Enhancing Circuit Trainability with Selective Gate Activation Strategy

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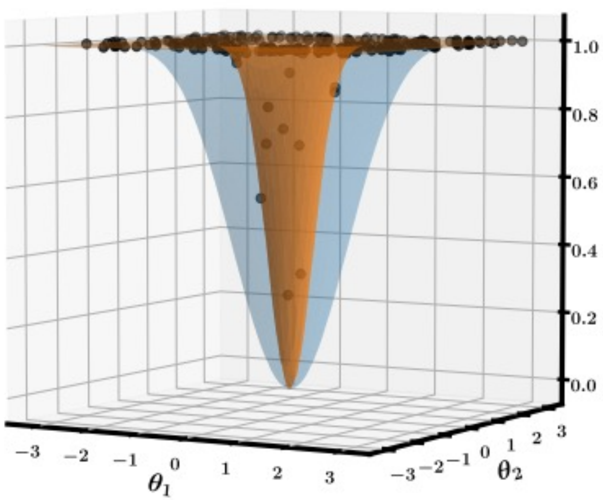
Introduction

- In Noisy Intermediate-Scale Quantum (NISQ) era, the quantum machine learning (QML) approach gained attention
- However, there are some problems that hinders usability of QML such as Barren Plateau and decreased trainability
- Some researches increased trainability by reducing effective parameter space of the circuit or using local cost function



Example of Barren Plateau, image credit from [1]

[1] Cerezo, M., Sone, A., Volkoff, T., Cincio, L., & Coles, P. J. (2021). Cost function dependent barren plateaus in shallow parametrized quantum circuits. *Nature communications*, *12*(1), 1791.

Introduction

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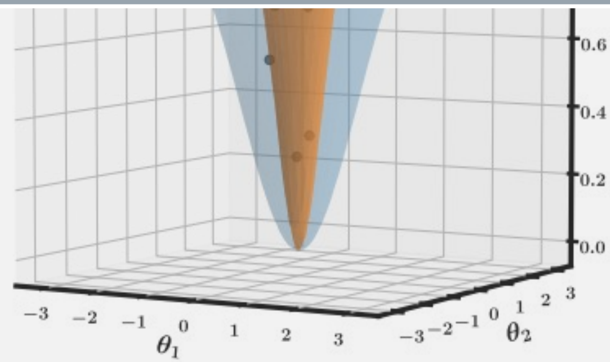
Decrease parameter space by selectively activating the gates being used



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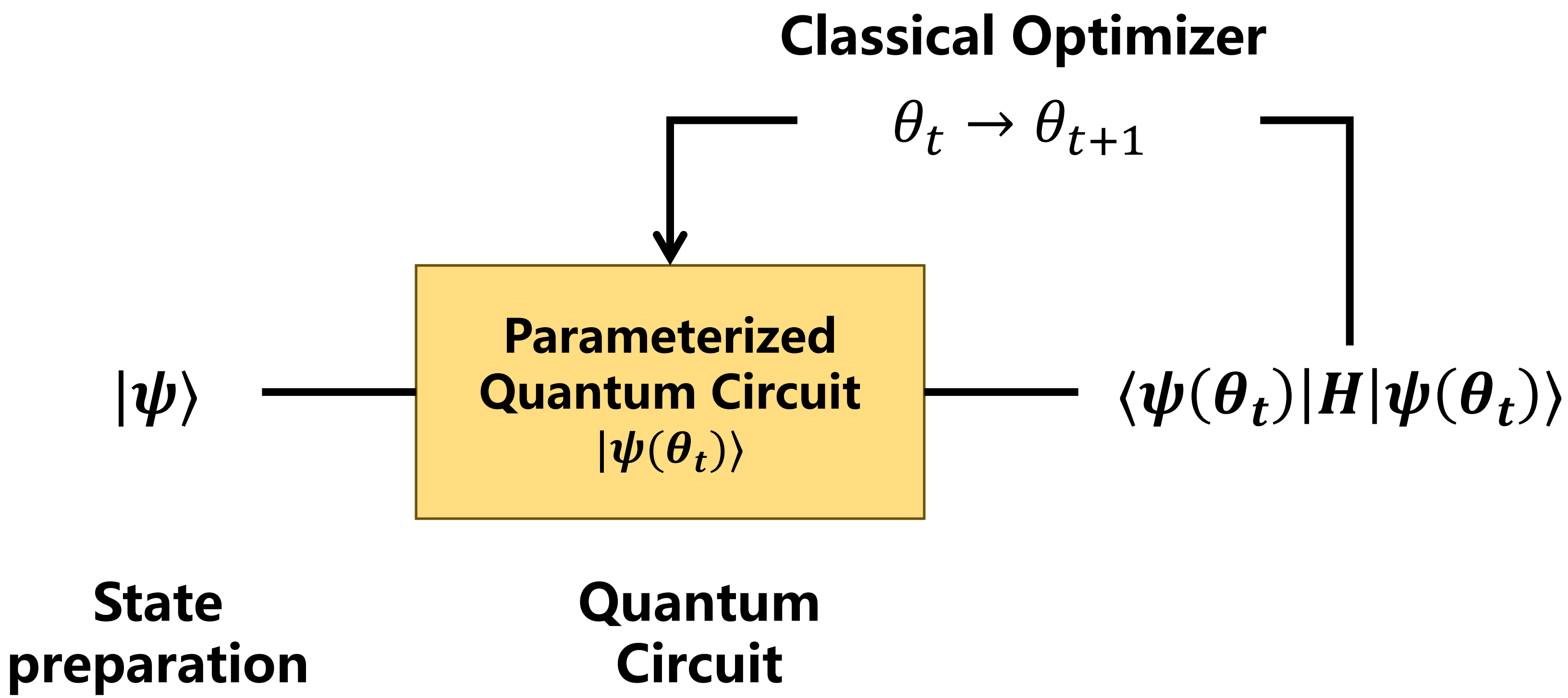
Method – Procedure

