QAOA: Reductions, Choice of Mixer Hamiltonians, and Convergence Guarantees

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Joint work with

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The problem

Let $\mathbb{D}^n := \{0, 1, \ldots, d-1\}^n$ be the set of n-element strings and $\mathcal{S}$ the group of permutations of these d^n elements.

Goal: given a function $F : \mathbb{D}^n \to \mathbb{R}$, find the elements in $\mathbb{D}^n$ on which it attains min (max) values.

Example

In case the function is quadratic (of type $F = a + \sum_{k=1}^{n} \beta_k \mathbf{x_k} + \sum_{1 \le i \le j \le n} \alpha_{ij} \mathbf{x_i} \mathbf{x_j}$ with coefficients $a, \alpha_{ij}, \beta_k \in \mathbb{R}$ and variables $\mathbf{x_i} \in \{0, 1\}$), the corresponding optimization problem is known as quadratic unconstrained binary optimization (QUBO).

The symmetries: level 1

If a permutation $g \in \mathcal{S}$ is '*undetectable*' by F, i.e. $F(g(x)) = F(x)$ for any $x \in \mathbb{D}^n$, then g is called a **symmetry** of F.
Such symmetries form a subgroup $G \subseteq \mathcal{S}$. The set $\mathbb{D}^n$ can be written as a disjoint union of G-orbits:

$$\mathbb{D}^n = \bigsqcup_{j=1}^{m} \mathcal{O}_j.$$

If the strings x and y are in the same G-orbit, then $F(x) = F(y)$.

Classical $\rightsquigarrow$ quantum

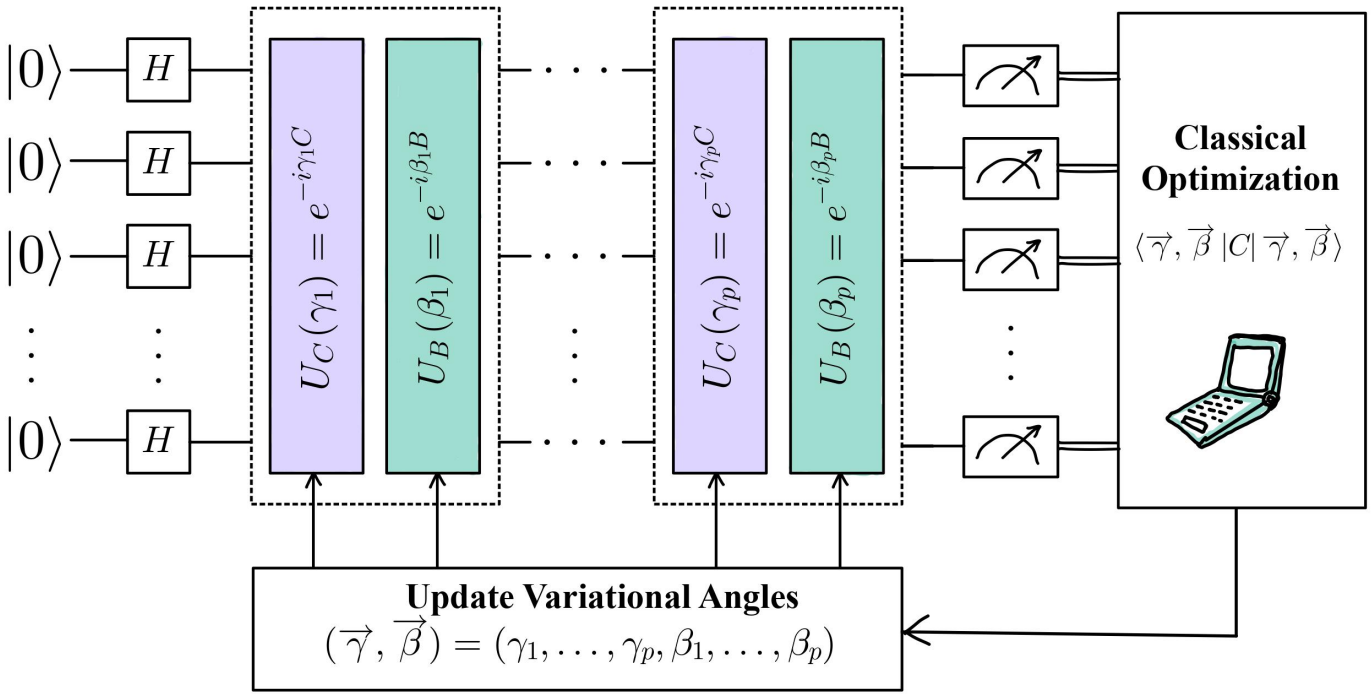
Let W be a vector space of dimension d^n with basis indexed by elements of $\mathbb{D}^n$, *standard basis*.
The Hamiltonian H_F is said to **represent** a function $F : \mathbb{D}^n \to \mathbb{R}$ if it satisfies $H_F(v_x) = F(x)v_x$ for any $x \in \mathbb{D}^n$.

