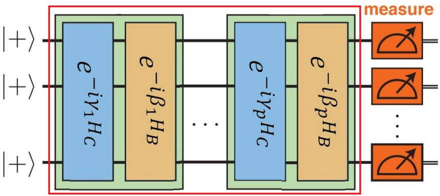
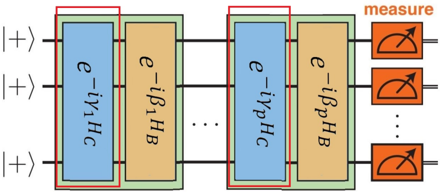
So the amplitude of every bit string is the same



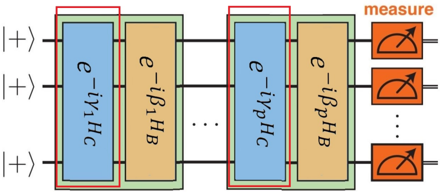
Next we alternately apply two gates, the **cost unitary** and the **mixer unitary**, derived from two Hamiltonians.

We repeat this p times



First of the two being the **cost unitary**. This unitary is derived from the **cost Hamiltonian** that encodes the objective function C

$$H_C \equiv \hat{C} = \begin{bmatrix} C(0,\ldots,0) & & \\ & \ddots & \\ & & C(1,\ldots,1) \end{bmatrix} \tag{9}$$



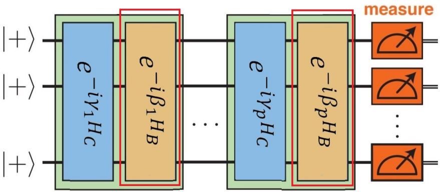
From the cost Hamiltonian we derive the **cost unitary**

$$H_C \longrightarrow U(H_C, \gamma) \tag{10}$$

with

$$U(H_C, \gamma) = e^{-i\gamma H_C} \tag{11}$$

for some real parameter $\gamma \in \mathbb{R}$

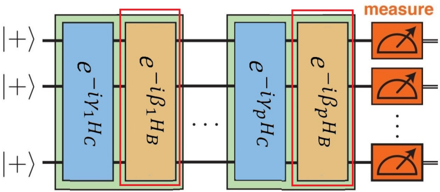


Secondly, the **mixer unitary**, derived from the **mixer Hamiltonian**

$$H_B = \sum_{k=1}^{n} \sigma_x^{(k)} \tag{12}$$

with $\sigma_x^{(k)}$ is the Pauli-X gate applied to the kth qubit, which is also called the quantum NOT-gate

$$\sigma_x = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \tag{13}$$



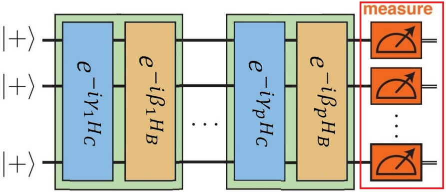
Analogous to the cost unitary we derive the **mixer unitary** is derived from the mixer Hamiltonian

$$H_B \longrightarrow U(H_B, \beta) \tag{14}$$

the mixer unitary is given by

$$U(H_B, \beta) = e^{-i\beta H_B} \tag{15}$$

for some real parameter $\beta \in \mathbb{R}$



In the end we prepared the parametrized state

$$|\gamma, \beta\rangle = \underbrace{U(H_B, \beta_p)U(H_C, \gamma_p) \dots \underbrace{U(H_B, \beta_1)U(H_C, \gamma_1)}_{\text{one layer}}}_{p \text{ layers}} |+\rangle^{\otimes n} \tag{16}$$

after which we measure the outcome.

The goal: maximize the expectation value

Our aim is to prepare a state such that the **expectation value of the cost Hamiltonian** is maximized

$$F_p(\boldsymbol{\gamma}, \boldsymbol{\beta}) = \langle \boldsymbol{\gamma}, \boldsymbol{\beta} | H_C | \boldsymbol{\gamma}, \boldsymbol{\beta} \rangle \tag{17}$$

for some sequences of parameters

$$\boldsymbol{\gamma} = (\gamma_1, \ldots, \gamma_p)$$

$$\boldsymbol{\beta} = (\beta_1, \ldots, \beta_p)$$

Applying QAOA to Max-Cut

We **translate** the objective function into a **Hamiltonian**

$$C = \sum_{\{i,j\}} w_{i,j}(1 - z_i z_j) \tag{18}$$

$$\downarrow$$

$$H_C = \sum_{\{i,j\}} w_{i,j}\left(I - \sigma_z^{(i)} \sigma_z^{(j)}\right) \tag{19}$$

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Using the fact σ_z has eigenvalues 1 and -1. Here $\sigma_z^{(i)}$ denotes the Pauli-Z matrix applied to the ith qubit.

