Quantum Machine Learning and Optimization on Real Devices

Benedek Hauer, Izuho Koyasu, Kosei Teramoto, Rudy Raymond, and Hiroshi Imai

Department of Computer Science
Graduate School of Information Science & Technology
The University of Tokyo

This talk summarizes recent research in our laboratory

1. Quantum Native Education using IBM Quantum Devices
2. Brief Summary of the following papers:
   - I. Koyasu, R. Raymond and H. Imai, "Distributed Coordinate Descent Algorithm for Variational Quantum Classification," 2023 IEEE International Conference on Quantum Computing and Engineering (QCE), Bellevue, WA, USA, 2023, pp. 457-467. (I)
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Introduction to Near-Term Quantum Information (2023)

Lecturers: Rudy Raymond, Yuri Kobayashi, Kifuni Numata
Lectures and exercise/projects on IBM Quantum device
up to 127qubit

東京大学 THE UNIVERSITY OF TOKYO

Date	Lecture Title	Lecturer	Date	Lecture Title	Lecturer
4/7	Unit 1: Understanding Quantum Information and Computation	John Watrous	6/9	Unit 8: Introduction to Qiskit Runtime and Primitives (Live only + recording will be shared later)	Ikko, Kifumi, Yuri
4/14	Unit 2: Multiple Systems **Introductory courses**	John Watrous	6/16	Unit 9: Quantum Applications – Optimization **Quantum Applications**	Takashi Imamichi
4/21	Unit 3: Quantum Circuits	John Watrous	6/23	Unit 10: Quantum Algorithms for Machine Learning	Rudy Raymond
4/28	Unit 4: Quantum Teleportation and Supderdense Coding	John W Kifumi N	6/30	Unit 11: Quantum Chemistry	Yukio Kawashima
5/19	Unit 5: Deutsch-Jozsa and Bernstein-Vazirani Algorithm	Yuri Kobayashi	7/7	Unit 12: Qiskit Runtime and Error Mitigation (Live only + recording will be shared later) **Quantum Error Mitigation**	Ikko, Kifumi, Yuri
5/26	Unit 6: Grover's Algorithm **Quantum Algorithms**	Atsushi Matsuo	7/14	Unit 13: Quantum Challenges with Qiskit Runtime Primitives	Ikko, Kifumi, Yuri
5/29 (Mon)	Unit 7: Quantum Fourier-Transformation and Phase Estimation	Tamiya Onodera			

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Lectures and exercise/projects on IBM Quantum devices up to 127qubit

Total students: 134

Weekly Homework: Submit to ITC-LMS

Date	Homework	Submit by	Date	Homework	Submit by
4/7 (Fri)	[Take Unit 1: Single Systems Quiz]() **Submit screen capture of finished quiz*	4/14 Quiz	6/9 (Fri)	Unit 8: Study, execute and submit Jupyter Notebook	6/16 jupyter
4/14 (Fri)	[Take Unit 2: Multiple Systems Quiz]() **Submit screen capture of finished quiz*	4/21 Quiz	6/16 (Fri)	Unit 9: Study, execute and submit Jupyter Notebook	6/23 jupyter
4/21 (Fri)	[Take Unit 3: Quantum circuits Quiz]() **Submit screen capture of finished quiz*	4/28 Quiz jupyter	6/23 (Fri)	Unit 10: Study, execute and submit Jupyter Notebook	6/30 jupyter
4/28 (Fri)	[Take Unit 4: Quantum Teleportation and Supderdense Coding Quiz]() **Submit screen capture of finished quiz*	5/19 Quiz jupyter	6/30 (Fri)	Unit 11: Study, execute and submit Jupyter Notebook	7/7 jupyter
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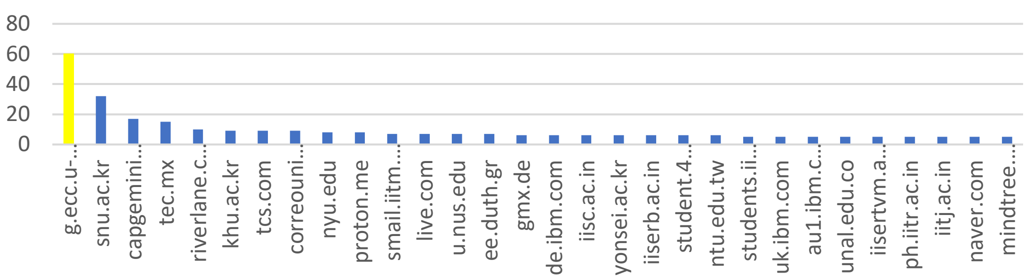
5/26 (Fri)	Unit 6: Study, execute and submit Jupyter Notebook	6/2 jupyter	7/14 (Fri)	Unit 13: Study, execute and submit Jupyter Notebook	7/21 jupyter
5/29 (Mon)	Unit 7: Study, execute and submit Jupyter Notebook	6/9 jupyter			
May TBD	Bonus Assignment I: Earn at least one badge from participating in IBM Quantum Challenge Spring 2023	OPTIONAL 			

IBM Quantum Challenge 2023 Top 30 Institutes



Introduction to Near-Term Quantum Information (2024)

