Testing the operation of the QAOA algorithm on the quantum testbed of the HybriLIT platform

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Variational Quantum Algorithms

VQA (gate based) 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.

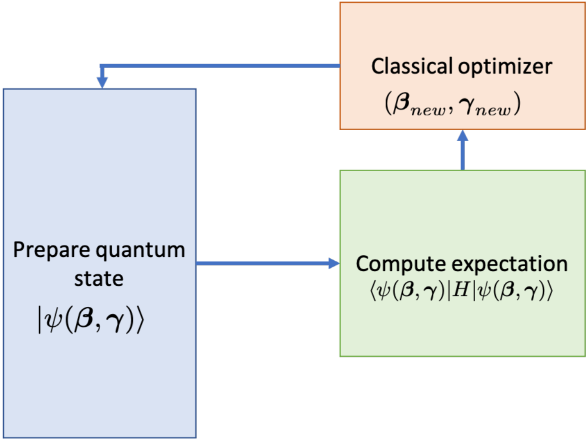
Quantum mechanical variational principle (Rayleigh-Ritz):
for any parametrized trial wave-function (state vector) $|\psi(\alpha)\rangle$, $\alpha = (\alpha_1, \ldots, \alpha_n)^T$

$$\langle\psi(\alpha)| \mathcal{H} |\psi(\alpha)\rangle \geq E_{Ground}.$$

The expectation value of the Hamiltonian plays the role of the cost function.

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

General Scheme of Variational Quantum Algorithms



Computation loop:

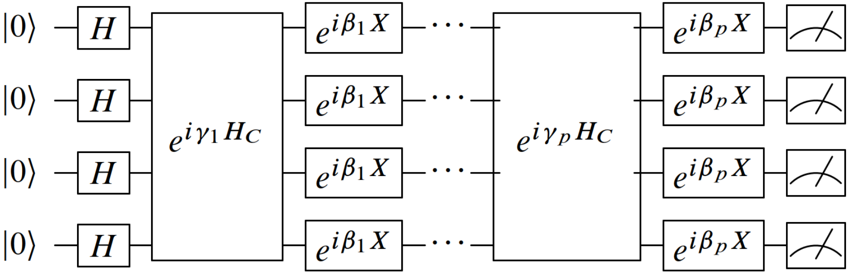
quantum computer : prepare $|\psi(\gamma, \beta)\rangle$ and measure observables,

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

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

The driver $U(\gamma_i,\mathcal{H})$ and mixing $U(\beta_i,B), i=1,\dots,p$, operators are arranged in p layers.

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



Main QAOA Theorem

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

Ising model Hamiltonian using Pauli strings

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

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

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

Variational Problem:
find the spin configuration on the lattice with the lowest expectation value of $H(Z)$, i.e. energy $E = \langle \psi(\alpha) | \mathcal{H} | \psi(\alpha) \rangle$, varying the set of parameters α.

Operators for construction of QAOA Variational Ansatz $|\psi(\gamma, \beta)\rangle$

- Driving operator with the Hamiltonian $\mathcal{H}(Z)$ (commutativity of the Hamiltonian terms is used the factorization),

$$
\begin{aligned}
U(\gamma, \mathcal{H}) =& e^{i\pi\gamma\mathcal{H}(Z)/2} \\
&= \prod_{\langle i,j\rangle} \exp\Big(-i\pi J\gamma Z^{(i)} \cdot Z^{(j)}/2\Big) \text{ (ZZ interaction of the neighbours } i \text{ and } j\text{)}, \\
&\prod_{i} \exp(-i\pi\gamma h Z^{(i)}/2) \qquad \text{(interaction of } i\text{th site with the magnetic field).}
\end{aligned}
$$

- Mixing operator with Pauli-X operators,

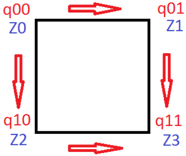
$$
U(\beta, B) = e^{i\pi\beta B(X)/2} = \prod_{j=1}^{n} e^{i\pi\beta X_j/2}, \qquad B(X) = \sum_{j=1}^{n} X_j.
$$

The variational parametersγ and β are "evolution times".

