基于 Pauli 路径积分模拟量子线路

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Introduction

Moore's law

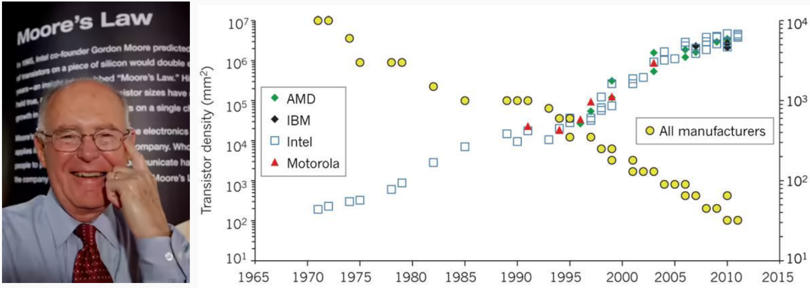
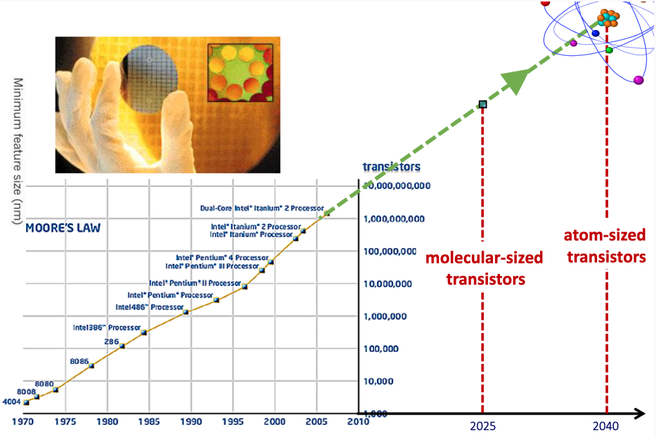


Figure 1: Moore's Law. Source: Liu, 2023

- Moore's Law: The number of transistors on a microchip would double every two years, while the cost would be halved.

The End of Moore's Law & Future of Computers



- The feature size of the transistor is approaching the atomic scale.
- Quantum effects become significant.
- The development of new technologies is required.

Quantum Computers VS Classical Computers

The New York Times

Google Claims a Quantum Breakthrough That Could Change Computing

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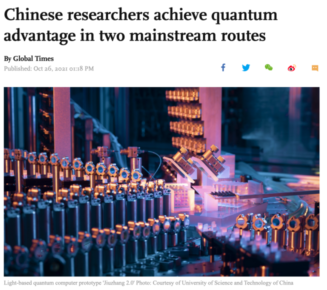
Google's quantum computer. The company said in a paper published on Wednesday that the machine needed only a few minutes to perform a task that would take a supercomputer at least 10,000 years. Google



Chinese researchers achieve quantum advantage in two mainstream routes

By Global Times

Published: Oct 26, 2021 01:18 PM

Light-based quantum computer prototype 'Jiuzhang 2.0' Photo: Courtesy of University of Science and Technology of China

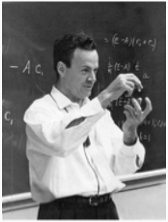
- Are quantum computers truly superior to classical computers?
    - Quantum Advantage VS Classical Simulation.

Simulation of quantum circuits based on Pauli path integral:

- **Part 1:** A classical simulation method for a broad class of quantum algorithms, with polynomial cost in the presence of noise.
- **Part 2:** A classical simulation method for near Clifford quantum circuits, with polynomial cost in noiseless case.
  - **Variational Quantum Algorithms (VQAs).**
  - Circuits with Clifford gates and Pauli rotation gates[1] under Pauli noise.

[1] Pauli rotation gates: $U(\theta) = e^{-i\frac{\theta}{2}P}$, where $P \in \{I, X, Y, Z\}^{\otimes n}$

Historical Background



- In the 1980s, Yuri Manin and Richard Feynman proposed the idea of quantum computing.
- **Motivation:** When classical computers simulate quantum systems, the cost grows exponentially with the number of particles.
- **Solution:** Build a computer based on quantum mechanics.

Key Questions:

- How do we develop **useful quantum algorithms**?
- How do we handle **quantum noise**?

