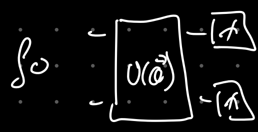
Class 3: PWF 2021 - QML 12/01/2021

$$C(\vec{\theta}) = \mathrm{Tr}[U(\vec{\theta})\rho_0 U^\dagger(\vec{\theta}) O]$$



O is usually of 2 forms

A) $O = \sum_i c_i \sigma_i$ $\quad \sigma_i \in \{X, Y, Z, \mathbb{1}\}^{\otimes n}$ set of Pauli strings

the summation has a polynomial number of terms

$$\underline{Z} \otimes \underline{Z} \otimes \underline{\mathbb{1}} \cdots \otimes \underline{\mathbb{1}} = Z_1 Z_2$$

$$Y_1 \otimes Z_2 \otimes Z_3 \otimes Z_4$$

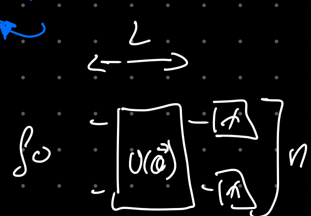
B) $O = \sum_i d_i |z_i\rangle\langle z_i|$ $\quad |z_i\rangle \in \{|0\rangle, |1\rangle\}^{\otimes n}$

$|0\cdots0\rangle, |10\cdots0\rangle, \ldots |1,\cdots1\rangle$

the summation has a polynomial number of terms

How do we estimate the cost through measurements that are usually projective measurements in the computational basis.

B) $\rightarrow$
$$C(\vec{\theta}) = \mathrm{Tr}[U(\vec{\theta})\rho_0 U^\dagger(\vec{\theta}) \sum_i d_i |z_i\rangle\langle z_i|$$
$$= \sum_i d_i \mathrm{Tr}[U(\vec{\theta})\rho_0 U^\dagger(\theta) |z_i\rangle\langle z_i|]$$
$$= \sum_i d_i \langle z_i| U(\vec{\theta})\rho_0 U^\dagger(\theta) |z_i\rangle$$
$$= \sum_i d_i \, p(z_i) \simeq \sum_i d_i \frac{N_{z_i}}{N}$$



n qubits

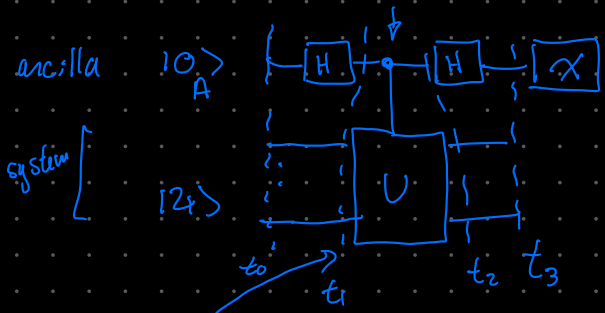
$$\sum_i d_i |z_i\rangle\langle z_i| \Rightarrow |0\cdots0\rangle\langle0\cdots0|$$

$$C(\vec{\theta}) = p(0\cdots0)$$

TIP #6   Hadamard Test

$|\psi\rangle$ is a general n-qubit state, and U is a unitary operator

$Re[\langle\psi|U|\psi\rangle]$ $\quad$ $Im[\langle\psi|U|\psi\rangle]$



$$H = \frac{1}{\sqrt{2}}\begin{pmatrix}1 & 1\\ 1 & -1\end{pmatrix}$$

$$\rightarrow \quad H|0\rangle = \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle) = |+\rangle$$

$$H|-\rangle = \frac{1}{\sqrt{2}}(|0\rangle - |1\rangle) = |-\rangle$$

$$C_U = |0\rangle\langle 0|_A \otimes \mathbb{1}_S + |1\rangle\langle 1|_A \otimes U$$

t_0 $\quad |0_A\rangle \otimes |\psi\rangle$

$$t_1 \xrightarrow{H} \frac{1}{\sqrt{2}}(|0_A\rangle + |1_A\rangle) \otimes |\psi\rangle = \frac{1}{\sqrt{2}}\left(|0_A\rangle \otimes |\psi\rangle + |1_A\rangle \otimes |\psi\rangle\right)$$

$$t_2 \xrightarrow{C_U} \frac{1}{\sqrt{2}}\left(|0_A\rangle \otimes |\psi\rangle + |1_A\rangle \otimes U|\psi\rangle\right)$$

$$t_3 \xrightarrow{H} \frac{1}{\sqrt{2}}\left(\frac{1}{\sqrt{2}}(|0_A\rangle + |1_A\rangle) \otimes |\psi\rangle + \frac{1}{\sqrt{2}}(|0_A\rangle - |1_A\rangle) \otimes U|\psi\rangle\right)$$

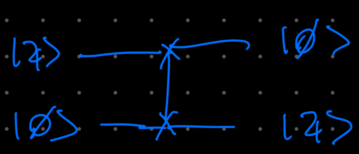
$$|\psi_f\rangle = \frac{1}{2}\left(|0_A\rangle \otimes (|\psi\rangle + U|\psi\rangle) + |1_A\rangle \otimes (|\psi\rangle - U|\psi\rangle)\right)$$

