Quantum Approximate Optimization Algorithm for Ising model

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Ising model presentation on quantum computer

A spin configuration on the lattice is a bitstring $z = z_1 z_2 \dots z_n$, $z_i = \pm 1$ where each z_i is spin orientation on the lattice i-th node.
The value of the variable z_i corresponds to the measurement outcome of the Pauli-Z operator on the i-th qubit of the quantum register in the computational basis:

$$|0\rangle = \begin{bmatrix} 1 \\ 0 \end{bmatrix} \leftrightarrow z = +1 \text{ and } |1\rangle = \begin{bmatrix} 0 \\ 1 \end{bmatrix} \leftrightarrow z = -1,$$

i.e. z_i are eigenvalues of $Z = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$ for the bases $|0\rangle$ and $|1\rangle$.

$$\text{bitstring } z = z_1 z_2 \dots z_n \longleftrightarrow \text{ register state } |z\rangle = |z_1 z_2 \dots z_n\rangle.$$

2^n states of the computational basis of the quantum register correspond to the 2^n possible assignments of the variables z_i on the lattice.

Ising Hamiltonian with nearest-neighbor interaction in an external magnetic field h:

$$\mathcal{H}_C(Z) = -J \sum_{\langle i,j \rangle} Z^{(i)} Z^{(j)} - h \sum_i Z^{(i)}$$

$Z^{(i)} = \mathbb{I} \otimes \cdots \otimes Z \otimes \cdots \otimes \mathbb{I}$ Pauli operator Z on i-th position acts on i-th qubit

Problem: find the spin configuration on the lattice with the lowest expectation value of $H_C(Z)$ (energy).

Variational Quantum Algorithms

VQA are hybrid quantum-classical algorithms, which employ a short-depth quantum circuit to efficiently evaluate a cost function depended on the parameters of a quantum gate sequence, and then leverage classical optimizers to minimize this cost function.

Rayleigh-Ritz variational principle:
for any parametrized trial wave-function $|x(\alpha)\rangle$, $\alpha = (\alpha_1, \ldots, \alpha_n)^T$

$$\langle x(\alpha)| \mathcal{H} |x(\alpha)\rangle \geq E_0.$$

Edward Farhi and Jeffrey Goldstone. ArXiv:1411.4028
A Quantum Approximate Optimization Algorithm
produces approximate solutions for combinatorial optimization problems.

The QAOA variational ansatz $|x(\alpha)$ consists of evolving an initial state

$$H^{\otimes n}|0\rangle^{\otimes n} = \frac{1}{2^{n/2}} \sum_{z \in \{0,1\}^n} |z\rangle \qquad \text{Hadamard operator } H,$$

which is an equal superposition of all bitstring, by two Hamiltonians (driver and mixer) for a specified number p of layers. The variational parameters $\alpha = (\gamma, \beta)$ are "times".

QAOA Variational Ansatz $|\psi(\gamma,\beta)\rangle$

- Driving operator with the cost Hamiltonian $\mathcal{H}_C(Z)$

$$U(\gamma,\mathcal{H}_C)=e^{i\pi\gamma\mathcal{H}_C}=\prod_{\langle i,j\rangle}e^{-i\pi\gamma Z_iZ_j}\prod_i e^{-i\pi\gamma h_iZ_i}$$

$$\exp(-i\pi\gamma Z\otimes Z)=\begin{bmatrix}e^{-i\pi\gamma}&0&0&0\\0&e^{i\pi\gamma}&0&0\\0&0&e^{i\pi\gamma}&0\\0&0&0&e^{-i\pi\gamma}\end{bmatrix}$$

The magnetic field terms

$$\exp(-i\pi\gamma hZ)=\begin{bmatrix}e^{-i\pi\gamma h}&0\\0&e^{i\pi\gamma}\end{bmatrix}$$