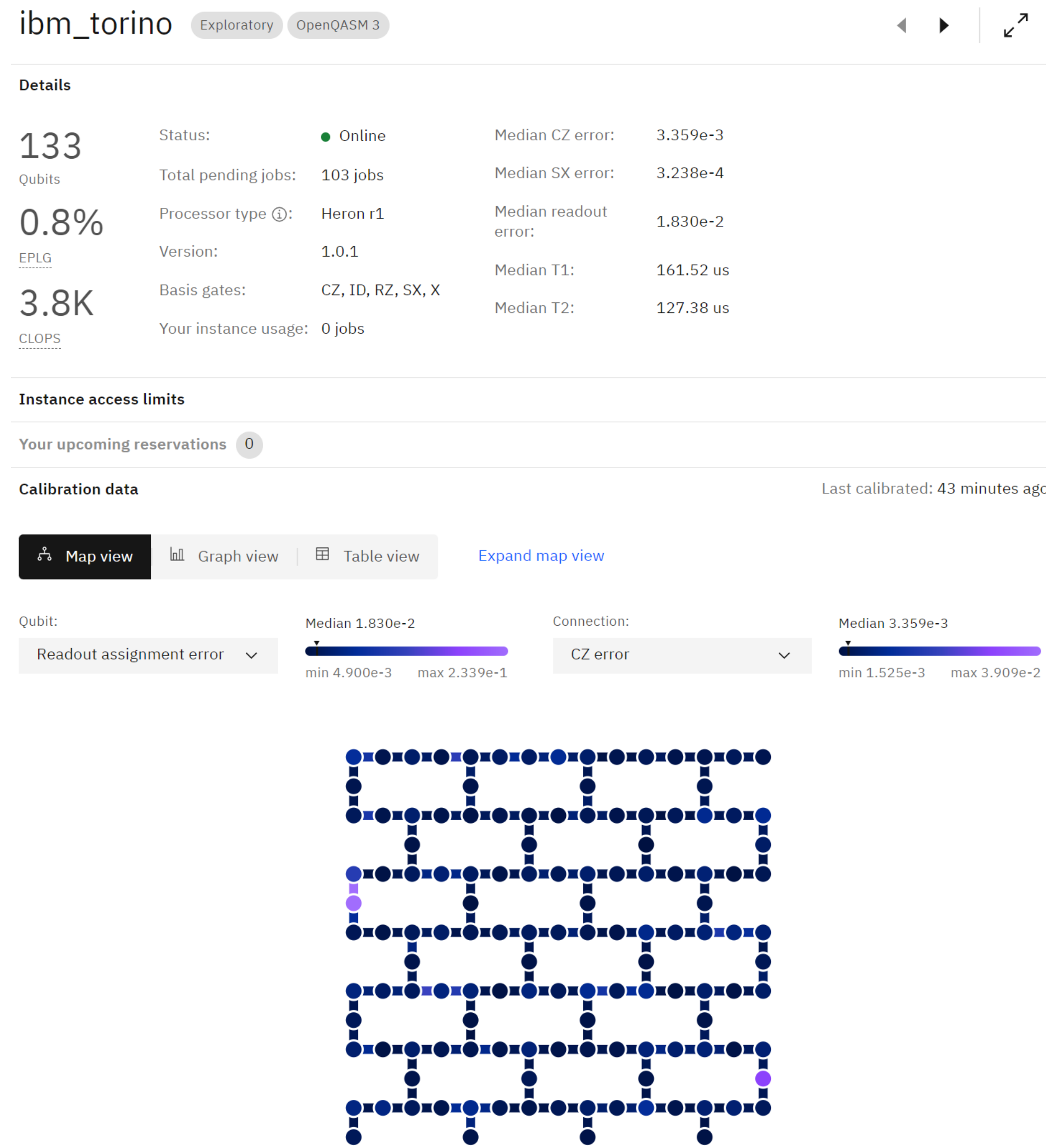
Plan for 2024

- Half: utility-level course

My personal view

- NISQ vs. near-term
  ノイズ有中規模 vs. 近々・短期
- Even in Error-Correction age, QC will be still noisy

Ex. 2 papers from Nature:
Google‘s `supremacy’ paper (2019)
random quantum circuit sampling:
$53\text{qubit}, \text{XEB} \approx 0.1\%$
Quera’s ‘error detecting’ paper (2023)
on IQP sampling circuits:
$48\text{logical qubit}, \text{XEB} \approx 0.1$



https://quantum.ibm.com/services/resources?tab=systems&view=table&limit=50&system=ibm_torino

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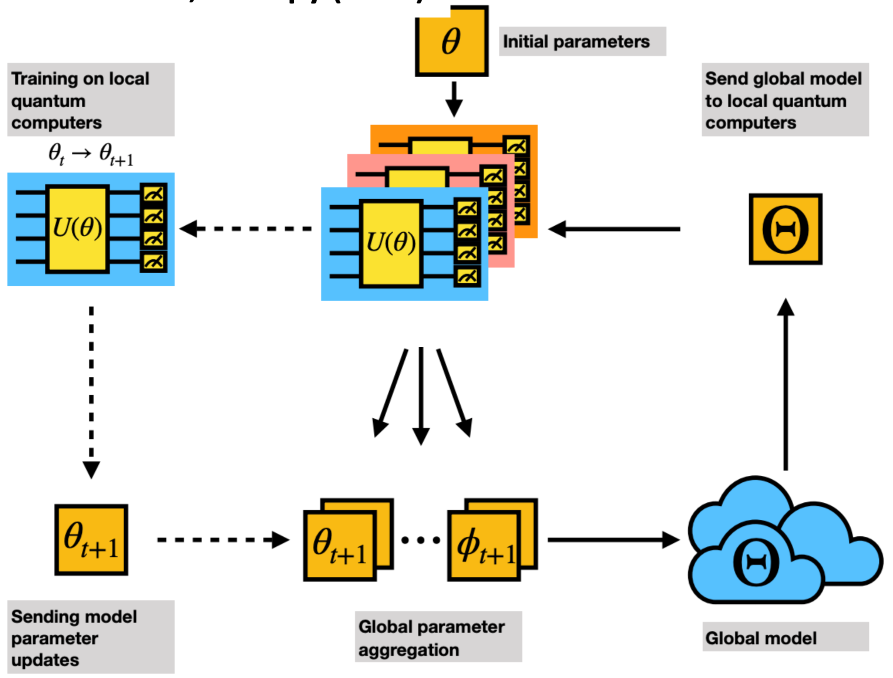
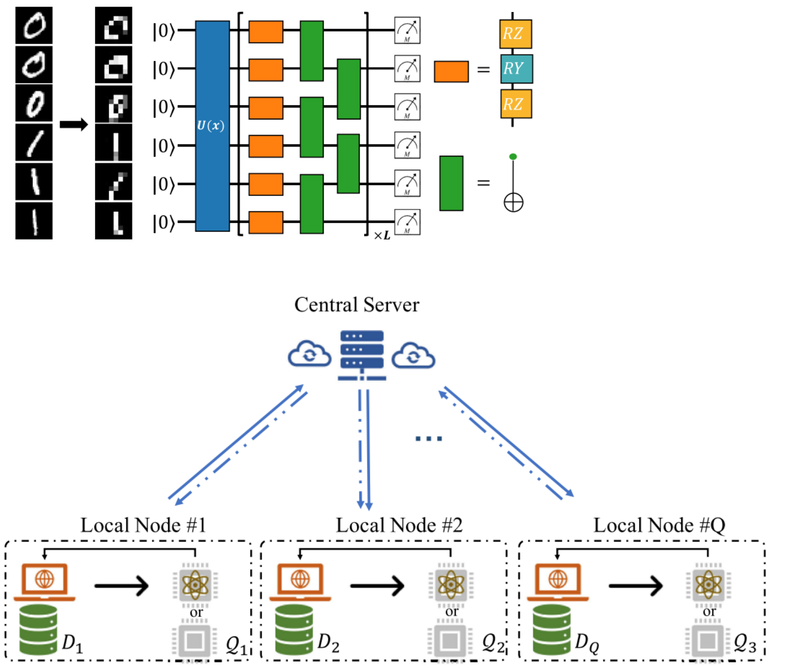
Previous Work: Distributed Variational Quantum Algorithms and Our Contributions