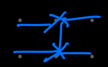
$$M_{0A} = [|0\rangle\langle 0|_A \otimes \mathbb{1}]$$

$$Tr[M_{0A}\, |\psi_f\rangle\langle\psi_f|] = P_A(0)$$

$$P_A(0) = \frac{1}{2}[1 + Re[\langle\psi|U|\psi\rangle]] \leftarrow$$

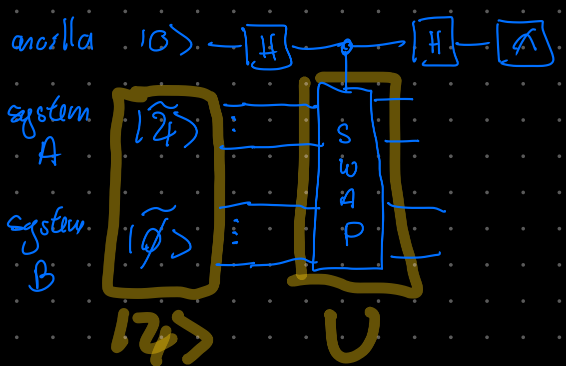
SWAP circuit



SWAP 

SWAP $|\psi\rangle\otimes|\phi\rangle = |\phi\rangle\otimes|\psi\rangle$

Hadamard-Swap test



probability ancilla being in zero

translating results

$|\psi\rangle = |\tilde\psi\rangle\otimes|\tilde\phi\rangle$

$U = SWAP$

$$|\psi_f\rangle = \frac{1}{2}\left(|0_A\rangle\otimes\left(|\tilde\psi\rangle|\tilde\phi\rangle + |\tilde\phi\rangle|\tilde\psi\rangle\right) + |1_A\rangle\otimes\left(|\tilde\psi\rangle|\tilde\phi\rangle - |\tilde\phi\rangle|\tilde\psi\rangle\right)\right)$$

$\langle\psi|U|\psi\rangle$

$$p_A(0) = \frac{1}{2}\left[1 + Re\left[\langle\tilde\psi|\langle\tilde\phi|\,\underline{SWAP\,|\tilde\psi\rangle|\tilde\phi\rangle}\right]\right]$$

$$= \frac{1}{2}\left[1 + Re\left[\langle\tilde\psi|\otimes\langle\tilde\phi|\tilde\phi\rangle\otimes|\tilde\psi\rangle\right]\right]$$

$$= \frac{1}{2}\left[1 + Re\left[\langle\tilde\psi|\tilde\phi\rangle\langle\tilde\phi|\tilde\psi\rangle\right]\right]$$

$(A\otimes B)\cdot(C\otimes D) = AC\otimes BD$

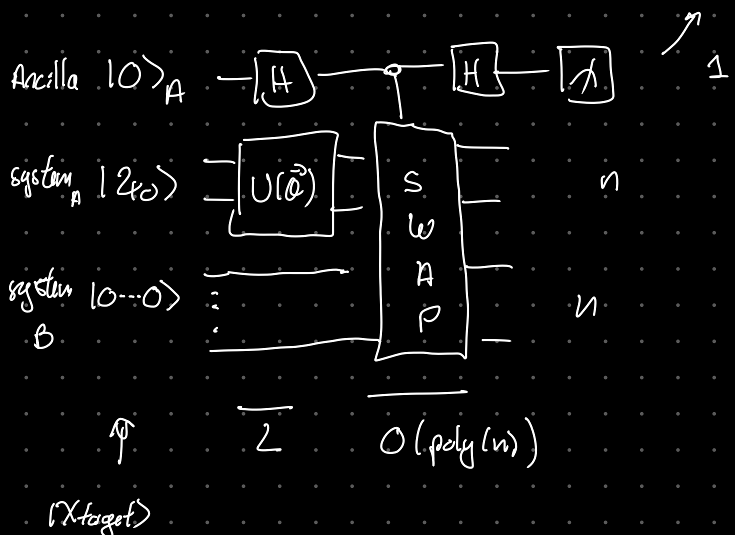
$$= \frac{1}{2}\left[1 + Re\left[|\langle\tilde\psi|\tilde\phi\rangle|^2\right]\right]$$

$$= \frac{1}{2}\left[1 + |\langle\tilde\psi|\tilde\phi\rangle|^2\right] \quad (*)$$

Our cost function $C(\vec\theta) = \underline{p(0\ldots0)} = \langle 0\ldots0|U(\vec\theta)\rho_0 U^\dagger(\vec\theta)|0\ldots0\rangle$

$\rho_0 = |\psi_0\rangle\langle\psi_0|$

$= |\langle 0\ldots0|U(\vec\theta)|\psi_0\rangle|^2 \quad (*)$



This requires $\underline{2n+1 \text{ qubits}}$

+ additional $O(poly(n))$ circuit depth.

