Discord Channel: https://discord.gg/UATwSfxy



Wifi:

• SSID 1:NTUIBM20241

PW: 20240819

• SSID 2:NTUIBM20242

PW: 20240821

• SSID 3: Hackathon2024

PW: IBMQHub@NTU

2024 Quantum Hackathon Projects introduction

1. Quantum image processing-FRQI (Flexible Representation of Quantum Images)-Yen Jui Chang

Introduction:

A Flexible Representation of Quantum Images (FRQI) has been introduced to provide a way to represent images on quantum computers. This method captures information about colors and their corresponding positions in the form of a normalized quantum state.

$$\begin{array}{c|c} \boldsymbol{\theta_0} & \boldsymbol{\theta_1} \\ \hline \boldsymbol{\theta_0} & \boldsymbol{\theta_1} \\ \hline \boldsymbol{\theta_2} & \boldsymbol{\theta_3} \\ \hline \boldsymbol{10} & \boldsymbol{11} \\ \end{array} |I\rangle = \frac{1}{2} \Big[\Big(\cos \theta_0 \, |0\rangle + \sin \theta_0 \, |1\rangle \Big) \otimes |00\rangle + \Big[\Big(\cos \theta_1 \, |0\rangle + \sin \theta_1 \, |1\rangle \Big) \otimes |01\rangle + \\ + \Big[\Big(\cos \theta_2 \, |0\rangle + \sin \theta_2 \, |1\rangle \Big) \otimes |10\rangle + \Big[\Big(\cos \theta_3 \, |0\rangle + \sin \theta_3 \, |1\rangle \Big) \otimes |11\rangle \Big]$$

Goal:

Fundamental: construct the 2x2, 4x8 digits image

Advance: Prepose other algorithm run on

Reference:

1. Le, P.Q., Dong, F. & Hirota, K. A flexible representation of quantum images for polynomial preparation, image compression, and processing operations. Quantum Inf Process 10, 63–84 (2011). https://doi.org/10.1007/s11128-010-0177-y

Quamtum Machine Learning for Imbalanced Data-Robin Huang

Introduction

 Imbalanced Data is a challenge for classical machine learning. Quamtum Machine Learning is potential to address some issues. The general strategies of Quamtum Machine Learning for Imbalanced Data are yet to be explored.

Goal

- Fundamental
 - Home Credit provides an imbalanced data to predict loan defaults (positive: 3%) [1].
 Build a novel Quamtum Machine Learning model with Home Credit data.
 Comprehensive evaluation is encouraged, e.g. sensitivity, specificity, F1, PPV, and NPV.
- Advanced
 - Propose a new general strategy for Quamtum Machine Learning for Imbalanced Data and test on multiple data types such as images, signals, or industrial data.

- [1] Daniel Herman, Tomas Jelinek, Walter Reade, Maggie Demkin, Addison Howard. (2024). Home Credit Credit Risk Model Stability. Kaggle. https://kaggle.com/competitions/home-credit-credit-risk-model-stability
- [2] Schetakis, N., Aghamalyan, D., Boguslavsky, M., Rees, A., Rakotomalala, M., & Griffin, P. R. (2024). Quantum machine learning for credit scoring. Mathematics, 12(9), 1391.
- o [3] Mancilla, J., Sequeira, A., Montalbán, I., Tagliani, T., Llaneza, F., & Beiza, C. (2024). Empowering Credit Scoring Systems with Quantum-Enhanced Machine Learning. arXiv preprint arXiv:2404.00015.

Application of Harrow-Hassidim-Lloyd Algorithm - YooYG

Introduction

HHL (Harrow-Hassidim-Lloyd) Algorithm is aimed to figure out solution of Linear System. This algorithm include QPE (Quantum Phase Estimation) and inversion of eigenvalue.