Training instances: $\{(x_i, y_i)\}_{i=1}^{N}$ and parameters: $|\theta| = M$

Chen and Yoo, Entropy (2021)



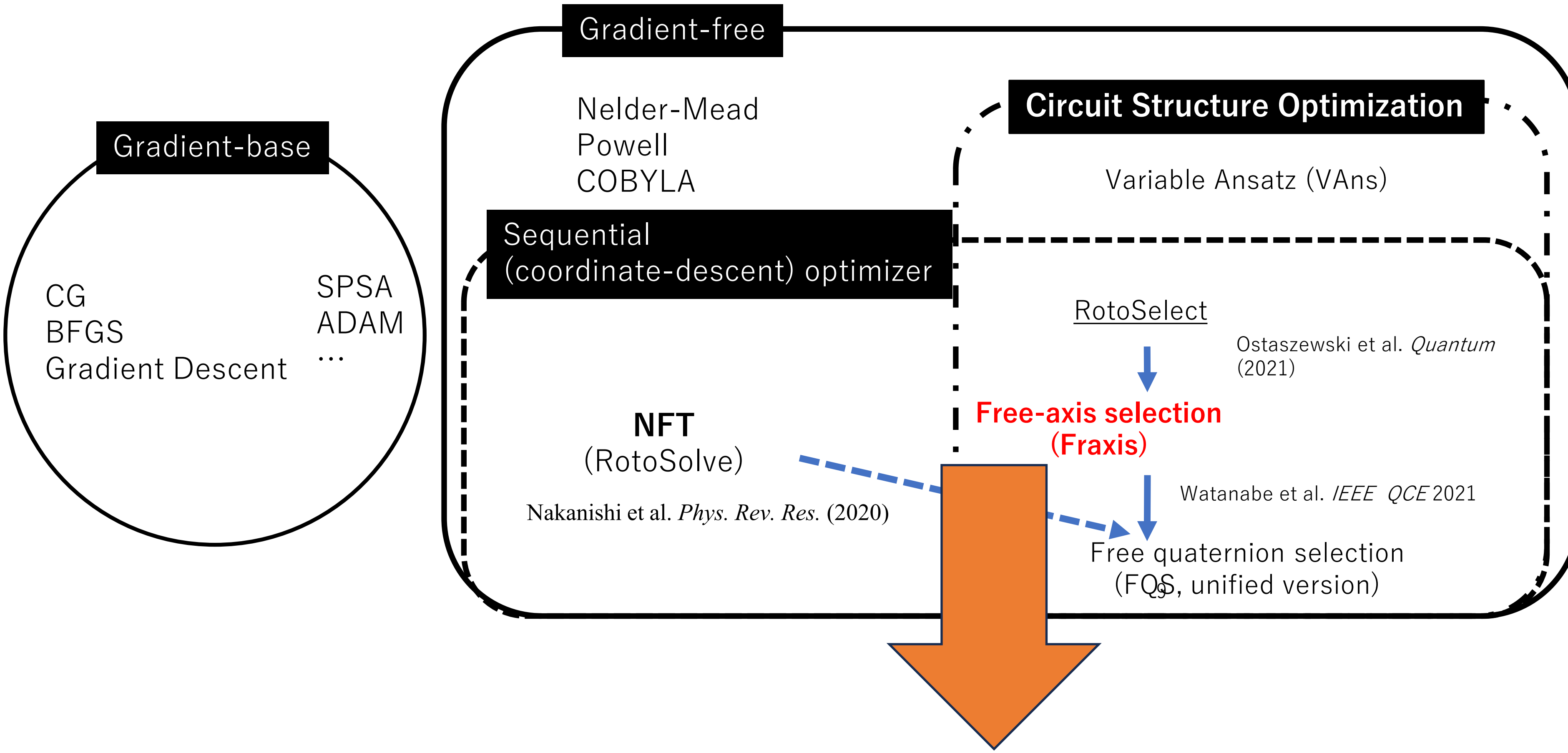
Du et al. , IEEE TQE (2022)



Our Contributions

- Devise a **distributed** coordinate descent algorithm with Free-axis selection (Fraxis)
- Experimental verifying its efficacy on IBM Quantum divices, including large ones

Optimizers for Parametrized Quantum Circuits



Distributed algorithm, with larger experiments

Gradient-free sequential optimizer can be better

From: K. M. Nakanishi, K. Fujii, and S. Todo (NFT), Sequential minimal optimization for quantum-classical hybrid algorithms, Physical Review Research 2, 043158 (2020)