Variational Quantum Algorithm

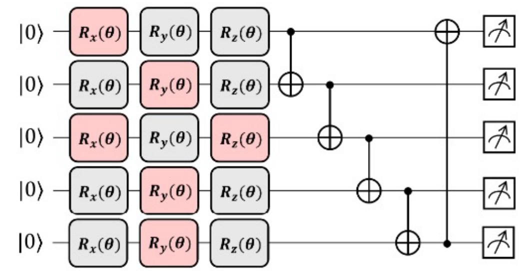
- Update parameter of the quantum circuit using classical optimizer
- Update parameter in every iteration



Method – Gate Activation Strategy

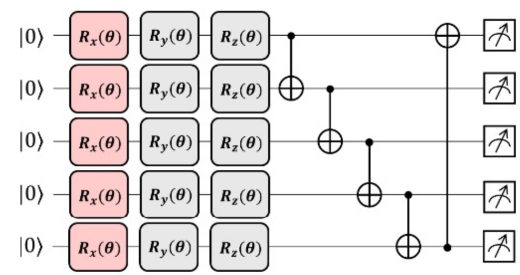
Fully Random

- Randomly select gates to activate without considering the size of the parameter



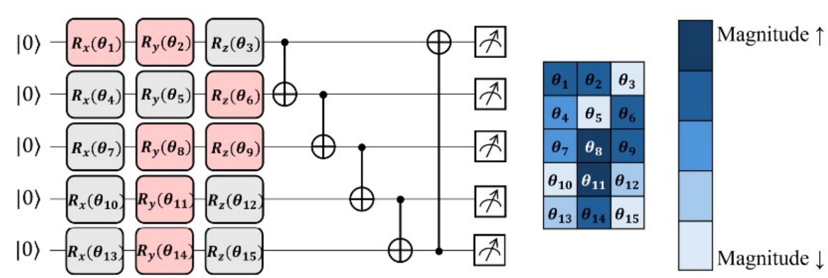
Gate Random

- First select gate type (rotation gate) to activate, and then randomly select gate



Magnitude-based

- Select gates based on the absolute magnitude of parameters
- Requires warm-up iteration



Method – Procedure

Gate activation strategy

- **Select gate to activate per iteration** based on following strategy
- For Magnitude-based activation strategy, it requires warm-up iteration for quantum circuit to gain information about the problem
- Hyperparameters
  - **Warm-up iteration**: # of iterations for full-quantum circuit training in Magnitude-based strategy
  - **Selection rate**: rate of gates being selected