Ressource Analysis

$$\boxed{C(\vec{\theta}) = 1 - |\langle \chi_{target} | \psi(\vec{\theta}) \rangle|^2}$$

if $|\psi(\vec{\theta})\rangle = e^{i\varphi} |\chi_{target}\rangle$ then $C(\vec{\theta}) = 0$

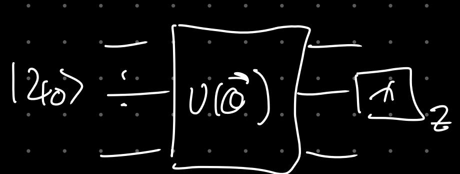
A) $\quad O = \sum_i c_i \sigma_i \qquad \sigma_i \in \{X, Y, Z, \mathbb{1}\}^{\otimes n}$

$$C(\vec{\theta}) = \sum_i c_i \; Tr\left[U(\vec{\theta}) |\psi_0\rangle\langle\psi_0| U^\dagger(\vec{\theta}) \sigma_i\right]$$

$$= \sum_i c_i \; \langle \psi_0 | U^\dagger(\vec{\theta}) \sigma_i U(\theta) | \psi_0 \rangle$$

$$= \sum_i c_i \; \langle \sigma_i \rangle_{U|\psi_0\rangle}$$

we know that if $\sigma_i = Z^{(k)}$

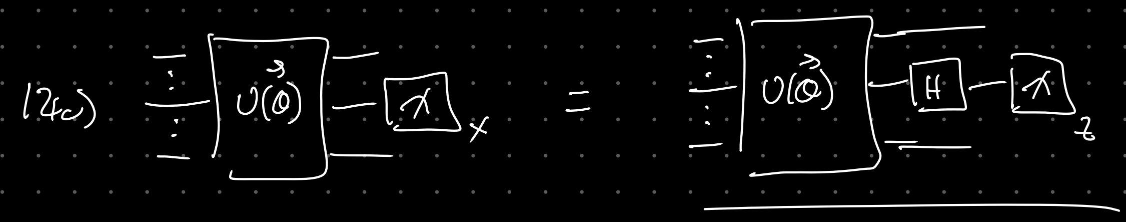


k-th qubit

$Z = |0\rangle\langle 0| - |1\rangle\langle 1|$

$$\langle Z^{(k)} \rangle = P_k(0) - P_k(1)$$

what happens if $\sigma_i = X^{(k)}$



$$P_k(0) = \mathrm{Tr}\Big[\underbrace{(H^{(k)} \otimes \mathbb{1}_{\bar{k}})\, U(\vec{\theta})\,|\psi_0\rangle\langle\psi_0|\,U^\dagger(\vec{\theta})\,(H^{(k)} \otimes \mathbb{1}_{\bar{k}})}\;\underbrace{(|0\rangle\langle 0|_k \otimes \mathbb{1}_{\bar{k}})}_{M_0^{(k)}}\Big]$$

$$= \mathrm{Tr}\Big[U(\vec{\theta})\,|\psi_0\rangle\langle\psi_0|\,U^\dagger(\vec{\theta})\,\underbrace{(H^{(k)} \otimes \mathbb{1}_{\bar{k}})(|0\rangle\langle 0|_k \otimes \mathbb{1}_{\bar{k}})(H^{(k)} \otimes \mathbb{1}_{\bar{k}})}\Big]$$

$$H^{(k)}|0\rangle\langle 0|_k H^k \otimes \mathbb{1}_k$$

$$\underbrace{|+\rangle\langle +|_k \otimes \mathbb{1}_k} \leftarrow M_+^{(k)}$$

$$= \mathrm{Tr}\Big[U(\vec{\theta})\,|\psi_0\rangle\langle\psi_0|\,U^\dagger(\vec{\theta})\,M_+^{(k)}\Big]$$

$$\langle X\rangle = P_k(0) - P_k(1)$$

Now let's compute the expectation value of 2-body Pauli operators

$$\langle Z_1 Z_2\rangle$$

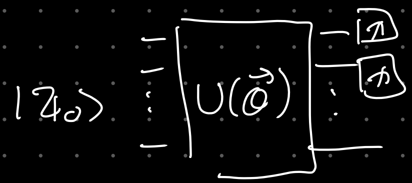
$$Z_1 = |0\rangle\langle 0|_1 - |1\rangle\langle 1|_1$$

$$Z_2 = |0\rangle\langle 0|_2 - |1\rangle\langle 1|_2$$

$$Z_1 Z_2 = (|0\rangle\langle 0|_1 - |1\rangle\langle 1|_1) \otimes (|0\rangle\langle 0|_2 - |1\rangle\langle 1|_2)$$