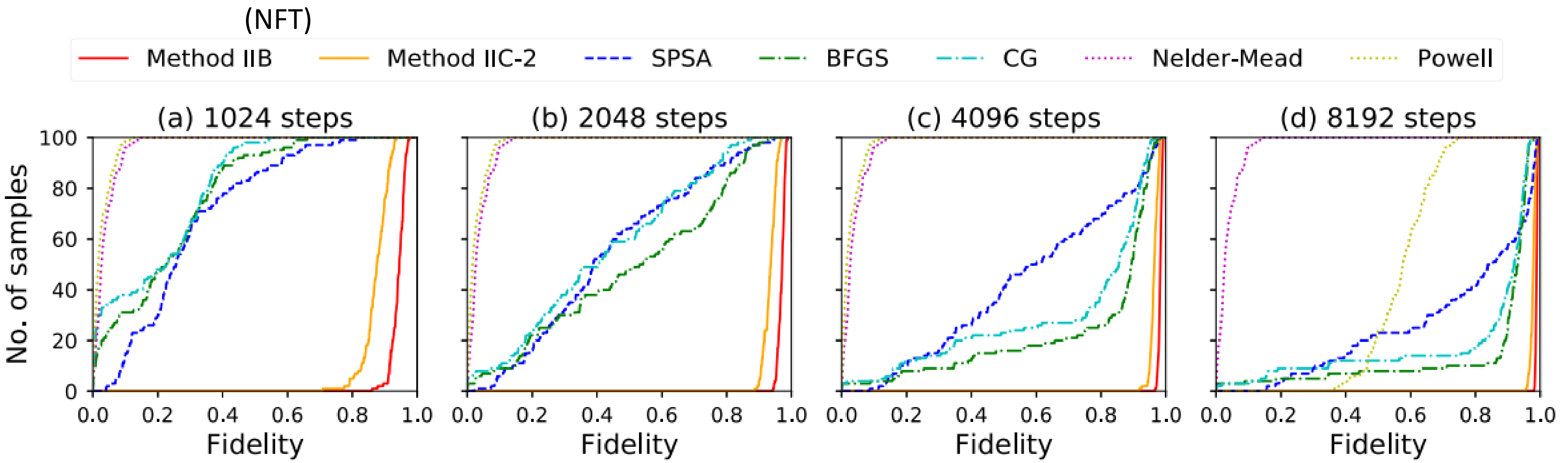


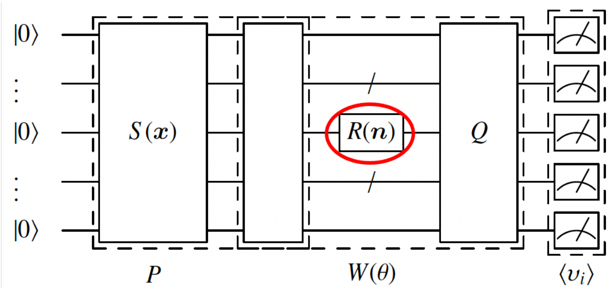
FIG. 3. Cumulative distribution function of fidelity after 1024, 2048, 4096, and 8192 steps in task 1. Method II B is denoted by the solid red (dark gray) lines. Method II C-2 is denoted by the solid orange (light gray) lines. The horizontal axes are the fidelity $|\langle 0|^{\otimes r} U^\dagger(\boldsymbol{\theta}^*)U(\boldsymbol{\theta})|0\rangle^{\otimes r}|^2$. The vertical axis shows the number of samples whose fidelity is under the value of x axis at particular steps.

In its conclusion,

`By numerical simulations, we demonstrate that our method converges to a better solution much faster than the existing ones.'

Coordinate-descent direction is simple/nice

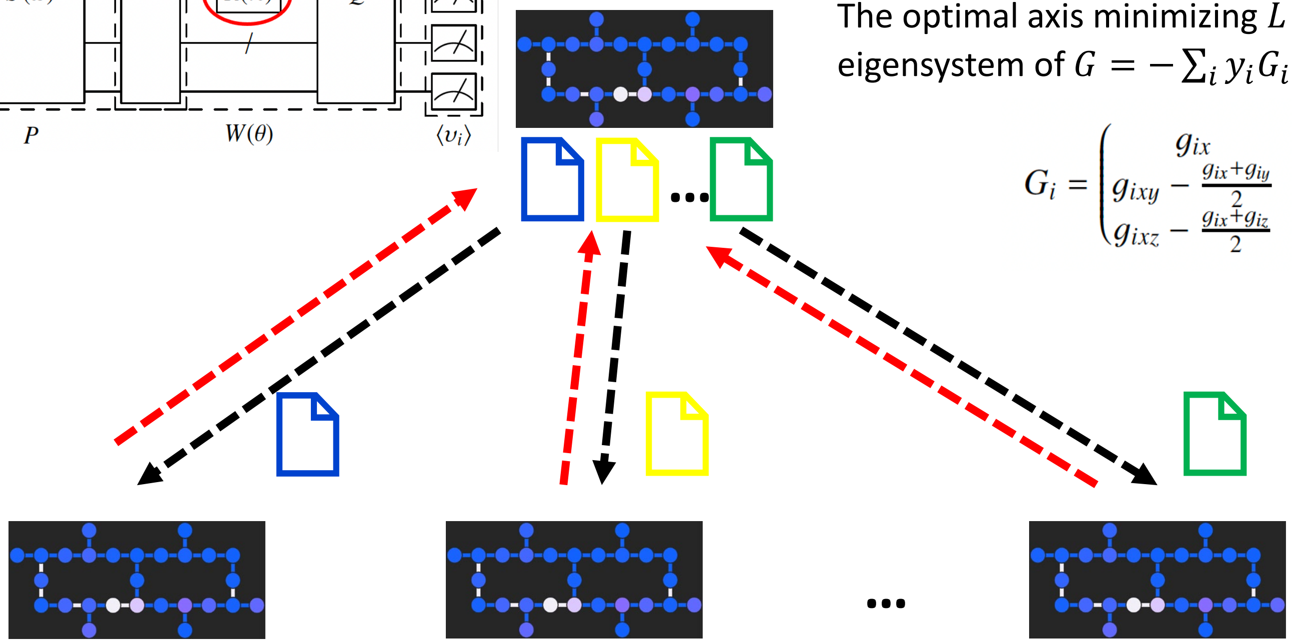
Data parallelization via distributed coordinate descent



Training instances: $\{(x_i, y_i)\}_{i=1}^{N}$ and parameters: $|\theta| = M$

The optimal axis minimizing $L = -\sum_i y_i \langle v_i \rangle$ is the eigensystem of $G = -\sum_i y_i G_i = G^{(1)} + \cdots + G^{(m)}$

$$G_i = \begin{pmatrix} g_{ix} & g_{ixy} - \frac{g_{ix}+g_{iy}}{2} & g_{ixz} - \frac{g_{ix}+g_{iz}}{2} \\ g_{ixy} - \frac{g_{ix}+g_{iy}}{2} & g_{iy} & g_{iyz} - \frac{g_{iy}+g_{iz}}{2} \\ g_{ixz} - \frac{g_{ix}+g_{iz}}{2} & g_{iyz} - \frac{g_{iy}+g_{iz}}{2} & g_{iz} \end{pmatrix}$$