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Experiments

Variational Quantum Eigensolver

- Find ground state energy of **Molecule Hamiltonian**
- Molecule Hamiltonian can be simplified as combination with coefficient and Pauli operations

$$H = \sum_j C_j \otimes_i \sigma_i^{(j)}$$

	C_2	HF	LiH	Li_2	OH^-
Charge	0	0	0	0	-1
Active Electrons	8	8	2	2	8
Bond Length (Å)	0.5, 0.7, 0.9, 1.1, 1.22, 1.3, 1.5, 1.7, 1.9, 2.1, 2.3, 2.5				
Active Orbitals	5				

- Use Pennylane package to obtain Molecule Hamiltonian with various bond length

Experiments – Hyperparameters

VQE training specification

Qubits	10
# of Layers	7
# of Parameters	210
Train Iteration	2000
Optimizer	Adam
Learning Rate	0.001

Gate activation specification

Warm-up iteration	0, 100, 200, 500
Selection rate (%)	10, 50, 90

Algorithms

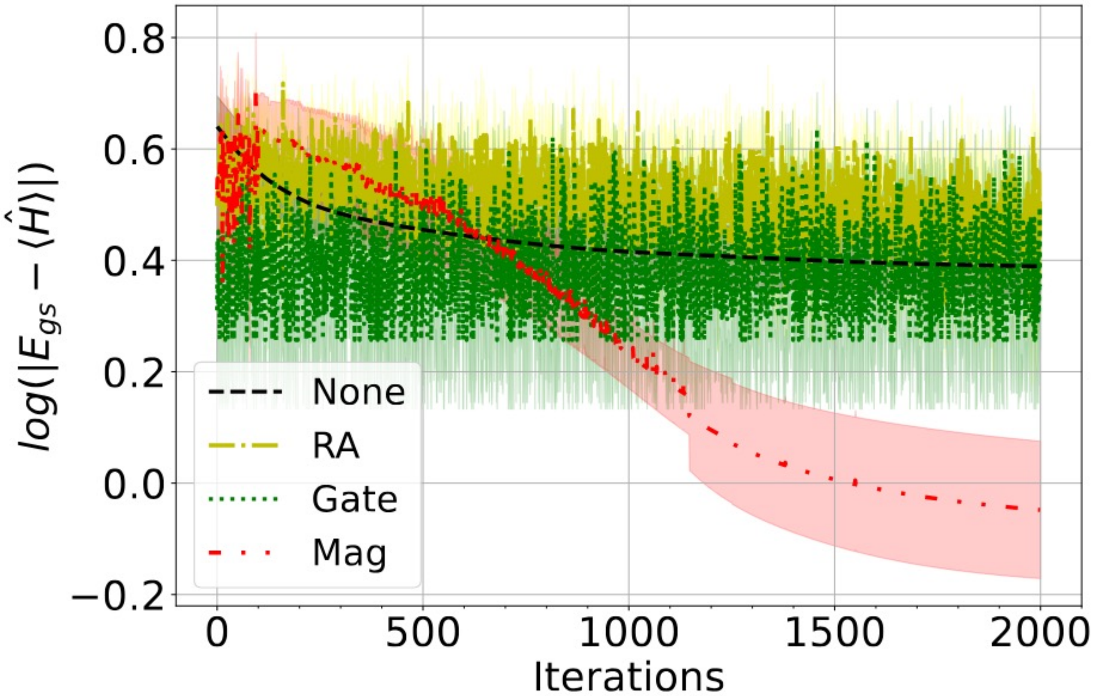
└ Random (RA), Gate Random (Gate), Magnitude-based (Mag)

└ Without gate activation (None)

