Predicting many properties of a quantum system from very few measurements

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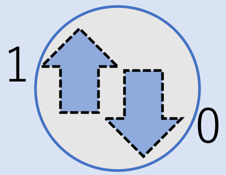
Reference : *Nat. Phys.* **16**, 1050–1057 (2020)

Authors : Hsin-Yuan Huang, Richard Kueng, and John Preskill

1. Introduction

Quantum computer

Unit of information:
→Qubit



$\alpha|0\rangle + \beta|1\rangle$

IBM Q

New computational methods that have been developed recently.

apply

Simulation of Quantum Physics

- Quantum many body system
- Lattice quantum field theory

When analytical calculations are not feasible, observables $\langle \mathcal{O} \rangle$ are computed numerically

Energy, correlation function etc

Today's topic :

Efficiently extracting many physical observables from a quantum computer.

1. Introduction

Why do we need quantum computers?

The sign problem

- In lattice QFT, people use the path-integral formalism and observables are typically evaluated using Monte Carlo integration
- At finite chemical potential or real-time dynamics, the path-integral weight becomes complex.
- As a result, important sampling breaks down → sign problem

1. Introduction

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- As a result, important sampling breaks down → sign problem

The limitations of tensor networks

- To circumvent the sign problem, researchers are turning to the Hamiltonian formalism.
- Tensor network methods work well in (1+1)D systems where the entanglement follows an area law.
- However, they become inefficient in higher dimensions or in systems exhibiting volume-law entanglement, where the required bond dimension grows rapidly.

1. Introduction

Why do we need quantum computers?

The sign problem

The limitations of tensor networks

Quantum computers can solve these problems.

Quantum computers

- Quantum computers are the computers built from quantum-mechanical components that obey the laws of quantum mechanics.
  =Qubits
- An n-qubit system can represent a 2^n-dimensional Hilbert space directly.
- They are free from the sign problem.
- Highly entangled states can be prepared naturally.
- Real-time quantum dynamics is implemented directly as unitary time evolution.

1. Introduction

Basics of quantum computer

Quantum states

Super position

1-qubit state : $|\psi\rangle = \alpha_1|0\rangle + \alpha_2|1\rangle$

2-qubits state : $\alpha_{00}|00\rangle + \alpha_{01}|01\rangle + \alpha_{10}|10\rangle + \alpha_{11}|11\rangle$

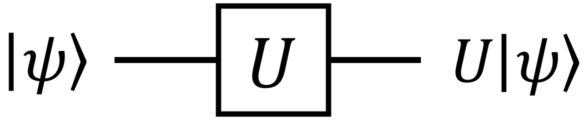
$\vdots$

Basic quantum gate operators

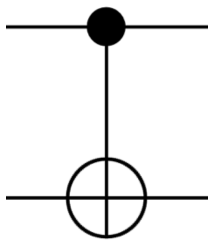
$$H = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}, X = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, Y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \dots$$

$$CNOT = |0\rangle\langle 0| \otimes 1 + |1\rangle\langle 1| \otimes X, \cdots$$

Quantum circuit notation



$U = H, X, Y \dots$ etc

$CNOT =$ 

※Arbitrary unitary operators can be written in terms of basic quantum gates.

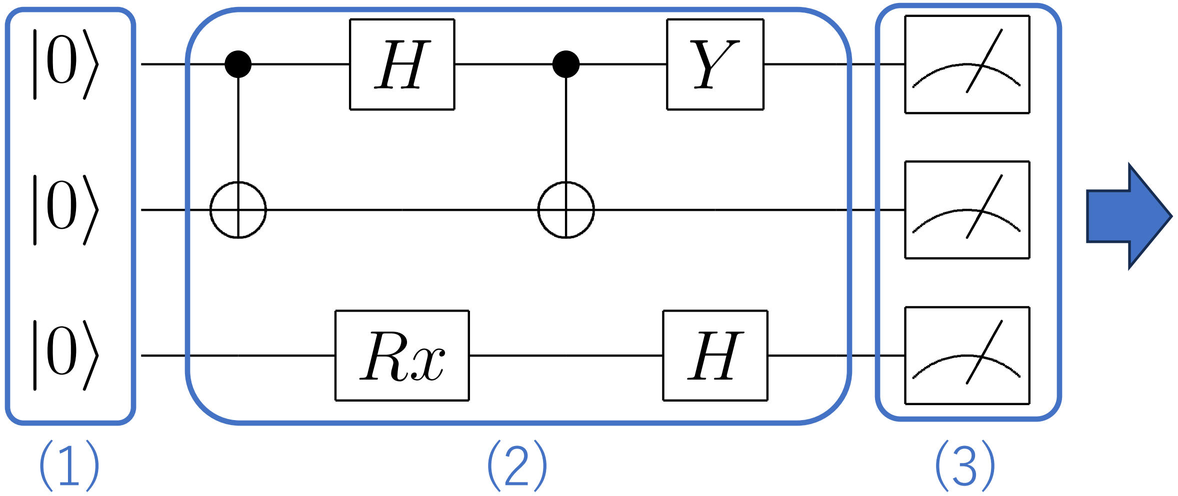
1. Introduction

Quantum computation consists of three essential steps:

(1) Prepare an initial state $|0\rangle^{\otimes n}$

(2) Apply a sequence of quantum gates

(3) Measure in the computational basis



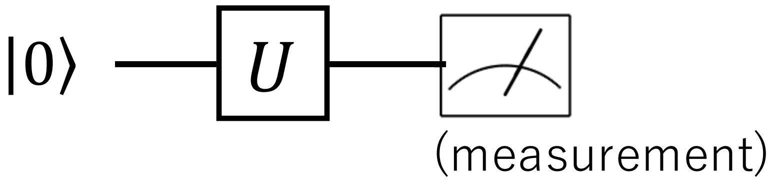
Outcome
$|b_1 b_2 \dots b_n\rangle$
↑ binary number

By repeatedly performing these three steps and collecting statistics from the measurement outcomes, we carry out quantum computation.

1. Introduction

The simple example : calculation of $\langle Z \rangle$

Let us consider estimating expectation value $\langle Z \rangle$ for the quantum state $|\psi\rangle = U\,|0\rangle$.