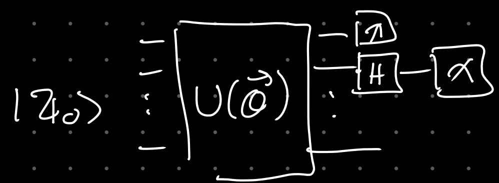
$$= |00\rangle\langle 00|_{12} - |01\rangle\langle 01|_{12} - |10\rangle\langle 10|_{12} + |11\rangle\langle 11|_{12}$$

$$\left[\langle Z_1 Z_2\rangle = p(0_1 0_2) + p(1_1 1_2) - p(0_1 1_2) - p(1_1 0_2)\right.$$



$$\langle Z_1 Z_2\rangle \simeq \frac{N_{00} + N_{11} - N_{01} - N_{10}}{N}$$

what happens $\langle Z_1 X_2\rangle$



$$\langle Z_1 X_2\rangle \simeq \frac{N_{00} + N_{11} - N_{01} - N_{10}}{N}$$

Ressource analysis

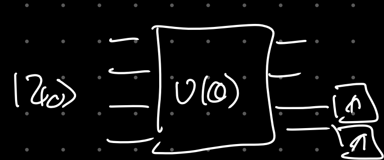
$$O = \underbrace{\sum_i c_i \sigma_i}_{\text{poly}(n)\text{-terms}}$$

estimating σ_i requires a circuit with (maybe) some change of basis, and local measurements

N shots

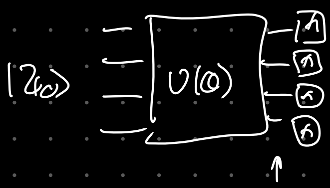
$\text{poly}(n) \times N$ measurement shots

Example I have a 4 qubit state $\langle Z_1 Z_2\rangle$ $\langle Z_3 Z_4\rangle$



$\langle Z_1 Z_2\rangle$ $\langle Z_3 Z_4\rangle$

N shots + N shots



$p(0000)$ $p(1000)$ $p(0100)$

$\dots$ $p(1111)$

$2^4 = 16$ outcomes

$p(x_i, y)$

$\downarrow$

$$p(x_i) = \sum_{y_\gamma} p(x_i, y_\gamma)$$

$$p(0_1 0_2) = p(0000) + p(0001) + p(0010) + p(0011)$$

This allows to compute both $\langle Z_1 Z_2 \rangle$ $\langle Z_3 Z_4 \rangle$ with N measurements?

$$Z_1 Z_2 = Z_1 \otimes Z_2 \otimes \mathbb{1}_3 \, \mathbb{1}_4 \qquad [Z_1 Z_2, Z_3 Z_4] = 0$$

$$Z_3 Z_4 = \mathbb{1}_1 \otimes \mathbb{1}_2 \otimes Z_3 \otimes Z_4$$

$X_2 X_3$ $\qquad [X_2 X_3, Z_1 Z_2] \neq 0$

$$[X_2 X_3, Z_3 Z_4] \neq 0$$

$X_3 X_4$ $\qquad [Z_1 Z_2, X_3 X_4] = 0$

$+1, -1$

$\frac{1}{\sqrt{N}}$

$$\langle Z_1 Z_2 \rangle = \sum q_\mu^{(ij)} \, p(ij)$$

n-length bitstrings)

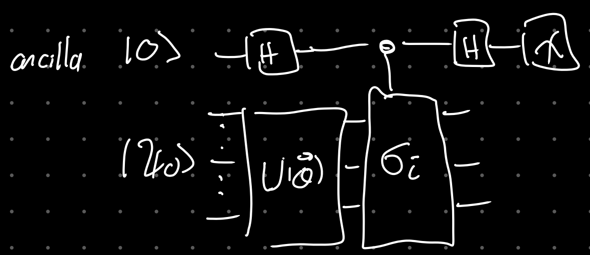
$$= \sum q_\mu^{ij} \, p(z \,/\, z_i = i \;\&\; z_j = j)$$

Error analysis:

$$\Delta(Z_1 Z_2) = \sum \Delta p$$

$$\Delta f(x_1 \dots x_n) = \sum_i \left| \frac{\partial f}{\partial x_i} \right| \Delta x_i$$

Note: we can also compute $\langle \sigma_i \rangle$ via the Hadamard Test



$\forall \quad \sigma_i \in \{X, Y, Z, \mathbb{1}\}^{\otimes n}$

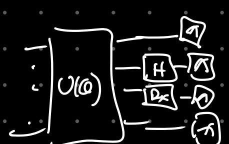
$\sigma_i \cdot \sigma_i^\dagger = \sigma_i \sigma_i = \underline{\mathbb{1}}$

$$Z_1 Z_2 \cdot Z_1 Z_2 = Z_1 Z_1 \otimes Z_2 \cdot Z_2 = \mathbb{1} \otimes \mathbb{1}$$