- $\mathbb{D}^n \rightsquigarrow W$
- $F \rightsquigarrow$ linear operator H_F acting on W
- Minima of F on $\mathbb{D}^n \rightsquigarrow$ lowest energy states of H_F in W.

QAOA

One of the widely employed algorithms for tackling the quantum version of the optimization problem is the Quantum Approximate Optimization Algorithm (QAOA). In the QAOA framework, the Hamiltonian H_F is commonly referred to as the *problem Hamiltonian* and is denoted by H_P.
The essence of the QAOA algorithm is in the gradual transformation of the mixer Hamiltonian H_M, one with a unique lowest energy state $|\xi\rangle$ into the problem Hamiltonian. This gradual transition ensures that the lowest-energy vector from the previous step becomes the lowest-energy vector in the subsequent step.

QAOA


$|0\rangle$
H
$U_C(\gamma_1) = e^{-i\gamma_1 C}$
$U_B(\beta_1) = e^{-i\beta_1 B}$
$U_C(\gamma_p) = e^{-i\gamma_p C}$
$U_B(\beta_p) = e^{-i\beta_p B}$
Classical Optimization
$\langle \vec{\gamma}, \vec{\beta} | C | \vec{\gamma}, \vec{\beta} \rangle$
Update Variational Angles
$(\vec{\gamma}, \vec{\beta}) = (\gamma_1, \ldots, \gamma_p, \beta_1, \ldots, \beta_p)$

