

Title: Learning to predict arbitrary quantum processes

Speakers: Hsin-Yuan Huang

Series: Perimeter Institute Quantum Discussions

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URL: <https://pirsa.org/23020031>

Abstract: We present an efficient machine learning (ML) algorithm for predicting any unknown quantum process over n qubits. For a wide range of distributions D on arbitrary n -qubit states, we show that this ML algorithm can learn to predict any local property of the output from the unknown process, with a small average error over input states drawn from D . The ML algorithm is computationally efficient even when the unknown process is a quantum circuit with exponentially many gates. Our algorithm combines efficient procedures for learning properties of an unknown state and for learning a low-degree approximation to an unknown observable. The analysis hinges on proving new norm inequalities, including a quantum analogue of the classical Bohnenblust-Hille inequality, which we derive by giving an improved algorithm for optimizing local Hamiltonians. Overall, our results highlight the potential for ML models to predict the output of complex quantum dynamics much faster than the time needed to run the process itself.

Zoom link: <https://pitp.zoom.us/j/93857777354?pwd=c044blZuQVhLS200ME4vN25uaGJudz09>

Learning to predict arbitrary quantum processes

Credit: DALL·E



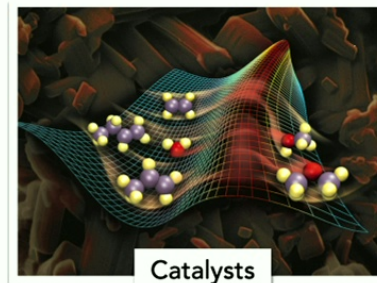
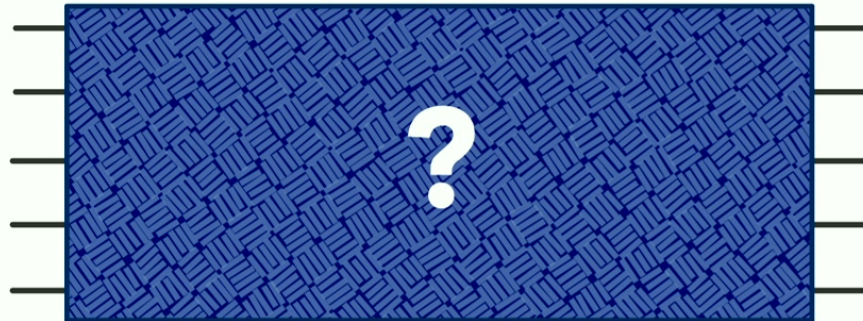
Presenter: Hsin-Yuan Huang (Robert)
Joint work with Sitan Chen and John Preskill



Motivation

- We have seen substantial recent progress on efficiently learning to predict quantum states.
- Are there efficient algorithms for learning to predict quantum circuits / processes?

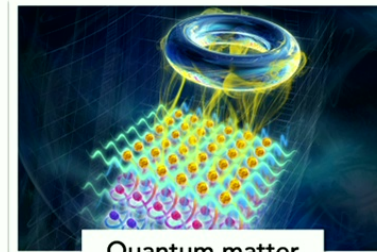
A high-complexity quantum process



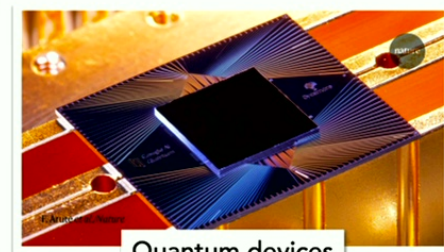
Catalysts



Pharmaceutics



Quantum matter



Quantum devices

Image credits: (Top left) <https://www.energy.gov/science/doe-explainscatalysts> (Top right) <https://theconversation.com/as-pharmaceutical-use-continues-to-rise-side-effects-are-becoming-a-costly-health-issue-105494> (Bottom left) <https://news.mit.edu/2019/ultra-quantum-matter-uqm-research-given-8m-boost-0529> (Bottom right) <https://www.nature.com/articles/d41586-019-03213-z>

The Setting

- In this work, we focus on training an ML model to learn and predict

$$\rho, O \mapsto f_{\mathcal{E}}(\rho, O) = \text{Tr}(O\mathcal{E}(\rho)),$$

where ρ is an input quantum state, \mathcal{E} is an (unknown) CPTP map, and O is an observable.

- This includes any function computable by a quantum computer (in exponential time).

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- This includes any function computable by a quantum computer (in exponential time).

Example 1

*Predicting outcomes of
physical experiments*

ρ : initial state given by classical input x

\mathcal{E} : the physical process in the experiment

O : what the scientist measure



Example 2

*Training
quantum neural networks*

ρ : input state encoding classical input x

\mathcal{E} : the quantum neural network to learn

O : a single fixed observable



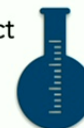
Example 3

*Speeding up
complex quantum dynamics*

ρ : initial state of the physical system

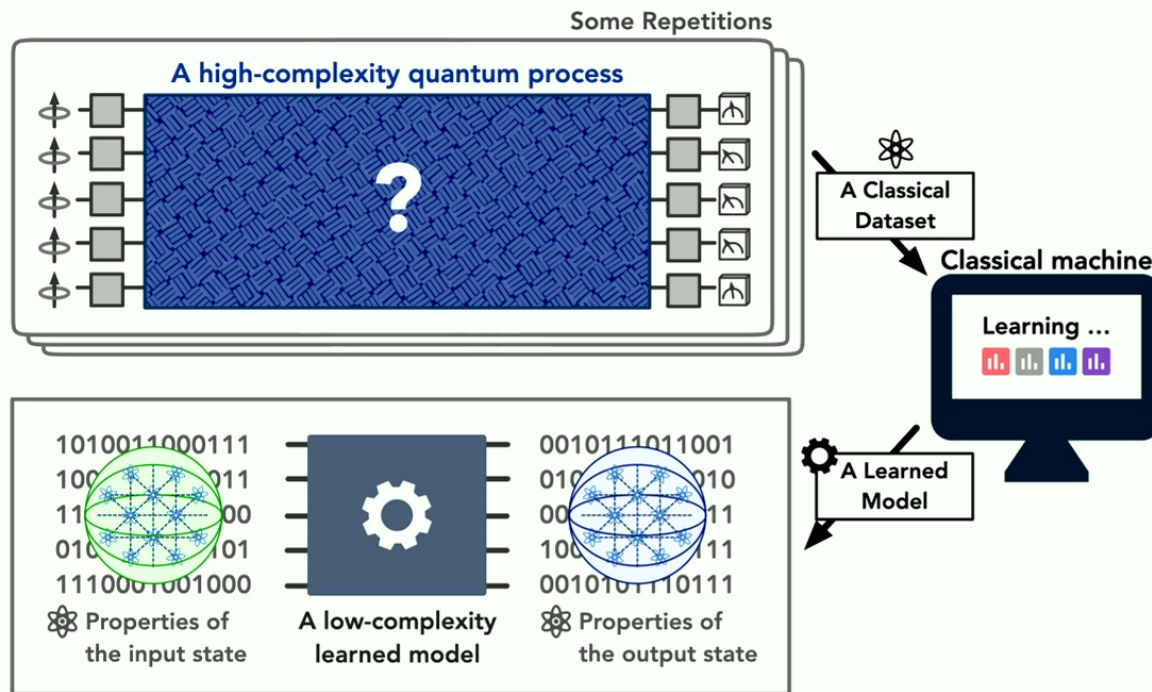
\mathcal{E} : the quantum dynamics to speed up

O : the property we want to predict



The goal of this work

Given an n -qubit CPTP map \mathcal{E} that represents a high-complexity quantum process



A Classical Problem

- Given an unknown classical Boolean circuit C mapping n bits to n bits.
- The input is now an n -bit string $x \in \{-1, 1\}^n$.
- The 1st output bit of C for input x is equal to $f_C(x) = \text{Tr}(Z_1 C(|x\rangle\langle x|))$.



Worst-case hardness

- The function f_C is equiv. to an exponentially long vector $\{-1,1\}^{2^n}$ with **no structure**.
- To learn a model $h(x)$, such that $\left| h(x) - f_C(x) \right|^2 < 0.5, \forall x \in \{-1,1\}^n$, we must query $f_C(x)$ for all input x . Query complexity: $\Theta(2^n)$.