$$\sigma_z = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} \tag{20}$$

Applying QAOA to Max-Cut

We can construct the necessary unitaries with local operators

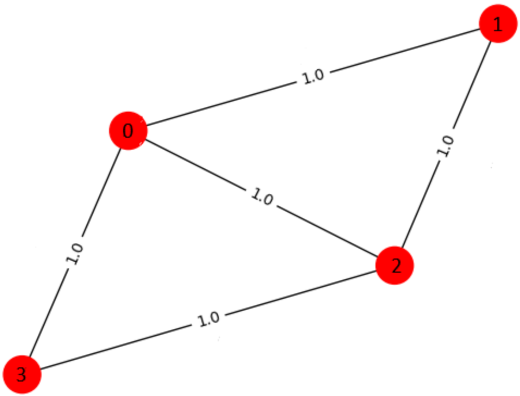
$$U(H_C,\gamma) = e^{-i\gamma H_C} = \prod_{\{i,j\}\in E} e^{-i\gamma w_{i,j}(1-\sigma_z^{(i)}\sigma_z^{(j)})} \tag{21}$$

$$U(H_B,\beta) = e^{-i\beta H_B} = \prod_{k\in V} e^{-i\beta\sigma_x^{(k)}} \tag{22}$$

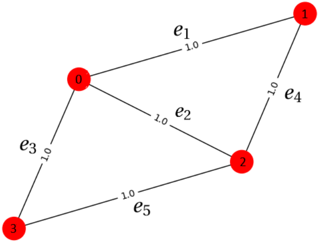
Note that the circuit is dependent on the graph $G = (V, E)$

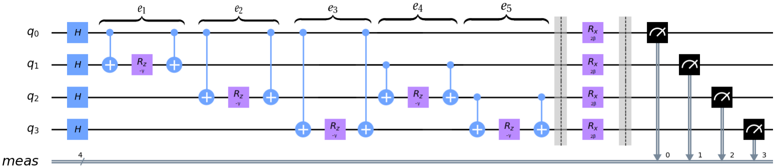
Now we are set to construct the circuit for Max-Cut!

Example - the Diamond graph

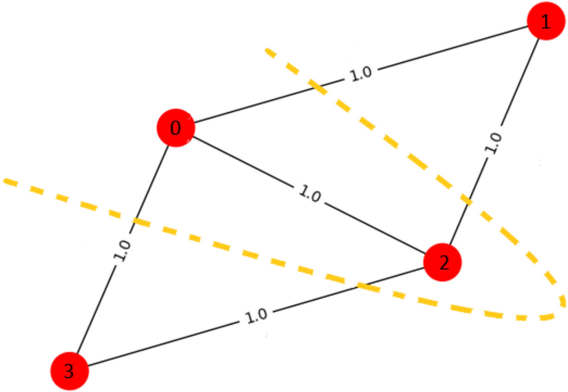


Example - the circuit



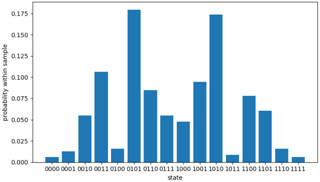


Example - the optimal cut

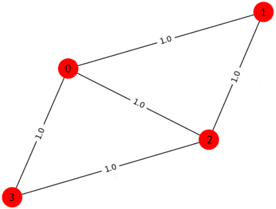


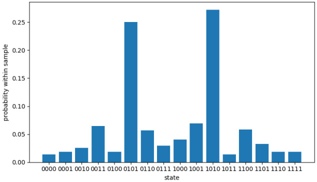
Note that the optimal cut is $S = \{0, 2\}, \bar{S} = \{1, 3\}$ or in terms of a binary string 0101 or 1010

Example - Maximizing the expectation value

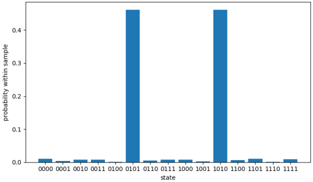


p=1, $F_1 = 3.24$



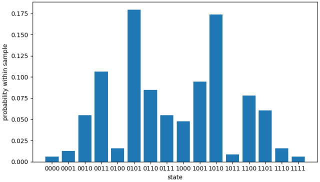


p=2, $F_2 = 3.39$



p=3, $F_3 = 3.87$

Example - Maximizing the expectation value



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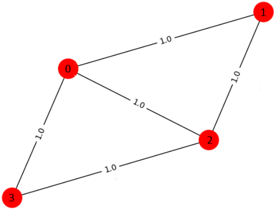