Useful quantum algorithms:

- In 1994[2], Peter Shor proposed a quantum algorithm that can factorize large numbers in polynomial time.
  - **Classical Algorithms:** Best known algorithm require sub-exponential time.

with a classical computer

# bits	1024	2048	4096
factoring in 2006	10^5 years	$5\text{x}10^{15}$ years	$3\text{x}10^{29}$ years
factoring in 2024	38 years	10^{12} years	$7\text{x}10^{25}$ years
factoring in 2042	3 days	$3\text{x}10^8$ years	$\boxed{2\text{x}10^{22}\text{ years}}$

with potential quantum computer
(e.g., clock speed 100 MHz)

# bits	1024	2048	4096
# qubits	5124	10244	20484
# gates	$3\text{x}10^9$	$2\text{X}10^{11}$	$\text{X}10^{12}$
factoring time	4.5 min	36 min	$\boxed{\text{4.8 hours}}$

R. J. Hughes, LA-UR-97-4986

[2] Shor, P. (1994). **Algorithms for quantum computation: Discrete logarithms and factoring.** *Proceedings 35th Annual Symposium on Foundations of Computer Science*, 124–134. https://doi.org/10.1109/SFCS.1994.365700

Quantum Error Correction

Protect quantum information from noise:

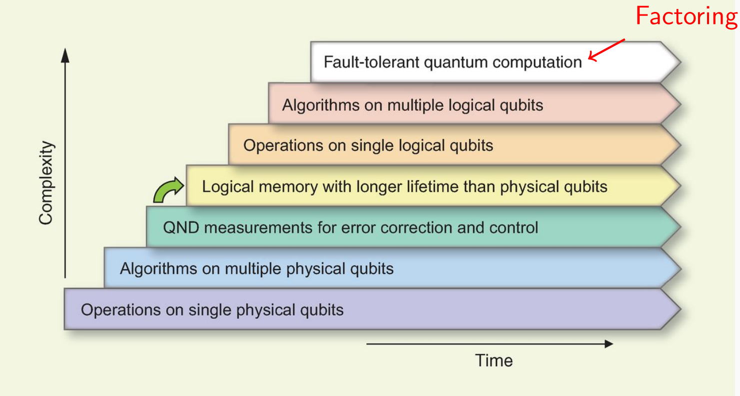
- Noise is inevitable in quantum systems.
- Peter Shor[3] proposed to use error correction codes to protect quantum information from noise.

[3] Shor, P. W. (1995). **Scheme for reducing decoherence in quantum computer memory.** *Physical review A*, *52*(4), R2493.

Error Correction is Expensive

The implementation of quantum error correction is described in seven stages, described in 2013.

Factoring Algorithm



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- After 10 years, Ni et al., 2023(USTC) and Acharya et al., 2024(Google) reached the fourth stage.

Noisy Intermediate-Scale Quantum (NISQ) Computers

Nowadays Quantum devices have entered the NISQ era, with the potential to achieve quantum advantages.

- **Qubit Count:** 50–1000 qubits
- **Gate Fidelity:** 99.9%–99.999% (still noisy)

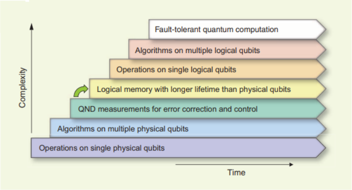
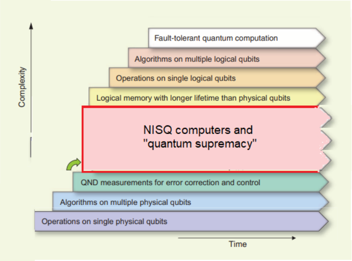


Fig. 1. Seven stages in the development of quantum information processing. Each advancement requires mastery of the preceding stages, but each also represents a continuing task that must be perfected in parallel with the others. Superconducting qubits are the only solid-state implementation at the third stage, and they now aim at reaching the fourth stage (green arrow). In the domain of atomic physics and quantum optics, the third stage had been previously attained by trapped ions and by Rydberg atoms. No implementation has yet reached the fourth stage, where a logical qubit can be stored, via error correction, for a time substantially longer than the decoherence time of its physical qubit components.

Quantum computation worldview 2010



Quantum computation worldview 2020 [5]

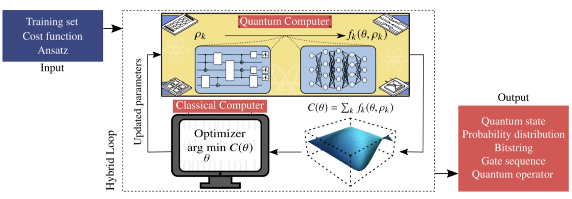
- Around 2020, exploring the potential of NISQ devices to achieve quantum advantages.

