

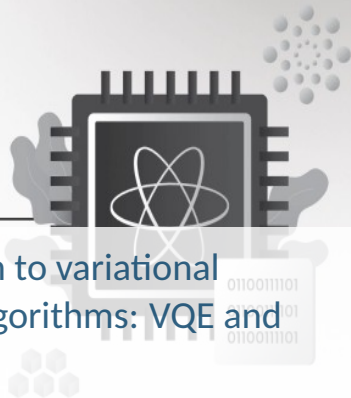
QUANTUM AUTUMN SCHOOL 2024



Introduction to variational quantum algorithms: VQE and QAOA

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Outline

- Projector Operators, Observables and Expectation values
- Variational Principle and VQE Theory
- QAOA and the Maxcut problem
- MaxKCut encodings:
 - k power of two
 - Degenerate color method
 - Constrained QAOA method

Projectors and exponentials

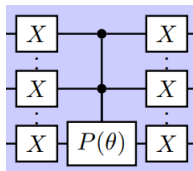
A projector operator acts on a quantum state of the Hilbert space and forces all components to zero, except those of the subspace it projects onto.

$$\Pi^2 = \Pi, \quad \Pi|_{\text{span}(\{\psi_i\}_{i=1}^d)} = \sum_i^d |\psi_i\rangle \langle \psi_i|, \quad \langle \psi_i | \psi_j \rangle = \delta_{ij} \quad (1)$$

$$e^{i\theta\Pi} = \sum_{n=0}^{\infty} \frac{(i\theta)^n}{n!} \Pi^n = \mathbb{I} + \left(\sum_{n=1}^{\infty} \frac{(i\theta)^n}{n!} \right) \Pi = \mathbb{I} + (e^{i\theta} - 1)\Pi \quad (2)$$

$$\begin{pmatrix} e^{i\theta} & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix}$$

$$e^{i\theta|0\rangle\langle 0|}$$



$$P(\theta) = Z^\theta = \begin{pmatrix} 1 & 0 \\ 0 & e^{i\theta} \end{pmatrix}$$

Observables

- An observable H is a **self-adjoint operator** on the Hilbert space $\mathbb{C}^{\otimes n}$.
- Spectral theorem: \exists orthonormal **basis** $\{|\psi_i\rangle\}_i$ of $\mathbb{C}^{\otimes n}$ consisting of eigenvectors of H , and all eigenvalues λ_i are **real**.
- We can write: $H = \sum_i \lambda_i |\psi_i\rangle \langle \psi_i|$
- To each energy λ_j corresponds to an **energy eigenstate**.
 - **ground state**: energy eigenstate $|\nu_1\rangle$ corresponding to the lowest energy
 - **first excited state, second excited state, ...**: $|\nu_2\rangle, |\nu_3\rangle, \dots$

Expectation values

Given

- a state $|\phi\rangle$ prepared on a quantum computer using the unitary U such that $U|0\rangle = |\phi\rangle$
- an observable H we are interested to measure

Then the expectation value of H respect to the state $|\phi\rangle$ is given by

$$\langle H \rangle_{|\phi\rangle} := \langle \phi | H | \phi \rangle = \langle 0 | U H U^\dagger | 0 \rangle \quad (3)$$

From the spectral theorem it follows:

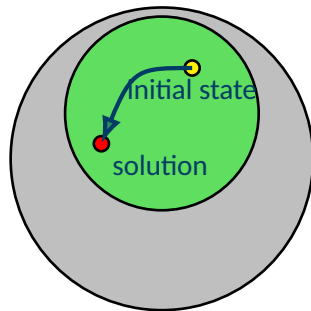
$$\langle H \rangle_{|\phi\rangle} = \langle \phi | \sum_i \lambda_i |\psi_i\rangle \langle \psi_i| \phi \rangle = \sum_i \lambda_i |\langle \phi | \psi_i \rangle|^2 = \sum_i \lambda_i |\langle 0 | U | \psi_i \rangle|^2. \quad (4)$$