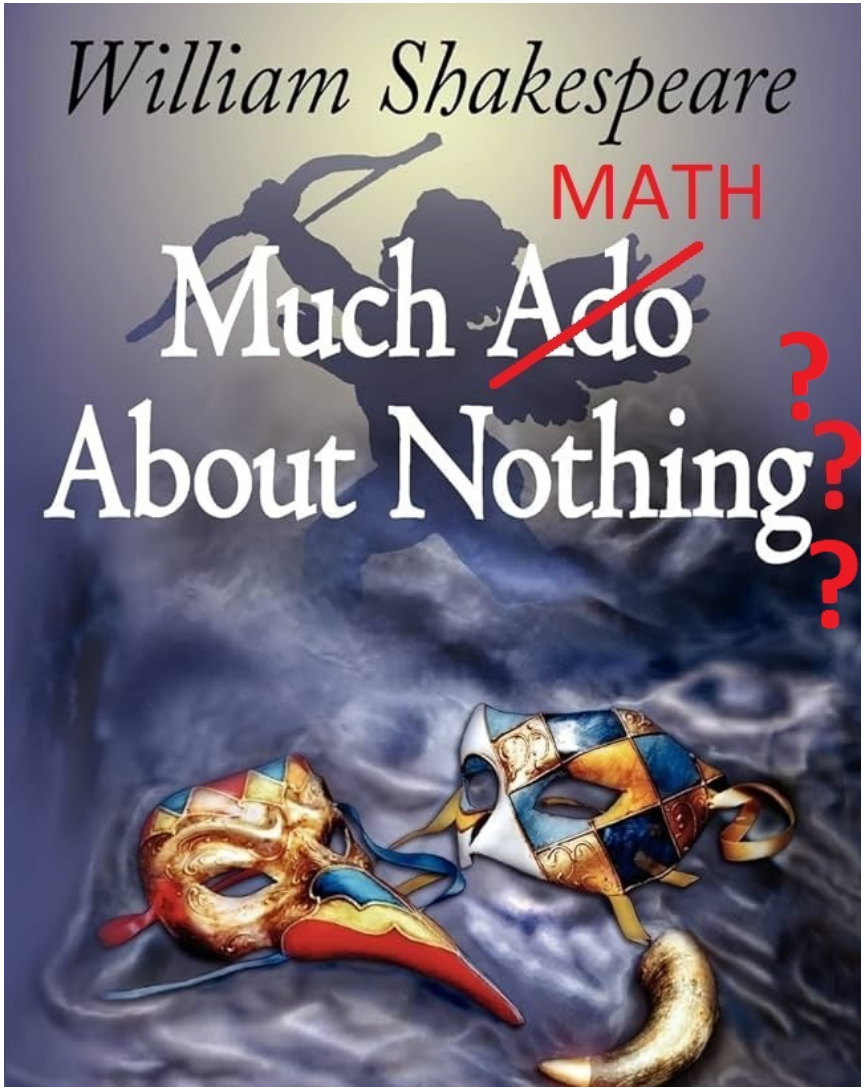
QAOA: a closer look

While the Hamiltonian H_P, representing the objective function, is uniquely determined by the classical problem, there is some flexibility in the choice of the mixer Hamiltonian.
The standard and most common choice of mixer Hamiltonian is $B = \sum_{0 \leq j \leq \ell - 1} X_j$. The corresponding ground state is $|\xi\rangle = |++\ldots+\rangle$.
The objective function in many optimization problems exhibits invariance under the action of the symmetric group $S_d = W(U_d)$ acting collectively on all qudits:

$$\sigma(x_1, x_2, \ldots, x_n) := (\sigma(x_1), \sigma(x_2), \ldots, \sigma(x_n)).$$

QAOA: a closer look

The **standard mixer Hamiltonian does not exhibit commutativity with the entire symmetric group** S_d, but only with a noticeably smaller subgroup. With this in mind, we explore an **alternative mixer Hamiltonian**, H_M, which maintains **commutativity** with the action of the **whole group**.


William Shakespeare
MATH
Much Ado
About Nothing???

A concrete application

Consider the problem of coloring the edges of a graph. A coloring is considered *proper* if no adjacent edges (sharing a vertex) have the same color. To each edge $e \in E$, one associates ℓ bits $e_0, e_1, \ldots, e_{\ell-1}$, the values of which uniquely determine its color.
The function χ_c is defined as follows:

$$\chi_c(c') := \begin{cases} 1, & \text{if } c'_i \equiv c_i \text{ for all } i \in \{1, \ldots, \ell\} \\ 0, & \text{otherwise} \end{cases}$$

This function serves as the characteristic function of a color: it has value 1 on color c and 0 on all other colors.
The objective function $F_\Gamma(C) := \sum_{e \bullet f} \sum_{c \in \mathfrak{C}} \chi_c(C(e))\chi_c(C(f))$ computes the number of adjacent edges of coinciding color.

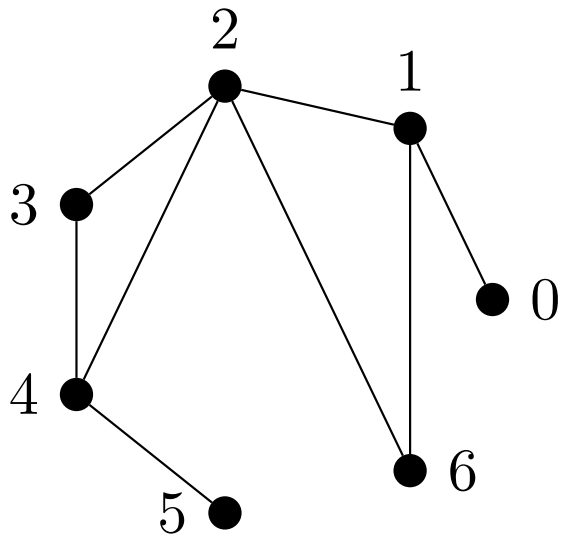
Remark

A coloring C is proper if and only if $F_\Gamma(C) = 0$.