[5] Kalai, 2022.

Variational Quantum Algorithms

Variational Quantum Algorithms

Variational quantum algorithms (VQAs) are a class of quantum algorithms designed for NISQ devices.



[6]

- **Parameterized Quantum Circuits**: Serve as the model, analogous to neural networks in deep learning.
- **Quantum Processor**: Executes the quantum circuits, acting as a co-processor.
- **Classical Optimizer**: Adjusts the circuit parameters to minimize the loss function, iteratively improving the solution.

[6] Cerezo et al., 2021.

Variational Quantum Algorithms

Many applications of variational quantum algorithms have been proposed, including:

- Hamiltonian simulation[7]
- Combinatorial optimization (QAOA)[8]
- Quantum chemistry (VQE)[9]
- Quantum machine learning (QDNN, QGAN, QCNN)[10]
- Quantum circuit compilation[11]
- Quantum error correction[12]
- ....

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[7] Chen et al., 2020.
[8] Farhi et al., 2014; Moll et al., 2018.
[9] **Kandala2017hardware**; Li et al., 2022; Peruzzo et al., 2014.
[10] Beer et al., 2020; Havlíček et al., 2019; Huang et al., 2021; Mitarai et al., 2018.
[11] Khatri et al., 2019.
[12] Johnson et al., 2017; Xu et al., 2021.

Simulating Noisy Variational Quantum Algorithms

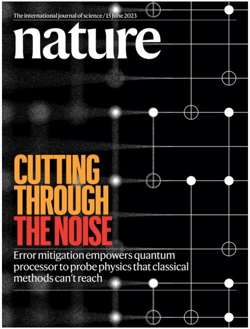
Whether the quantum advantage of variational quantum algorithms can be maintained in the presence of noise?

Shao, Y., Wei, F., Cheng, S., & Liu, Z. (2024).**Simulating noisy variational quantum algorithms: A polynomial approach.** *Physical Review Letters*, *133*(12), 120603

- **Simulation Method:** A method to simulate the noisy observable value of variational quantum algorithms without assumptions of locality, low entanglement entropy, or circuit depth.
- **Cost:** Prove that the simulation cost is polynomial scale when simulation error is bounded by a given threshold with high probability.

IBM's 127-qubit expriments

In 2023, IBM[13] demonstrated a 2D Ising model simulation task on a 127-qubit quantum computer and claimed it as evidence of the utility of quantum computing.



Evidence for the utility of quantum computing before fault tolerance

https://doi.org/10.1038/s41586-023-06096-3

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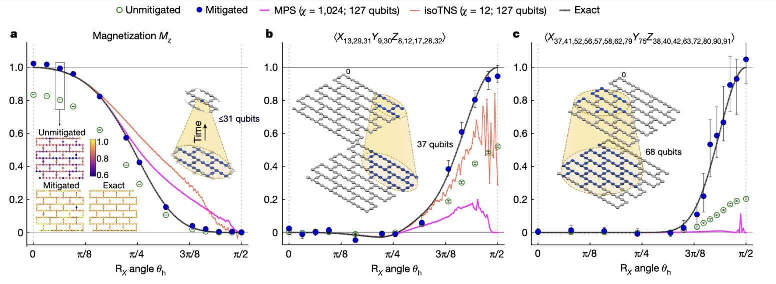
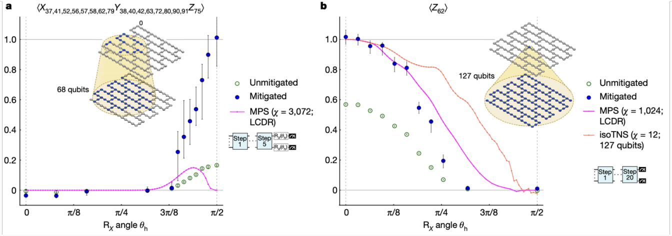
Youngseok Kim[1,6]✉, Andrew Eddins[2,6]✉, Sajant Anand[3], Ken Xuan Wei[1], Ewout van den Berg[1], Sami Rosenblatt[1], Hasan Nayfeh[1], Yantao Wu[3,4], Michael Zaletel[3,5], Kristan Temme[1] & Abhinav Kandala[1]✉