The Quantum Circuit for the Variational Ansatz $|\psi(\gamma, \beta)\rangle$

one layer, $p = 1$, $J = 1, h = 0.5$ prepared with Google package Cirq (Python).

```
(0, 0): ───H───ZZ────────ZZ──────────────────────────────────────Z^(0.5*γ)───X^(β)───
               │         │
(0, 1): ───H───┼─────────ZZ^(γ)───ZZ─────────────────────────────Z^(0.5*γ)───X^(β)───
               │                  │
(1, 0): ───H───ZZ^(γ)─────────────┼─────────ZZ───────────────────Z^(0.5*γ)───X^(β)───
                                  │         │
(1, 1): ───H──────────────────────ZZ^(γ)───ZZ^(γ)────────────────Z^(0.5*γ)───X^(β)───
```



Search in Parameter Space using the direct access to the state vector $|\psi(\gamma,\beta)\rangle$.

- One-layer Variational Ansatz

$$|\psi(\gamma,\beta)\rangle = U(\beta,B)U(\gamma,\mathcal{H})H^{\otimes 4}|0\rangle^{\otimes 4}$$

- Energy as expectation value of the Hamiltonian is a function of the variational parameters γ,β,

$$E(\gamma,\beta) = \langle\psi(\gamma,\beta)|\,\mathcal{H}\,|\psi(\gamma,\beta)\rangle,$$

or, if we use the diagonal form of the Hamiltonian,

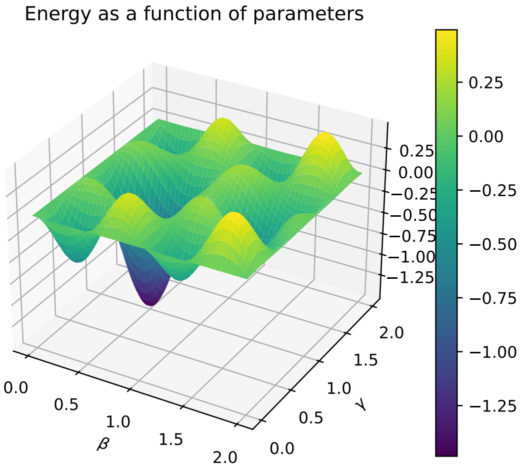
$$E(\gamma,\beta) = \sum_{i=0}^{2^4-1} |\alpha_i(\gamma,\beta)|^2 E_i.$$

QAOA ansatz (parametrized state vector describing the quantum register)

$$|\psi(\gamma,\beta)\rangle = \alpha_0(\gamma,\beta)|0000\rangle + \alpha_1(\gamma,\beta)|0001\rangle + \ldots + \alpha_{15}(\gamma,\beta)|1111\rangle$$

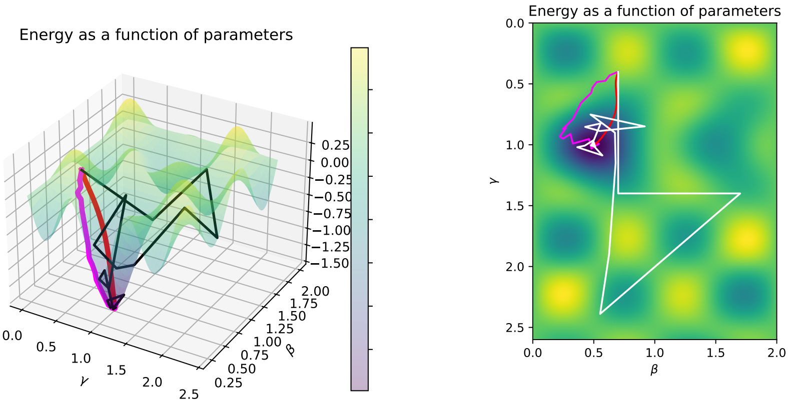
Energy per site for each spin configuration (main diagonal of $\mathcal{H}$)