Examples

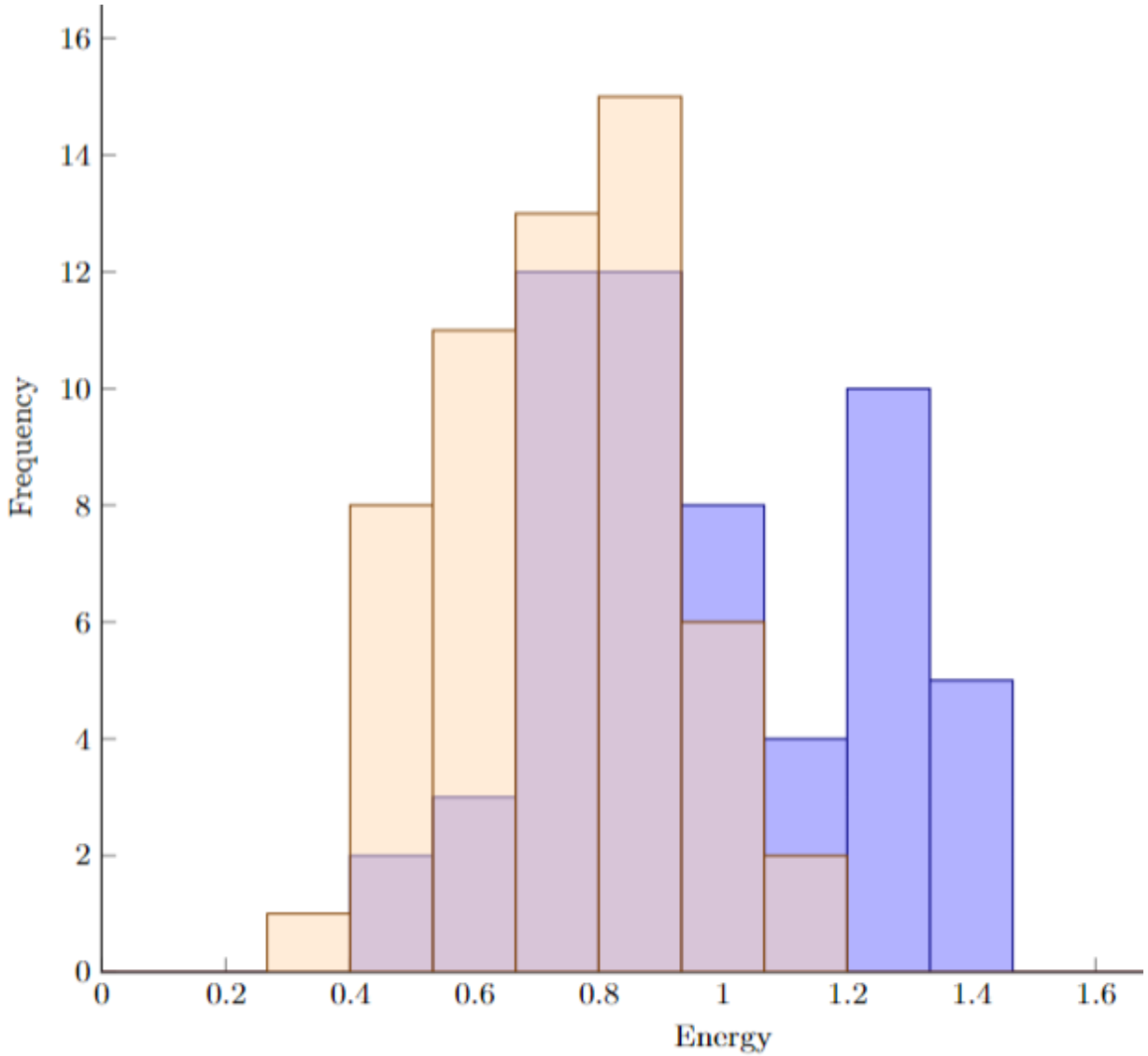
We would like to showcase a performance comparison between two versions of QAOA (standard and the newly proposed one) in determining appropriate edge colorings for the graph. Both algorithms are configured iteratively with a depth parameter of $p = 9$. Through over 50 independent trials for each scenario, we observe statistically significant differences in mean values at the 1.5% significance level, with the new variant consistently demonstrating lower means. Moreover, we note **considerably lower median and minimal values** in the experiments utilizing the **newly introduced mixer Hamiltonian** compared to the classical one.

Graph 1 (4 colors)

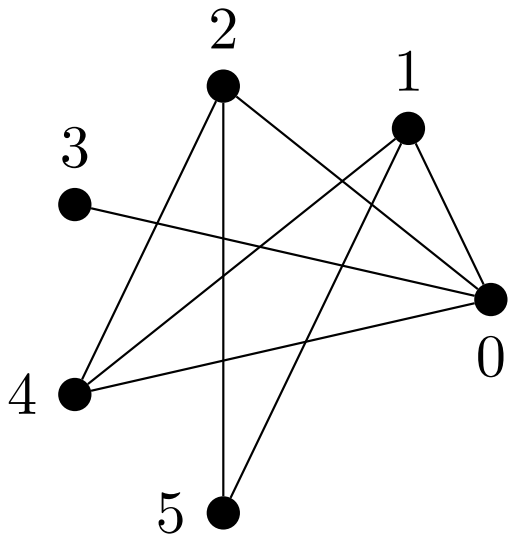


	Mean	Median	Min	Energy < 1
QAOA	0.9696	0.9316	0.4814	33/56
QAOA_{new}	0.7437	0.7388	0.3691	51/56