[13]Kim, Y., Eddins, A., Anand, S., Wei, K. X., van den Berg, E., Rosenblatt, S., Nayfeh, H., Wu, Y., Zaletel, M., Temme, K., & Kandala, A. (2023).**Evidence for the utility of quantum computing before fault tolerance.** *Nature*, *618*(7965), 500–505. https://doi.org/10.1038/s41586-023-06096-3





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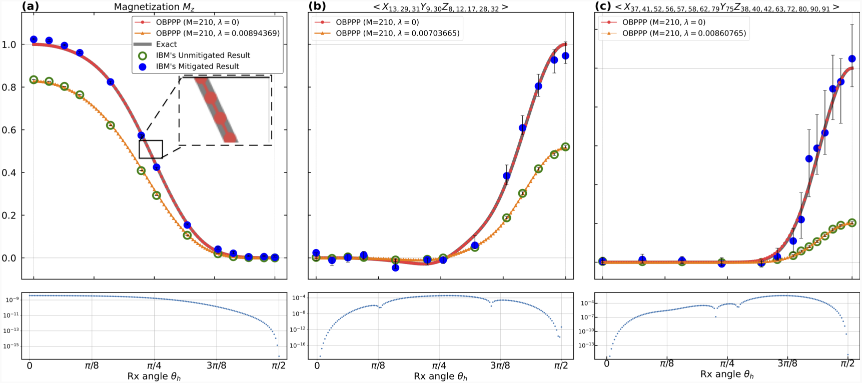
[14]Experimental data:

Blue points Mitigated results: Use Zero noise extrapolation (ZNE) to estimate noiseless results from noisy experimental data.

Green points Unmitigated results: Noisy raw experimental data.



Our Simulation results:

- Red(noiseless):Faster and more accurate than the Quantum computer.
- Outputs are **analytical expressions**, with the entire curve obtained in a **single run**.
- Orange(noisy):Use unmitigated results to fit the noise rate, which is consistent with the noise rate reported by IBM. (0.007-0.009) 15

[15] Blue points Mitigated results.
Green points Unmitigated results: Noisy raw experimental data.
Runtime: Classical 13s, 146s, 29s vs Quantum 5 minutes(without post-processing).

Properties

Key properties of our simulation method:

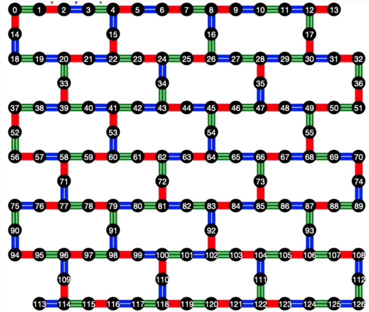
- **Analytical Outputs:** The simulation provides analytical expressions as functions of both the rotation angles and the noise rate.
  1. **Efficiency:** The entire curve can be computed in a single run. Bring in different rotation angles to get points on the curve.
  2. **Noise Mitigated and Unmitigated Results:**
     - By setting the noise rate to zero, the noise effects are mitigated, providing an estimate of the noiseless results.
     - The noise rate can be optimized to fit the noisy unmitigated results, simulating the noisy raw experimental data.
- **No Structural Assumptions:** The approach does not rely on the layout of Quantum Chip or low entanglement-entropy constraints.

Low-entanglement and Tensor Network Simulation

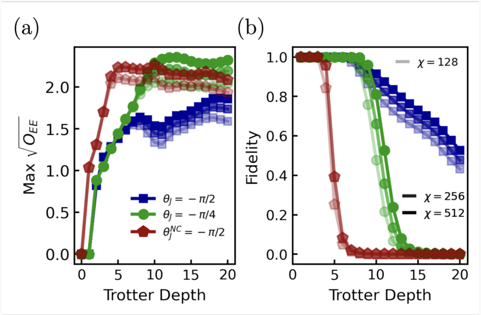
- **Limited Gate Locality:**
  - Qubits can only interact with their nearest neighbors.
  - **Low Entanglement Entropy.**

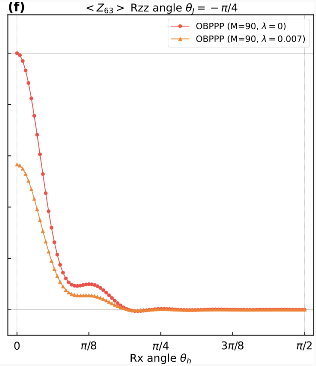
Improved tensor-network based simulation:

- Tindall et al., 2023
- Begušić et al., 2024
- Liao et al., 2023
- Patra et al., 2024



Anand et al., 2023[16] proposed an improved experimental setting, which is more challenging for tensor network based simulation methods.

