Improving Classical Shadows with Grouping Strategies

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Motivation

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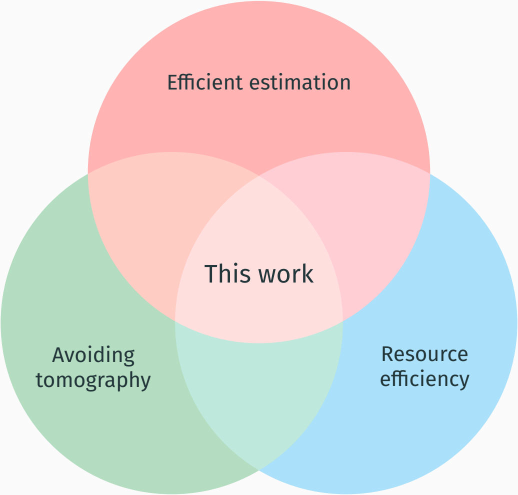
Quantum computing faces three key bottlenecks:



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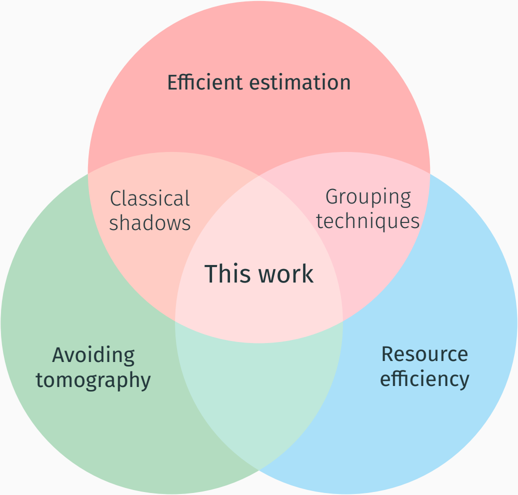

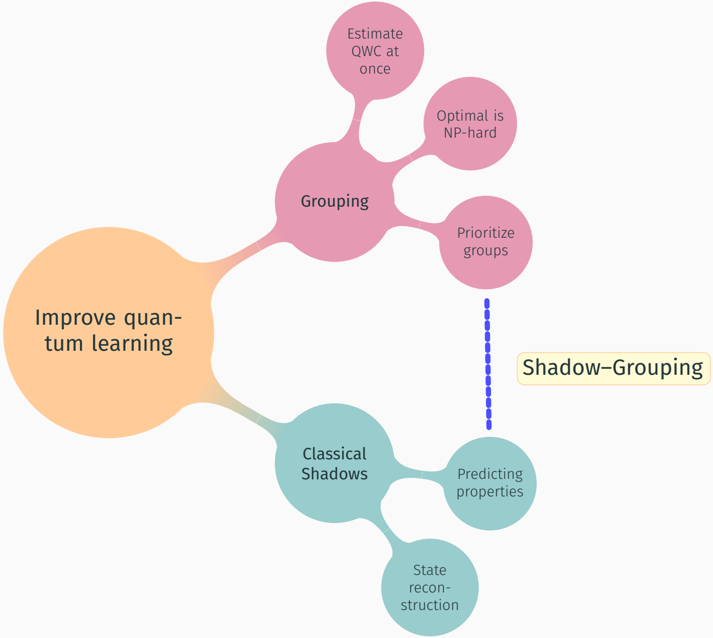
Improve quantum learning
Grouping
Estimate QWC at once
Optimal is NP-hard
Prioritize groups
Classical Shadows
Predicting properties
State reconstruction
Shadow–Grouping

Grouping via Qubit-wise Commutativity

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Two tensor-product observables

$$A = A_1 \otimes \cdots \otimes A_n \qquad \text{and} \qquad B = B_1 \otimes \cdots \otimes B_n$$

qubit-wise commute (QWC) if $[A_i, B_i] = 0$ for all $i = 1, \ldots, n$.

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$$\text{QWC} \implies \text{commutativity} \implies \boxed{\text{common eigenbasis}}$$

Grouping QWC terms allows simultaneous measurement [1].

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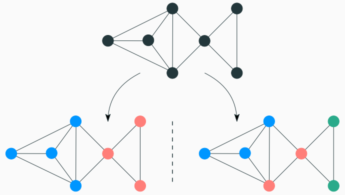
Formulated as a Minimum Clique Cover (MCC) problem on a *graph*:

- Nodes: observables
- Edges: QWC relation
- Find minimal number of *complete subgraphs* (NP-hard [1])



Classical Shadows

Classical Shadows — Basics

Given a quantum state ρ:

- Learn the expectation value of multiple observables $\{O_i\}_{i=1}^{M}$ from a small number of randomized measurements [2].
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Procedure

Given a state ρ, choose an ensemble $\mathcal{U}$ of unitaries. Then:

1. Randomly **choose** $U \in \mathcal{U}$ and **evolve** ρ by U. — $\rho \longmapsto U\rho U^\dagger$
2. **Measure** rotated state in the comp. basis. — $|b\rangle = |0110\ldots101\rangle$
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If $\mathcal{U} = \{\text{single-qubit Clifford gates}\}$, then step 2 is equivalent to measuring in a Pauli basis P_U.

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Problem:

no matches $\implies$ measurements are discarded! [3]

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Suppose we want to estimate the energy $\langle H \rangle$ of a state ρ, where

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Adaptively choose measurement bases that QWC with multiple Hamiltonian terms [4, 5].
Prioritize terms in H by **weights**:

$$\mathrm{weight}\big(O^{(i)}\big) \begin{cases} \uparrow \text{ with } |h_i|, \\ \downarrow \text{ with the } \textbf{number of times } O^{(i)} \text{ has been measured} \end{cases}$$

Algorithm Sketch and Numerical Demonstrations

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Inputs: Hamiltonian decomposition $H = \sum_{i=1}^{M} h_i O^{(i)}$, measurement budget N.