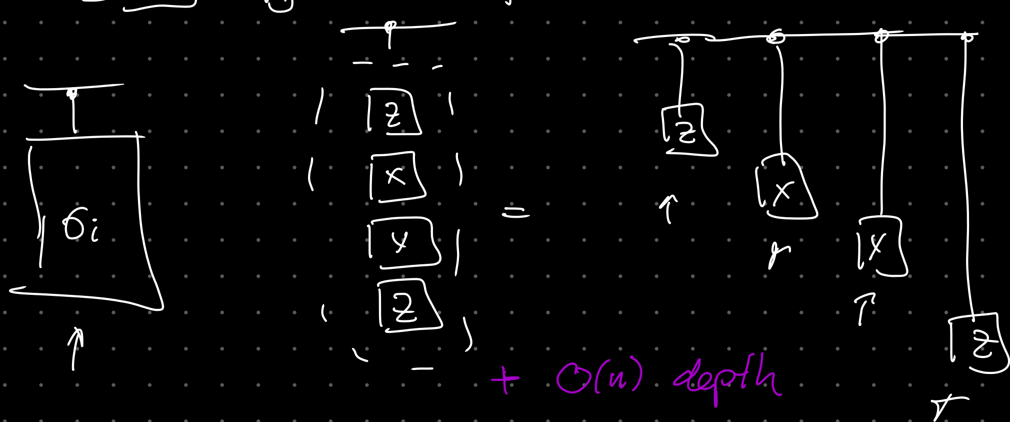
$$p_A(0) = \frac{1}{2}\left[1 + \langle \sigma_i \rangle\right]$$

$Z_1 Z_2$

Assume σ_i acts <u>non-trivial</u> on <u>all</u> n-qubits



if we use the hadamard test



+ $O(n)$ depth

$$\left(|0\rangle\langle 0| \otimes \mathbb{1} + |1\rangle\langle 1| \otimes X_2\right) \cdot \left(|0\rangle\langle 0| \otimes \mathbb{1} + |1\rangle\langle 1| \times Z_1\right)$$

$$\left(|0\rangle\langle 0| \otimes \mathbb{1} + |1\rangle\langle 1| \otimes X_2 Z_1\right)$$

k-body Pauli string

$O(n)$

QAOA : Quantum Approximation Optimization Algorithm

Farhi et al arxiv 1411.4028

Solving combinatorial problemin in Quantum computers.

Used logistics, supply chains, developping networks
sending taxis & fixing rate, optimal delivering routes
water & electricity supply.

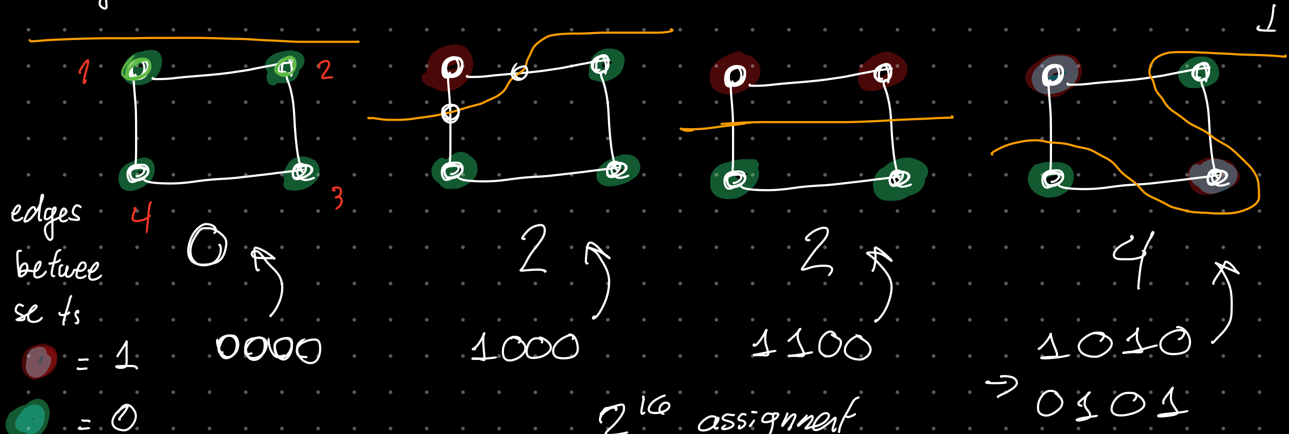
General : Hard to solve

formally speaking a Combinatorial optimization is defined as a task of determining optimal object out of a finite set of objects.

We will focus: we find an optimal bitstring, optimal sequence of 0's and 1's.

Graphs → Max-cut problem

Partinioning nodes on a graph into 2 sets, such that the number of edges between the sets is maximum.



2^{16} assignment

As the # of nodes increases, the number of possible assignments increases exponentials.