Particularly: $\langle H \rangle_{|\psi_i\rangle} = \lambda_i$

The Variational Principle

$$\langle H \rangle_{|\phi\rangle} = \sum_i \lambda_i |\langle \phi | \psi_i \rangle|^2 \geq \sum_i \lambda_{\min} |\langle \phi | \psi_i \rangle|^2 = \lambda_{\min} \quad (5)$$

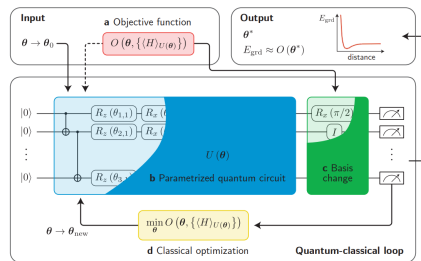
- H can encode a problem as ground state
- Prepare parametrized state $|\psi(\theta)\rangle$
- Find θ^* s.t. $|\langle H \rangle_{|\phi(\theta^*)} - \lambda_{\min}|$ minimal



The Variational Quantum Eigensolver

$$E_0 \leq \langle \psi(\theta) | H | \psi(\theta) \rangle \quad (6)$$

- $H = \sum_{\alpha} w_{\alpha} \sigma_{\alpha}, \quad \sigma_{\alpha} \in I, X, Y, Z^{\otimes N},$
- $|\psi(\vec{\theta})\rangle = \prod_i U_{\theta_i} |0\rangle = U(\vec{\theta}) |0\rangle$
- $E_{VQE} = \min_{\vec{\theta}} \sum_{\alpha} w_{\alpha} \langle 0 | U^{\dagger}(\vec{\theta}) \sigma_{\alpha} U(\vec{\theta}) | 0 \rangle$



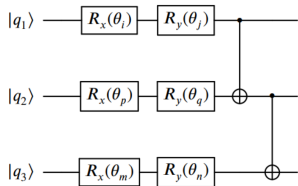
The Ansatz problem

The right choice of ansatz is critical to obtain a solution that is close to the ground state.

- Expressability: Refers the range of feasible states that the ansatz can achieve.
- Trainability: Refers to the ability to find the best set of parameters of the ansatz respect to expectation values of the Hamiltonian in a finite amount of time.
- Depth of the circuit: Refers to the number of sequential operations required for the implementation, which impacts the overall runtime of the method and its resilience to noise

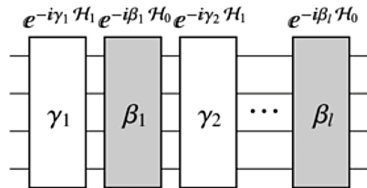
Hardware Efficient Ansatz

$$|\psi(\theta)\rangle_{HEA} = \prod_{i=1}^d U_{ent} U_{rot}(\theta_i) |0\rangle$$



Hamiltonian Variational Ansatz $|\psi(\theta)\rangle =$

$$\prod_{l=1}^P (\prod_j e^{i\theta_{lj} H_j}) |\psi_0\rangle, \quad H = \sum_j H_j$$



The Classical Optimizer choice

Gradient Descent Based

Use the analytical property of the ansatz, the gradient of observables can be directly computed on a quantum computer.

Gradient Descent,
Quantum Natural Gradient

Stochastic Gradient Based

Approximated the true gradient using random sampled data at each iteration.

SPSA, QNSPSA, Adam

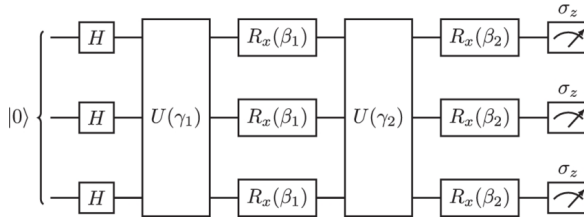
Gradient-free searching

Do not rely on gradient information and instead explore the parameter space using alternative techniques as random search, evolutionary algorithms or Bayesian optimization.