$$E = [-1.5, -0.25, -0.25, 0, -0.25, 0, 1, 0.25, -0.25, 1, 0, 0.25, 0, 0.25, 0.25, -0.5]$$



Learned optimal values $\gamma = 1.0,\ \beta = 0.5$.
define the state vector $|\psi(\gamma,\beta)\rangle = [\alpha_0(\gamma,\beta) \approx -0.999, 0, \ldots, 0]$,
which corresponds to the basis vector $|0000\rangle$
providing the minimal value $E(\gamma = 1.0,\ \beta = 0.5) = E_{min} = -1.5$.

Minimization in 2-dim Parameter Space for 2×2 lattice.

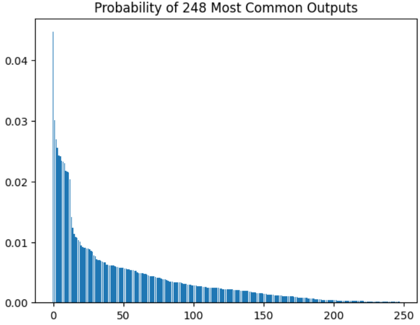


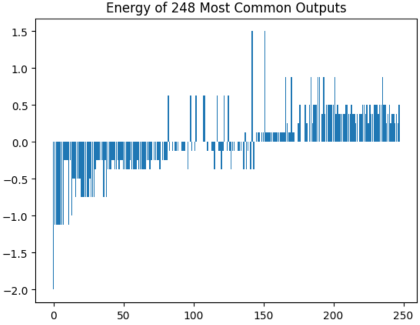
Minimization trajectories:
- red curved arrow, gradient optimization;
- magenta broken line, gradient-free optimization (Nelder - Mead, simplex method);
- black and white broken lines (COBYLA, simplex method).

One-layer Ansatz for $2 \times 2 \times 2$ lattice. Sampling (register state measurement).

Sampling data for a set of $n_{meas} = 10000$ measurements at the point $(\gamma, \beta) = (0.8, 1.2)$:

output enumeration	0	1	2	...	248
basis state	$\|00000000\rangle$	$\|00001000\rangle$	$\|10000000\rangle$	...	$\|10010011\rangle$
occurrences, n_{state}	447	301	269	...	1
energy, E_{state}	-2.0	-1.125	-1.125	...	0.5





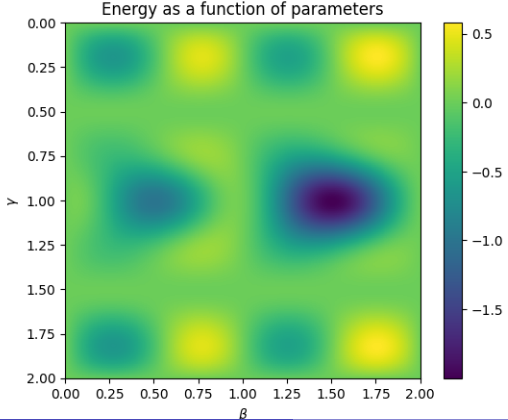
$$E_1^{Sampl}(0.8, 1.2) = \sum_{states} E_{state}\, n_{state}/n_{meas} = -0.5187 \text{ vs } E_1^{State\ Vctor}(0.8, 1.2) = -0.5184$$

2x2x2 lattice. One-layer Ansatz. Sampling Search in Parameter Space

Energy evaluation with sampling data instead of direct using of $|\psi(\vec{\gamma}, \vec{\beta})\rangle$.