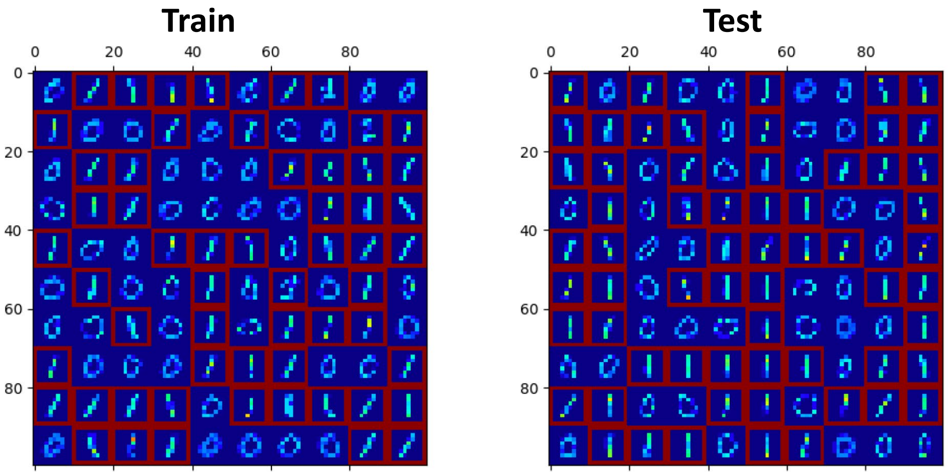
Local node 1
Evaluate $G^{(1)}$

Local node 2
Evaluate $G^{(2)}$

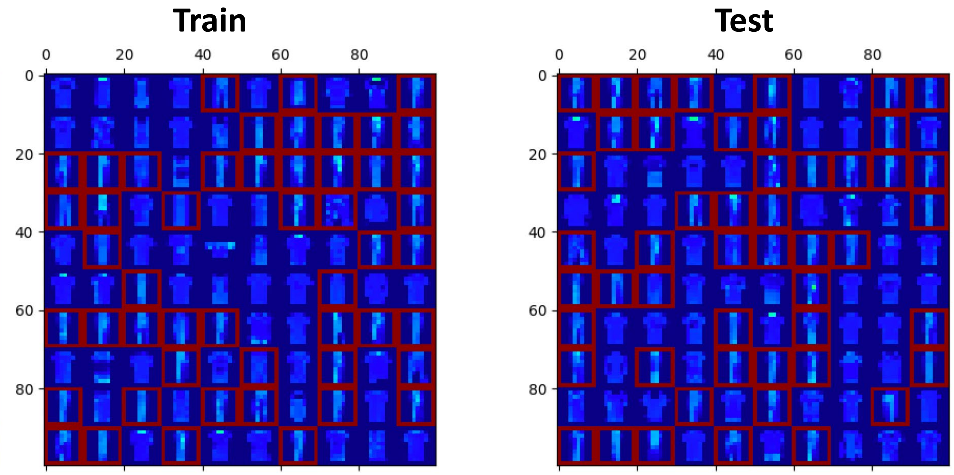
Local node m
Evaluate $G^{(m)}$

almost linear speed-up

Experiments: Datasets



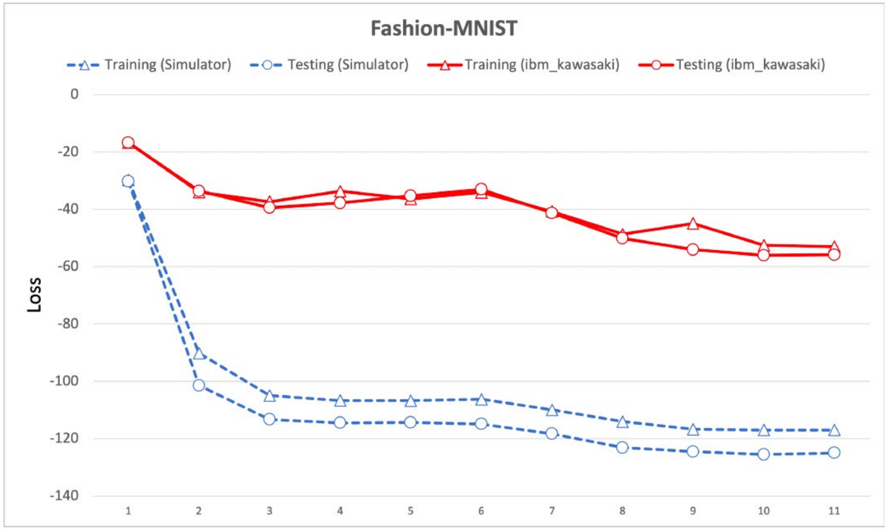
0-1 MNIST

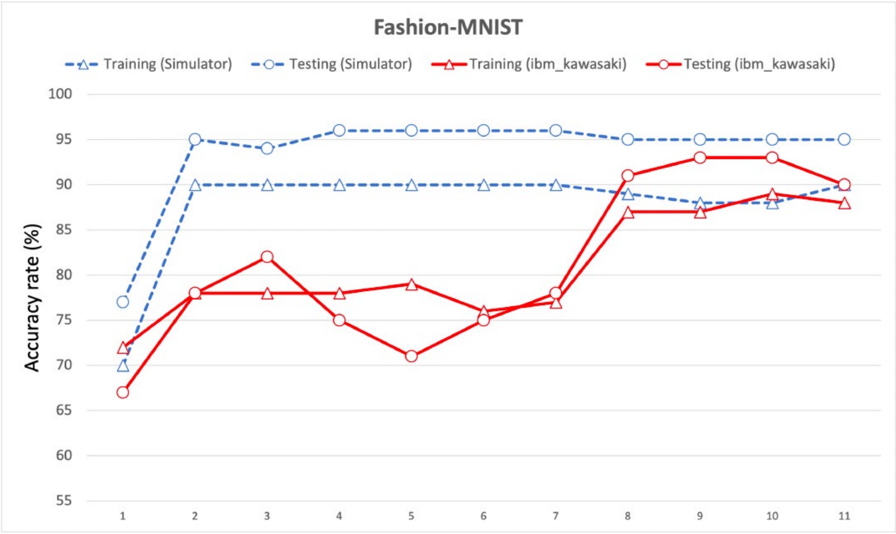


T-S Fashion MNIST

- 28 x 28 grayscale images are transformed into 8 x 8 images by OpenCV
- 100 images for train and test
- MNIST: slightly imbalanced (57, 62), Fashion MNIST: balanced

Experiments: Fashion MNIST





On ibm_kawasaki (9x3), we confirmed similar patterns of training/testing loss with perfect simulators.