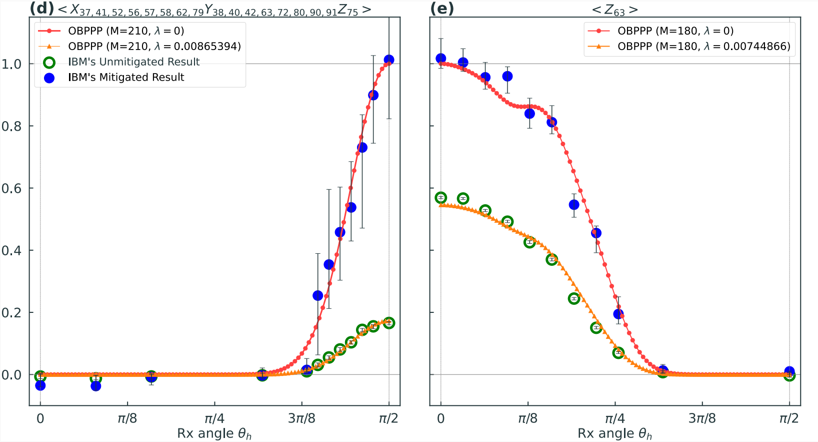




- Theoretical prediction of mitigated results and noisy unmitigated results. [17]
- Noise rate (0.007) is estimated from previously experimental data.

[16] Anand et al., 2023.

[17] Red line: Theoretical prediction of mitigated results.
Orange line: Theoretical prediction of noisy unmitigated results.



- **No Exact References Available:** For deeper circuits, exact results are not available for comparison.
- **Simulation Consistency:**
  - Noisy simulation results (orange) align closely with noisy unmitigated results (green points).

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[18] Runtime: 137s and 262s.

Numerical Simulation for Non-locality Circuits

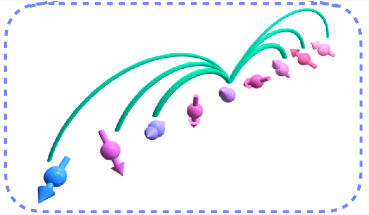
Pagano et al., 2020[19] used a 1D array of ions to perform a low-depth long-range Quantum Approximate Optimization Algorithm (QAOA).

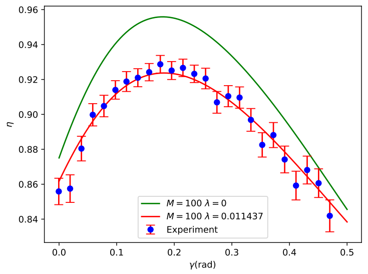
Quantum approximate optimization of the long-range Ising model with a trapped-ion quantum simulator

Guido Pagano, Aniruddha Bapat, Patrick Becker, +12, and Christopher Monroe Authors Info & Affiliations

Contributed by Christopher Monroe, July 30, 2020 (sent for review April 13, 2020; reviewed by John Bollinger, James Freericks, and Vito Scarola)

October 6, 2020 | 117 (41) 25396-25401 | https://doi.org/10.1073/pnas.2006373117





Theoretical Analysis

Not only practical utility, we also provide

- A theoretical analysis of computational complexity.
- Error analysis of the simulation method.
- Rigorous proof of the polynomial scale cost.

For arbitrary $\varepsilon, \delta > 0$, the simulation ensures that the error is less than ε with a probability of at least $1 - \delta$.

Time Complexity:

- $\mathrm{Poly}(n)\mathcal{O}(L)\left(\frac{c}{\varepsilon\sqrt{\delta}}\right)^{\mathcal{O}(1/\gamma)}$ for Case 1
- $\mathrm{Poly}(n)\mathcal{O}\left((nL)^{\frac{1}{2\gamma}\ln\frac{c}{\varepsilon\sqrt{\delta}}+1}\right)$ for Case 2

- Considering current experimental capabilities, the cost scales polynomially with n and L in both cases[20].
- As noise vanishes ($\gamma \to 0$), the cost becomes uncontrolled due to the exponential dependency on γ^{-1}.