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For each shot $k \in \{1, \dots, N\}$:

1. Compute **weights** based on $|h_i|$ and previous measurements.
2. **Sort** terms by decreasing weight.
3. **Construct a measurement setting** that QWC with as many terms as possible.
4. Measure and **estimate**.

Numerical Demonstrations

- **Tools:** *PennyLane*'s Python library [6].
- **Test cases**: ground state energy estimation of $\mathrm{H_2}$ and LiH molecules [7].

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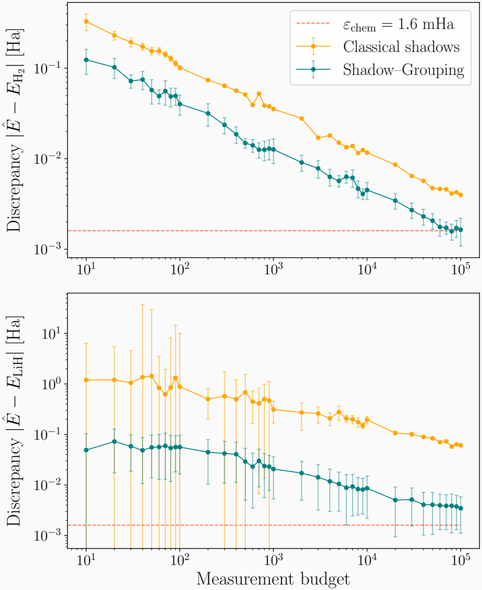
Results

- Up to 18x improvement in accuracy for a fixed measurement budget.
- Reached chemical precision with orders of magnitude fewer measurements.



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All code and data are publicly available in a GitHub repository [8].

Acknowledgements

Acknowledgements

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- Family, friends.

References

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Backup Slides

Classical Shadows + Grouping

Problem: more settings Q that QWC with $O^{(i)} \implies$ better estimation of $\langle O^{(i)} \rangle$. But what about other terms?

Possible solution: **prioritize** QWC-settings.

Assign a **weight** to each term and update it after every shot.

Recall: $H = \sum_{i=1}^{M} h_i O^{(i)}$, with $O^{(i)} \in \mathcal{P}$.

Desirable properties of $\mathrm{weight}\big(O^{(i)}\big)$:

1. Should be **proportional** to $|h_i|$.
2. Should **decrease** if we have estimated $\langle O^{(i)} \rangle$ many times.

In [4], authors propose:

$$\mathrm{weight}\big(O^{(i)}\big) := |h_i| \frac{\sqrt{N_i + 1} - \sqrt{N_i}}{\sqrt{N_i(N_i+1)}},$$

where $N_i \equiv \#$ times we have estimated $\langle O^{(i)} \rangle$ before.

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How do we construct a measurement setting Q?

Recall: Q is a Pauli word and has to QWC with as many terms of H as possible.

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Algorithm ([4]): 4-qubit system. At a certain shot $k \in \{1, \ldots, N\}$:

	Terms				Meas. setting Q_k				
					$\mathbb{I}$	$\mathbb{I}$	$\mathbb{I}$	$\mathbb{I}$	$\longleftarrow$ Initialize
w_1	X	$\mathbb{I}$	Y	$\mathbb{I}$					
w_2	Y	Z	$\mathbb{I}$	$\mathbb{I}$					
w_3	X	Z	$\mathbb{I}$	$\mathbb{I}$					
w_4	Z	Y	$\mathbb{I}$	X					
w_5	X	$\mathbb{I}$	$\mathbb{I}$	Y					
		$\ldots$							

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\begin{array}{c|cccc||cccc|l}
 & \multicolumn{4}{c}{\text{Terms}} & \multicolumn{4}{c}{\text{Meas. setting } Q_k} & \\
\hline
 & & & & & \boxed{\mathbb{I}} & \mathbb{I} & \boxed{\mathbb{I}} & \mathbb{I} & \longleftarrow \text{Initialize} \\
w_1 & \boxed{X} & \mathbb{I} & \boxed{Y} & \mathbb{I} & X & \mathbb{I} & Y & \mathbb{I} & \longleftarrow \text{Change matches} \\
w_2 & Y & Z & \mathbb{I} & \mathbb{I} & & & & & \\
w_3 & X & Z & \mathbb{I} & \mathbb{I} & & & & & \\
w_4 & Z & Y & \mathbb{I} & X & & & & & \\
w_5 & X & \mathbb{I} & \mathbb{I} & Y & & & & & \\
 & & \ldots & & & & & & &
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w_3	X	Z	$\mathbb{I}$	$\mathbb{I}$					
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w_3	X	Z	$\mathbb{I}$	$\mathbb{I}$	X	Z	Y	$\mathbb{I}$	$\longleftarrow$ Change matches
w_4	Z	Y	$\mathbb{I}$	X	X	Z	Y	$\mathbb{I}$	$\longleftarrow$ No changes
w_5	X	$\mathbb{I}$	$\mathbb{I}$	Y	X	Z	Y	Y	$\longleftarrow$ Change matches

No more changes available

$$\Longrightarrow \boxed{Q_k = X_1 \otimes Z_2 \otimes Y_3 \otimes Y_4.}$$

Now update weights of terms that QWC with Q_k and compute setting for shot $k+1$.

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We programmed this algorithm:

$$H = h_1 X_1 Z_2 + h_2 Y_1 Z_3 + h_3 Z_2 Z_3 + h_4 X_1 Y_2 Z_3, \quad 0 < h_1 < h_2 < h_3 < h_4.$$