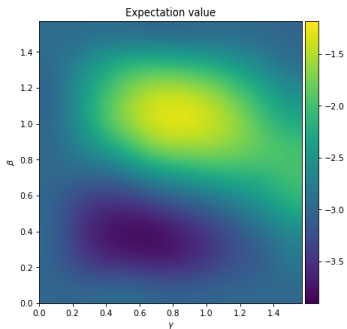
COBYLA, Nelder-Mead

The Quantum Alternating Operator Ansatz

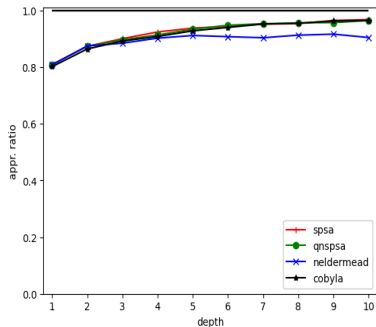
- Objective function $f : \{0, 1\}^n \rightarrow \mathbb{R}$
- Where are looking for the optimal vector $x^* = \operatorname{argmin}_{x \in \{0,1\}^n} f(x)$
- Problem Hamiltonian $H_P |z\rangle = f(z) |z\rangle$, $\langle H_P \rangle_{|z\rangle} = f(z)$
- Ground states of H_P minimize the objective function.
- Ansatz: $|\vec{\gamma}, \vec{\beta}\rangle = U_M(\beta_p) U_P(\gamma_p) \cdots U_M(\beta_1) U_P(\gamma_1) |\phi_0\rangle$
- Find $\gamma, \beta \in \mathbb{R}^p$, such that $\langle \gamma, \beta | H_P | \gamma, \beta \rangle$ is minimized.



Energy Landscape $p=1$



Multiple layers QAOA performance



Combinatorial Optimization: MaxKcut

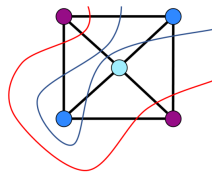
$$\max_{\mathbf{x} \in \{1, \dots, k\}^n} C(\mathbf{x}), \quad C(\mathbf{x}) = \sum_{(i,j) \in E} w_{ij} \begin{cases} 1, & \text{if } x_i \neq x_j \\ 0, & \text{otherwise.} \end{cases} \quad (7)$$

Solving NP hard optimization problems.

- **Heuristic algorithms.** No polynomial run time guarantee; appear to perform well on some instances.
- **Approximate algorithms.** Efficient and provide provable guarantees. With high probability we get a solution x^* such that

$$\frac{C(x^*) - \min_x C(x)}{\max_x C(x) - \min_x C(x)} \geq \alpha, \quad (8)$$

where $0 < \alpha \leq 1$ is the approximation ratio.



k	2	3	4	5
α	.878567	.836008	.857487	.876610
k	6	7	8	9
α	.891543	.903259	.912664	.920367

The problem Hamiltonian

For a given k we encode the information of a vertex belonging to one of the sets by $|i\rangle_{L_k}$, which requires

$$L_k := \lceil \log_2(k) \rceil \quad (9)$$

qubits.

$$H_P = \sum_{e \in E} w_e H_e, \quad H_e = I - \hat{H}_e, \quad U_P(\gamma) = e^{i\gamma H_P} = \prod_{e \in E} e^{i\gamma w_e \mathbb{I}} e^{-i\gamma w_e \hat{H}_e} \quad (10)$$

$$\hat{H}_e = \sum_{i,j=1}^{2^{L_k}} |i\rangle \langle i| \otimes |j\rangle \langle j| = \sum_{i,j=1}^{2^{L_k}} |ij\rangle \langle ij| \quad (11)$$

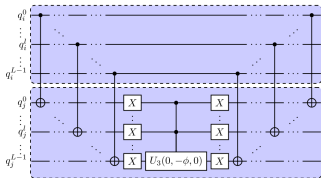
Here, \sim_{clr} is an equivalence relation $\text{clr} = \{\text{sets of equivalent colors states}\}$. With this, it is clear that $H_{i,j}$ has eigenvalue 0 for a state $|i\rangle |j\rangle$ if $i \sim_{\text{clr}} j$ and +1 if not.