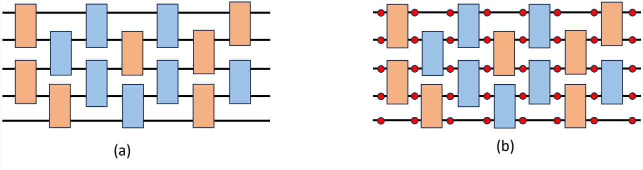
[20] Here n is the number of qubits, L is the circuit depth, c is a constant and γ is a noise-related value.

Pauli Noise Model

Single-qubit Pauli noise model, which is defined as follows:

$$\mathcal{N}(\phi) = (1 - p_x - p_y - p_z)\phi + p_x X\phi X + p_y Y\phi Y + p_z Z\phi Z, \quad (1)$$

p_x, p_y, p_z denote the probabilities of X, Y, Z error occuring, respectively.



It is assumed that single-qubit Pauli noise $\mathcal{N}$ acts independently before each layer and the final observable.

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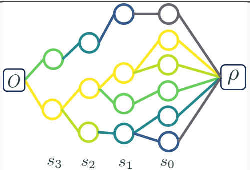
- Case 1: At least two non-zero elements in $\{p_x, p_y, p_z\}$.
- Case 2: Only one non-zero element in $\{p_x, p_y, p_z\}$.

Pauli Path

A Pauli path(Aharonov et al., 2023) for an L-layer circuit is a sequence:

$$s = (s_0, \ldots, s_L) \in \boldsymbol{P}_n^{L+1}, \text{where } \boldsymbol{P}_n = \left\{ \frac{\mathbb{I}}{\sqrt{2}}, \frac{X}{\sqrt{2}}, \frac{Y}{\sqrt{2}}, \frac{Z}{\sqrt{2}} \right\}^{\otimes n}, \tag{2}$$

which describes the evolution path of the quantum state through the quantum circuit.



The observable value can be expressed as the sum (Fourier transform):

$$\langle O \rangle = \sum_{s \in \boldsymbol{P}_n^{L+1}} f(\mathcal{U}(\boldsymbol{\theta}), s, O, \rho), \tag{3}$$

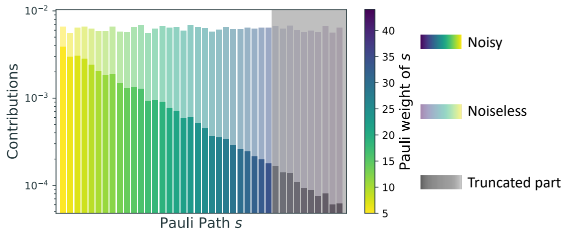
where $f(\mathcal{U}(\boldsymbol{\theta}), s, O, \rho)$ denotes the contribution of a specific Pauli path $s = (s_0, \cdots, s_L) \in \boldsymbol{P}_n^{L+1}$:

$$f(\mathcal{U}(\boldsymbol{\theta}), s, O, \rho) = \mathrm{Tr}\{O s_L\} \left(\prod_{i=1}^{L} \mathrm{Tr}\left\{ s_i \mathcal{U}_i s_{i-1} \mathcal{U}_i^{\dagger} \right\} \right) \mathrm{Tr}\{s_0 \rho\}, \tag{4}$$

Truncated Pauli Paths

When noise is present, contributions from Pauli paths are suppressed:[21]

$$\left|\hat{f}(\mathcal{U}(\boldsymbol{\theta}), s, O, \rho)\right| \leq \gamma^{|s|_{\mathcal{N}}} |f(\mathcal{U}(\boldsymbol{\theta}), s, O, \rho)|, \quad \text{where } \gamma := \min\{p | p \in \{p_x, p_y, p_z\}, p \neq 0\} < 1. \tag{5}$$



This inspires calculates all contributions of the Pauli paths with $|s|_{\mathcal{N}} \leq M$ to approximate $\langle O \rangle$:

$$\widetilde{\langle O \rangle} := \sum_{|s|_{\mathcal{N}} \leq M} \hat{f}(\mathcal{U}(\boldsymbol{\theta}), s, O, \rho). \tag{6}$$

Taking the low-order terms of a Fourier-like expansion.

[21] $|s|_{\mathcal{N}}$ is noise-related Hamming weight.