On ibm_kawasaki (9x3), we saw accuracies on real devices were initially lower but became better with the number of updates

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(Teramoto, Taymond, I IEICE QCE 2023)

Quantum-Relaxation Based Optimization Algorithm

- **MaxCut problem** $\max_{x \in \{-1,+1\}^{|V(G)|}} \frac{1}{2} \sum_{e_{i,j} \in E(G)} (1 - x_i x_j)$

(cf) problem Hamiltonian in QAOA [4]

$$H \coloneqq \frac{1}{2} \sum_{e_{i,j} \in E(G)} (I - Z_i Z_j)$$

- **Algorithm**

1. Convert the problem into a **relaxed Hamiltonian**.

$$H_{relax} \coloneqq \frac{1}{2} \sum_{e_{i,j} \in E(G)} (I - 3P_i P_j) \quad (P_i \in \{X, Y, Z\})$$

Quantum Random Access Codes (QRAC) is used to encode three classical bits into a single qubit by using not only the Pauli Z operator but also Pauli X and Y operators

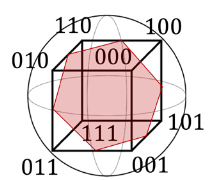
more QRACs!

2. Search for the maximum eigenstate (**relaxed state**) with variational methods.

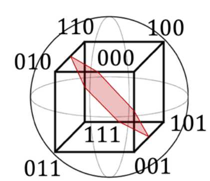
※ In typical quantum oprimizers such as QAOA [4] or VQE [5], found state corresponds to the solution to the orignal problem.

3. Perform a **quantum state rounding** algorithm to extract classical solution from the relaxed state.

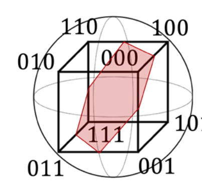
- For each qubit, choose the measurement basis randomly from the following four types, and decode the encoded three bits simultaneously.



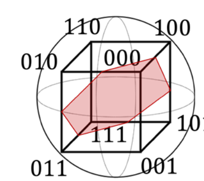
000 or 111



100 or 011



010 or 101



110 or 001

- Repeat this procedure and output the best solution.

Quantum power is expected to provide better solutions!

Result 1: Better Approximation Ratio

Trade-off

Trade-off

Decoding success prob.	Space compression ratio	Approximation ratio
1.0	1.0x	(1.0)
0.85	2.0x	0.625
0.79	3.0x	0.555
0.908	1.5x	**0.722** Our result (3,2)-QRAC

Our result

Formulate a quantum relaxation using (3,2)-QRAC

Prove that the approximation ratio is 0.722…

※ Assumption

(Relaxed state energy) ≥ **(classical MaxCut value)**

(No need to obtain maximum eigenstate)

Conjecture (Open)

r: space compression ratio

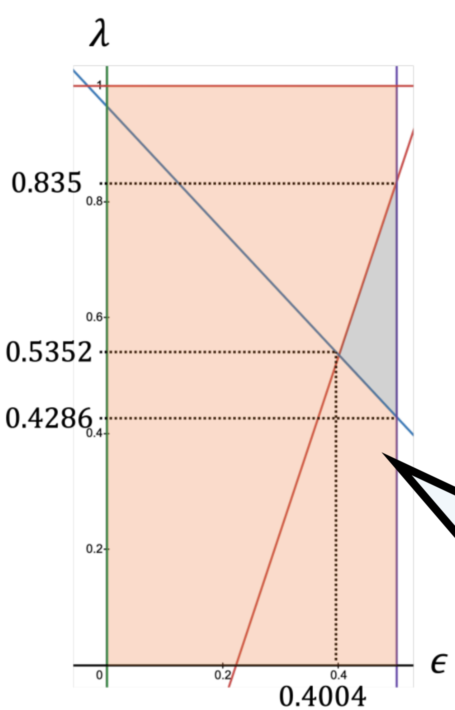
Approximation ratio seems to be

$$\frac{1}{2}(1 + r^{-2})$$

Result 2: Space Compression Ratio Preservation

Our result

- Formulate a new quantum relaxation whose space compression ratio is always 2x (and some more constants>2)
- Finding cases with merits of having the expected approx. ratio>1/2



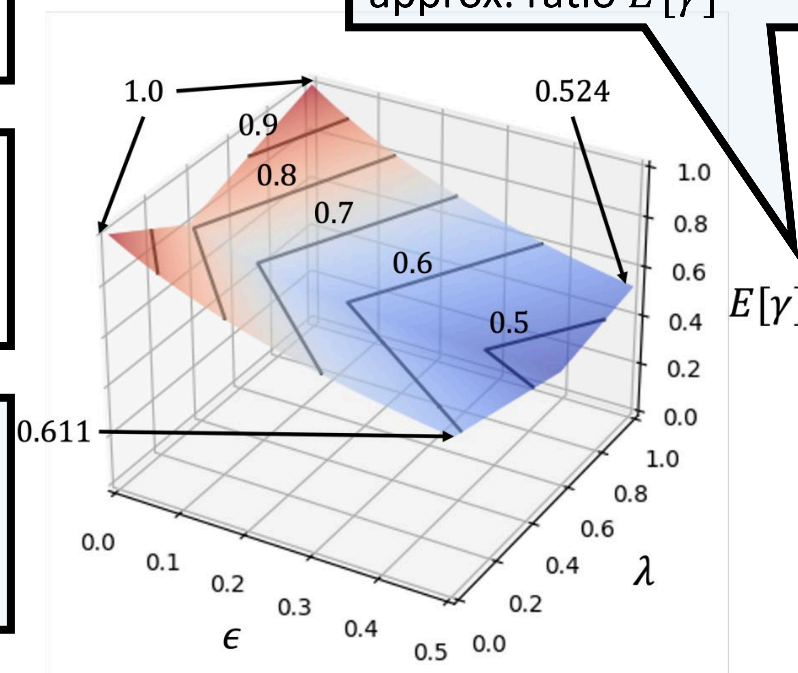
ϵ: gain

$$OPT = \left(\frac{1}{2} + \epsilon\right) |E(G)|$$

λ: The ratio of edges whose endpoints are with different qubits.