t-test p-value is $3.053993311768478 \cdot 10^{-7}$

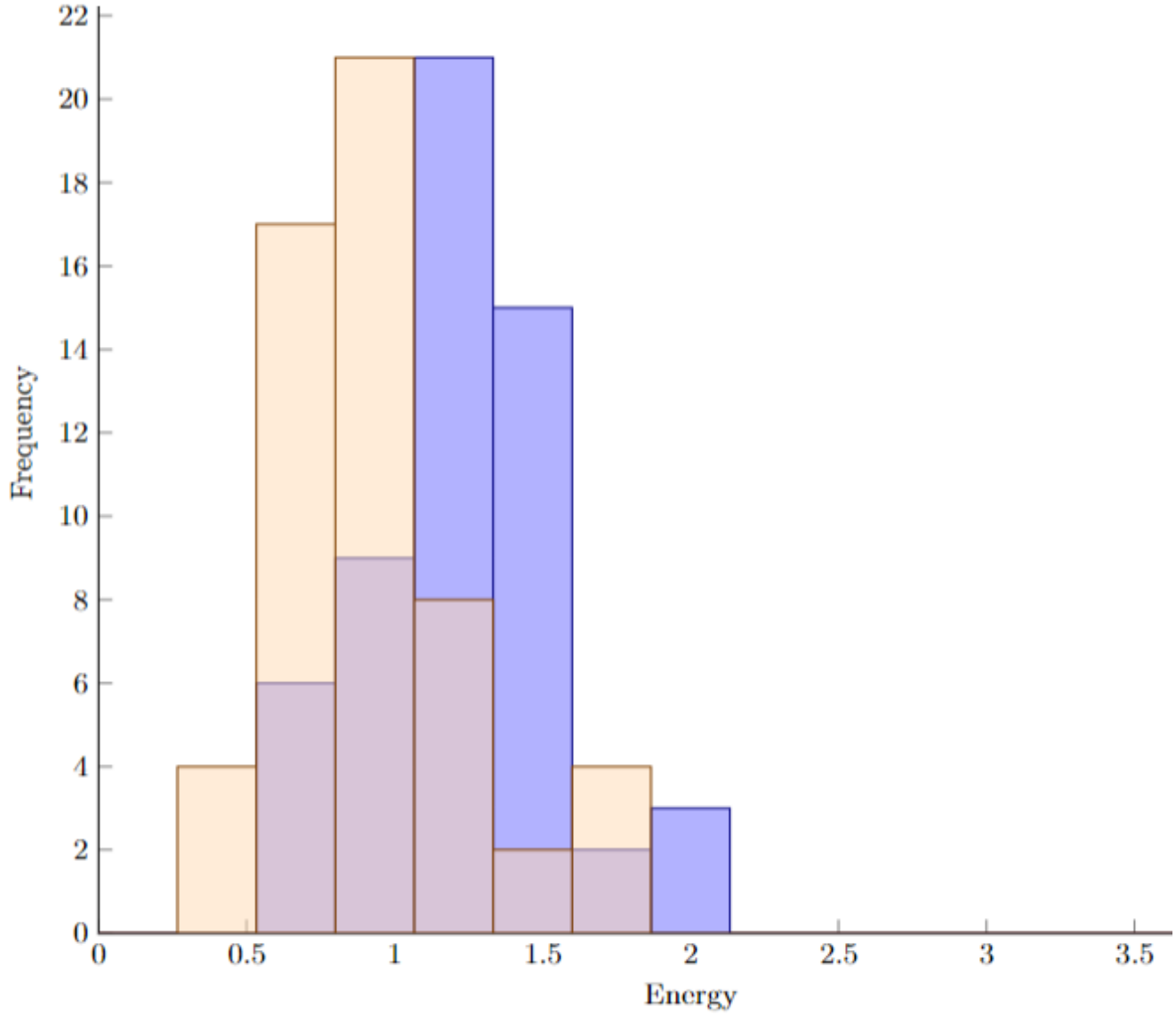

16
14
12
10
8
6
4
2
0
Frequency
0
0.2
0.4
0.6
0.8
1
1.2
1.4
1.6
Energy

Graph 2 (4 colors)