A Polynomial-Time Classical Algorithm for Noisy Random Circuit Sampling

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The idea of the truncated Pauli path is inspired by the above wonderful work. Different in the noise model and the quantum circuits.

- **Their: Depolarizing noise + Random Circuit Sampling** (2-design).
- **Ours: Pauli-type noise + Typical parameterized quantum circuits** (Clifford gates + Rotation gates).

We also provide an efficient practical simulation method and conclude the efficiency is due to the choices of noise model and quantum circuits.

Find a new "easy island" in the "hard ocean" of quantum circuits simulations.

Error Analysis

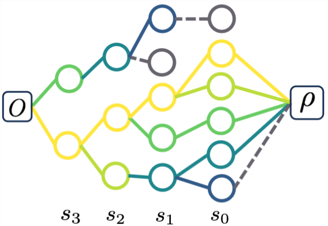
Lemma

Suppose the quantum circuit $\mathcal{U}(\boldsymbol{\theta})$ *is splittable, for* $\forall \nu > 0$*, given* $M \geq \frac{1}{4\gamma} \ln \frac{\|O\|_\infty^2}{\nu}$*, where* $\gamma := \min\{p | p \in \{p_x, p_y, p_z\}, p \neq 0\}$*. Then* **the mean-square error** $\mathbb{E}_{\boldsymbol{\theta}} \left| \widetilde{\langle O \rangle} - \langle O \rangle \right|^2 \leq \nu$*, where* $\boldsymbol{\theta}$ *satisfies uniformly distributed in* $[0, 2\pi]^{\sum_{i=1}^{L} R_i}$*.*

- M is independent of the number of qubits n, the circuit depth L and circuit construction.

Observable's back-propagation on Pauli paths (OBPPP)

To calculate the sum of contributions from Pauli paths with $|s|_{\mathcal{N}} \leq M$, we propose the OBPPP algorithm.



The time complexity of OBPPP is

- $\mathrm{Poly}(n)\mathcal{O}(L)2^M$ for Case 1
- $\mathrm{Poly}(n)\mathcal{O}\left((nL)^{M+1}\right)$ for Case 2

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- Case 1: At least two non-zero elements in $\{p_x, p_y, p_z\}$.
- Case 2: Only one element in $\{p_x, p_y, p_z\}$ non-zero.

n : number of qubits, L : number of layers.

Main Results

Theorem

Suppose the quantum circuit $\mathcal{U}(\boldsymbol{\theta})$ *is splittable and* O, ρ *are (pauli-)sparse. For a fixed* $\gamma := \min\{p | p \in \{p_x, p_y, p_z\}, p \neq 0\}$ *and arbitrary truncation error* ε*, there exists a classical algorithm to determine the truncated noisy observable value* $\widetilde{\langle O \rangle}$*. This value satisfies* $\left| \widetilde{\langle O \rangle} - \langle O \rangle \right| \leq \varepsilon$ *with a probability of at least* $1 - \delta$ *over a uniform distribution of* $\boldsymbol{\theta} \in [0, 2\pi]^{\sum_{i=1}^{L} R_i}$.

The time complexity is

- $\mathrm{Poly}(n)\mathcal{O}(L)\left(\frac{\|O\|_\infty}{\varepsilon\sqrt{\delta}}\right)^{\mathcal{O}(1/\gamma)}$ *for Case 1*
- $\mathrm{Poly}(n)\mathcal{O}\left((nL)^{\frac{1}{2\gamma}\ln\frac{\|O\|_\infty}{\varepsilon\sqrt{\delta}}+1}\right)$ *for Case 2.*

[21]
- Case 1: At least two non-zero elements in $\{p_x, p_y, p_z\}$.
- Case 2: Only one element in $\{p_x, p_y, p_z\}$ non-zero.

O is the observable operator, $\boldsymbol{\theta}$ is the rotation angles, n is the number of qubits, L is the circuit depth.

Corollary

For depolarizing noise, assume the quantum circuit $\mathcal{U}(\boldsymbol{\theta})$ is splittable and both O, ρ are (pauli-)sparse, with $\|O\|_\infty$ fixed. To estimate $\widetilde{\langle O \rangle}$ with $\mathbb{E}_{\boldsymbol{\theta}}\left|\widetilde{\langle O \rangle} - \langle O \rangle\right|^2$ less than a sufficiently small constant, we have

1. If $\gamma = \Omega(\frac{1}{\log L})$, a classical algorithm exists that can simulate the circuit in time $\mathrm{Poly}\,(n, L)$.