$|\psi\rangle = \alpha|0\rangle + \beta|1\rangle$

Outcomes : $\begin{cases} |0\rangle \text{ with probability } |\alpha|^2 \\ |1\rangle \text{ with probability } |\beta|^2 \end{cases}$

Repeating this experiment many times, we can estimate $|\alpha|^2$ and $|\beta|^2$ by

$$|\alpha|^2 \approx \frac{N_0}{N_{\text{shots}}}, \qquad |\beta|^2 \approx \frac{N_1}{N_{\text{shots}}}$$

N_{shots} : the total number of experiments
$N_{0/1}$: the number of measurement outcome 0/1

Then, the expectation value $\langle Z \rangle$ is estimated as follows;

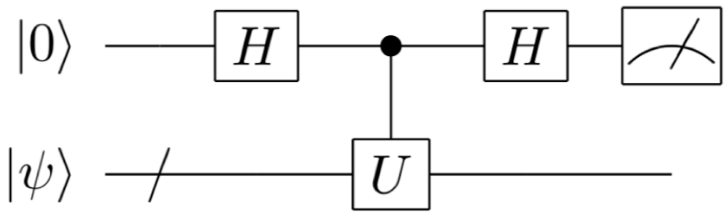
$$\langle Z \rangle = |\alpha|^2 - |\beta|^2 \approx \frac{N_0 - N_1}{N_{\text{shots}}}$$

1. Introduction

When we extend to multi-qubits systems, the computational possibilities expand dramatically.

By introducing ancilla qubits (auxiliary qubits), we can implement more sophisticated operations.

Hadamard test : ancilla qubits→



$\rightarrow \langle U \rangle$

Examples of quantum algorithms:

- Hadamard test : estimation of $\langle U \rangle$ for arbitrary unitary U
- SWAP test : estimation of $\langle \psi | \phi \rangle$
- Quantum Fourier transform : discrete Fourier transformation
- Phase estimation : estimation of eigenvalue of unitary operator
- Grover's algorithm : search algorithm for solution $f(x) = 1$

These quantum algorithms enable us to estimate relevant quantities and address specific computational tasks.

1. Introduction

Let me consider the following goal.

Goal : Estimating M different physical observables, where M is large.

$$\langle \mathcal{O}_i \rangle = \mathrm{Tr}[\mathcal{O}_i \, \rho], \qquad i = 1,2, \ldots M \gg 1$$

We can estimate individual $\langle \mathcal{O}_i \rangle$ by known quantum algorithm (e.g. Hadamard test)
However…

Problems

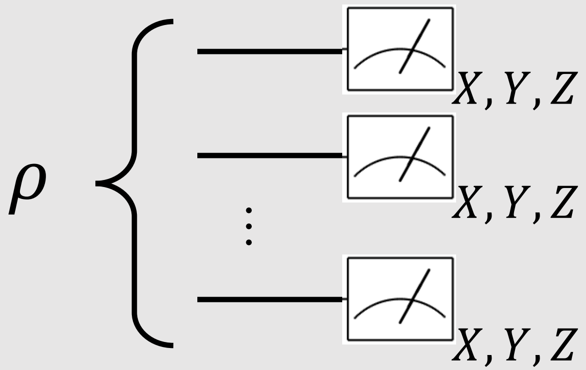
- Naively, we need to design and execute M different quantum circuits.
  →△We must perform $\mathcal{O}(M)$ measurements.

- Many algorithms also require ancilla qubits, increasing the total number of qubits and circuit depth.
  →△Current quantum computers are still small and contain noise.

- The required gate are often complex and difficult to implement on near term quantum computers.

1. Introduction

Quantum state tomography : reconstructing the full density matrix ρ of a quantum system.
[Sugiyama-Turner-Murao 2013]



$$\rho = \frac{1}{2^n} \sum_{i=1}^{4^n} \langle P_i \rangle P_i$$

$$P_i \in \{I, X, Y, Z\}^n$$

Problems

- Needs to measure in many different basis (Pauli X, Y, Z)

  →△Required the number of measurements is $\mathcal{O}(3^n)$ for n-qubits system.
- Postprocessing is computationally expensive $(= \mathcal{O}(4^n))$

  →△Impractical for large system.

Quantum state tomography is Not efficient for estimating many observables

1. Introduction

Goal : Estimating M different physical observables, where M is large.

$$\langle \mathcal{O}_i \rangle = \mathrm{Tr}[\mathcal{O}_i\, \rho], \qquad i = 1,2, \dots M \gg 1$$

Estimating $\langle \mathcal{O}_i \rangle$ by know quantum algorithm

- M different quantum circuits
- # of measurement $\sim\mathcal{O}(M)$
- Ancilla qubits
- Complex gate operation

➡ ❌ **challenging**

Quantum state tomography

We can estimate ρ directly but,

- # of measurement $\sim\mathcal{O}(3^n)$
- Classical postprocessing cost $\sim\mathcal{O}(4^n)$

➡ ❌ **challenging (Not scalable)**

Are there efficient ways to estimate many observables from a quantum system?

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Are there efficient ways to estimate many observables from a quantum system?

➡ **Classical shadow** [Huang-Kueng-Preskill 2020]

1. Introduction

Short summary of classical shadow

- Estimates M different physical observables from only $\mathcal{O}(\log M)$ measurements.
  →**Exponential speed up**
- Dones not use ancilla qubits or multiple copies of system.
  → **The number of required qubits is minimal.**
- Requires only shallow randomized circuits
  → **Suitable for current quantum devices**
- The authors demonstrate its effectiveness across various observables, including two-point correlation functions, energy, and entanglement entropy.

Outline

1. Introduction
2. Classical shadow
3. Applications and numerical results
4. Summary

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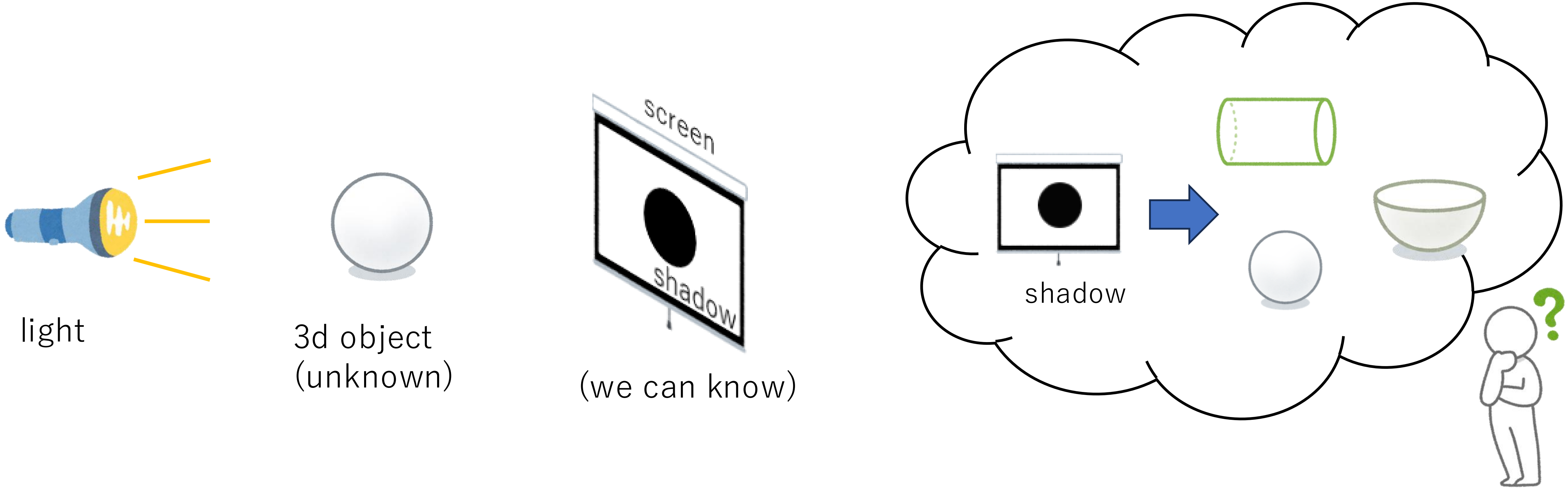
2. Classical shadow