Performance metric: gap between exact energy and expectation

Experiments

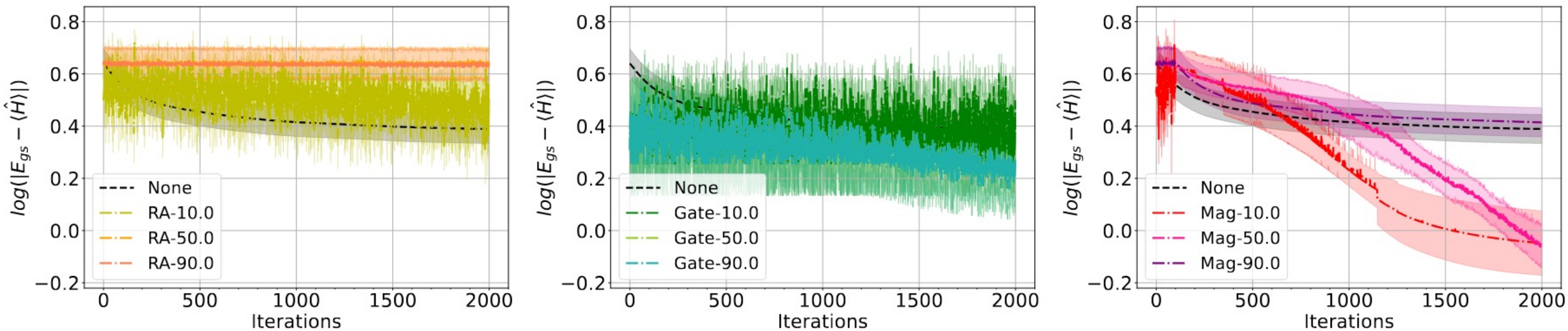
Performance relative to Strategy



- Lower the better
- Mag shows the best and enhance performance compared to others

Experiments

Trainability relative to Selection rate



(a) Fully random activation (b) Gate random activation (c) Magnitude-based activation

- As the number of gates being selected, it shows performance closer to None
- Except Mag, all failed to training as the selected gates are modified per iteration

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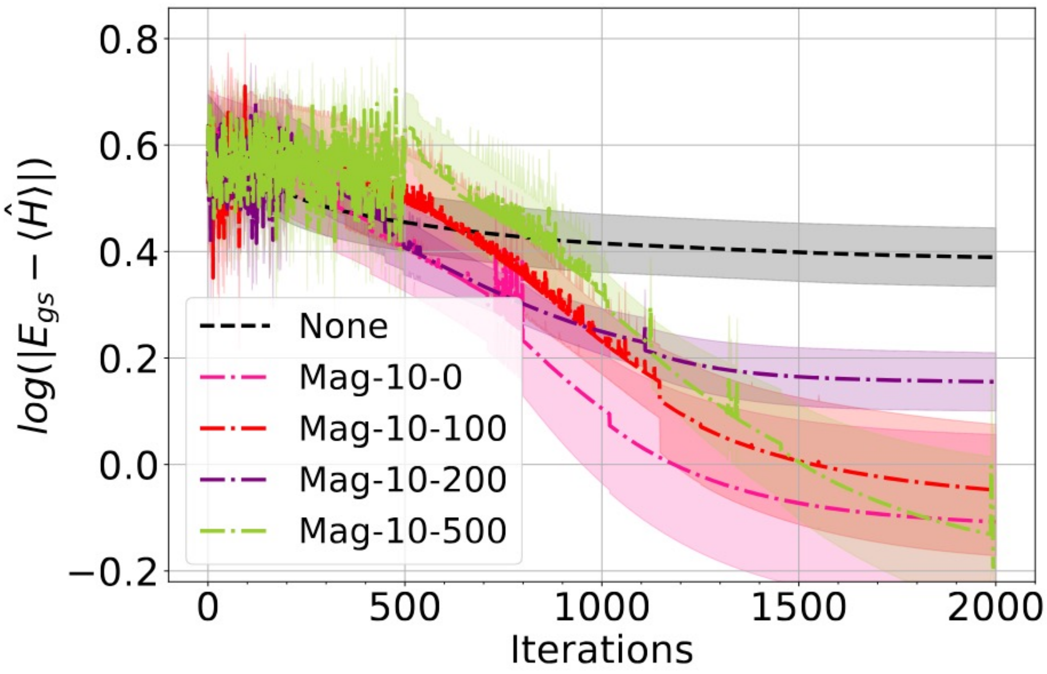
Experiments

Performance relative to warm-up iteration



- Using different warm-up iteration results in different performance, but it still shows better performance than without gate activation

Conclusion and Future Work

- **Gate activation can increase the trainability of the quantum circuit and therefore can achieve better performance than whole circuit**

- **Future work**
  - **Adaptive gate selection**: instead of fixed number of gates being activated, use adaptive gate selection that considers optimization landscape or training progress
  - **New metric for selecting gate**: simple magnitude-based shows better performance than random, but there can be a better metric/rule for gate selection

Thank You! Questions?

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