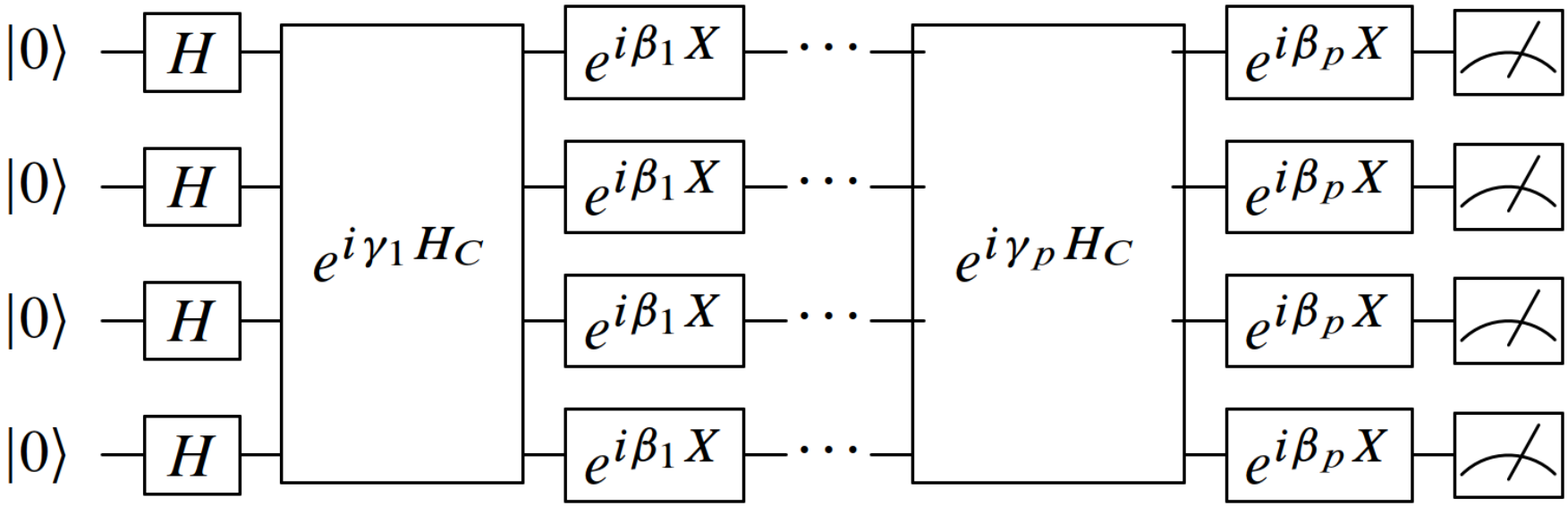
- Mixing operator with Pauli-X operators

$$U(\beta,B)=e^{i\pi\beta B}=\prod_{j=1}^{n}e^{i\pi\beta X_j},\qquad B=\sum_{j=1}^{n}X_j$$

The total circuit consists of repeating these two operators $p\geq 1$ times with independent parameters γ_i and $\beta_i,\ i=1,\ldots,p$,

$$|\psi(\gamma,\beta)\rangle=\underbrace{U(\beta_p,B)U(\gamma_p,\mathcal{H}_C)}_{p}\underbrace{\ldots}_{\ldots}\underbrace{U(\beta_1,B)U(\gamma_1,\mathcal{H}_C)}_{1}H^{\otimes n}|0\rangle^{\otimes n}$$