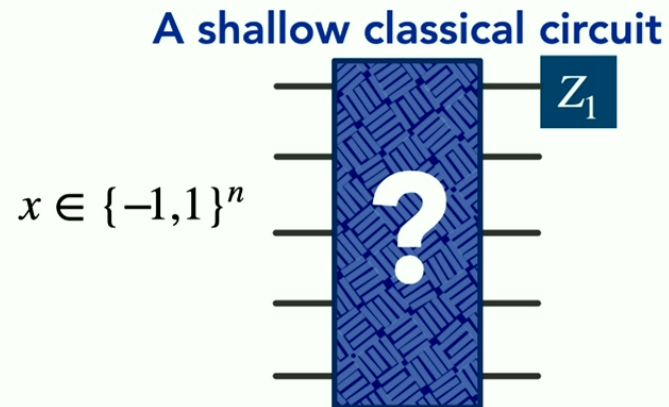
Average-case hardness

- The function f_C is equiv. to an exponentially long vector $\{-1,1\}^{2^n}$ with **no structure**.
- To learn a model $h(x)$, such that $\mathbb{E}_{x \sim \{-1,1\}^n} |h(x) - f_C(x)|^2 < 0.5$, we must query $f_C(x)$ for at least half of all x . Query complexity: $\Theta(2^n)$.



Average-case hardness for shallow classical circuits

- [AGS19] showed that learning $h(x)$, such that $\mathbb{E}_{x \sim \{-1,1\}^n} |h(x) - f_C(x)|^2 < 0.5$, is computationally hard (for both classical & quantum computers), even when the classical Boolean circuit is **constant-depth** (with majority gates, i.e., TC_0).

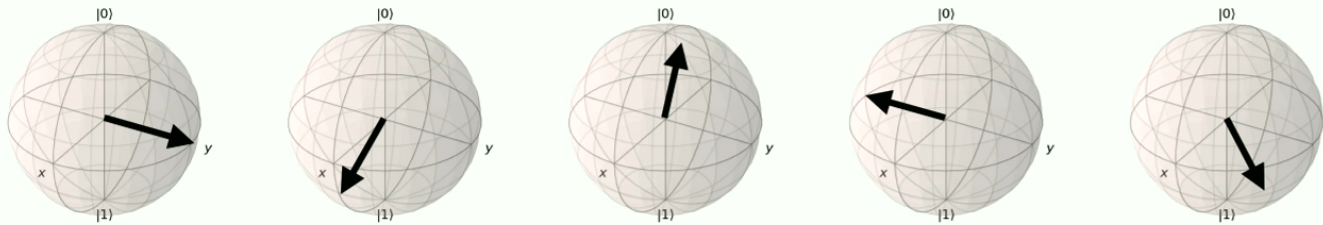


Overview

- A classical version of the quantum problem
- A restricted version of the quantum problem
- Generalization to the original quantum problem

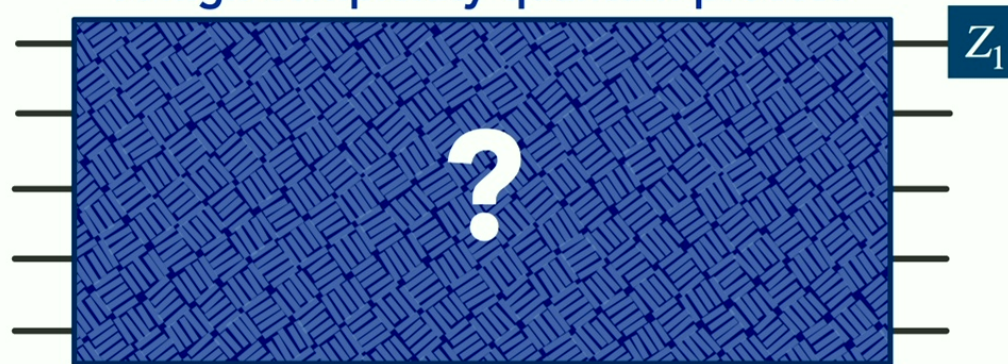
A Quantum Problem

Input:



A high-complexity quantum process

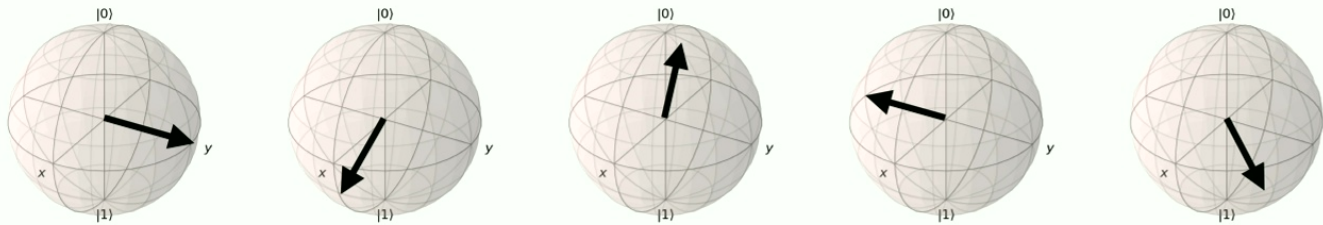
$$\bigotimes_{i=1}^n |\psi_i\rangle \in (\mathbb{C}^2)^{\otimes n}$$



Is this harder?

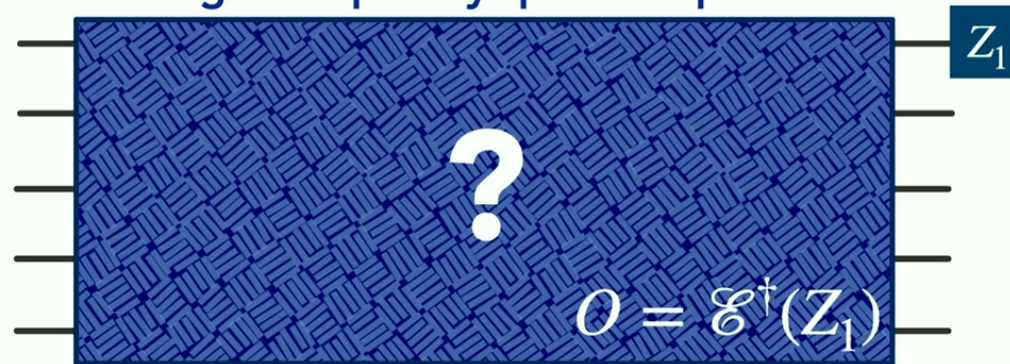
A Quantum Problem

Input:



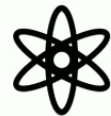
A high-complexity quantum process

$$\bigotimes_{i=1}^n |\psi_i\rangle \in (\mathbb{C}^2)^{\otimes n}$$



Is this harder?

A Classical Dataset



Classical Dataset about O

$$|\psi_\ell\rangle = \bigotimes_{i=1}^n |\psi_{\ell,i}\rangle \mapsto y_\ell, \quad \mathbb{E}[y_\ell] = \langle \psi_\ell | O | \psi_\ell \rangle$$

for $\ell = 1, \dots, N$.

Each repetition prepares a random product state, and measures the 1st qubit in the Z basis

The Prediction Task

 Classical Dataset about O

$$|\psi_\ell\rangle = \bigotimes_{i=1}^n |\psi_{\ell,i}\rangle \mapsto y_\ell, \quad \mathbb{E}[y_\ell] = \langle \psi_\ell | O | \psi_\ell \rangle$$

for $\ell = 1, \dots, N$.

Given a new state $|\psi\rangle = \bigotimes_{i=1}^n |\psi_i\rangle \in (\mathbb{C}^2)^{\otimes n}$,
how to predict $\langle \psi | O | \psi \rangle$ accurately?

Worst-case hardness

- To learn a model $h(|\psi\rangle)$, such that $\left| h(|\psi\rangle) - \langle \psi | O | \psi \rangle \right|^2 < 0.5, \forall |\psi\rangle = \bigotimes_{i=1}^n |\psi_i\rangle$, the problem is at least as hard as the classical problem.
- Hence, the query complexity is $\Omega(2^n)$.



Average-case hardness?

- To learn a model $h(|\psi\rangle)$, such that $\mathbb{E}_{|\psi\rangle=\bigotimes_{i=1}^n |\psi_i\rangle} \left| h(|\psi\rangle) - \langle \psi | O | \psi \rangle \right|^2 < 0.5$, is the problem still exponentially hard?
- Surprisingly, the answer is **no**. The problem can be done in quasi-polynomial time.