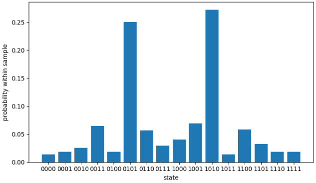

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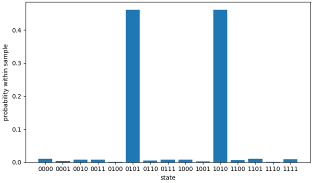

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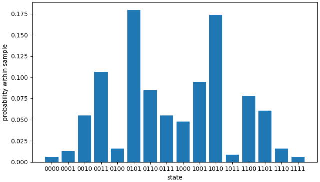
Example - Maximizing the expectation value



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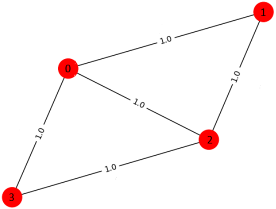

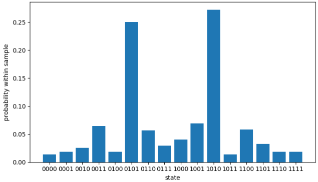

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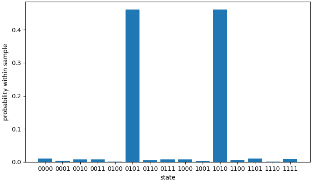

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Determining the parameters γ, β

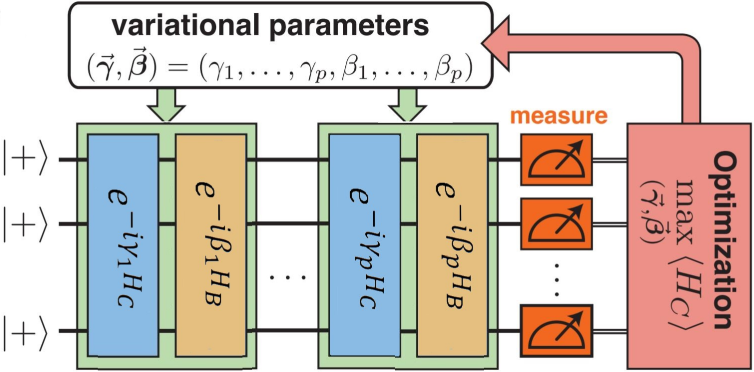


Figure: Schematic of the QAOA circuit using VQE optimization.[1]

[1] Figure adapted from Zhou et al. Quantum Approximate Optimization Algorithm: Performance, Mechanism, and Implementation on Near-Term Devices (2018)

Relation to Quantum Adiabatic Algorithm

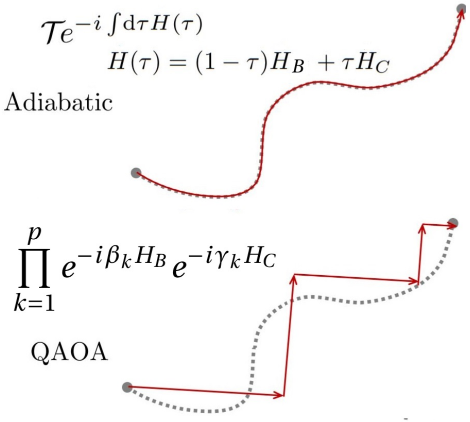


Figure adapted from Verdon et al. A quantum algorithm to train neural networks using low-depth circuits (2017)

Relation to Quantum Adiabatic Algorithm

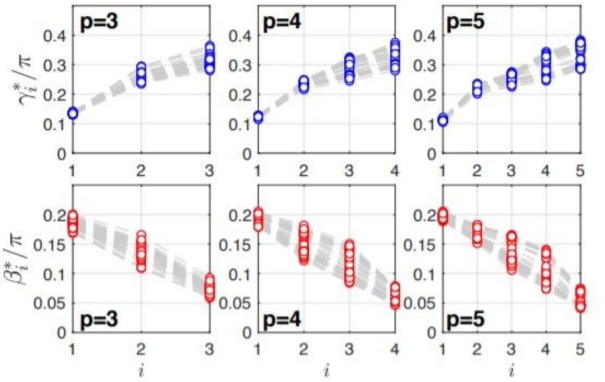
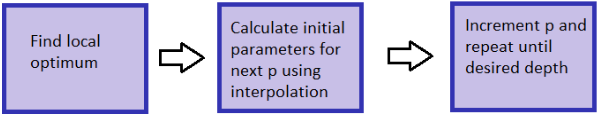


Figure: Optimal parameter patterns for unweighted 3-regular graphs with 16 nodes[2]

[2]Zhou et al. Quantum Approximate Optimization Algorithm: Performance, Mechanism, and Implementation on Near-Term Devices (2018)