The power of two case

When $k = 2^L$ the equivalence relation for the problem Hamiltonian becomes trivial because each color $c_i \rightarrow |bin(i)\rangle$ we assigned the related binary state

$$\hat{H}_e = \sum_{i=0}^{k-1} |i\rangle \langle i| \otimes |i\rangle \langle i| = \sum_{i=0}^{k-1} |ii\rangle \langle ii| = CX_{A \rightarrow B} (I_A \otimes |0\rangle_B \langle 0|_B) CX_{A \rightarrow B}. \quad (12)$$

$$CX_{A \rightarrow B} |q_A\rangle |q_B\rangle = |q_A^0\rangle \dots |q_A^{L-1}\rangle |q_B^0 \oplus q_A^0\rangle \dots |q_B^{L-1} \oplus q_A^{L-1}\rangle \quad (13)$$

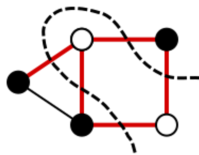


Where the \oplus operation is modulo 2.

This means that the state of the qubits belonging to j has zero entries if and only if all qubits have the same state as in the register i .

$$e^{-i\phi\hat{H}_e} = CX_{A \rightarrow B} (I_A \otimes e^{-i\phi|0\rangle_B \langle 0|_B}) CX_{A \rightarrow B}$$

The Maxcut case



$$\hat{H}_e = |00\rangle\langle 00| + |11\rangle\langle 11| = \frac{\mathbb{I} - Z \otimes Z}{2} \Rightarrow H_{Maxcut} = \sum_{(i,j) \in E} w_{ij} \frac{1 - Z_i Z_j}{2} \quad (14)$$

$$e^{-i\theta Z \otimes Z} = \begin{pmatrix} e^{-i\theta/2} & 0 & 0 & 0 \\ 0 & e^{i\theta/2} & 0 & 0 \\ 0 & 0 & e^{i\theta/2} & 0 \\ 0 & 0 & 0 & e^{-i\theta/2} \end{pmatrix} = \begin{array}{c} \text{---} \bullet \text{---} \\ | \\ \oplus \\ \text{---} \oplus \text{---} \\ | \\ \text{---} \oplus \text{---} \\ | \\ \bullet \text{---} \end{array} \begin{array}{c} \text{---} \\ \boxed{R_z(-\theta)} \\ \text{---} \end{array} \begin{array}{c} \text{---} \bullet \text{---} \\ | \\ \oplus \\ \text{---} \oplus \text{---} \\ | \\ \bullet \text{---} \end{array} \quad (15)$$

EXERCISE 1.1) Try to implement the Max4cut Hamiltonian H_e for one edge.

EXERCISE 1.2): Plot landscape for $p = 1$ and performance up to depth $p = 5$.

The degenerate color method

When $k \neq 2^{L_k}$ we can think to encode the k colors into all the computational basis states with some equivalence class degeneracy for some choices of colors. One possible choice is to assign $c_0 \rightarrow |0\rangle, c_1 \rightarrow |1\rangle, \dots, c_{k-2} \rightarrow |k-2\rangle, c_{k-1} \rightarrow \cup_{i=k-1}^{2^{L_k}-1} \{|i\rangle\}$.

$$\hat{H}_e = \sum_{i,j=1}^{2^{L_k}} |i\rangle \langle i| \otimes |j\rangle \langle j| = \sum_{i,j=1}^{2^{L_k}} |ij\rangle \langle ij|. \quad (16)$$

We should find a way to construct the exponential $U_P(\gamma) = e^{i\gamma H_P}$ using the minimum amount of resources for the specific choices of k and the equivalence class clr .