Low-weight approximation

$$O = \sum_{P \in \{I, X, Y, Z\}^{\otimes n}} \alpha_P P$$

$$O^{(\text{low})} = \sum_{|P| \leq k} \alpha_P P$$

Lemma (Low-weight approximation): $\mathbb{E}_{|\psi\rangle = \bigotimes_{i=1}^n |\psi_i\rangle} \left| \langle \psi | O | \psi \rangle - \langle \psi | O^{(\text{low})} | \psi \rangle \right|^2 < \frac{1}{3^k}.$

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Lemma (Low-weight approximation): $\mathbb{E}_{|\psi\rangle = \bigotimes_{i=1}^n |\psi_i\rangle} \left| \langle \psi | O | \psi \rangle - \langle \psi | O^{(\text{low})} | \psi \rangle \right|^2 < \frac{1}{3^k}.$

Interpretation: For most product state $|\psi\rangle = \bigotimes_{i=1}^n |\psi_i\rangle$, $\langle \psi | O | \psi \rangle \approx \langle \psi | O^{(\text{low})} | \psi \rangle$.

Low-weight approximation **does not** hold in the classical version of this problem

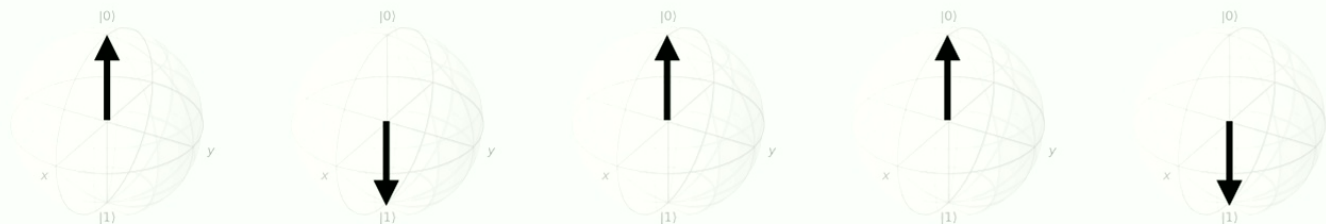
Low-weight approximation

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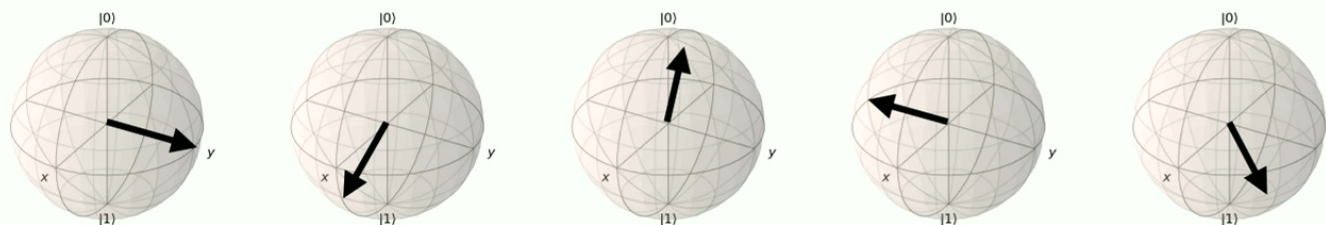
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Classical inputs are perfectly distinguishable.
But quantum state inputs are not.

Classical Input:



Quantum Input:



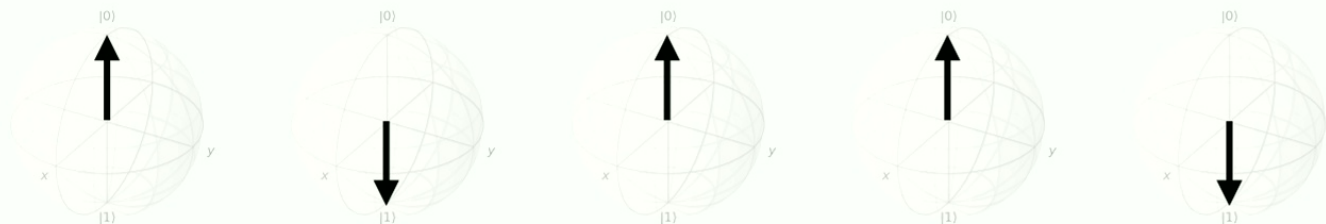
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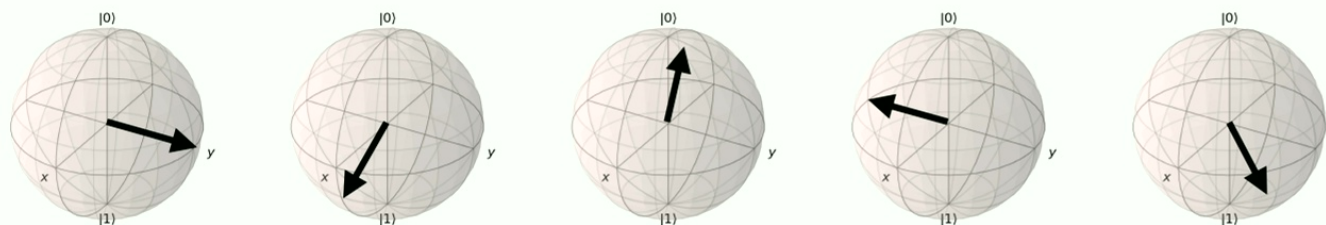
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Classical Input:



Quantum Input:



Basic Idea for the ML model

Basic idea: Learn the low-weight observable $O^{(\text{low})} = \sum_{|P| \leq k} \alpha_P P$ for a small k .

Lemma (Fourier transform): $\alpha_P = \mathbb{E} \left[\frac{3^{|P|}}{N} \sum_{\ell=1}^N y_\ell \langle \psi_\ell | P | \psi_\ell \rangle \right], \forall P \in \{I, X, Y, Z\}^{\otimes n}$



Classical Dataset

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for $\ell = 1, \dots, N$.

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Lemma

We only need $N = \mathcal{O}(\log n)$!

$\{Z\}^{\otimes n}$



Classical Dataset

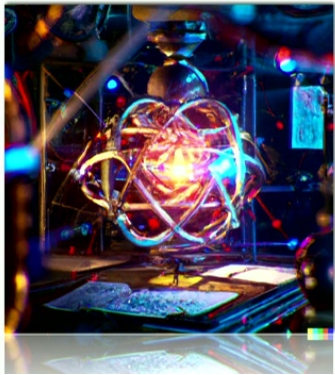
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An interlude

Optimizing Quantum Hamiltonians

Credit: DALL·E



Presenter: Hsin-Yuan Huang (Robert)
Joint work with Sitan Chen and John Preskill



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The Task

Given an n -qubit, k -local Hamiltonian $H = \sum_{|P| \leq k} \alpha_P P$.

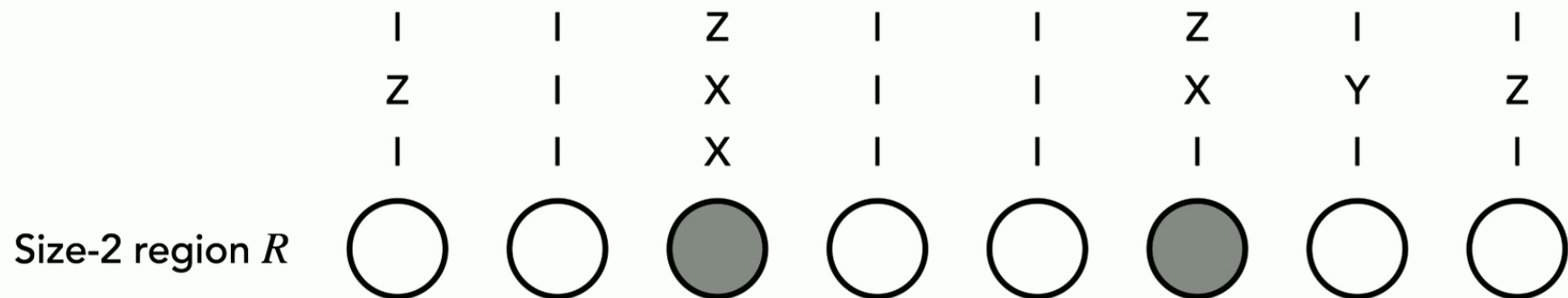
Find a state $|\psi\rangle$ that maximizes or minimizes $\langle\psi|H|\psi\rangle$.

**We want a guarantee on $\langle\psi|H|\psi\rangle$
based on the description of $H = \sum_{|P| \leq k} \alpha_P P$**

Expansion property

Given an n -qubit, k -local Hamiltonian $H = \sum_{|P| \leq k} \alpha_P P$.