Before introducing the algorithm of classical shadow, let me explain a intuition.
Reconstructing a 3d object from 2d shadows.

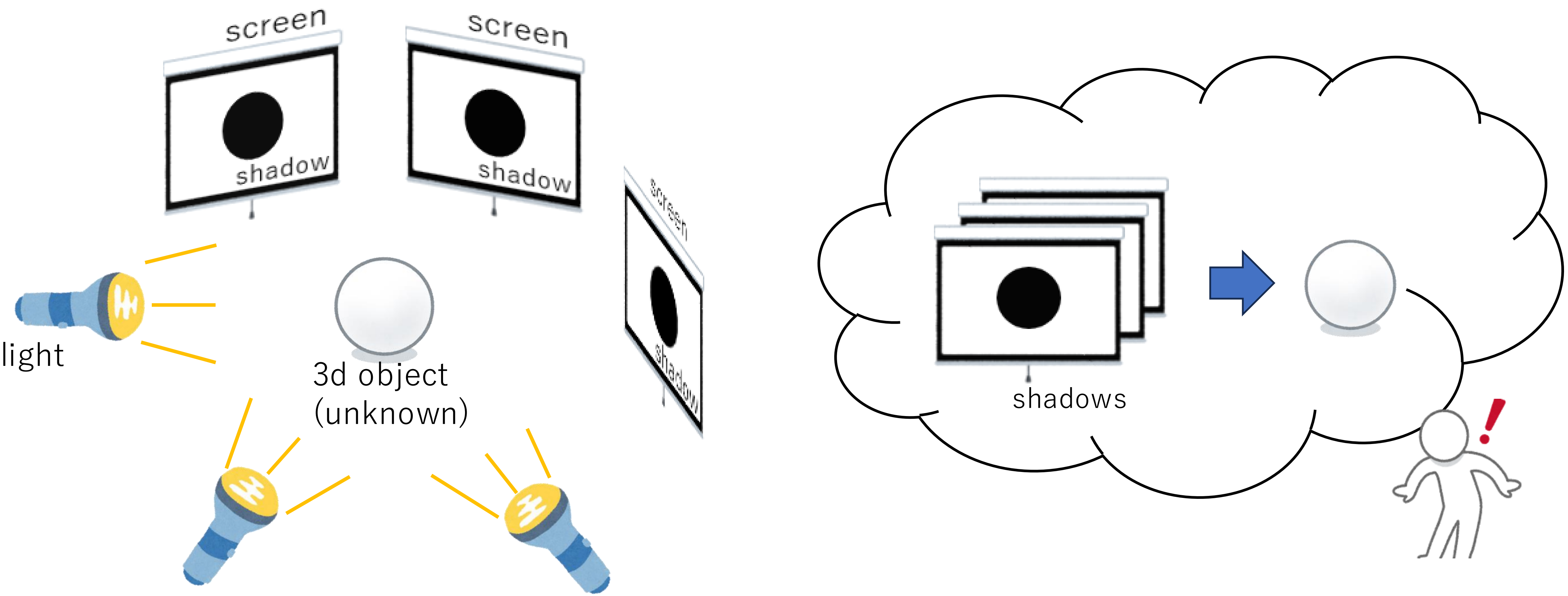


We cannot reconstruct the 3d object from single shadow.

2. Classical shadow

Before introducing the algorithm of classical shadow, we get intuition.

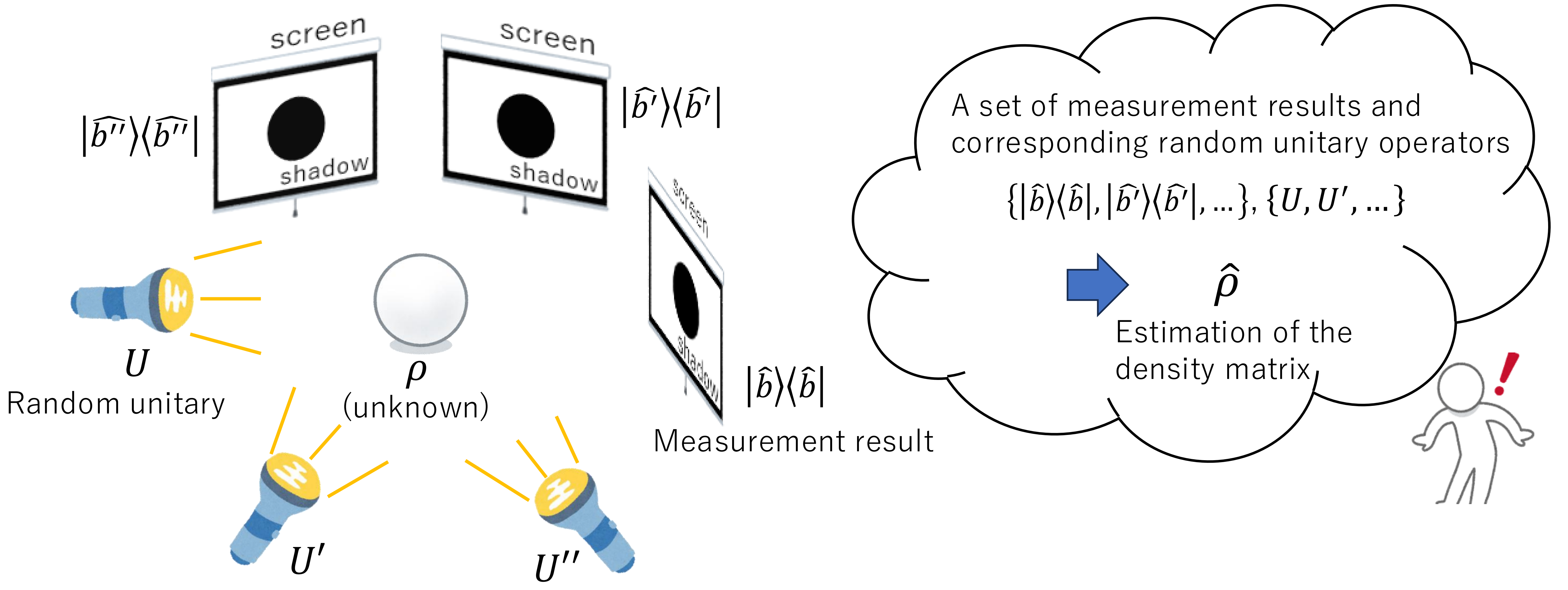
<u>Reconstructing a 3d object from 2d shadows.</u>



If we collect many shadows from various directions, we can estimate the 3d object.