Variational Ansatz for QAOA

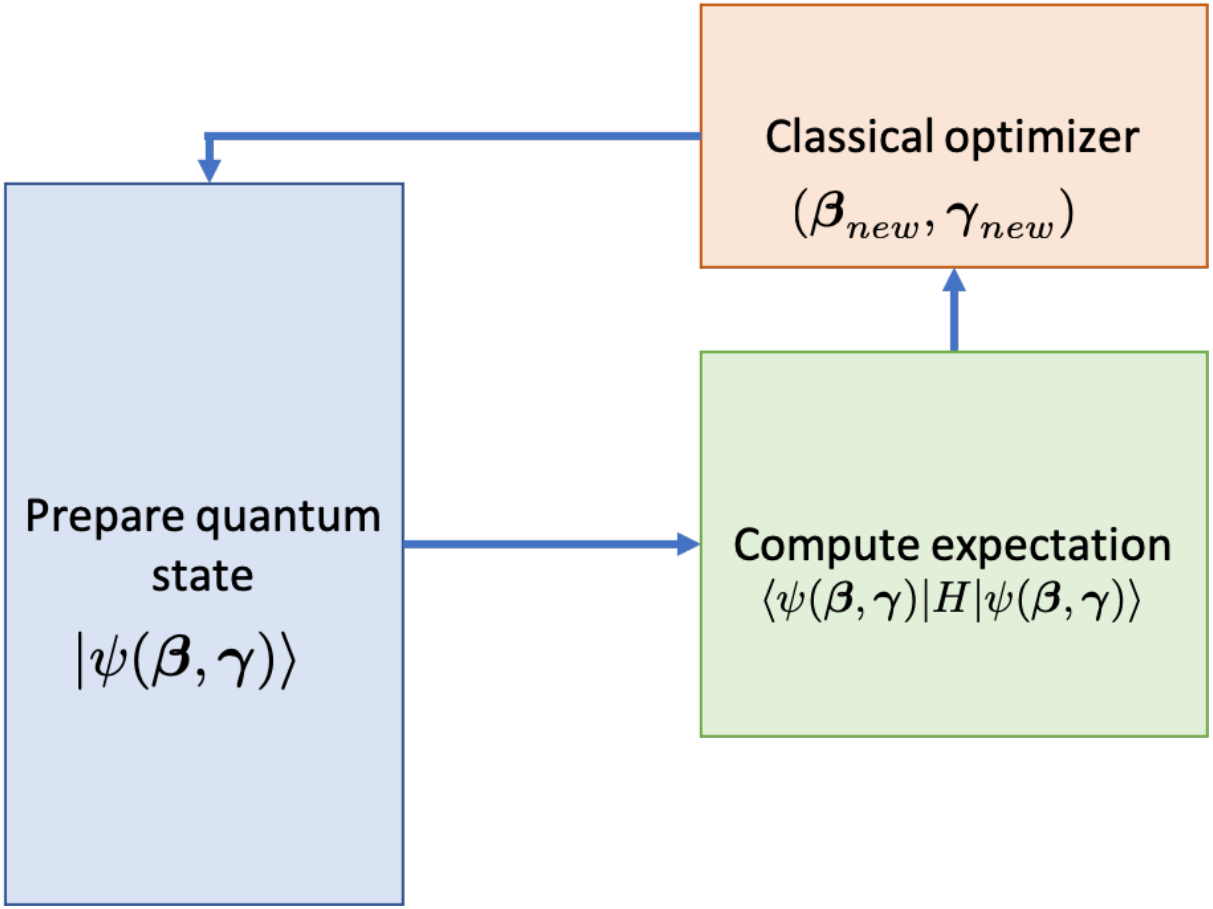


Jack D. Hidary, Quantum Computing, 2nd ed.

Main QAOA Theorem

$$\lim_{p\to\infty} \min_{\gamma,\beta} E_p(\gamma,\beta) = \min_z \mathcal{H}_C(z), \qquad E_p(\gamma,\beta) \equiv \langle\psi(\gamma,\beta)|\mathcal{H}_C|\psi(\gamma,\beta)\rangle$$

Quantum Approximate Optimization Algorithm QAOA

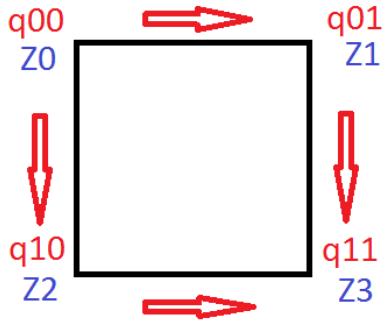


Computation loop:

quantum computer : prepare $|\psi(\gamma, \beta)\rangle$ and measure observables,

classical computer : update the parameters γ, β with an optimization algorithm to reduce the expectation value of the cost Hamiltonian.