Exploiting the relation to QAA - the INTERP method



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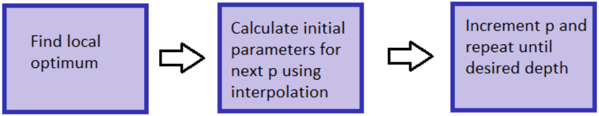
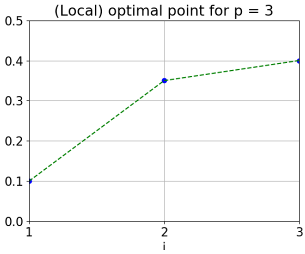
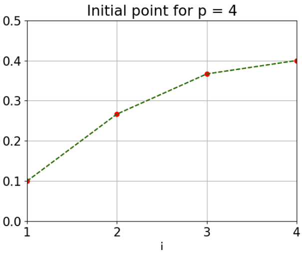


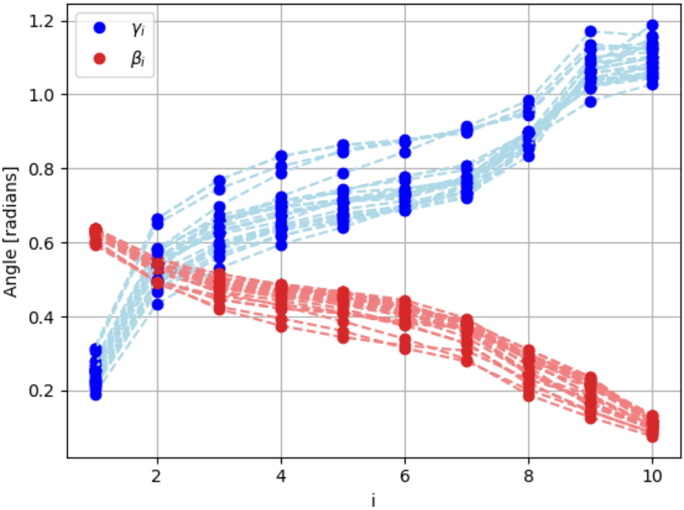




My work

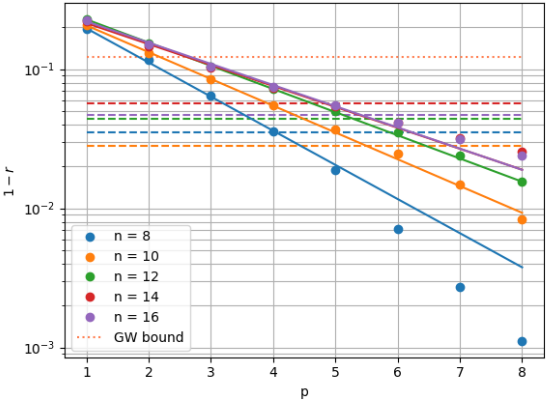
1. analysis on **INTERP method** on different graphs
   - cyclic graphs
   - 3-regular graphs, weighted and unweighted
   - Erdős-Rényi graphs
2. benchmark against **Goemans-Williamson**, the best known classical approximation algorithm
3. polynomial time

Found patterns



Unweighted 3-regular graphs

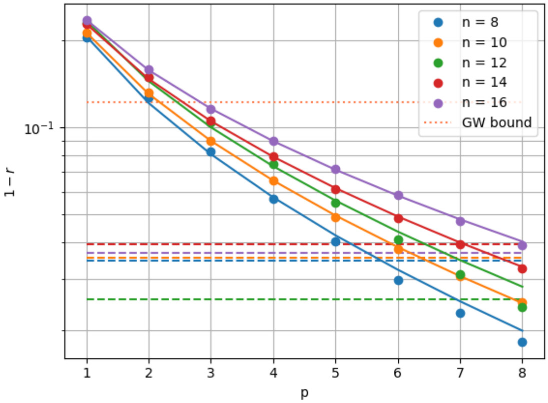
Fractional error $1 - r$ decays exponentially with p



The horizontal lines indicate the average performance of the classical Goemans-Williamson

Weighted 3-regular graphs

Fractional error $1 - r$ decays exponentially with $\sqrt{p}$



The horizontal lines indicate the average performance of the classical Goemans-Williamson

Similar relations were found for the Erdős-Rényi graphs

Conclusions

- INTERP beats the classical Goemans-Williamson for relatively low $p \approx 7$ for small graphs
- The method needs a lot of function evaluations to determine good angles
- However, this number increases polynomially with p and n so it might offer advantages for large graphs

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Thank you!

Questions?

Time complexity

In Zhou et al. (2018) it was claimed the INTERP method is polynomial in p, and since the quantum circuit has depth $3m + n$, we find that the complete INTERP method is polynomial in both n and p, but is this true in practice?