1) we need to define a cost function

Maxcut problems are defined of a graph

$$G = (\underset{\text{nodes}}{V}, \underset{\text{edges}}{E})$$

Object function for the classical problem is defined on bitstrings of lenght n.

$$S(z) = \sum_{\alpha=1}^{E} S_\alpha(z) \qquad z \in \{0,1\}^{\otimes n}$$

here $S_\alpha(z) = 1$ if z satisfies a clause

$S_\alpha(z) = 0$ otherwise

we want to promote the classical object function a quantum cost function

1 -1

$$\boxed{H_P = \sum_{\langle jk \rangle} H_{\langle jk \rangle}}$$

edges on the graph

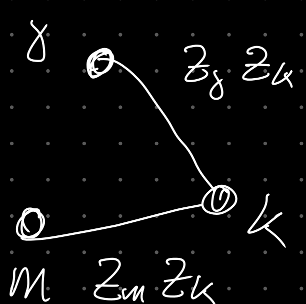
where $H_{\langle jk \rangle} = \frac{1}{2}\left(1 - Z_j Z_k\right)$

$|z\rangle$ k-th qubit is in 0 $\}$ 1
j-th qubit is in 0 $\}$ 1

$\left[\langle z | H_{\langle jk \rangle} | z \rangle = 0\right.$

k-th qubit in 0 $\}$ 1
j-th qubit in 1 $\}$ 0

$\left[\langle z | H_{\langle jk \rangle} | z \rangle \; 1\right.$



The QAOA cost function

$$C(\vec{\theta}) = \mathrm{Tr}\left[U(\vec{\theta}) |\psi_0\rangle\langle\psi_0| U^\dagger(\vec{\theta}) \, H_p \right]$$

2) Ansatz for $U(\vec{\theta})$ loosely base on the adiabatic theorem

$$H_M \qquad\qquad\qquad\qquad H_p$$

$$|GS_M\rangle \longrightarrow |GS_p\rangle$$

$$H(t) = (1-s(t))H_M + s(t)H_p \qquad s(0)=0, \quad s(t_f)=1$$

$e^{-iH(t)t}$ hard to implement

1) Discretize t into p, Δt intervals

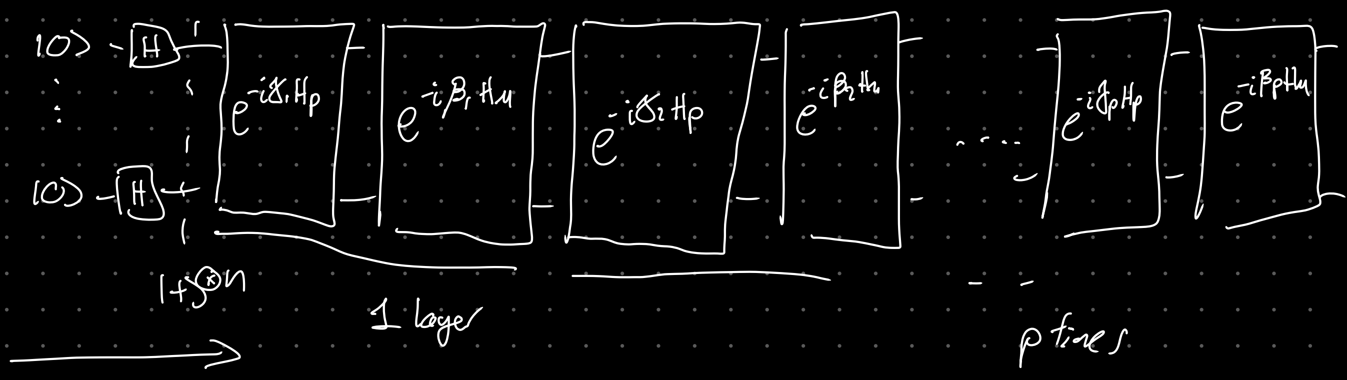
$$U(t_f,0) = U(t_f, t_f-\Delta t)\cdots U(\Delta t, 0)$$
$$= \prod_{j=1}^{p} U(j\Delta t, (j-1)\Delta t)$$
$$\simeq e^{-iH(j\Delta t)\Delta t}$$

$$e^{i(A+B)x} \approx e^{iAx}e^{iBx} + O(x^2)$$

$$U(t_f,0) = \prod_{j=1}^{p} e^{-i(1-s(j\Delta t))H_M\Delta t} \, e^{-is(j\Delta t)H_p\Delta t}$$

Our "mixer" $H_M = \sum_i X_i$ $\qquad |GS_M\rangle = |+\rangle^{\otimes n}$

"driver"



$$U(\vec{\gamma},\vec{\beta}) = U(H_M,\beta_p)\,U(H_p,\gamma_p)\dots U(H_M,\beta_1)\,U(H_p,\gamma_1)$$

$$U(\vec{\gamma},\vec{\beta})|\psi_0\rangle =$$

$$\underline{A.B.|x\rangle}$$

③ How do we compute the cost ?