$$c_0 \rightarrow |00\rangle, c_1 \rightarrow |01\rangle, c_2 \rightarrow |10\rangle, |11\rangle \quad (17)$$

$$\hat{H}_e = |0000\rangle \langle 0000| + |0101\rangle \langle 0101| + |1010\rangle \langle 1010| \quad (18)$$

$$+ |1111\rangle \langle 1111| + |1110\rangle \langle 1110| + |1011\rangle \langle 1011| \quad (19)$$

Realizing exponentials of diagonal Projectors operators

We want to realize the exponential of a *diagonal square binary* matrix Λ , i.e.,

$$\Lambda_{i,j} \in \begin{cases} \{0, 1\}, & \text{if } i = j \\ \{0\}, & \text{otherwise,} \end{cases} \quad \forall 0 \leq i, j \leq 2^n - 1 \quad (20)$$

with quantum gates. Let's start with the case of where the number of ones elements in Λ are m , a power of two. There exists a permutation P_π , such that

$\Lambda = P_\pi (|0\rangle_A \langle 0|_A \otimes I_B) P_\pi^{-1}$ where $|B| = \log(m)$ and $|A| = n - |B|$. From this it follows that

$$\begin{aligned} e^{i\theta\Lambda} &= \left(\sum_{l=0}^{\infty} \frac{(i\theta)^l}{l!} \Lambda^l \right) = I + \left(\sum_{l=1}^{\infty} \frac{(i\theta)^l}{l!} \Lambda \right) = I + (e^{i\theta} - 1)\Lambda = \\ &= P_\pi \left((I_A + (e^{i\theta} - 1) |0\rangle_A \langle 0|_A) \otimes I_B \right) P_\pi^{-1}. \end{aligned} \quad (21)$$

In general we can rewrite m as $m = 2^{q_1} + 2^{q_2} + \dots + 2^{q_p}$ and consequently divide Λ into a sum of diagonal matrices with corresponding many non-zero elements, i.e.,

$$\Lambda = \Lambda_{q_1} + \Lambda_{q_2} + \dots + \Lambda_{q_p}. \quad (22)$$

For all matrices Λ_{q_i} in the above sum the number of non-zero elements is a power of two, then

$$e^{-i\theta\Lambda} = \prod_{j=1}^p e^{-i\theta\Lambda_j} = \prod_{j=1}^p P_{\pi_j} (I_{A_j} \otimes D_{z_j}) P_{\pi_j}^{-1} = \hat{P}_{\pi_0} \prod_{j=1}^p \hat{D}_j \hat{P}_{\pi_j}. \quad (23)$$

Each permutation P_{π} can be in principle implemented using only gates from the set $\{X, CX, CCX\}$.

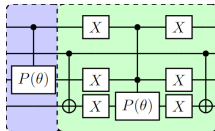
The k=3 case

In the edge Hamiltonian $|0000\rangle, |0101\rangle, |1010\rangle, |1111\rangle, |1011\rangle, |1110\rangle$ are the +1 eigenstates so the number of ones in \hat{H}_e is $m = 6 = 2^2 + 2^1$. Dividing $\hat{H}_e = H_1 + H_2$, where H_1 represent the first two colors and H_2 the remaining ones.

$$H_1 = \sum_{(i,j) \in \text{clr}_{<3}^3 |i,j \leq 1} |ij\rangle \langle ij| = CX_{2,4} (|0\rangle \langle 0| \otimes I \otimes |0\rangle \langle 0| \otimes |0\rangle \langle 0|) CX_{2,4}, \quad (24)$$

$$H_2 = \sum_{(i,j) \in \text{clr}_{<3}^3 |i,j \geq 2} |ij\rangle \langle ij| = X_1 X_3 (|0\rangle \langle 0| \otimes I \otimes |0\rangle \langle 0| \otimes I) X_1 X_3, \quad (25)$$

where $CX_{a,b}$ denotes a CX gate with control index a and target index b .



EXERCISE 2.1) Realize the quantum circuit for the cost function for the partition $\{|0000\rangle, |0101\rangle, |1010\rangle, |1111\rangle\} \cup \{|1011\rangle, |1110\rangle\}$.