Example: Ising Model on 2×2 lattice



$$\mathcal{H}_C(Z) = -J\left(Z^{(0)}Z^{(1)} + Z^{(0)}Z^{(2)} + Z^{(1)}Z^{(3)} + Z^{(2)}Z^{(3)}\right) - h\sum_{i=0}^{3} Z^{(i)}$$

$Z^{(i)} = \mathbb{I} \otimes \cdots \otimes Z \otimes \cdots \otimes \mathbb{I}$ Pauli operator Z on i-th position

Matrix $Z^{(i)}$ has diagonal z_i

$$\begin{bmatrix} z_0 \\ z_1 \\ z_2 \\ z_3 \end{bmatrix} = \begin{bmatrix} 1 & 1 & 1 & \dots & -1 & -1 & -1 \\ 1 & 1 & 1 & \dots & -1 & -1 & -1 \\ 1 & 1 & -1 & \dots & 1 & -1 & -1 \\ 1 & -1 & 1 & \dots & -1 & 1 & -1 \end{bmatrix}$$

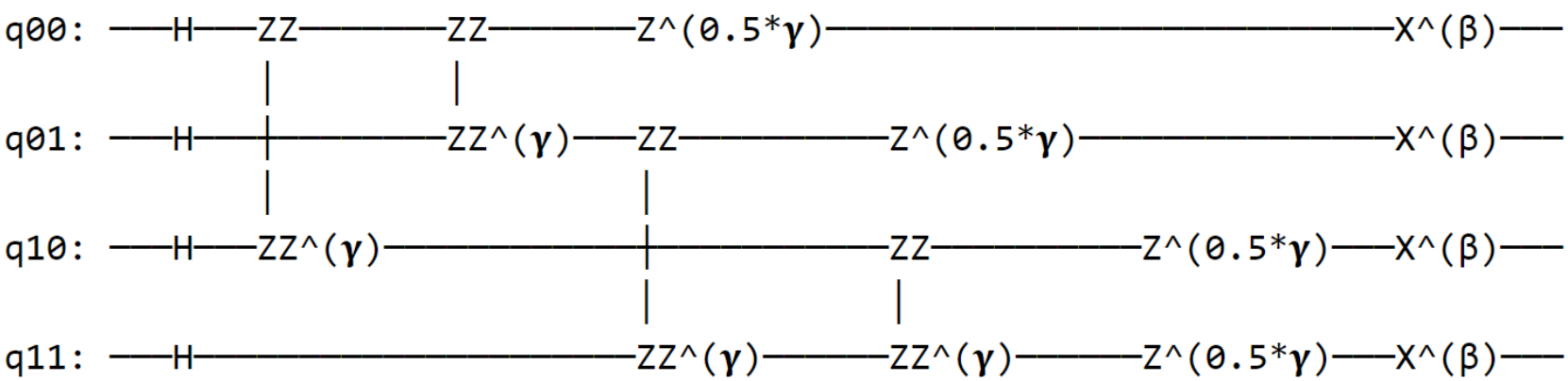
Binary number table 2^n, $n = 4$ with substitution $1 \to 0$ and $-1 \to 1$
Energy per site for each spin configuration ($J = 1,\ h = 0.5$)

$$[-1.5, -0.25, -0.25, -0., -0.25, -0., 1., 0.25, -0.25, 1., -0., 0.25, -0., 0.25, 0.25, -0.5]$$

Note: the bitstring $|0000\rangle$ provides the minimum energy.