H has an expansion coefficient c_e and dimension d_e if for every size- d_e region R , the number of P with $\alpha_P \neq 0$, $\text{dom}(P) \subseteq R$, $R \subseteq \text{dom}(P)$ is at most c_e .



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Example 1

Geometrically-local Hamiltonian

$$c_e = \mathcal{O}(1), d_e = 1$$

Example 2

General k -local Hamiltonian

$$c_e = 4^k, d_e = k$$

Example 3

Degree- d 2-body Hamiltonian

$$c_e = 16d, d_e = 1$$

Theorem

Given an n -qubit, k -local Hamiltonian $H = \sum_{|P| \leq k} \alpha_P P$.

If H has an expansion coefficient c_e and dimension d_e , then for $r = 2d_e/(d_e + 1) \in [1, 2)$, we have an algorithm that either finds a maximizing product state $|\psi\rangle$,

$$\langle \psi | H | \psi \rangle \geq \mathbb{E}_{|\phi\rangle: \text{Haar}} \langle \phi | H | \phi \rangle + \frac{1}{c_e^{1/2d_e} 2^{\Theta(k \log k)}} \left(\sum_{P \neq I} |\alpha_P|^r \right)^{1/r},$$

or finds a minimizing product state $|\psi\rangle$ with a similar guarantee ($+ \rightarrow -$, $\geq \rightarrow \leq$).

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Theorem

Improved over existing results

Given an n -qubit, k -local Hamiltonian $H = \sum_{|P| \leq k} \alpha_P P$.

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The Algorithm

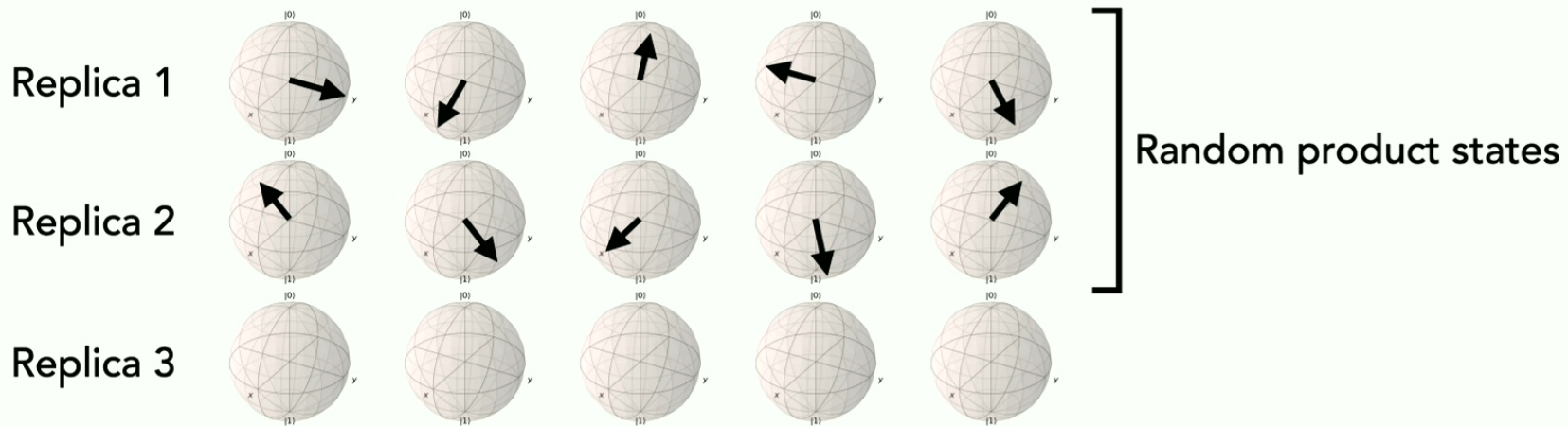
Select a slice with the largest value of α_P

Given an n -qubit, k -local Hamiltonian $H = \sum_{|P|=k} \alpha_P P$.

Find a product state $|\psi\rangle$ that approximately optimizes $\langle\psi|H|\psi\rangle$.

The Algorithm

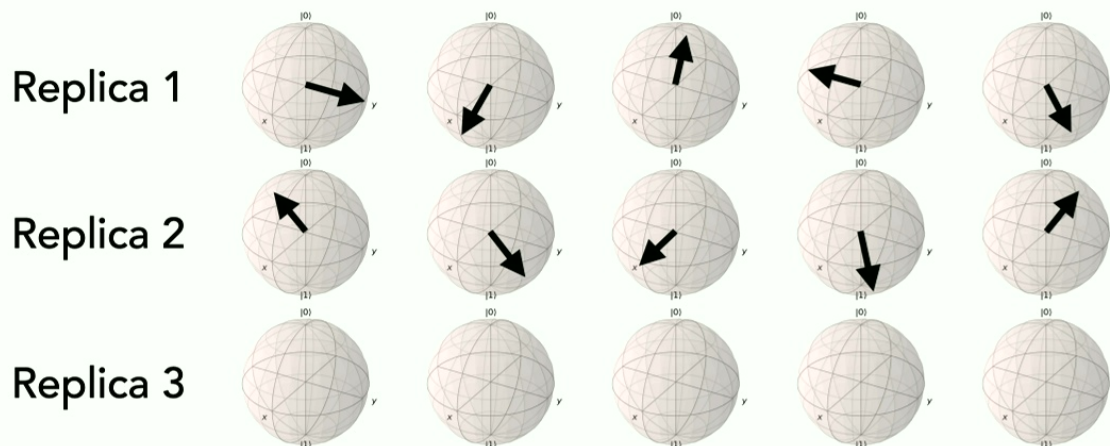
Given an n -qubit, k -local Hamiltonian $H = \sum_{|P|=k} \alpha_P P$.



The Algorithm

Lift n -qubit H to nk qubits

Given an n -qubit, k -local Hamiltonian $H = \sum_{|P|=k} \alpha_P P$.

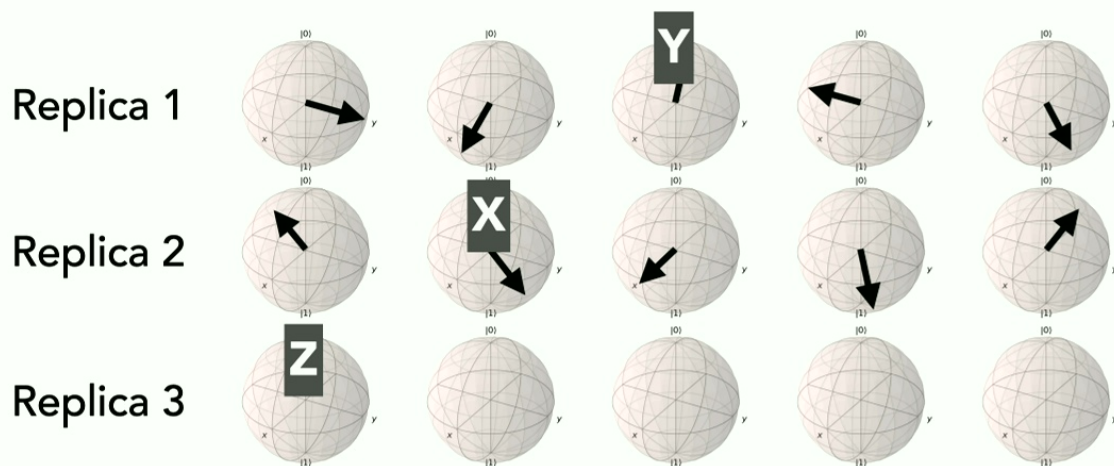


$$\text{pol}(H) = \sum_{|P|=k} \alpha_P \text{pol}(P) \in \mathbb{C}^{2^{nk} \times 2^{nk}}$$