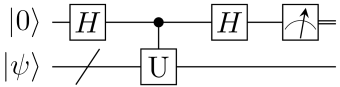
$$E_p(\gamma, \beta) \approx \sum_{i=0}^{n-1} \mathcal{P}_{i,p}(\gamma, \beta) E_i, \qquad \sum_{i=0}^{n-1} \mathcal{P}_{i,p}(\gamma, \beta) = 1, \qquad \mathcal{P}_{i,p}(\gamma, \beta) = n_{ith\ state} / n_{meas}$$

where $\mathcal{P}_{i,p}(\gamma, \beta)$ is the probability to find the register in i-th basis state (with energy E_i) given p-layer ansatz and a fixed set of the parameters $\vec{\gamma}, \vec{\beta}$.



parameter step 1/100,
10000 measurements for each point.
Coincidence of state vector search and sampling search.

Evaluation of an average $\langle\psi(\boldsymbol{\alpha})|U|\psi(\boldsymbol{\alpha})\rangle$. Hadamard Test



$$H = \frac{1}{\sqrt{2}}\begin{bmatrix}1 & 1\\ 1 & -1\end{bmatrix}, \quad |0\rangle = \begin{bmatrix}1\\0\end{bmatrix}, \quad |1\rangle = \begin{bmatrix}0\\1\end{bmatrix}$$

$$\begin{aligned}
|0\rangle \otimes |\psi\rangle &\xrightarrow{H} \frac{1}{\sqrt{2}}\left(|0\rangle \otimes |\psi\rangle + |1\rangle \otimes |\psi\rangle\right)\\
&\xrightarrow{contr-U} \frac{1}{\sqrt{2}}\left(|0\rangle \otimes |\psi\rangle + |1\rangle \otimes U|\psi\rangle\right)\\
&\xrightarrow{H} \frac{1}{2}\Big((|0\rangle + |1\rangle) \otimes |\psi\rangle + (|0\rangle - |1\rangle) \otimes U|\psi\rangle\Big) =\\
&= \frac{1}{2}\Big((|0\rangle \otimes (\mathbb{I} + U)|\psi\rangle + |1\rangle \otimes (\mathbb{I} - U)\psi\rangle\Big)
\end{aligned}$$

Measurements of the ancilla qubit $|0\rangle$ allow to evaluate the average $\langle\psi|U|\psi\rangle$.

$$P(1) = \frac{1}{2}\langle\psi(\boldsymbol{\alpha})|(\mathbb{I} - Re\, U)|\psi(\boldsymbol{\alpha})\rangle, \qquad P(0) = 1 - P(1) = \frac{1}{2}\langle\psi(\boldsymbol{\alpha})|(\mathbb{I} + Re\, U)|\psi(\boldsymbol{\alpha})\rangle$$

$$Re\,\langle\psi(\boldsymbol{\alpha})|U|\psi(\boldsymbol{\alpha})\rangle = 1 - 2P(1), \qquad 2Re\, U = U + U^\dagger$$

Evaluation an average $\langle\psi(\boldsymbol{\alpha})|U|\psi(\boldsymbol{\alpha})\rangle$ needs measuring only the ancilla qubit!

Optimization

SciPy optimize

We fulfilled minimization with two parameters (one-layer ansatz) and six parameters (three-layer ansatz).

Local (multivariate) optimization

Direct search algorithms (gradient-free optimization). Gradient-based failed.

COBYLA, Powell, Nelder-Mead

Global optimization

(Typically, global minimizers efficiently search the parameter space, while using a local minimizer (e.g., minimize) under the hood.)

- Dual Annealing (with COBYLA and Powell as local minimizers),
- SHGO (simplicial homology global optimization) with COBYLA and Powell. *sampling_method='sobol'*.

Computations with large number of qubits (e.g. Ising model on $3 \times 3 \times 3$ lattice, 27 qubits) become time and memory consuming.

The situation is especially hard for the schemes with the Hadamard test and when the number of repetitions for sampling is large.

Solution: the quantum testbed of the HybriLIT platform

Полигон для квантовых вычислений

http://hlit.jinr.ru/quantum-polygon/