2. Classical shadow

The idea of classical shadow:

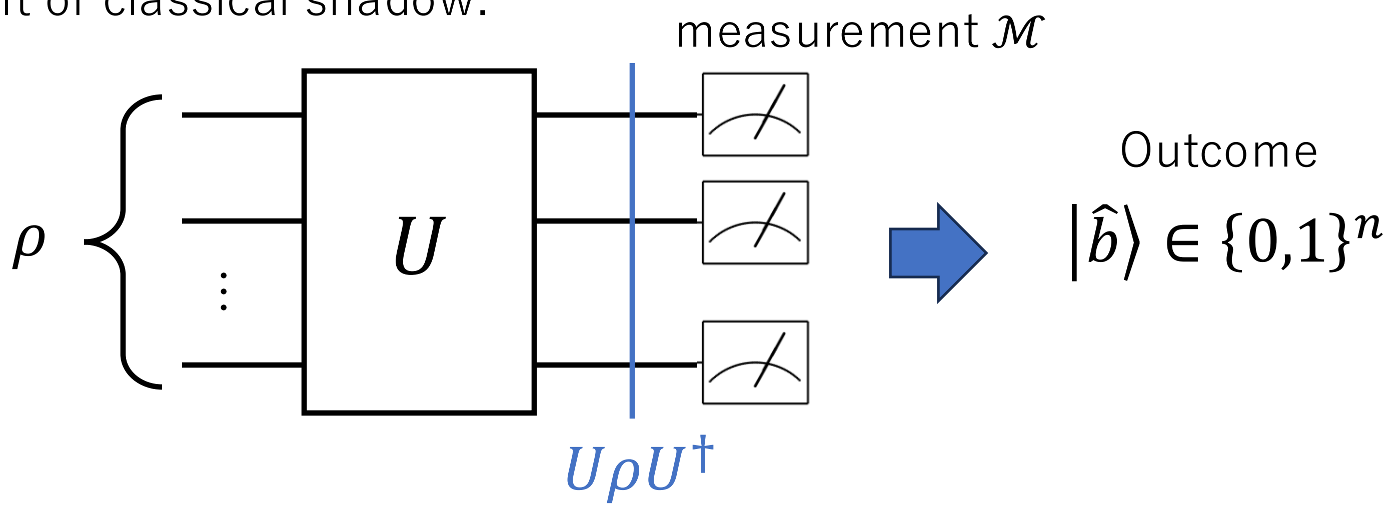


If we collect many measurements results with various basis, we can estimate the density matrix.

2. Classical shadow

Consider the n qubits system.

The quantum circuit of classical shadow:



Procedures

1. Choose a random unitary $U \in \mathcal{U}$ and apply to the state :$\rho \mapsto U\rho U^\dagger$
2. Perform a computational basis measurement $\mathcal{M}$ and get outcome $|\hat{b}\rangle$
3. Restore the classical snapshot $U^\dagger|\hat{b}\rangle\langle\hat{b}|U$

Repeating this procedures N times,

$$\mathbb{E}_{\mathcal{U},b}\left[U^\dagger|\hat{b}\rangle\langle\hat{b}|U\right] = \mathcal{M}(\rho)$$

Ensemble average over $\mathcal{U}$ and outcome $b \in \{0,1\}^n$

True density matrix

2. Classical shadow

$$\rho \xrightarrow{\text{random unitary}} U\rho U^\dagger \xrightarrow[\text{(state collapses)}]{\text{measurement } \mathcal{M}} |\hat{b}\rangle\langle\hat{b}|$$

The idea of classical shadow

Classical shadow : $\hat{\rho} = \mathcal{M}^{-1}\left(U^\dagger|\hat{b}\rangle\langle\hat{b}|U\right)$

"A classical guess of the density matrix based on a single measurement outcome"

(where $\mathcal{M}^{-1}$ depends on the unitary ensemble $\mathcal{U}$)

$$\rho = \mathbb{E}_{\mathcal{U},b}[\hat{\rho}]$$

The ensemble average gives the true density matrix

Classical shadow is a classical approximation of the density matrix constructed from a measurement outcome.

2. Classical shadow

Example of 1-qubit classical shadow $\hat{\rho}$

For $n = 1$ case, we can choose $\mathcal{U}$ as Clifford random unitaries $\mathrm{Cl}(2)$:

$$\mathrm{Cl}(2) = \{U \in \mathrm{U}(2) | \forall P \in \mathcal{P}, UPU^\dagger \in \mathcal{P}\}$$,where $\mathcal{P}$ is Pauli group

Classical shadow per single measurement:

$$\hat{\rho} = \mathcal{M}^{-1}\left(U^\dagger \left|\hat{b}\right\rangle\left\langle\hat{b}\right| U\right) = 3U^\dagger \left|\hat{b}\right\rangle\left\langle\hat{b}\right| U - I$$, where $U \in \mathrm{Cl}(2)$

It is mathematically shown that this classical shadow reproduces the density matrix ρ.

$$\mathbb{E}_{\mathcal{U},b}[\hat{\rho}] = \rho$$

(※This result follows from the fact that Clifford unitaries form a unitary 2-design.

$$\mathbb{E}_{\mathcal{U},b}[\hat{\rho}] = \underbrace{\mathbb{E}_{\mathcal{U}}\left[\sum_b \underbrace{\langle b|U\rho U^\dagger|b\rangle}_{\text{probability}} \left(3U^\dagger|b\rangle\langle b|U - I\right)\right]}_{\text{Unitary 2-design}} = \rho$$)

2. Classical shadow

Based on this idea, the following algorithm was proposed: [Huang-Kueng-Preskill 2020]

Algorithm

1. Perform the experiment N times and collect the classical shadows:

   $\{\hat{\rho}_1, \hat{\rho}_2, \ldots, \hat{\rho}_N\}$, where $\hat{\rho}_k = \mathcal{M}^{-1}\left(U_k^\dagger |\widehat{b_k}\rangle\langle\widehat{b_k}| U_k\right)$, for $k = 1, \ldots N$

2. Estimate the expectation values of M observables using a classical computer :

   $\langle \hat{\mathcal{O}}_i \rangle = \frac{1}{N} \sum_{k=1}^{N} \mathrm{Tr}[\mathcal{O}_i \hat{\rho}_k]$, for $i = 1, \ldots, M$

3. Increase the number of experiments N until the statistical error reaches the desired accuracy ϵ .

※ The required classical memory is $\mathcal{O}(NM)$

A finite number of classical shadows is sufficient to estimate observables.