$$C(\theta) = \Big\langle \sum_{\langle jk\rangle} H_{\langle jk\rangle} \Big\rangle = \sum_{\langle jk\rangle} \langle H_{jk}\rangle = \sum_{\langle jk\rangle} \frac{1}{2}\left(1-\langle Z_j Z_k\rangle\right)$$

$$H_{\langle jk\rangle} = \frac{1}{2}(1-Z_j Z_k)$$

$$[Z_j Z_k, Z_m Z_p] = 0 \quad \forall j,k,m,p$$

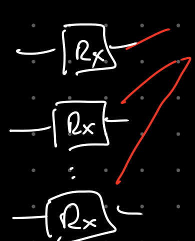
$$[X_i, X_j] = 0 \quad \forall i,j$$

$$e^{A+B} = e^A e^B$$

if $[A,B]=0$

2.1

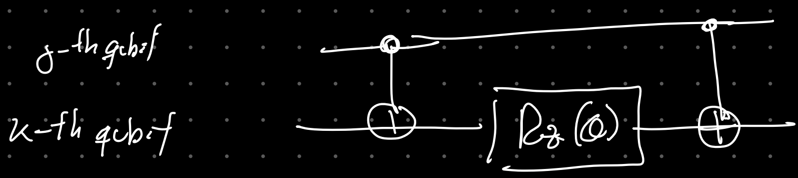
$$e^{-iH_M\beta} = e^{-i\beta\sum_i X_i} = \prod_{i=1}^{n} \underbrace{e^{-i\beta X_i}}_{R_X(\beta)}$$



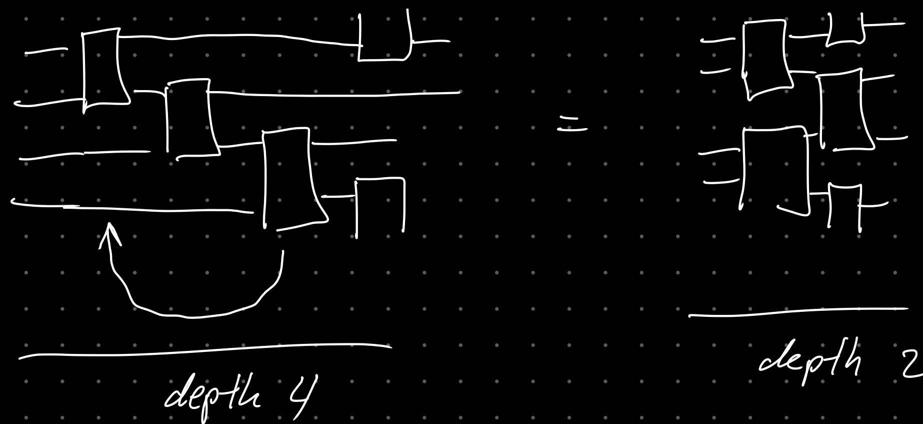
same param. β

$$\Sigma_{jk} \neq \Sigma_{\langle jk \rangle}$$

$$
\begin{aligned}
\underline{e^{-i\gamma H_p}} &= e^{-i\gamma \sum_{\langle jk \rangle} \frac{1}{2}(1 - Z_j Z_k)} \\
&= e^{-i\gamma/2\, \underline{\mathbb{1}} + i\gamma \sum_{\langle jk \rangle} \underline{Z_j Z_k} /2} \\
&= e^{-i\gamma/2} \prod_{\langle jk \rangle} e^{i\gamma/2\, \underline{Z_j Z_k}}
\end{aligned}
$$



$$= e^{-i\theta Z_j Z_j}$$



The generalization of the ansatz of $U(\theta)$

Hadfield et al Algorithms 12(2). 34 (2019)

arXiv 1709.0348

Given H_M, H_p

find $|GS\rangle$

QAOA = Quantum Alternating Operator Ansatz

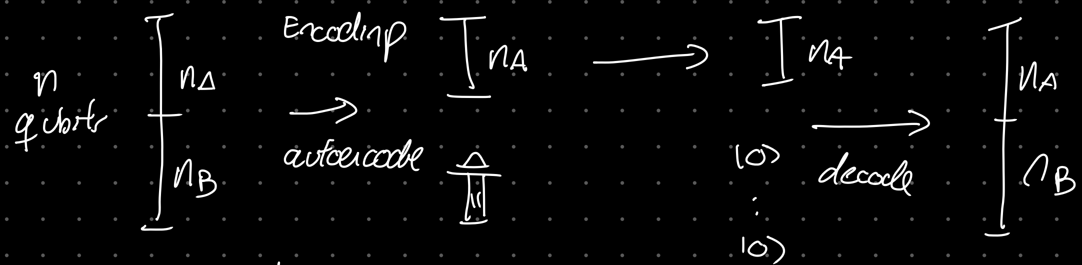
Quantum Autoencoder

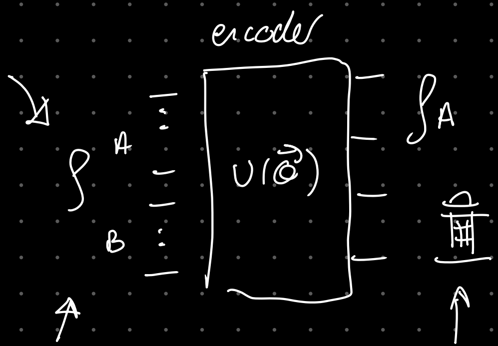
Romero et. al
Quantum Sci Tech
2 045001, (2017)
arxiv 1612.02806