By Separating Oracle split into each Function and Operator, considering Complexity and runtime, we could shorten depth of circuit and error rate. but decompose make runtime longer. as a result, Hybrid HHL is Trade off from Accuracy and Runtime

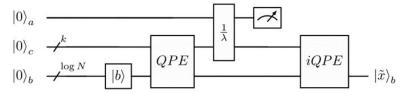


Figure 1. high level diagram of an HHL Circuit

Goal1. Construct HHL Circuit to solve most small System A (use N<2 System Matrix of A)

Goal2. Construct Hybrid HHL Circuit with using Classical Bits to improve Circuit. i.e) Eigenvalue estimation, Fourier Transform... then extend scale of System A also (2x2, 4x4,...,2ⁿn x 2ⁿn)

Reference

Harrow, A. W., Hassidim, A., & Lloyd, S. (2009). Quantum algorithm for linear systems of equations. *arXiv preprint arXiv:0811.3171v3*. Retrieved from http://arxiv.org/abs/0811.3171v3

Morgan, J., Ghysels, E., & Mohammadbagherpoor, H. (2024). An Enhanced Hybrid HHL Algorithm. *arXiv preprint arXiv:2404.10103v1*. Retrieved from http://arxiv.org/abs/2404.10103v1

Randomized benchmarking - Eugene Hsu

Introduction

 To improve qubit fidelity, characterizing noise becomes a important issue. Randomized benchmarking (RB) is the most widely-used technique in experiment.

Goal

- Fundamental
 - Execute 1-qubit and 2-qubit RB
- Advanced
 - Try different methods based on RB. e.g. interleaved RB, Simultaneous RB, ...
 - Try different way of decomposing RB.

- [1] https://github.com/qiskit-community/qiskit-textbook/blob/main/content/ch-quantum-hardware/randomized-benchmarking.ipynb
- o [2] https://arxiv.org/abs/2010.07974
- o [3] https://youtu.be/d6TMuTH4qdo

Generate Classical Neural Network Weights by Quantum Machine Learning - Chen-Yu Liu

Introduction

Quantum neural networks can be considered as generative models to produce data. But what if we use them to generate the weights of classical neural networks? And how many quantum parameters are needed to generate a certain number of classical parameters? This is the basic idea behind the proposed Quantum-Train approach.

Goal

- Fundamental: Implement the basic idea of generating classical neural network weights using quantum neural networks. Specifically, generate some numbers from the QNN and input them into a classical NN. Perform basic learning tasks, such as binary classification, to assess the applicability of this model.
- Advanced: Investigate the parameter reduction behavior. Can we generate more parameters than our controlling parameters (QNN parameters)? If so, what does this reduction look like?

- 1. https://ieeexplore.ieee.org/document/9321551
- https://arxiv.org/abs/2402.16465
- 3. https://arxiv.org/abs/2405.11304
- 4. https://github.com/Hon-Hai-Quantum-Computing/QuantumTrain

Quantum stochastic walks - Wei-Ting Wang

Introduction:

Quantum Stochastic Walks (QSW) is a theoretical framework that extends classical random walks (RW) and continuous-time quantum walks (CTQW) to incorporate both quantum and classical dynamics. They are used to model processes where coherent quantum evolution and incoherent stochastic processes are present, such as in open quantum systems.

Goal:

Fundamental: Generating a distribution via QSW with different coupling strength Advanced: Optimizing Energy Transfer in Quantum Networks

- 1. https://arxiv.org/abs/0905.2942
- 2. Hu, Z., Xia, R. & Kais, S. A quantum algorithm for evolving open quantum dynamics on quantum computing devices. *Sci Rep* **10**, 3301 (2020).
- 3. https://arxiv.org/abs/2101.05287v3

Calculation of metal corrosion processes using Simplify VQE- Ran-Yu Chang

Introduction:

We will use Density Functional Theory (DFT) integrated with the Variational Quantum Eigensolver (VQE) for simulating metalinhibitor absorption process, to enhance the simulation quality of corrosion inhibition on aluminum alloy surfaces. We introduced AA6061 and AA6063 as the metal substrate and MSDP to be our choice of inhibitor. VQE calculation will be a possible approach, aiming to address the limitations of DFT methods by improving accuracy and efficiency in computational simulations.