2. Classical shadow

Theoretical guarantee of Classical shadows:

Theorem 1 [Huang-Kueng-Preskill 2020]

To estimate M observables up to accuracy ϵ, the required number of measurements N is given by:

$$N = \mathcal{O}\left(\frac{\log(M)}{\epsilon^2} \max_i \|O_i\|_{\text{shadow}}\right)$$

where $\|O_i\|_{\text{shadow}}$ depends on the unitary ensemble $\mathcal{U}$ used to generate the classical shadows.

Examples of shadow norms for different unitary ensembles:

$$\begin{cases} \mathcal{U} = \mathrm{Cl}(2^n) \quad \Rightarrow \|O_i\|^2{}_{\text{shadow}} \leq \mathrm{Tr}\left[O_i^2\right] \\ \mathcal{U} = \mathrm{Cl}(2)^{\otimes n} \Rightarrow \|O_i\|^2{}_{\text{shadow}} \leq 4^k \|O_i\|^2 \end{cases}$$

$\|O_i\|$: operator norm

where k denote the locality of O_i , e.g. $O_i = X_1 \otimes Y_2 \Rightarrow \mathrm{k} = 2$.

- The number of required measurements **scales only logarithmically** with the number of observables M.
- The shadow norm determines the difficulty of estimating each observable.

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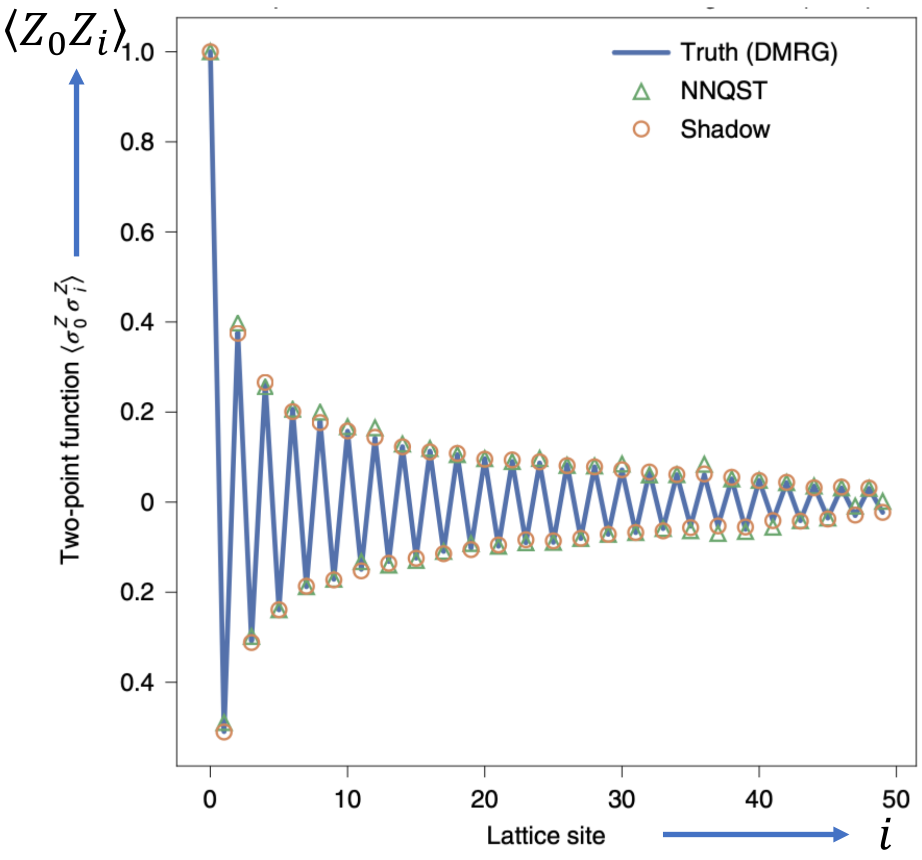
3. Applications and numerical results

Application 1 : 1d transverse Ising model

$$H = J \sum_j Z_j Z_{j+1} + h \sum_j X_j$$,where we set $J = h$.



Goal : two-point functions $\langle Z_0 Z_i \rangle$ for $i = 1, \ldots, N_{\mathrm{site}} = 50$

Exact results(DMRG)

Quantum state tomography [Torlai, et al 2018]

Classical shadow

We use $\mathcal{U} = \mathrm{Cl}(2)^{\otimes N_{\mathrm{site}}}$ and $N = 2^{19}$ measurement snapshots.

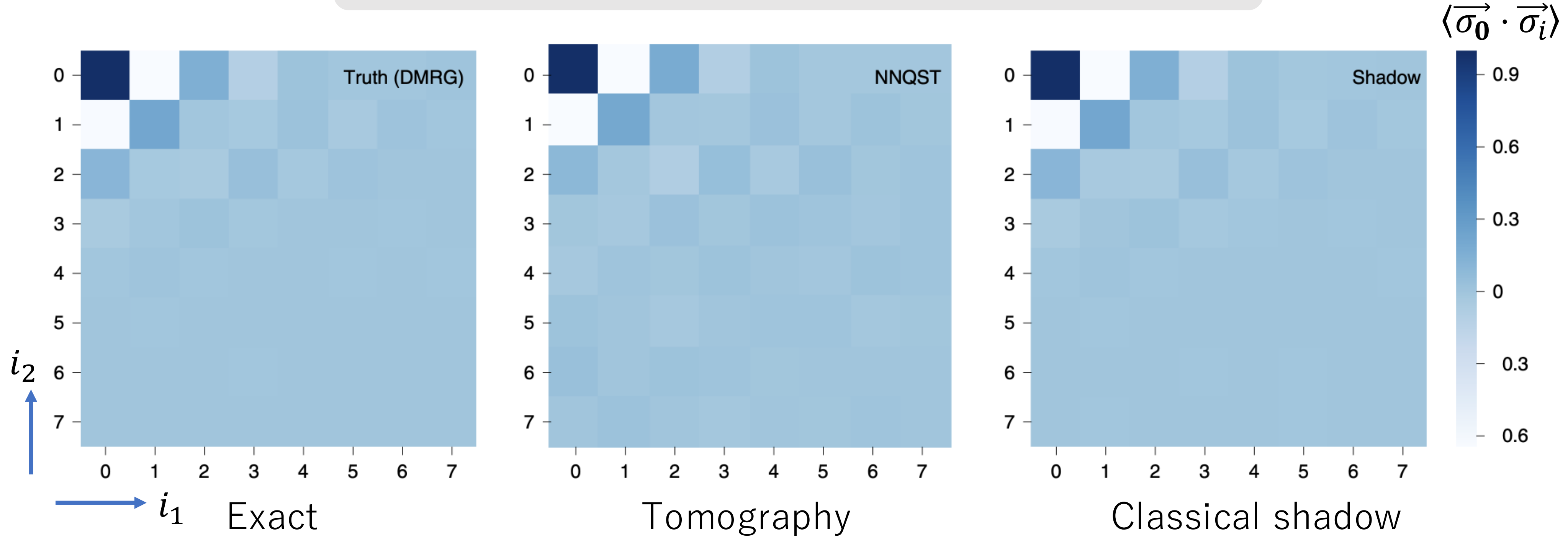
The classical shadow predictions perfectly match the exact results.