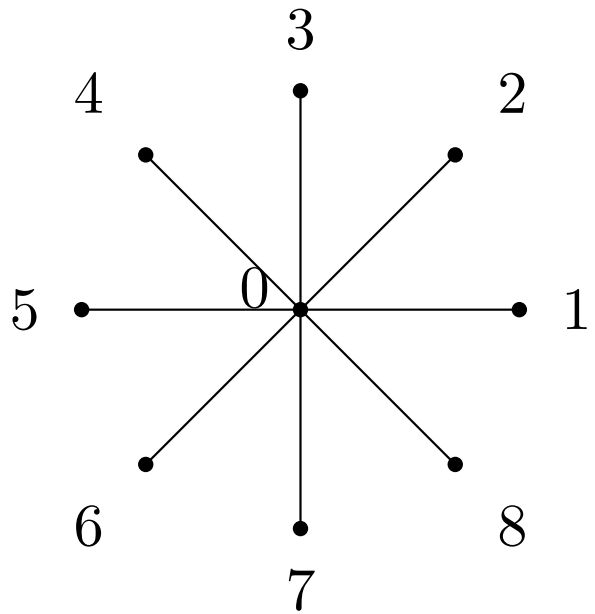


	Mean	Median	Min	Energy < 1
QAOA	1.2495	1.2417	0.6533	11/56
QAOA_{new}	0.9344	0.8857	0.3691	35/56