The Algorithm

Lift n -qubit H to nk qubits

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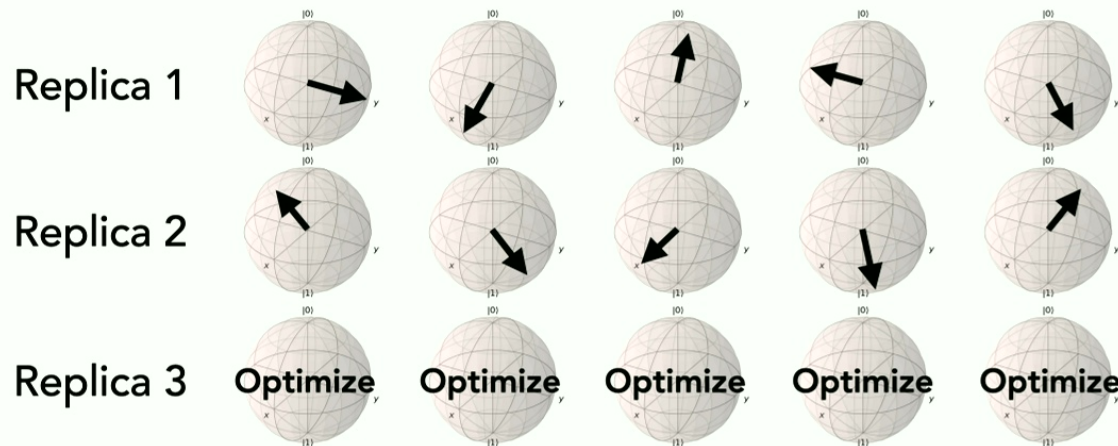


$$\text{pol}(H) = \sum_{|P|=k} \alpha_P \text{pol}(P) \in \mathbb{C}^{2^{nk} \times 2^{nk}}$$

$$P = ZXYII$$

The Algorithm

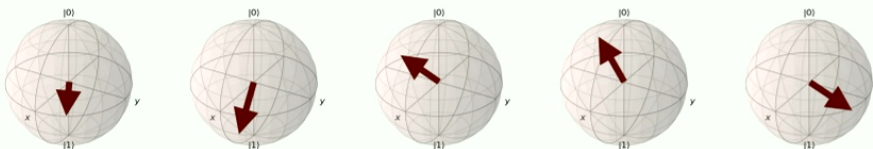
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The Algorithm

Given an n -qubit, k -local Hamiltonian $H = \sum_{|P|=k} \alpha_P P$.



Combine the Bloch vectors
using a weighted sum

Theorem

Given an n -qubit, k -local Hamiltonian $H = \sum_{|P| \leq k} \alpha_P P$.

If H has an expansion coefficient c_e and dimension d_e , then for $r = 2d_e/(d_e + 1) \in [1, 2)$, we have an algorithm that either finds a maximizing product state $|\psi\rangle$,

$$\langle \psi | H | \psi \rangle \geq \mathbb{E}_{|\phi\rangle: \text{Haar}} \langle \phi | H | \phi \rangle + \frac{1}{c_e^{1/2d_e} 2^{\Theta(k \log k)}} \left(\sum_{P \neq I} |\alpha_P|^r \right)^{1/r},$$

or finds a minimizing product state $|\psi\rangle$ with a similar guarantee ($+ \rightarrow -$, $\geq \rightarrow \leq$).

Another interlude

Generalized Quantum Bohnenblust-Hille Inequality

Credit: DALL·E



Presenter: Hsin-Yuan Huang (Robert)

Joint work with Sitan Chen and John Preskill



Caltech



Theorem

Given an observable $O = \sum_{|P| \leq k} \alpha_P P$ with an expansion coefficient c_e and dimension d_e .

$$\|O\|_{\infty} \geq \frac{1}{c_e^{1/2d_e} 2^{\Theta(k \log k)}} \left(\sum_P |\alpha_P|^r \right)^{1/r} \text{ for } r = \frac{2d_e}{d_e + 1} \in [1, 2).$$

Proof ideas:

- (1) Use the guarantee from the algorithm for optimizing quantum Hamiltonians.
- (2) Adapt by noting that $\|O\|_{\infty} \geq |\langle \psi | O | \psi \rangle|$, where $|\psi\rangle$ is the state found by the algo.

Theorem

Given an observable $O = \sum_{|P| \leq k} \alpha_P P$ with an expansion coefficient c_e and dimension d_e .

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Example 1

A sum of geometrically-local terms

$$c_e = \mathcal{O}(1), d_e = 1$$

$$\sum_P |\alpha_P| \leq \mathcal{O}(\|O\|_{\infty})$$

Theorem

Given an observable $O = \sum_{|P| \leq k} \alpha_P P$ with an expansion coefficient c_e and dimension d_e .

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Example 2

A sum of k -local terms

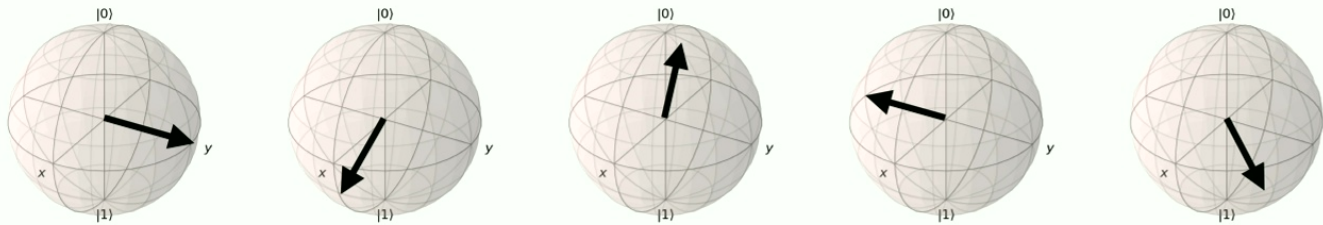
$$c_e = 4^k, d_e = k$$

$$\|\vec{\alpha}\|_{\frac{2k}{k+1}} \leq 2^{\mathcal{O}(k \log k)} \|O\|_{\infty}$$

A quantum analogue of
the Bohnenblust-Hille inequality

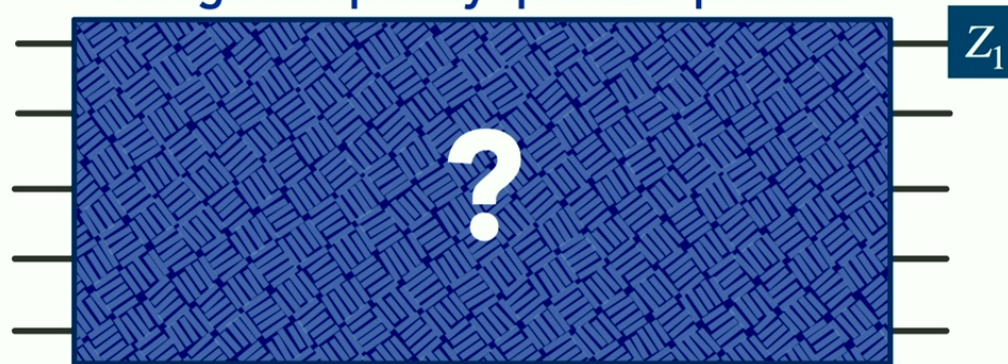
A Quantum Problem

Input:



A high-complexity quantum process

$$\bigotimes_{i=1}^n |\psi_i\rangle \in (\mathbb{C}^2)^{\otimes n}$$



Basic Idea for the ML model

Basic idea: Learn the low-weight observable $O^{(\text{low})} = \sum_{|P| \leq k} \alpha_P P$ for a small k .

Lemma (Fourier transform): $\alpha_P = \mathbb{E} \left[\frac{3^{|P|}}{N} \sum_{\ell=1}^N y_\ell \langle \psi_\ell | P | \psi_\ell \rangle \right], \forall P \in \{I, X, Y, Z\}^{\otimes n}$



Classical Dataset

$$|\psi_\ell\rangle = \bigotimes_{i=1}^n |\psi_{\ell,i}\rangle \mapsto y_\ell, \quad \mathbb{E}[y_\ell] = \langle \psi_\ell | O | \psi_\ell \rangle$$

for $\ell = 1, \dots, N$.

Insight from Quantum BH inequality

Insight 1: Learn the low-weight observable $O^{(\text{low})} = \sum_{|P| \leq k} \alpha_P P$ for a small k .

Insight 2: The Pauli coef. in $O^{(\text{low})}$ is approximately sparse as $\|\vec{\alpha}\|_{\frac{2k}{k+1}} \leq 2^{\mathcal{O}(k \log k)} \|O^{(\text{low})}\|_{\infty}$.

This idea is also used in classical learning theory [AI22]



Classical Dataset

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Basic Idea for the ML model

Basic idea: Learn the low-weight observable $O^{(\text{low})} = \sum_{|P| \leq k} \alpha_P P$ for a small k .

Lemma

How large should the data size N be?

$\{Z\}^{\otimes n}$



Classical Dataset

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The ML algorithm

Insight 1: Learn the low-weight observable $O^{(\text{low})} = \sum_{|P| \leq k} \alpha_P P$ for a small k .

Insight 2: The Pauli coef. in $O^{(\text{low})}$ is approximately sparse as $\|\vec{\alpha}\|_{\frac{2k}{k+1}} \leq 2^{\mathcal{O}(k \log k)} \|O^{(\text{low})}\|_{\infty}$.