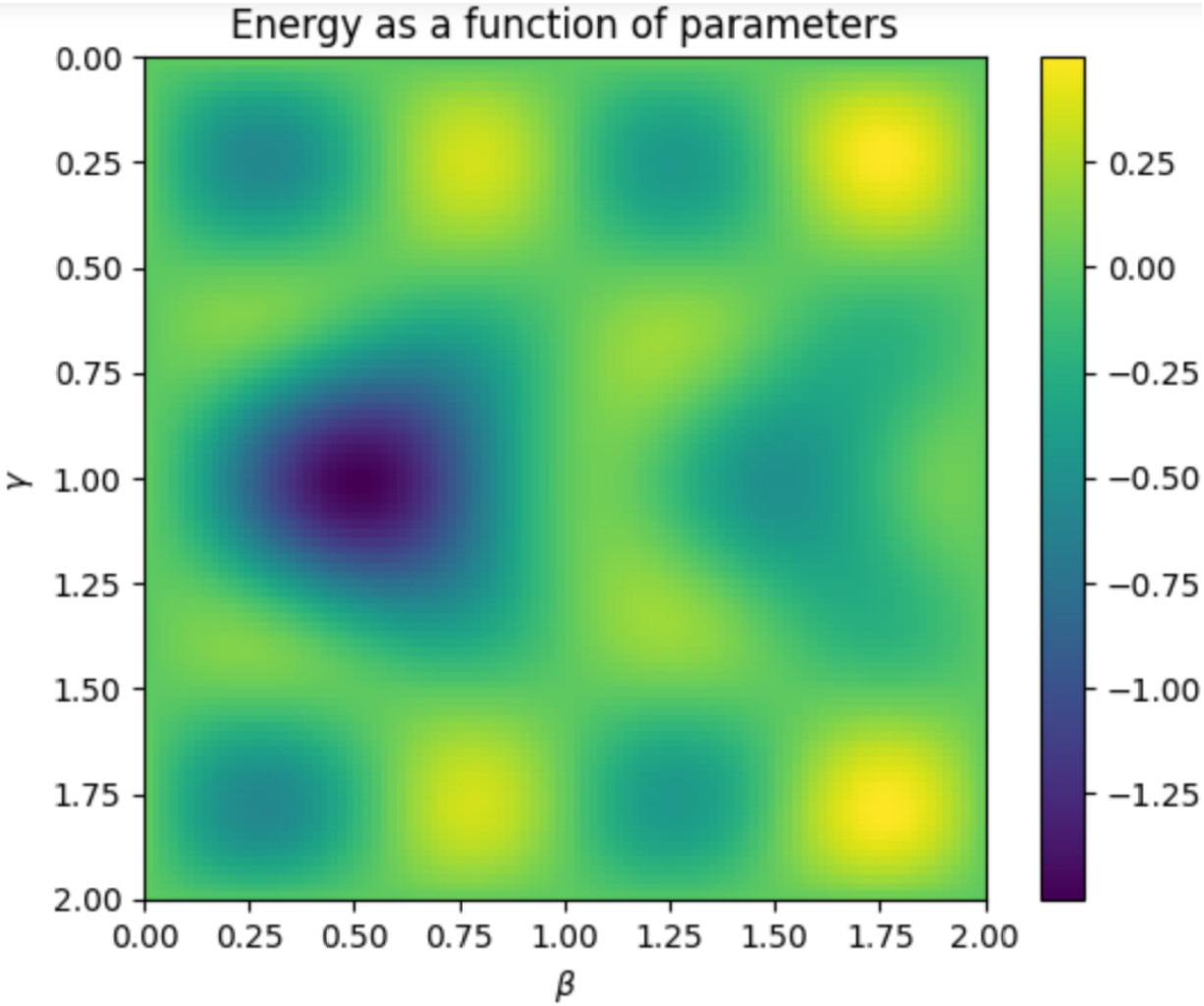
Variational Ansatz (Google package Cirq)

$h = 0.5$



Grid Search in Parameter Space (Wave Function used)

$h = 0.5$, grid size 100



Learned optimal values $\gamma \approx 1.0,\ \beta \approx 0.5$

Wave Function $|\psi(\gamma, \beta)\rangle$ approximate components $[-0.9999999, 0, \ldots, 0]$,

i.e. approximately, the basis vector $|0000\rangle$

Gradient Descent Optimization and Sampling with found parameters

Gradient Descent Optimization (Wave Function used) found parameters
starting point $\gamma_0 = 0.4,\ \beta_0 = 0.7$,
learned optimal values $\gamma = 0.978,\ \beta = 0.532$.
Wave Function $|\psi(\gamma, \beta)\rangle$ approximate components
$[-9.9217653e-01 + 0.00937j, -1.3227567e-02 + 0.04896933j, \ldots]$
i.e. a linear combination of all bases $|ijkl\rangle,\ i, j, k, l = 0, 1$

Sampling with $\gamma,\ \beta$. Number of shots : 100:
Result: 0000 : 98, 0011 : 1, 1010 : 1.