The range of λ and ϵ with the non-trivial approx. ratio > 0.5

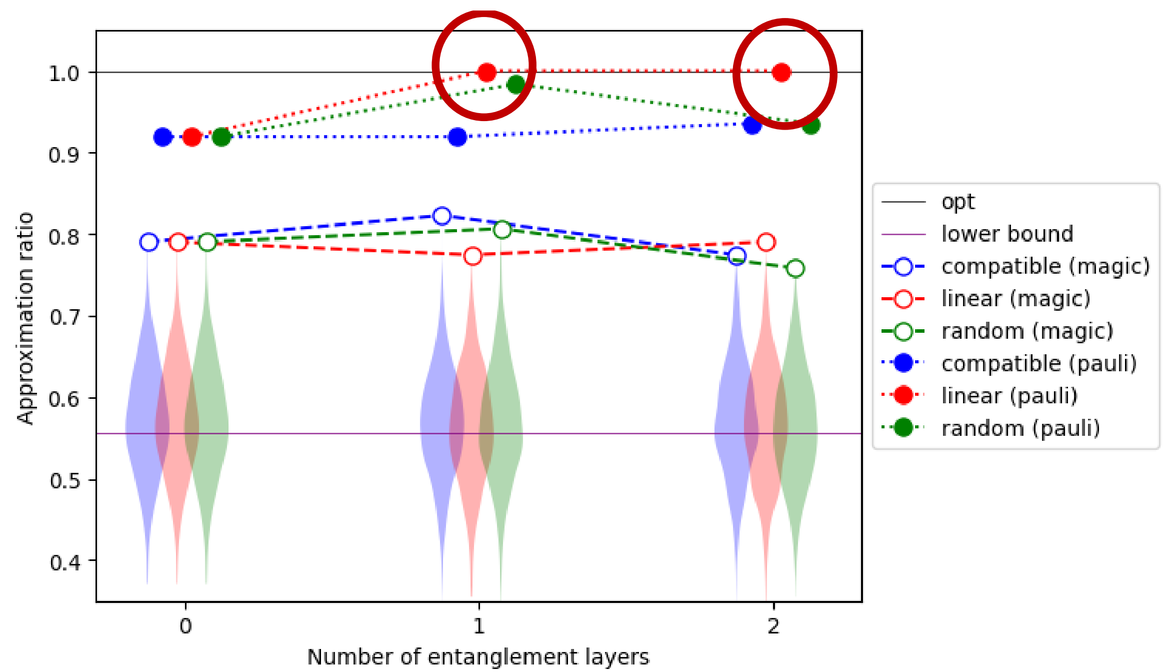
3D plot of the expected approx. ratio $E[\gamma]$



Recent experimental extensions of Quantum Random Access Optimization (QRAO) https://arxiv.org/abs/2302.09481

Experimental Analysis by Simulation (poster@QIP23)

- Analyze the performance of quantum relaxation by simulation
- Though quantumness (entanglement) does not always improve the result, there exists some instances whose optimal solutions are found with the help of quantumness
  - Unweighted: 17-21%
  - Weighted: 18-20%



(e.g.) one of the instances (46 nodes)

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JFQI 2023

Solving Not-All-Equal 3SAT using Quantum Random Access Optimization

Benedek Hauer, Imai Laboratory
The University of Tokyo

Outline

- Not-All-Equal (NAE-3SAT) Problem
- Transforming NAE-3SAT to Max-Cut
- Experiments and Results
- Conclusion and Future Work

Not-All-Equal 3SAT Problem

The NAE-3SAT problem [1] is a combinatorial optimization problem, which is the same as the regular 3SAT problem, except that it has an additional constraint:

- For each clause, we cannot have all variables evaluate to True at the same time.

For example, for the following (very simple) CNF: $x_1 \vee x_2 \vee \neg x_3$

- $x_1 = 1, x_2 = 1, x_3 = 0$ would not be a correct solution because all literals evaluate to 1
- However, $x_1 = 0, x_2 = 0, x_3 = 0$ would be a correct solution.

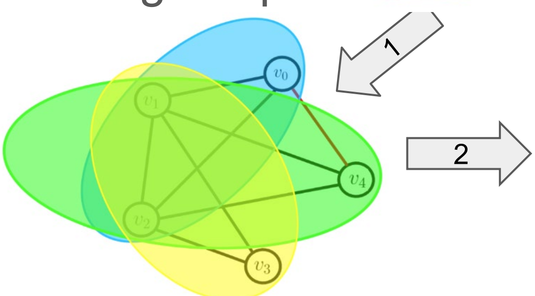
Why NAE-3SAT?

- Variant of the famous 3-SAT Problem
- Interesting Property: It can be reduced to the Max-Cut Problem
- It can be interpreted as a Constraint Satisfaction Problem (CSP)
- While quantum computers can solve unconstrained binary optimization problems, implementing constraints into quantum computers is not an easy task, and this is a nice first step towards solving constrained problems using variational quantum algorithms.
- To my knowledge this the first implementation of solving a constraint problem using Quantum Random Access Optimization and using the ground state energy value for predicting un/satisfiability.