t-test p-value is $1.9806919304846427 \cdot 10^{-6}$

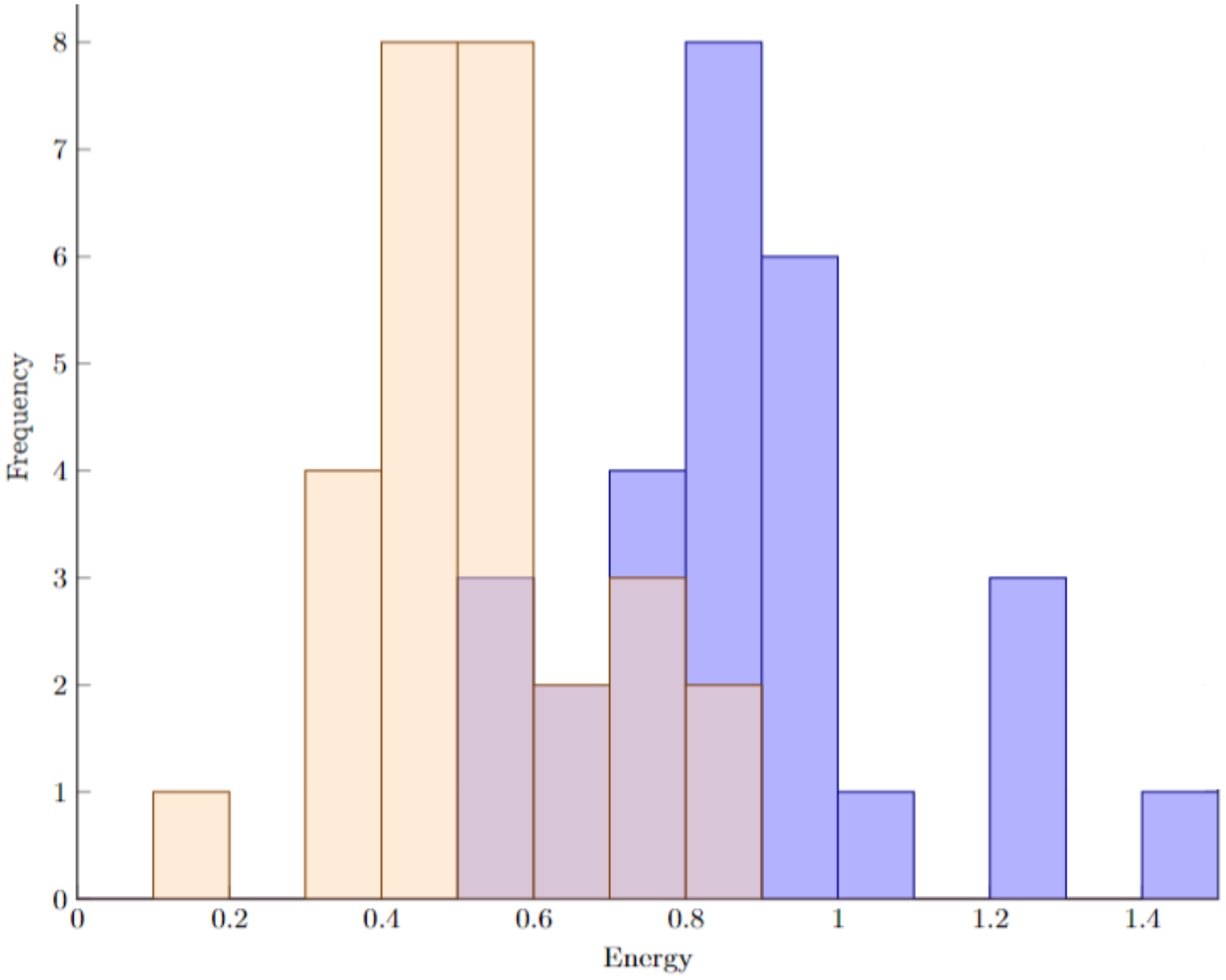

Frequency
Energy
0
2
4
6
8
10
12
14
16
18
20
22
0
0.5
1
1.5
2
2.5
3
3.5

Graph 3 (8 colors)



	Mean	Median	Min
QAOA	0.8726	0.8569	0.502
QAOA_{new}	0.5227	0.5073	0.17

t-test p-value is $1.2230598272375008 \cdot 10^{-8}$


Frequency
Energy
0
1
2
3
4
5
6
7
8
0
0.2
0.4
0.6
0.8
1
1.2
1.4

The symmetries: level 2

The action of G on the set $\mathbb{D}^n$ extends to an action on W.
Actions of G and H_F on W commute:

$$H_F(g(w)) = g(H_F(w)) \ \forall w \in W, \ \forall g \in G.$$

According to the G-action, W can be written as a direct sum of subspaces:

$$W = \bigoplus W_i.$$

Here one of the subspaces is the **subspace of G-invariants**:

$$W^G = \{w \in W \mid g(w) = w, \forall g \in G\}.$$

The decomposition is preserved by H_F:

$$H_F(W_i) \subseteq W_i.$$

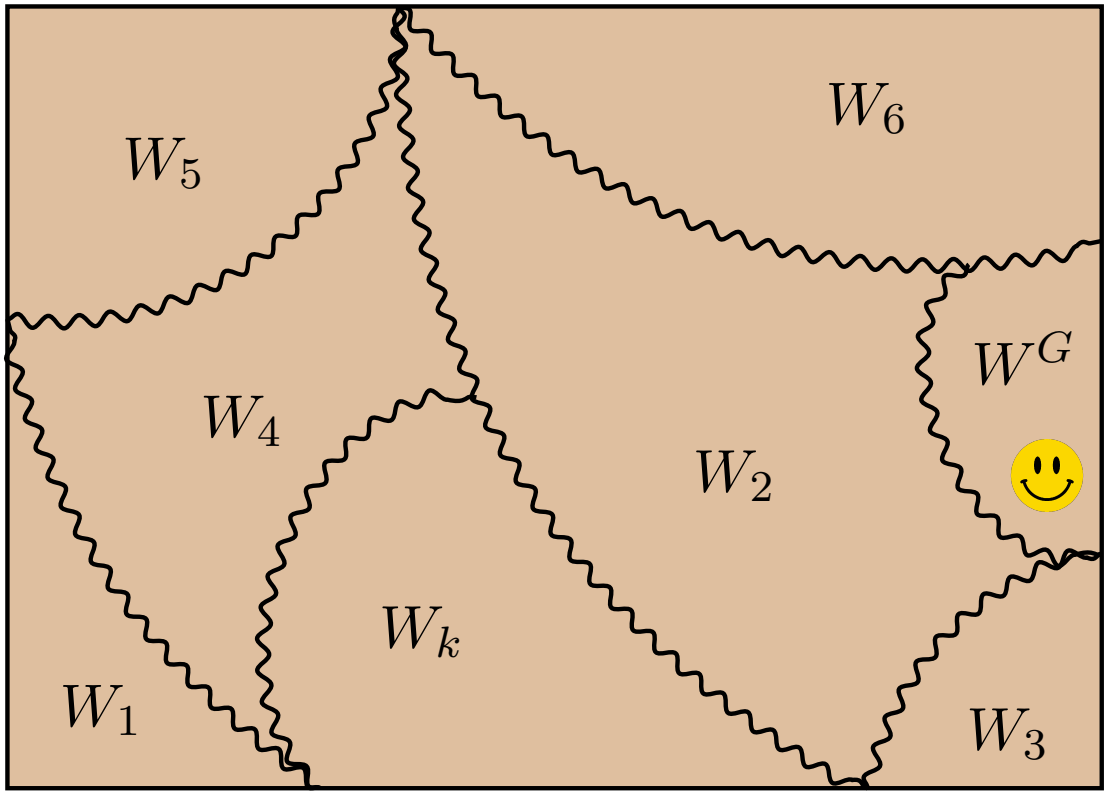


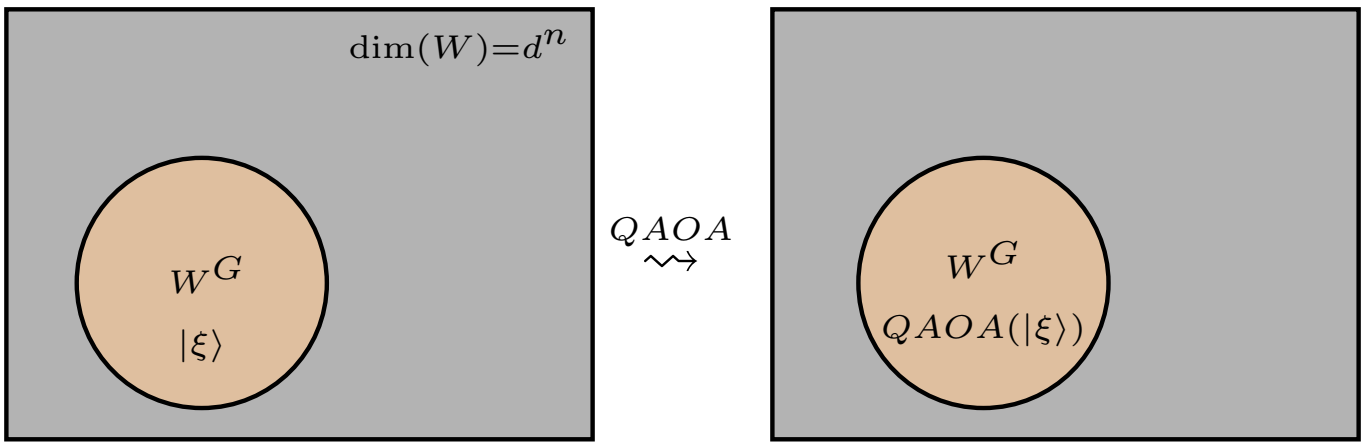
Figure: Decomposition of $W = V^{\otimes d}$

Where does QAOA 'live'?

Remark

Notice that the uniform superposition $\xi = |++\ldots+\rangle$ is inside W^G for any $G \subseteq \mathcal{S}$.

Suppose we employ a QAOA algorithm with the initial state ξ, and the objective function has a group of symmetries G. If the mixer Hamiltonian commutes with G, then the algorithm will operate within the subspace W^G prior to the final measurement.
In case $G = S_d$ acting as described before, we have $\dim(W^G) \approx \frac{d^n}{d!}$.



Where does QAOA 'live'?

Question

Is it possible to pick an initial state and mixer Hamiltonian so that QAOA *effectively* runs in a different W_i?

Yes, but there is something to keep in mind...

Remark

The ground state for a mixer Hamiltonian, satisfying the assumptions of the **Perron-Frobenius theorem**, *must be* a superposition of all classical states with nonzero amplitudes. Consequently, the standard argument for guaranteeing the convergence of QAOA as $\mathbf{p} \to \infty$ to an optimal classical solution is **inapplicable** unless the initial state is a superposition of all classical states with **positive amplitudes**.

Where does QAOA 'live'?

The only subspace for which this holds is W^G...
However, there is hope 

Graph	Mean	Median	Min	$\mathcal{E}_9 < 1$
Γ_1, W	0.726	0.7056	0.3584	41/50
Γ_1, W^G	0.5692	0.4673	0.1923	47/50
Γ_1, W_1	0.5726	0.5142	0.1621	47/50
Γ_2, W	0.9696	0.9316	0.4814	33/56
Γ_2, W^G	0.7437	0.7388	0.3691	51/56
Γ_2, W_1	0.8688	0.7148	0.3964	47/56
Γ_3, W	1.2495	1.2417	0.6533	11/56
Γ_3, W^G	0.9344	0.8857	0.3691	35/56
Γ_3, W_1	0.7334	0.6763	0.2598	50/56
Γ_4, W	1.4857	1.5313	0.7382	6/56
Γ_4, W^G	1.1959	1.1074	0.5117	21/56
Γ_4, W_1	1.2415	1.1489	0.4395	20/56
Γ_5, W	1.3469	1.3066	0.6162	14/50
Γ_5, W^G	0.9149	0.9507	0.3516	30/50
Γ_5, W_1	0.94123	0.9375	0.2939	27/50

Table: QAOA energy for edge coloring problem with $p = 9$