Classical Dataset

$$|\psi_{\ell}\rangle = \bigotimes_{i=1}^n |\psi_{\ell,i}\rangle \mapsto y_{\ell}, \quad \mathbb{E}[y_{\ell}] = \langle \psi_{\ell} | O | \psi_{\ell} \rangle$$

for $\ell = 1, \dots, N$.

For all $|P| \leq k$,

$$\text{set } \hat{\alpha}_P \leftarrow \frac{3^{|P|}}{N} \sum_{\ell=1}^N y_{\ell} \langle \psi_{\ell} | P | \psi_{\ell} \rangle.$$

If $\hat{\alpha}_P$ is small, set $\hat{\alpha}_P \leftarrow 0$.

The learned observable is $\hat{O}^{(\text{low})} = \sum_{|P| \leq k} \hat{\alpha}_P P$.

Guarantee for learning O

For any small constant ϵ, ϵ' , given a training set size $N = \mathcal{O}(\log n)$, the prediction error is

$$\mathbb{E}_{|\psi\rangle = \bigotimes_{i=1}^n |\psi_i\rangle} \left| \langle \psi | \hat{O}^{(\text{low})} | \psi \rangle - \langle \psi | O | \psi \rangle \right|^2 < \epsilon + \epsilon' \|O^{(\text{low})}\|_{\infty}^2.$$



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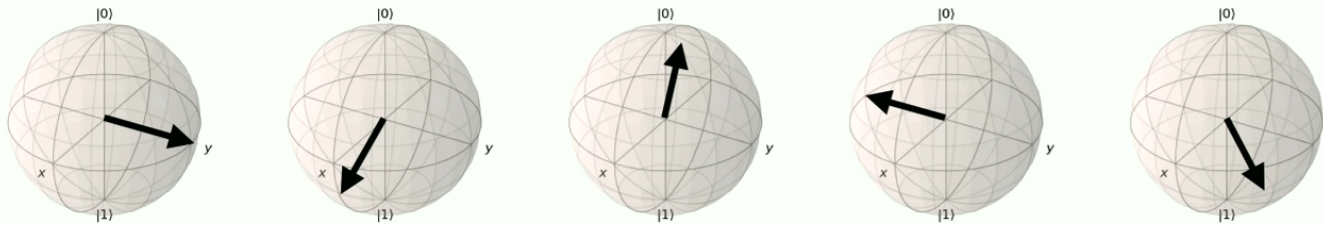
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A Quantum Problem

Input:



A high-complexity quantum process

$$\bigotimes_{i=1}^n |\psi_i\rangle \in (\mathbb{C}^2)^{\otimes n}$$



Quasi-polynomially
easy!

Guarantee for learning O

For any ϵ, ϵ' , given a training set size $N = \log(n) 2^{\tilde{O}(\log(1/\epsilon)\log(1/\epsilon'))}$, the prediction error is

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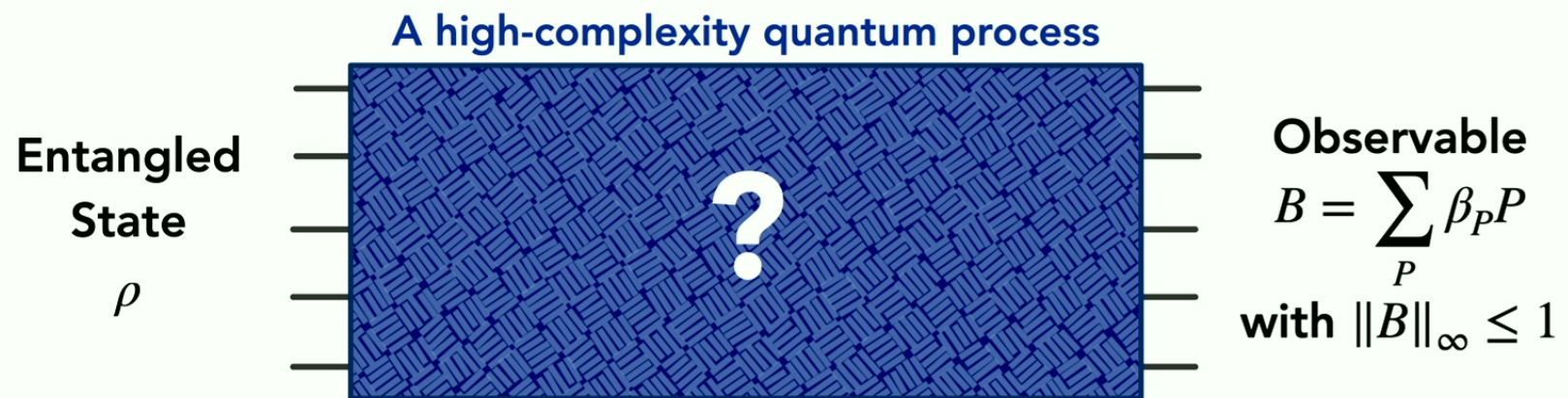
Overview

- A classical version of the quantum problem
- A restricted version of the quantum problem
- Generalization to the original quantum problem