3. Applications and numerical results

Application 2: 2d Heisenberg model

$$H = J \sum_{\langle i,j \rangle} \vec{\sigma_i} \cdot \vec{\sigma_j}$$ with an 8×8 triangular lattice

Goal: two-point functions $\langle \vec{\sigma_0} \cdot \vec{\sigma_i} \rangle$ for $i = (i_1, i_2)$



Exact

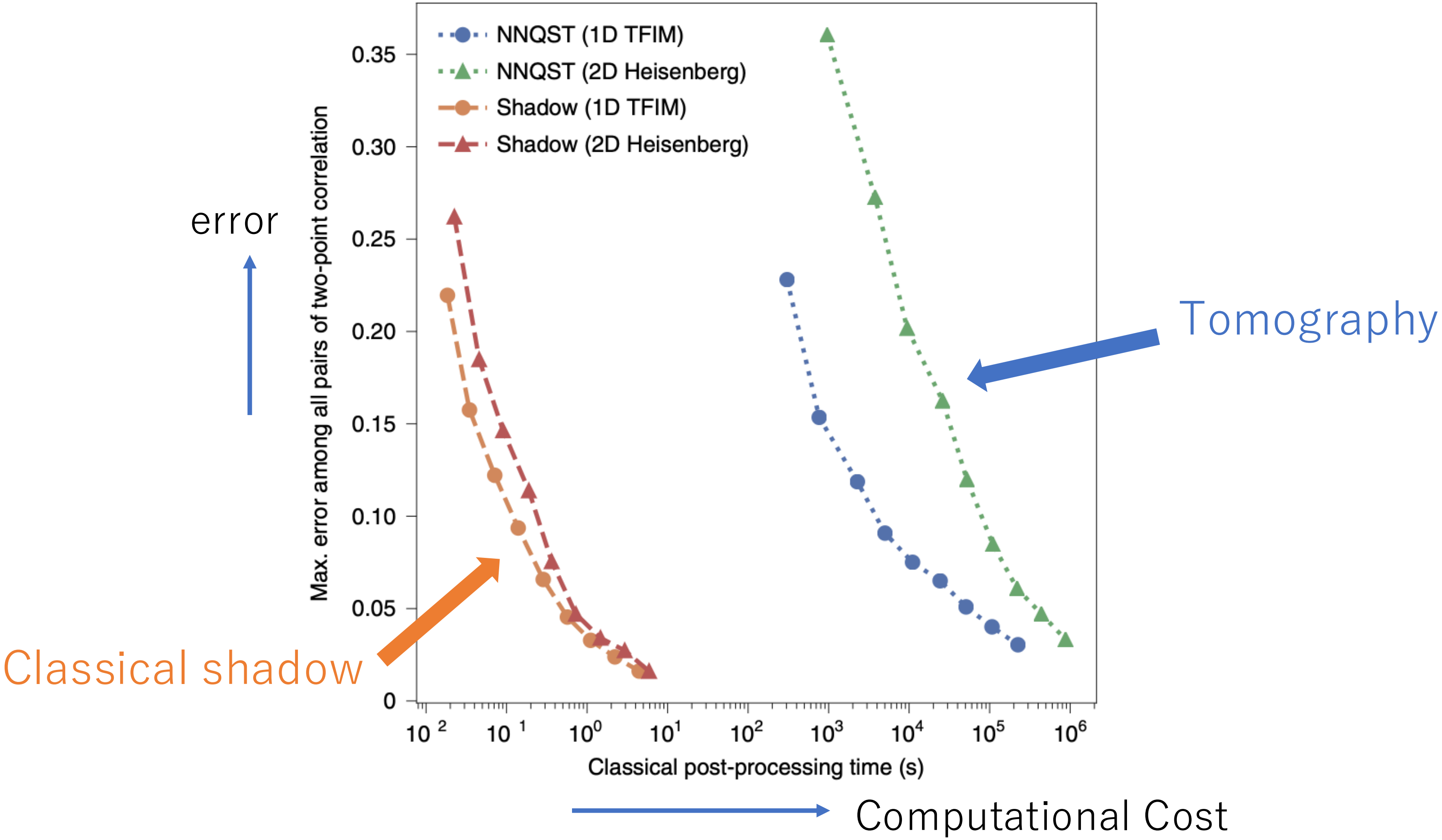
Tomography
[Torlai, et al 2018]

Classical shadow

The classical shadow predictions perfectly match the exact results.