Goal:

Fundamental: Successfully calculated the energy of this system

Advanced: For macromolecular systems, Hamiltonian matrix cutting can be used to convert them into small molecule systems for calculation, simplifying the calculation process resources.

- 1. <u>CORROSION INHIBITION OF AA6061 AND AA6063 ALLOY IN HYDROCHLORIC ACID MEDIA BY SCHIFF BASE</u> <u>COMPOUNDS</u>
- **2.** T.L.P. Galv ao, I. Ferreira, A. Kuznetsova, et al. Cordata: an open data management web application to select corrosion inhibitors. npj Materials Degradation, 6:48, 2022. doi: 10.1038/s41529-022-00259-9
- 3. Benchen Huang, Simulating the Electronic Structure of Spin Defects on Quantum Computers
- 4. Molecular Structure PySCF
- 5. https://journals.aps.org/prxquantum/abstract/10.1103/PRXQuantum.3.010339

Randomized measurements (Classical Shadow)

Introduction:

Full characterization of quantum states and channels usually exponentially-scaled resources. However, it's possible to estimate certain quantum state properties (e.g. fidelity, observables) with polynomially scaled random measurements, or called "Shadow Tomography".

Applications:

- Fidelity Estimation:
 - O The randomized measurement toolbox | Abstract (arxiv.org)
- improved VQE
 - O Predicting Many Properties of a Quantum System from Very Few Measurements | Abstract (arxiv.org)
 - O <u>Efficient estimation of Pauli observables by derandomization | Abstract (arxiv.org)</u>
- Shadow Estimation under noise
 - O Robust Shadow Estimation with Mitig Mitig 0.38.0 documentation
 - O Robust shadow estimation | Abstract (arxiv.org)
 - O Quantum Error Mitigated Classical Shadows | Abstract (arxiv.org)

Distributed Quantum Computing - Kuo-Chin Chen

Introduction:

Quantum computing has reached the engineering phase, with processors now utilizing hundreds of noisy qubits. The next challenge is scaling up to thousands or millions of noise-free qubits. There is a consensus in academia and industry that distributed computing, which involves using multiple smaller quantum processors, is essential for this scalability. This project aims to address whether a given quantum algorithm or circuit is naturally suited for distributed execution.

Goal:

Fundamental: Variational Quantum Algorithms Advanced: Fault-Tolerant Quantum Algorithms

- 1. Caleffi, Marcello, et al. "Distributed quantum computing: a survey." arXiv preprint arXiv:2212.10609 (2022).
- 2. DiAdamo, Stephen, Marco Ghibaudi, and James Cruise. "Distributed quantum computing and network control for accelerated vqe." *IEEE Transactions on Quantum Engineering* 2 (2021).
- 3. Neumann, Niels MP, Roy van Houte, and Thomas Attema. "Imperfect distributed quantum phase estimation." *Computational Science–ICCS 2020: 20th International Conference, Amsterdam, The Netherlands, June 3–5, 2020, Proceedings, Part VI 20.* Springer International Publishing, 2020.

Error mitigation (Ming-Chien Hsu)

Introduction:

To utilize the full power of quantum computers, it is essential to reduce the errors that occurs when executing the quantum circuits. The project is to characterize the error behaviours and/or mitigate the errors.

Goal:

characterize the errors do the error mitigation / error correction

- 1. General error mitigation for quantum circuits | Quantum Information Processing (springer.com)
- 2. [2202.12408] Quantum Error Correction Scheme for Fully Correlated Noise (arxiv.org)
- 3. [2011.07064] Virtual Distillation for Quantum Error Mitigation (arxiv.org)

Efficient measurement of molecular Hamiltonians via double-factorization (Kevin)

Introduction: Measuring the expectation value of a Hamiltonian is a common task in quantum algorithms. A fermionic Hamiltonian can be measured by mapping the Hamiltonian to a linear combination of Pauli strings. A naive mapping will have ~N^4 terms, but by using a double-factorized (low-rank) decomposition of the two-body tensor, the total number of terms can be reduced to ~N (References [1, 2]).