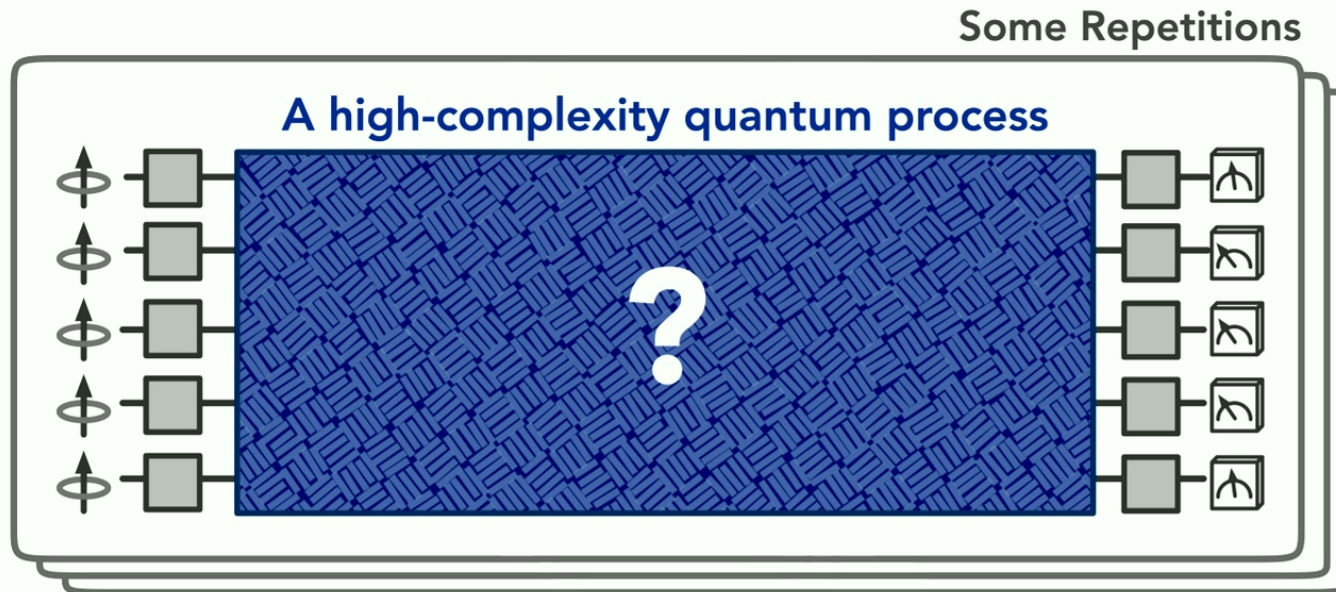
The Restricted Problem



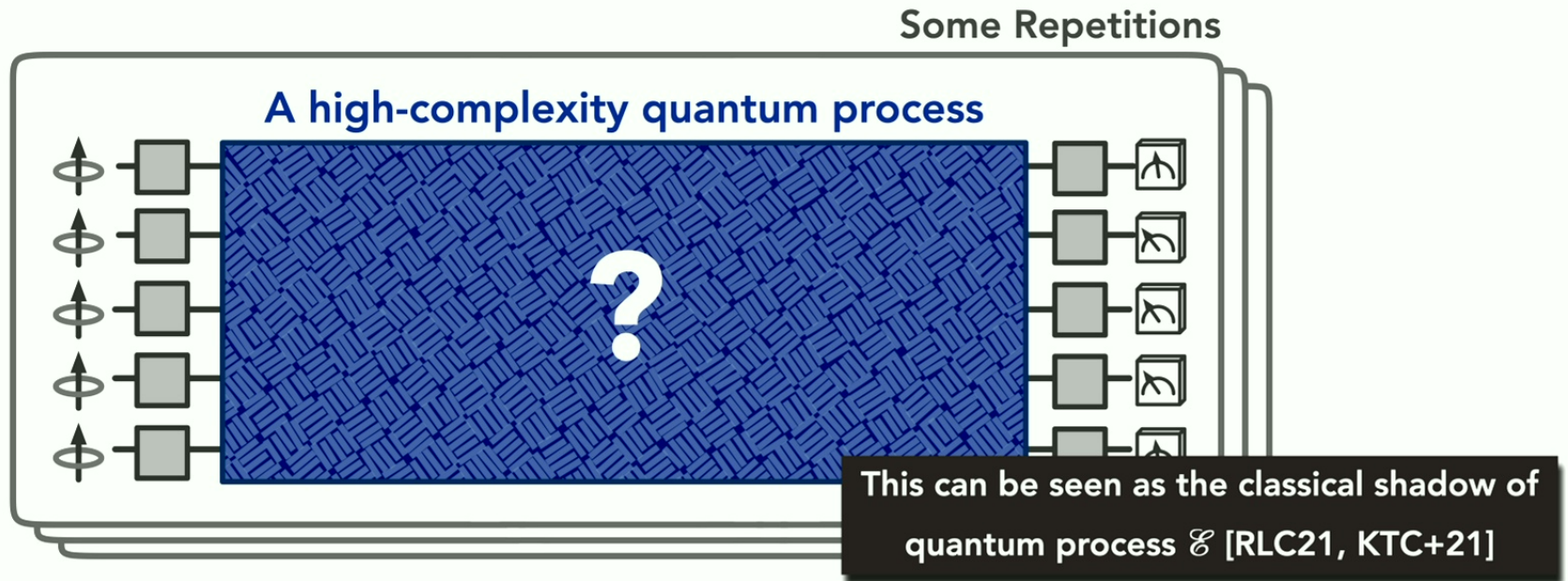
The Original Problem



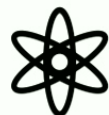
A Classical Dataset for Learning \mathcal{E}



A Classical Dataset for Learning \mathcal{E}



A Classical Dataset for Learning \mathcal{E}



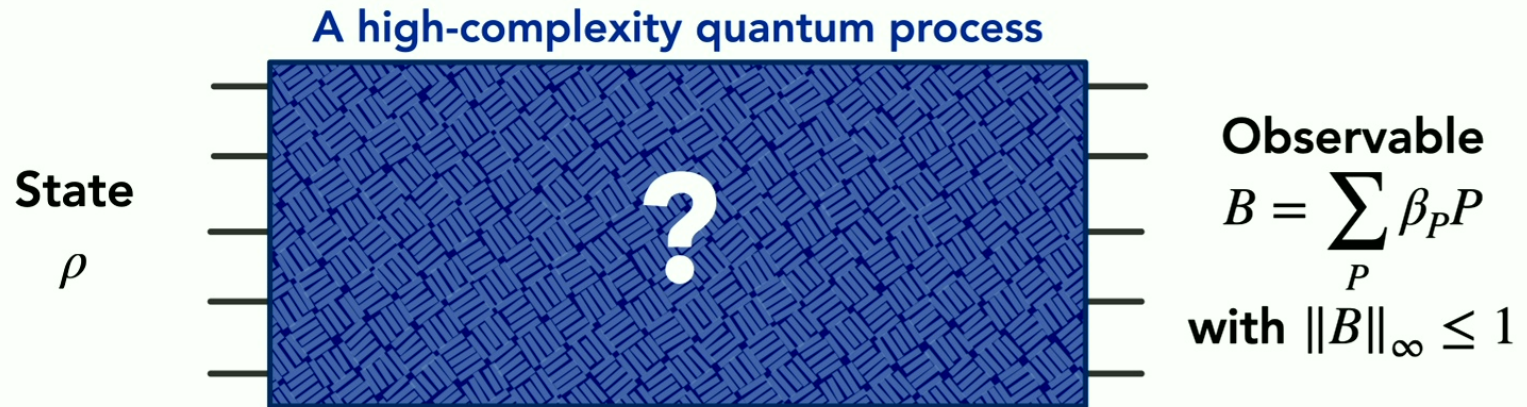
Classical Dataset

$$|\psi_\ell\rangle = \bigotimes_{i=1}^n |\psi_{\ell,i}\rangle \mapsto |\phi_\ell\rangle = \bigotimes_{i=1}^n |\phi_{\ell,i}\rangle$$

for $\ell = 1, \dots, N$.

This can be seen as the classical shadow of quantum process \mathcal{E} [RLC21, KTC+21]

How to make prediction?

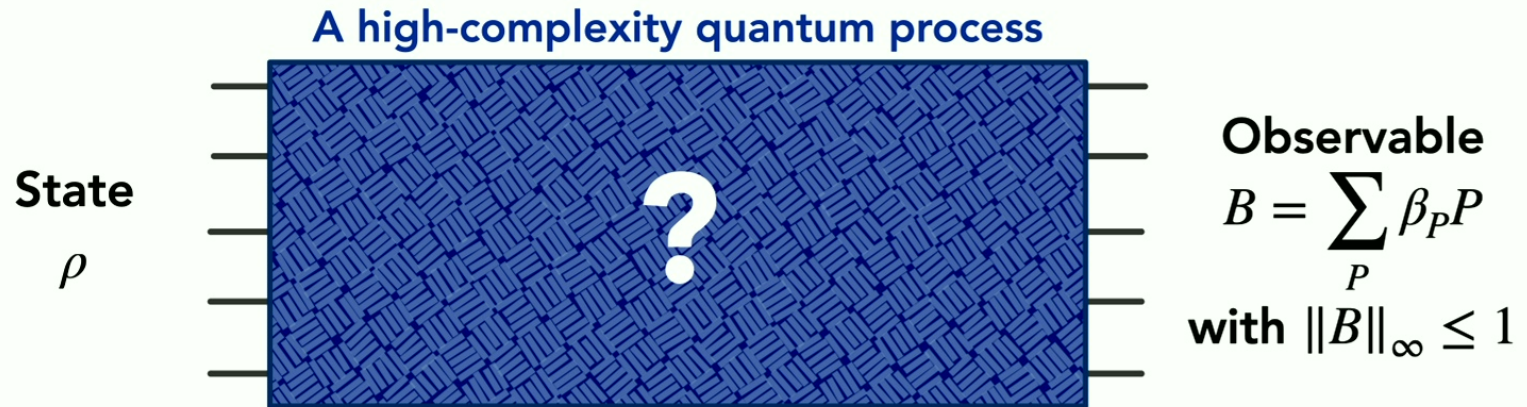


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Construct a dataset with classical shadow



A New Classical Dataset

$$|\psi_\ell\rangle = \bigotimes_{i=1}^n |\psi_{\ell,i}\rangle \mapsto y_\ell = \text{Tr} \left(B \bigotimes_{i=1}^n (3|\phi_{\ell,i}\rangle\langle\phi_{\ell,i}| - I) \right)$$

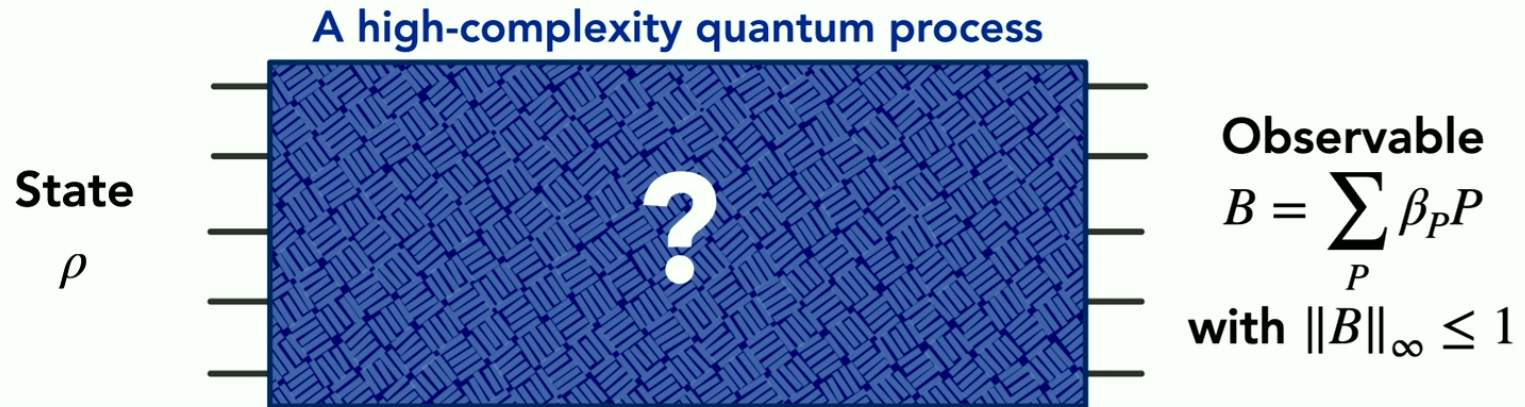
for $\ell = 1, \dots, N$.