EXERCISE 2.2) Plot Landscape for $p=1$ and performance up to depth $p=5$.

The Constrained to a Subspace method

When k is not a power of two instead of using equivalence color classes we can define the feasible set B and constraint the QAOA ansatz to explore only this set. We then need to initialize a feasible initial state and define a constraint Mixer.

For each vertex the feasible set of color states can be defined as

$$B_k = \{|i\rangle \mid 0 \leq i \leq k - 1\}.$$

Since the feasible bit-strings admit a Cartesian product structure (the vertices are independent), the feasible subspace becomes a tensor product of the form

$$B = B_k^1 \otimes \cdots \otimes B_k^{|V|}. \quad (26)$$

We observe that

$$H_P^{\text{bin}}(2^{L_k})|_{\text{span}(B)} = H_P^{\text{bin}}(k), \quad (27)$$

Using this approach we shift the complexity from the Phase or Cost Hamiltonian to the Mixer Hamiltonian.

Constrained QAOA

The solutions constrained to a feasible subspace $\text{span}(B) \subset \mathcal{H} = (\mathbb{C}^2)^{\otimes n}$:

$$B = \{ |z_j\rangle, 1 \leq j \leq J, z_j \in \{0, 1\}^n \}. \quad (28)$$

Definition valid mixer

- Preserve the feasible subspace

$$U_M(\beta) |v\rangle \in \text{span}(B), \quad \forall |v\rangle \in \text{span}(B), \forall \beta \in \mathbb{R}, \quad (29)$$

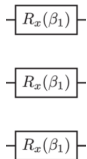
- Provide transitions between all pairs of feasible states, i.e., for each pair of computational basis states $|x\rangle, |y\rangle \in B$ there exist $\beta^* \in \mathbb{R}$ and $r \in \mathbb{N} \cup \{0\}$, such that

$$| \langle x | \underbrace{U_M(\beta^*) \cdots U_M(\beta^*)}_{r \text{ times}} | y \rangle | > 0. \quad (30)$$

Example of Valid Mixers

Unconstrained case: X mixer

$$U_X(\beta) = \prod_i RX_i(\beta) = \prod_i (\cos(\beta)\mathbb{I} + i\sin(\beta)X_i) \quad (31)$$

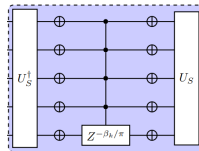


$$U_X\left(\frac{\pi}{2}\right) = \frac{1}{2\sqrt{2}}(\mathbb{I} + i(X_1 + X_2 + X_3) - (X_1X_2 + X_2X_3 + X_1X_3) - iX_1X_2X_3)$$

Constrained case: Grover mixer

$$|F\rangle = \frac{1}{\sqrt{|B|}} \sum_{i \in B} |i\rangle = |F\rangle = U_S |O\rangle \Rightarrow \quad (32)$$

$$U_{\text{Grover}}(\beta) = e^{i\beta|F\rangle\langle F|} = U_S e^{i\beta|O\rangle\langle O|} U_S^\dagger \quad (33)$$



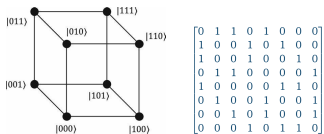
$$(|F\rangle\langle F|)^2 = |F\rangle\langle F| \Rightarrow U_{\text{Grover}}(\beta) = \sum_i \frac{(i\beta)^n}{n!} (|F\rangle\langle F|)^n = \mathbb{I} + (e^{i\beta} - 1) |F\rangle\langle F|$$

EXERCISE 3.1) Pen and paper exercise: Prove that the Grover mixer and the X mixer are valid mixer .

EXERCISE 3.2) Try to prove that the mixer are valid choosing different pair of comp states and check the overlap for a certain range of parameters.