Goal: Implement the measurement scheme for a molecular Hamiltonian using the double-factorized (low-rank) representation. Consider implementing it using the Estimator primitive interface in Qiskit (Reference [3]). The linear algebra for the double-factorization is already implemented in ffsim (Reference [4]).

Advanced goal: Measure a molecular Hamiltonian on an IBM quantum processor using the double-factorized measurement scheme, as well as a naive Pauli decomposition scheme, and compare the results.

- [1] https://arxiv.org/abs/1907.13117
- [2] https://giskit-community.github.io/ffsim/explanations/double-factorized.html
- [3] https://docs.quantum.ibm.com/api/qiskit/qiskit.primitives.BaseEstimatorV2
- [4] https://giskit-community.github.io/ffsim/

Solving the weight clique problem with the hybrid algorithm (Chien-Hung, Cho)

Introduction:

The weight clique problem has many applications in different fields, such as molecule design, biology. This project aims to solve this problem via the hybrid algorithm on quantum computers.

Goal:

Formulate the weight clique problem

Use the quantum computers to find the solution.

- 1. The partial constraint satisfaction problem: Facets and lifting theorems. Oper. Res. Lett, 23(3-5):89–97, 1998.
- 2. Quantum bridge analytics I: a tutorial on formulating and using QUBO models. Ann. Oper. Res, 314:141–183, 2022.
- 3. https://youtube.com/watch?v=YpLzSQPrgSc

Pathsum based Quatum Circuits Verification (Wei-Jia Huang)

Introduction:

As quantum algorithms become more and more complex, verification of quantum circuits is an important issue. The verification of quantum circuits can ensure that the quantum circuit has behavior that indeed satisfies the quantum algorithm. Pathsum is one of method which can verification quantum circuits.

Goal:

- 1. Build Pathsum Based Quantum Circuits Representaion.
- 2. Reproduce Pathsum Reduction Rules.
- 3. Implement Quatum Circuits Equivalence Checking.

$$U_{\xi}: |\mathbf{x}\rangle \mapsto \frac{1}{\sqrt{2^m}} \sum_{\mathbf{y} \in \mathbb{Z}_2^m} e^{2\pi i P(\mathbf{x}, \mathbf{y})} |f(\mathbf{x}, \mathbf{y})\rangle.$$

- Amy, M. (2018). Towards large-scale functional verification of universal quantum circuits. arXiv preprint arXiv:1805.06908.
- 2. Hietala, K., Rand, R., Hung, S. H., Li, L., & Hicks, M. (2020). Proving quantum programs correct. arXiv preprint arXiv:2010.01240.
- 3. Chareton, C., Bardin, S., Bobot, F., Perrelle, V., & Valiron, B. (2021). An automated deductive verification framework for circuit-building quantum programs. ETAPS 2021, Proceedings 30 (pp. 148-177).
- 4. Vilmart, R. (2021, March). The Structure of Sum-Over-Paths, its Consequences, and Completeness for Clifford. In FoSSaCS (pp. 531-550).
- 5. Amy, M., Bennett-Gibbs, O., & Ross, N. J. (2022). Symbolic synthesis of Clifford circuits and beyond. arXiv preprint arXiv:2204.14205.
- 6. Amy, M. (2023). Complete equational theories for the sum-over-paths with unbalanced amplitudes. arXiv preprint arXiv:2306.16369.

Quantum Circuit Compression (Huai-Chun Chang)

> Introduction

Quantum computing is a powerful tool for simulating physics problems, such as many-body problems. We can represent these problems as Hamiltonians and map them to quantum circuits using Trotter decomposition. However, sometimes this process results in quantum circuits with large circuit depths. While this is acceptable for quantum simulators, for current quantum computers, it not only increases the calculation time but also introduces more noise due to the circuit's depth..