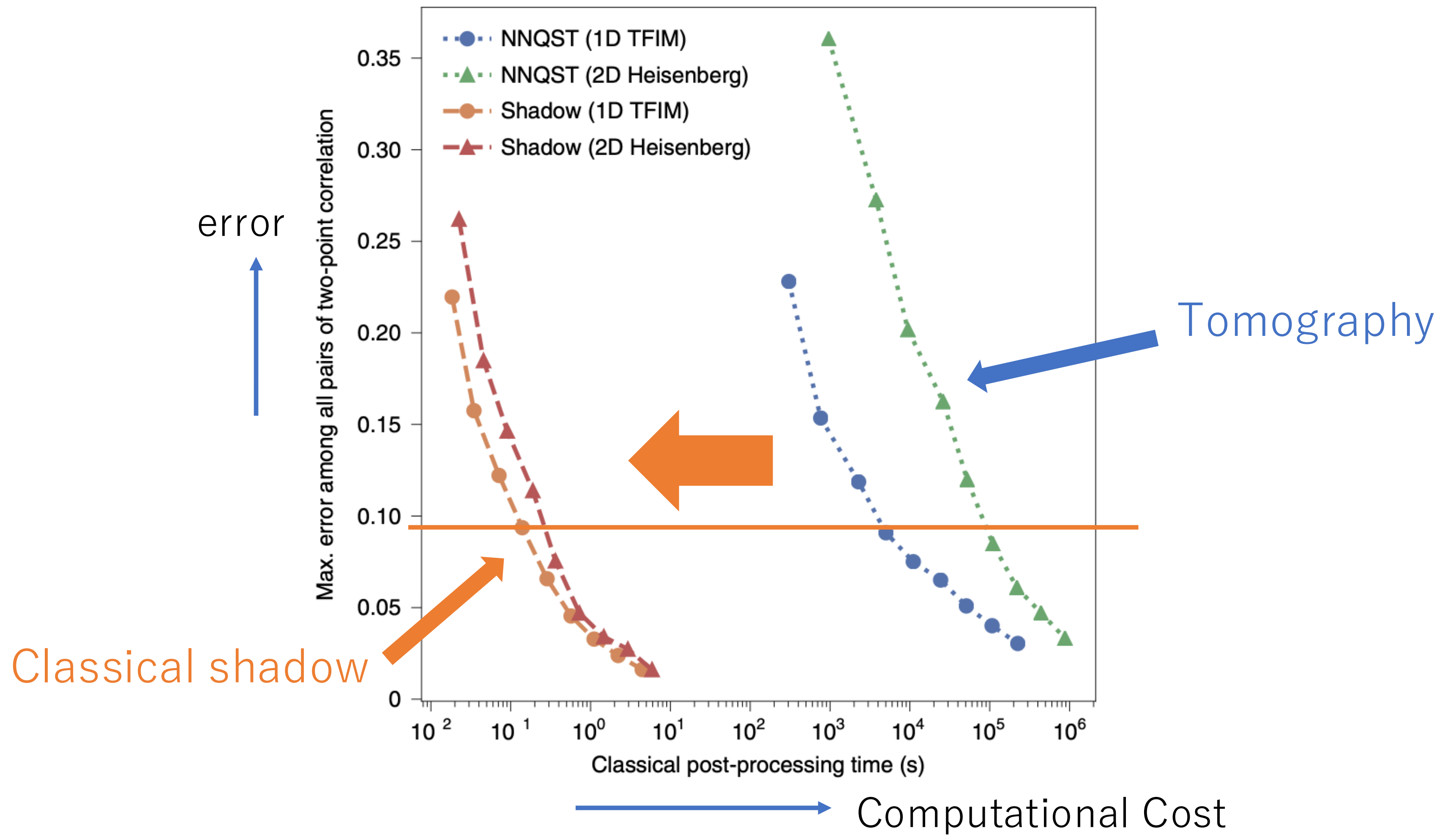
3. Applications and numerical results

Computational cost of application 1 and 2



3. Applications and numerical results

Computational cost of application 1 and 2



Classical shadows achieve comparable accuracy with significantly fewer measurements.

Application 3: Ground state energy estimation in the Schwinger model

$$\mathcal{L} = -\frac{1}{4} F_{\mu\nu}F^{\mu\nu} + i\bar{\psi}\gamma^{\mu}(\partial_{\mu} + igA_{\mu})\psi - m\bar{\psi}\psi \xrightarrow{\text{Jordan-Wigner transformation}} H_{\mathbf{spin}}$$

$H_{\mathbf{spin}}$: spin Hamiltonian

Goal: ground state energy

The ground state of the Schwinger model was studied by VQE in [Kokail, C. et al. 2019].

VQE

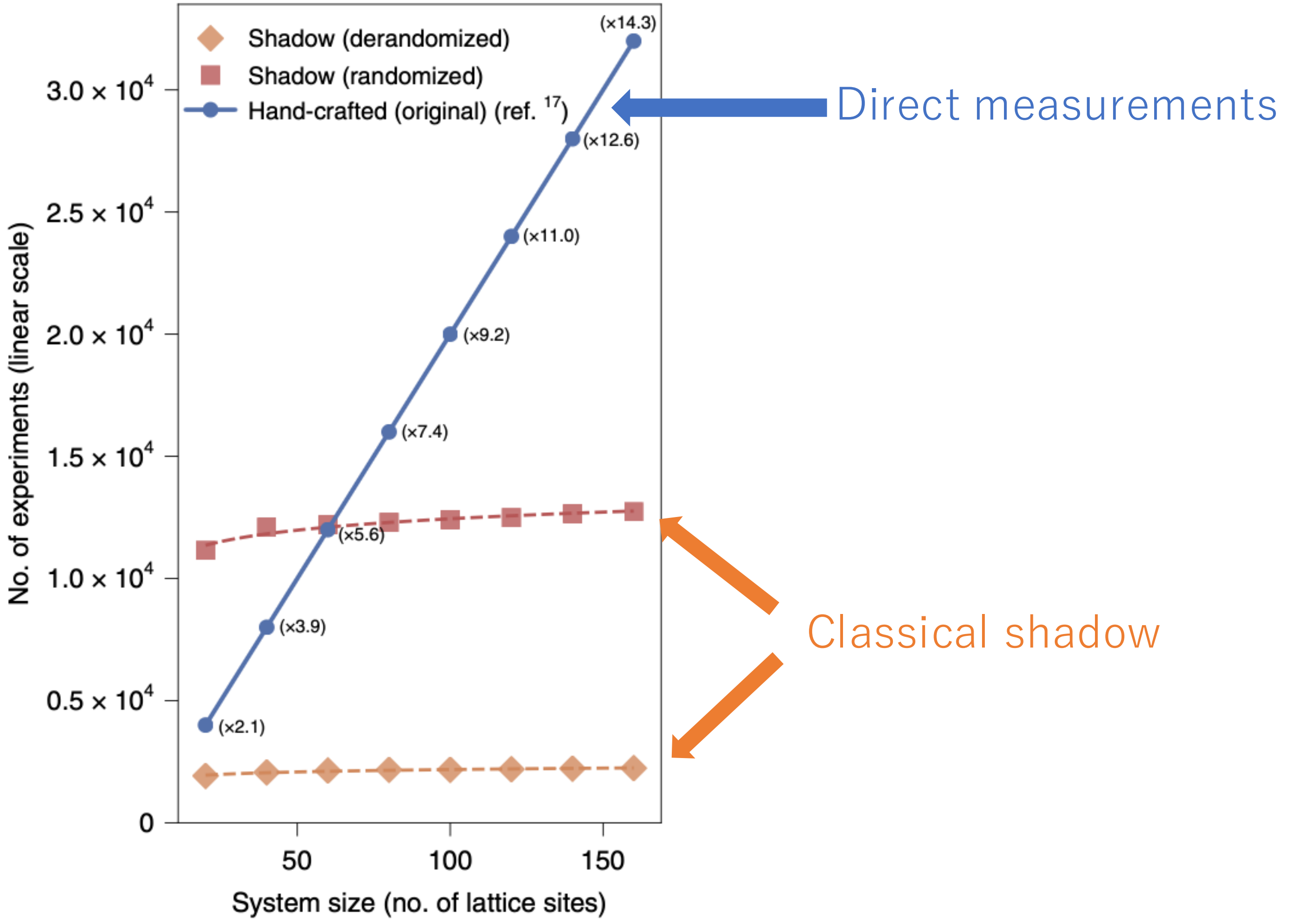
1. Set ansatz $|\psi(\theta)\rangle$, θ: parameters
2. Calculate $\langle H_{\mathbf{spin}}\rangle_{\theta}$ by a quantum computer
3. Update parameters θ to minimize the energy $\langle H\rangle_{\theta}$