Examples of Graphs and mixers

X mixer as Hypercube graph



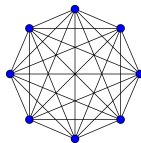
$$\begin{bmatrix} 0 & 1 & 1 & 0 & 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 1 & 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 1 & 0 & 0 & 1 & 0 \\ 0 & 1 & 1 & 0 & 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 & 0 & 1 & 1 & 0 \\ 0 & 1 & 0 & 0 & 1 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 & 1 & 0 & 0 & 1 \\ 0 & 0 & 0 & 1 & 0 & 1 & 1 & 0 \end{bmatrix}$$

$$R_x(\beta_1)$$

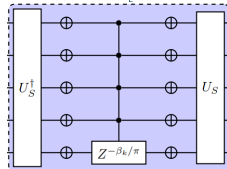
$$R_x(\beta_1)$$

$$R_x(\beta_1)$$

Grover mixer as Complete Graph



$$\begin{bmatrix} 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \end{bmatrix}$$



Initial state preparation

Given the independence of the different color constraints for each vertex of the problem the initial state can be prepared as the uniform superposition of all feasible basis state as follows:

$$\left| \Phi_0^{<k} \right\rangle^{\otimes |V|} = U_S \otimes \cdots \otimes U_S |0\rangle, \text{ where } \left| \Phi_0^{<k} \right\rangle = U_S |0\rangle = \frac{1}{k} \sum_{i=0}^{k-1} |i\rangle. \quad (36)$$

Where we prepare independently on each vertex the equal superposition of all feasible colors due to the property of the tensor product:

$$\left(\sum_{i \in B_k} a_i |i\rangle \right) \otimes \left(\sum_{j \in B_k} b_j |j\rangle \right) = \sum_{i \in B_k, j \in B_k} a_i b_j |ij\rangle = \sum_{m \in B_k \otimes B_k} c_m |m\rangle \quad (37)$$

Grover Mixer construction

Now we need to define a valid mixer for the feasible subspace B.

The first possibility is to use directly the initial state preparation circuit $U_S \otimes \dots \otimes U_S$ to implement the Grover mixer

$$U_{Grover}(\beta) = (U_S \otimes \dots \otimes U_S) e^{i\beta(|0\rangle\langle 0|)^{\otimes |V|}} (U_S^\dagger \otimes \dots \otimes U_S^\dagger) \quad (38)$$

The total cost of this mixer is $2|V|$ times the cost of implementing the initial state for a vertex and the cost of implementing the $|V|L_k - 1$ control phase operator.

Alternative we can take advantage from the structure of B and define the Grover Mixer independently for each vertex

$$U_M(\beta) = U_S e^{i\beta|0\rangle\langle 0|} U_S^\dagger \otimes \dots \otimes U_S e^{i\beta|0\rangle\langle 0|} U_S^\dagger \quad (39)$$

This Grover mixer can be obtained by exponentiation of the following Hamiltonian Mixer

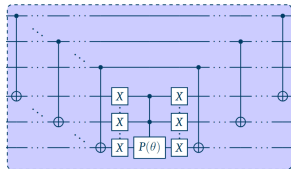
$$H_M = G^{\square |V|} = G \square G \cdots \square G, \quad G = |F\rangle \langle F| \quad (40)$$

where the Cartesian or Box product is defined as

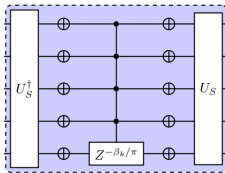
$$G \square H = G \otimes \mathbb{I} + \mathbb{I} \otimes H. \quad (41)$$

If G and H are connected graphs then $G \square H$ is connected too and the mixer is valid.

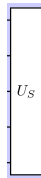
Cost Circuit for an edge of the Maxkcut problem



Grover Mixer for a $16 < k \leq 32$ MaxkCut vertex



Initial state for a $16 < k \leq 32$ MaxkCut vertex



EXERCISE 3.3) Implement the tensorize or box product Grover mixer for $k=3$.

EXERCISE 3.4) Computing landscapes and performance up to depth $p=5$ and compare it with the degenerate color case.

References I

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