$\{p_i, |\psi_i\rangle\}$

n-qubit quantum

$\rho = \sum_i p_i |\psi_i\rangle\langle\psi_i|$



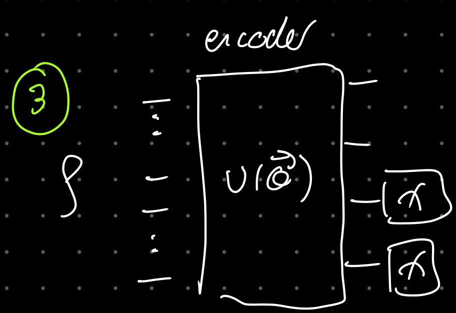


1 $C(\vec\theta) = 1 - p_B(0\cdots0)$

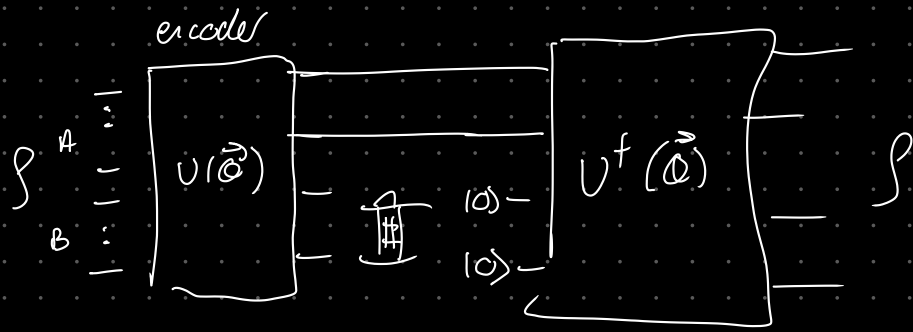
$M^{(B)} = \mathbb{1}_A \otimes |0..0\rangle\langle 0..0|_B$

$$C(\vec\theta) = 1 - p_B(0..0) = \mathrm{Tr}\left[U(\vec\theta)\rho U^\dagger(\vec\theta)\left(\mathbb{1}_A \otimes |0..\rangle\langle 0..0|_B\right)\right]$$

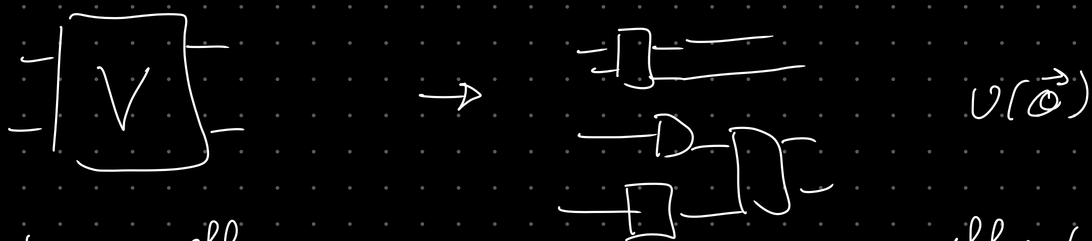
3



cost-evaluating circuit



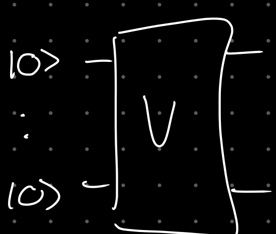
Compilation Algorithm



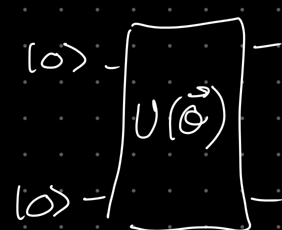
- has no efficient quantum circuit description
- unknown

e^{-iHt}

Task: we learn an efficient quantum circuit
Goal: representation of a unitary V



$V|\vec{0}\rangle$ & $U(\vec{\theta})|\vec{0}\rangle$



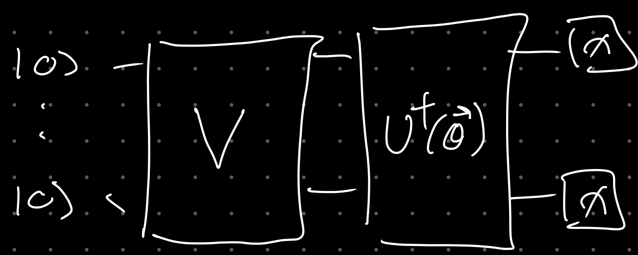
we want $U(\vec{\theta})|0\rangle$ to match $V|\vec{0}\rangle$

1 → 3

$$C(\vec{\theta}) = 1 - |\langle\vec{0}|U^\dagger(\vec{\theta})\, V|\vec{0}\rangle|^2$$

$$C(\vec{\theta}) = 1 - |\langle \vec{0} | U^{\dagger}(\vec{\theta}) \, V | \vec{0} \rangle|^2$$

How do we evaluate $C(\vec{\theta})$: 1 SWAP TEST



$$C(\vec{\theta}) = 1 - p(\vec{\theta})$$

(2) For the autoencoder & the compilation task: what ansatz should we use for $U(\vec{\theta})$?

Ansatz design
Problem