➤ Goal

- Fundamental: Demonstrate a quantum circuit compression with any problem which original circuit depth larger than 500 gates.
- Advanced: Demonstrate the compressed quantum circuit on real machine.

➤ Reference

- a. The Quantum Autoencoder
- b. [2108.03283] An Algebraic Quantum Circuit Compression Algorithm for Hamiltonian Simulation
- c. Real- and Imaginary-Time Evolution with Compressed Quantum Circuits

Discrete-time quantum walk optimization algorithm - Aurél Gábris

Introduction:

Discrete-time quantum walks (DTQW) have been observed to be useful also for optimization by applying an position-dependent phase shift that corresponds to an external potential [1]. The canonical definition of DTQW on a 2D lattice, requires the use of a four-dimensional coin operator.

Goal:

Implement and explore performance of DTQW optimization using a simplified model called split-step walk, which uses only a two coin dimensions. The effect of additional randomness, i.e. a classical random walk, on performance could also be interesting to evaluate.

- 1. Liliopoulos et al, Discrete-time quantum walk-based optimization algorithm. *Quantum Inf. Process*. 23:23 (2024). https://doi.org/10.1007/s11128-023-04234-4
- 2. https://arxiv.org/abs/1010.2470
- 3. https://arxiv.org/abs/0706.0304

Quantum Circuit Optimization Challenge: Beyond Al Transpilation with Qiskit (Vishal)

Introduction:

Recent advancements in quantum circuit optimization have led to AI-assisted techniques and tools like the Qiskit AI Transpiler service. This challenge invites you to push the boundaries of Qiskit's transpilation capabilities by developing advanced custom passes and exploring the limits of current optimization techniques.

Goal [Fundamental]:

Develop a custom transpilation workflow using custom Qiskit transpiler passes for a specific class of quantum circuits of your choice on ibm_kyoto (127 qubits). Compare performance against:

- Qiskit default transpiler options (optimization levels 0-3)
- Qiskit Al Transpiler service
- Optimal solutions (where feasible)

Focus on metrics such as CNOT count, SWAP count, total circuit depth and demonstrate scalability to 100+ qubit regime. [Advanced] Achieve atleast 5-10% reduction in both two qubit gate count and circuit depth compared to AI Transpiler service or optimal solution, while maintaining or improving transpilation time complexity.

References and helpful links:

- Practical and efficient quantum circuit synthesis and transpiling with Reinforcement Learning (Kremer et al., 2024)
- Documentation and tutorials: Qiskit <u>transpiler documentation</u>, Qiskit <u>transpiler service docs</u> and <u>AI assisted Transpilation</u>,
 Transforming Quantum circuits using Qiskit's transpiler <u>Matthew Trenish</u>
- Helpful notebooks on Transpilation and Transpiler service: QGSS <u>Lab 1</u>, Qiskit community <u>qopt optimal transpilation</u>, IBM Quantum Challenge 2024 <u>Lab 3</u>

2024 Quantum Hackathon Logistics & Rules

Originality and Uniqueness (15%)

o Compared to what you've seen before, how unique is this project? How interesting do you find it? Did the team attempt something new or difficult?

Usefulness and Complexity (25%)

o Will other people be able to use this project? Was the project thoughtful in how it was designed? How functional is the project as of judging?

Quantum Community Benefit (25%)

o Will this project help the community at large? Can people use this for research or further develop it? Will this project help others learn and understand quantum computing?

Presentation (35%)

o Did the team represent their project well? Was the team able to explain why they made certain decisions? Did the entire team get a chance to speak?



Remarks

- IBM Quantum Computing Resource. Ask your mentor for tokens if you need additional computing resource.
- Each team has 10 minute (8min + 2min Q&A) to present about the outcome of their projects.
- Presentation Slides due on 8/21 11AM. Upload to the Discord Channel.