2. If $\gamma = \mathcal{O}\left(\frac{1}{L}\right)$, there are instances where OBPPP method exhibits exponential time complexity with respect to L.

- γ is essential to keep below $o(\frac{1}{\log L})$ to ensure the quantum circuit simulation is hard.

Simulating noiseless near-Clifford circuits

Can we use the Pauli path integral method to simulate the ideal noiseless quanrum circuits?

Zhang, R., Shao, Y., Wei, F., Cheng, S., Wei, Z., & Liu, Z. (2024).**Clifford perturbation approximation for quantum error mitigation.** *arXiv preprint arXiv:2412.09518*

- **Simulation Method:** A method to simulate the noiseless observable value of near-Clifford circuits (small angle space): Sparse Pauli Dynamics (SPD)[22].
- **Application:** The near-Clifford circuits noiseless simulation results can be used to mitigate the noise in real quantum experiments.

[22]Begušić et al., 2024.

Pauli Path Integral For Noiseless Circuits

When the rotation parameters are located in the small angle space $\Theta = \{\boldsymbol{\theta} \mid |\theta_i| \leq \theta_*, i = 1, \cdots, L\}$, the truncation error can be upper bounded, as summarized in the following theorem.

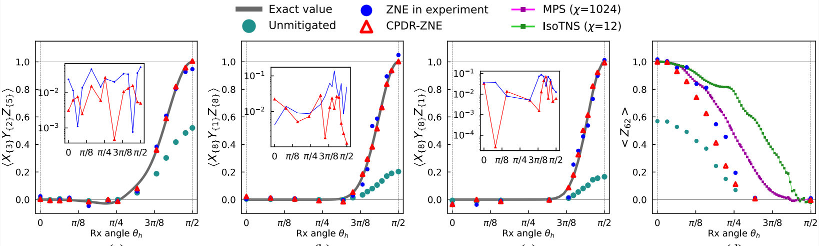
Theorem

For any given $\delta > 0$, $M > 0$ satisfies $\frac{\ln 1+\frac{\delta}{2}}{L-M} \leq \frac{\ln 2}{M}$, and Pauli observable O:

- *If $\theta_* = \frac{\ln 1+\frac{\delta}{2}}{L-M} = \mathcal{O}\left(\frac{1}{L-M}\right)$, then the truncation error satisfies $\left|\langle O\rangle - \langle O\rangle^{(M)}\right| \leq \delta$ for all $\boldsymbol{\theta} \in \Theta$.*
- *In average case, if $\theta_* = \sqrt{\frac{3\ln 1+\frac{\delta}{2}}{L-M}} = \mathcal{O}\left(\frac{1}{\sqrt{L-M}}\right)$, then the mean square error $\mathbb{E}_{\boldsymbol{\theta}\in\Theta}[(\langle O\rangle - \langle O\rangle^{(M)})^2] \leq \delta$.*

[22] O is the observable operator, $\boldsymbol{\theta}$ is the rotation angles, n is the number of qubits, L is the circuit depth.

Clifford Perturbation Data Regression (CPDR)



(a) (b) (c) (d)

Conclusion

Summary

- We propose a polynomial-scale classical algorithm to simulate the observable value of the noisy quantum circuits.
- Containing most variational quantum algorithms.
- The efficiency of the algorithm is verified by IBM's 127-qubit experiments, and can be used to fit the raw experimental data.
- The algorithm is also efficient for the improved experimental setting proposed by Anand et al., 2023.
- The efficiency of the algorithm is irrelevant to the locality of the gates and the entanglement entropy.
- For noiseless circuits, Pauli path integral method can also be used to simulate the noiseless observable value of near-Clifford circuits.

Future Work

- Consider other circuit ensembles (local scrabling) and noise models (non-unital).
- Combing with tensor network (stablizer tensor network).
- Find noise bottleneck in quantum circuits.
- Worst-case analysis, noise threshold, monte-carlo method?

Thank you

Backup slides

Sometimes, it is useful to add slides at the end of your presentation to refer to during audience questions.

The best way to do this is to include the `appendixnumberbeamer` package in your preamble and call `\appendix` before your backup slides.

metropolis will automatically turn off slide numbering and progress bars for slides in the appendix.