We compare classical shadow-based energy estimation with the standard method using direct measurements as implemented in [Kokail, C. et al. 2019].

3. Applications and numerical results

Application 3: Ground state energy estimation in the Schwinger model

Scaling of the number of measurements required to achieve a fixed error.



3. Applications and numerical results

Application 3: Ground state energy estimation in the Schwinger model

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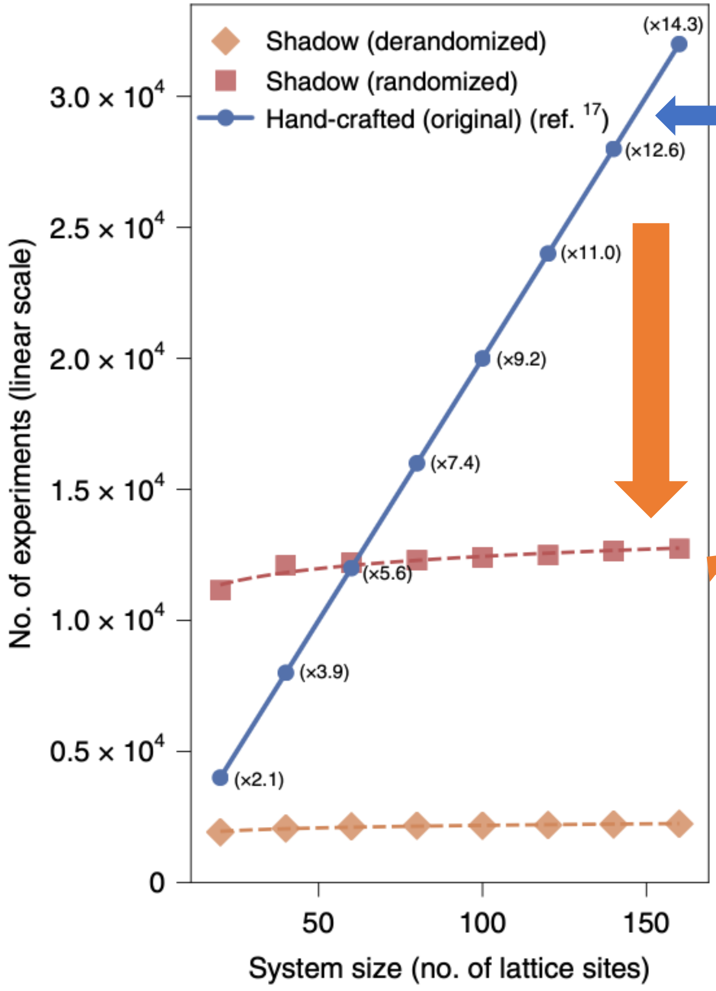

Direct measurements

Classical shadow significantly reduce the required number of measurements

Classical shadow

3. Applications and numerical results

Application 4: Estimating entanglement Rényi entropy

Using classical shadows, one can estimate the purity $\mathrm{Tr}[\rho_A^2]$,which is related to the second Rényi entanglement entropy.

Estimation of purity by classical shadows

$$\mathrm{Tr}[\rho_A^2] \approx \frac{1}{N(N-1)} \sum_{i \neq j}^{N} \mathrm{Tr}\left[\hat{\rho}_{A,i} \hat{\rho}_{A,j}\right]$$

$\{\hat{\rho}_{A,1}, \ldots, \hat{\rho}_{A,N}\}$: classical shadows on subsystem A.

Calculated via pairwise trace overlaps between shadow estimates.

The number of required measurements:

$$N = \mathcal{O}\left(\frac{2^n}{\epsilon^2}\right)$$

n: number of qubits
ϵ: desired statistical error

This cost arises from the non-local nature of entanglement, and the authors showed that it is unavoidable due to fundamental information-theoretical bounds.

Outline

1. Introduction

2. Quantum Algorithm : Classical shadow

3. Applications and numerical results

4. Summary

4. Summary

- Classical shadow efficiently estimates many observables from quantum states.
- Only $\mathcal{O}(\log M)$ measurements are needed to estimate M observables $\langle \mathcal{O}_i \rangle = \mathrm{Tr}[\mathcal{O}_i\, \rho]$.
  →**Exponential speed up!** $i = 1,2, \dots M$
- Requires only shallow quantum circuits →**Suitable for near-term quantum computer**
- Estimating non-local properties such as entanglement requires many measurements, but it is efficient among methods that do not use ancilla or additional qubits.
- **Classical shadows are promising tools for studying quantum many-body systems and quantum field theory simulations on near-term quantum computers.**

Appendix

Appendix

The concrete form of classical shadows

$$\mathcal{U} = \mathrm{Cl}(2^n) \quad \Rightarrow \quad \hat{\rho} = (2^n + 1) U^\dagger |\hat{b}\rangle\langle\hat{b}| U - \mathbb{I}$$

$$\mathcal{U} = \mathrm{Cl}(2)^{\otimes n} \Rightarrow \quad \hat{\rho} = \bigotimes_{j=1}^{n} \left(3 U_j^\dagger |\hat{b}_j\rangle\langle\hat{b}_j| U_j - \mathbb{I} \right)$$

Appendix

Random unitary ensemble $\mathcal{U}$ should be tomographically complete.

For $\rho \neq \sigma$, there exist $U \in \mathcal{U}$ and b s.t.

$$\langle b|U\rho U^\dagger|b\rangle \neq \langle b|U\sigma U^\dagger|b\rangle$$