Transforming NAE-3SAT to Max-Cut

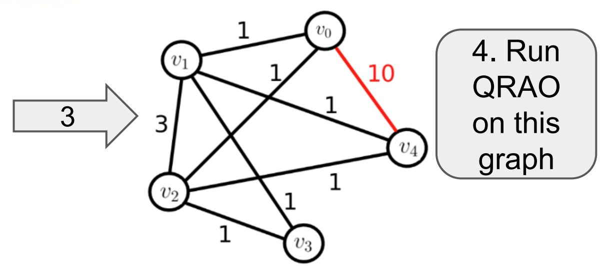
The Max-Cut problem can be solved using Quantum Random Access Optimization. Here is an example of a graph, and setting the per

$$(x_0 \vee x_1 \vee x_2) \wedge (\neg x_0 \vee x_1 \vee x_2) \wedge (x_1 \vee x_2 \vee x_3)$$



Literal Pair	Count
(x_0, x_1)	1
(x_0, x_2)	1
$(x_1, x_2$	3
$(\neg x_0, x_1)$	1
$(\neg x_0, x_2$	1
(x_1, x_3)	1
(x_2, x_3)	1

compute and add weights



Note: A CNF of n variables and m clauses will be transformed into a graph of at most 2*n nodes and at most 3*m + n edges.

Experiments and Results (*ibmq_qasm_simulator*)

1. Solve 38 random Not-All-Equal satisfiable CNFs using QAOA and QRAO
2. Use QRAO to classify 500 random CNFs into “satisfiable” or “unsatisfiable” based on the obtained energy value. (Lemma: If the cut value is lower than some threshold, then we know for sure that the CNF is not satisfiable with the Not-All-Equal constraint)

weights in the graph

number of clauses

theoretical max-cut value

compute before VQE

$$\mathtt{TMCV} = \frac{1}{2}\left(\sum_{(i,j)\in E} W_{ij} + C + M|\mathtt{NEGVAR}|\right)$$

number of variables such that both the variable and its negation appear in the CNF

We can infer unsatisfiability from the energy value alone (no need for rounding)

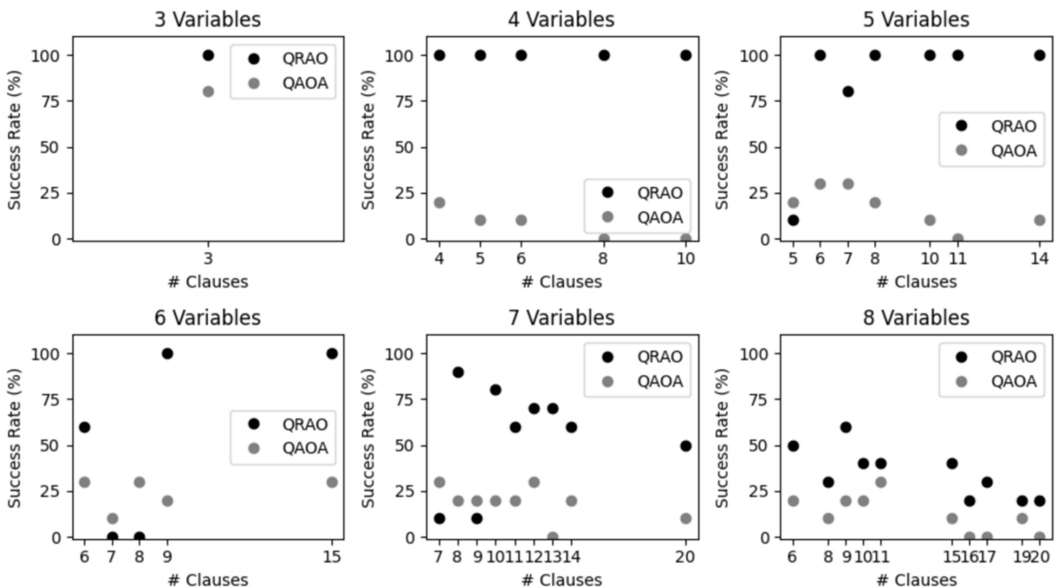
computed using VQE

$$\mathtt{RMCV} < \mathtt{TMCV} \implies \text{CNF is not NAE-3SAT}$$

Lemma

Experiments and Results

Experiment 1 Results



Experiments and Results

Experiment 2 Results

For QAOA

	Actual NAE-3SAT	Actual not NAE-3SAT
Predicted NAE-SAT	71	0
Predicted not NAE-3SAT	227	202

Accuracy: 54.6%   Recall: 23.8%

For QRAO

	Actual NAE-3SAT	Actual not NAE-3SAT
Predicted NAE-SAT	201	52
Predicted not NAE-3SAT	97	150

Accuracy: 70.2%   Recall: 67.4%

Advantage of QRAO over QAOA

- If the number of variables of a CNF is n, then QAOA requires 2n qubits, while QRAO may require as few as 2n/3 qubits, as QRAO's core idea is encoding multiple classical bits into one qubit. [5]
- QRAO performs better when classifying Not-All-3SAT CNFs because it is not necessary for it to find the exact ground state energy of the Hamiltonian in order to make an accurate prediction. For QAOA, however, it is necessary to find the exact ground state energy of the Hamiltonian in order to make an accurate prediction.

Note: Downside of QRAO: It can sometimes mispredict an unsatisfiable NAE-3SAT CNF as *satisfiable*, while that case is not possible for QAOA.

Conclusion and Future Work

Research summary:

- Solved Not-All-Equal 3SAT using QRAO
- Proved a lemma that enables us to infer unsatisfiability from the energy value alone.
- Showed performance improvement of QRAO over QAOA for small instances at least.

Future Work:

- Increase the number of variables to have better insight on the performance of QRAO
- Run the experiments on real devices
- Improve the rounding step to lower the consistency error of solutions

Thank you very much for your attention!

References

[1] Sean McCulloch, Discussions of NP-Complete Problems, 2014 (https://npcomplete.owu.edu/2014/07/22/not-all-equal-3sat/)

[2] Teramoto, Raymond and Imai, The Role of Entanglement in Quantum-Relaxation Based Optimization Algorithms (https://arxiv.org/pdf/2302.00429.pdf)

[3] Peruzzo et al., A variational eigenvalue solver on a photonic quantum processor, 2014 (https://arxiv.org/pdf/1304.3061.pdf)

[4] Farhi et al., A quantum approximate optimization algorithm, 2014 (https://arxiv.org/pdf/1411.4028.pdf)

[5] Fuller et al., Approximate Solutions of Combinatorial Problems via Quantum Relaxations, 2021 (https://arxiv.org/pdf/2111.03167.pdf)