Properties [HKP20]:

$$\mathbb{E}[y_\ell] = \text{Tr}(B \mathcal{E}(|\psi_\ell\rangle\langle\psi_\ell|))$$

$$\text{Var}[y_\ell] \leq \|B\|_{\text{shadow}}^2$$

Construct a dataset with classical shadow



For any sum of local observables B , $\|B\|_{\text{shadow}} \leq \mathcal{O}(\|\vec{\beta}\|_1) \leq \mathcal{O}(\|B\|_\infty)$ using the generalized quantum BH inequality.

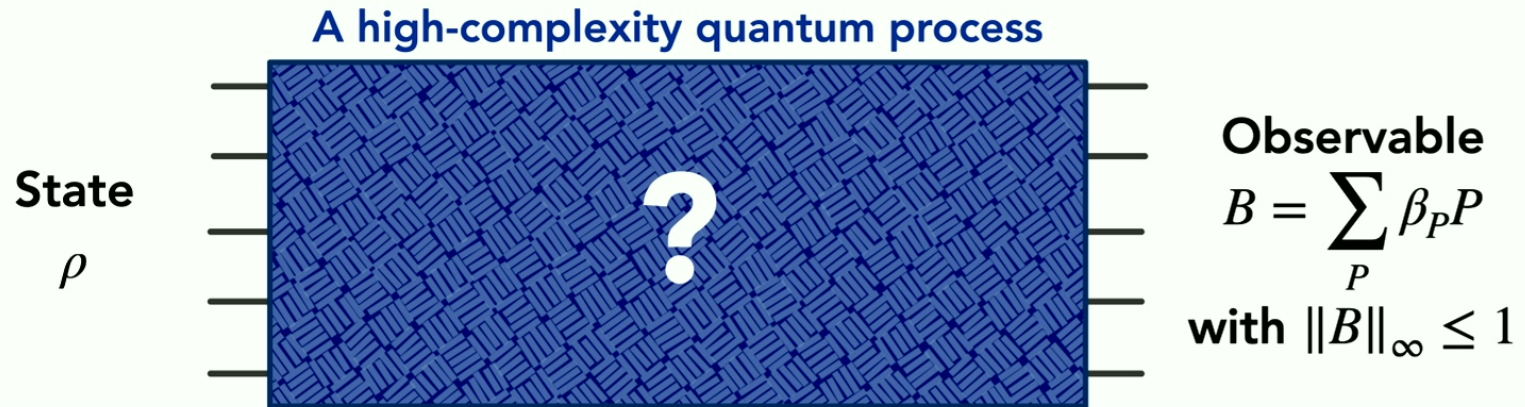
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$$\mathbb{E}[y_\ell] = \text{Tr}(B \mathcal{E}(|\psi_\ell\rangle\langle\psi_\ell|))$$

$$\text{Var}[y_\ell] = \mathcal{O}(1)$$

Low-weight approximation

$$O = \sum_{P \in \{I, X, Y, Z\}^{\otimes n}} \alpha_P P$$

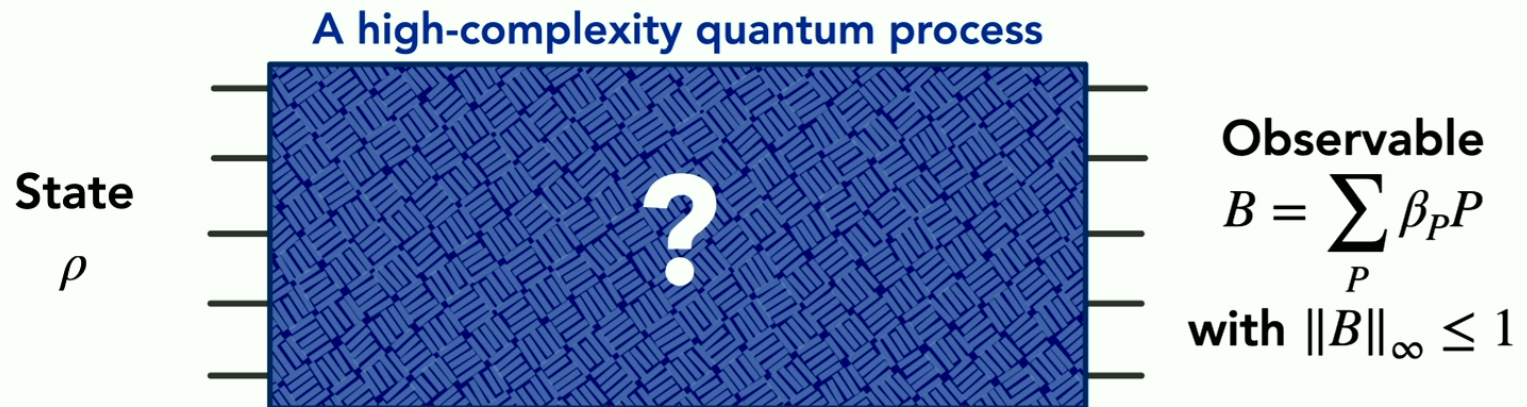
$$O^{(\text{low})} = \sum_{|P| \leq k} \alpha_P P$$

Lemma (Low-weight approximation): $\mathbb{E}_{\rho \sim \mathcal{D}} \left| \text{Tr}(O\rho) - \text{Tr}(O^{(\text{low})}\rho) \right|^2 < \frac{1}{1.5^k}.$

The lemma holds for any distribution \mathcal{D} over any quantum state ρ
as long as \mathcal{D} is flat under single-qubit rotations.

Example: ρ is the ground/thermal state of a generic geometrically-local Hamiltonian.

The ML algorithm

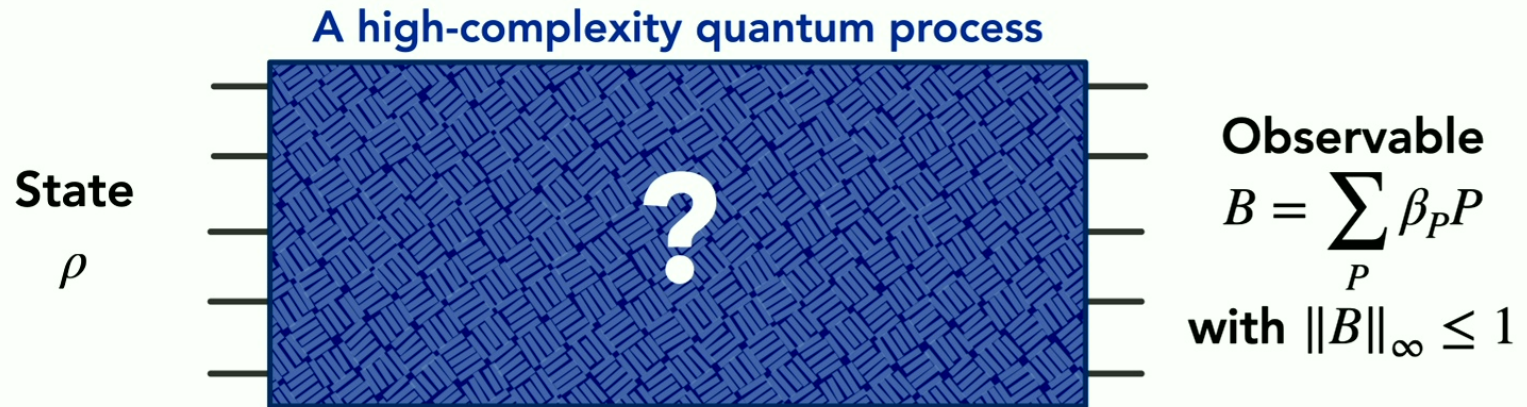


 **Classical Dataset**

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for $\ell = 1, \dots, N$.

The ML algorithm



✱ Classical Dataset for $O = \mathcal{E}^\dagger(B)$

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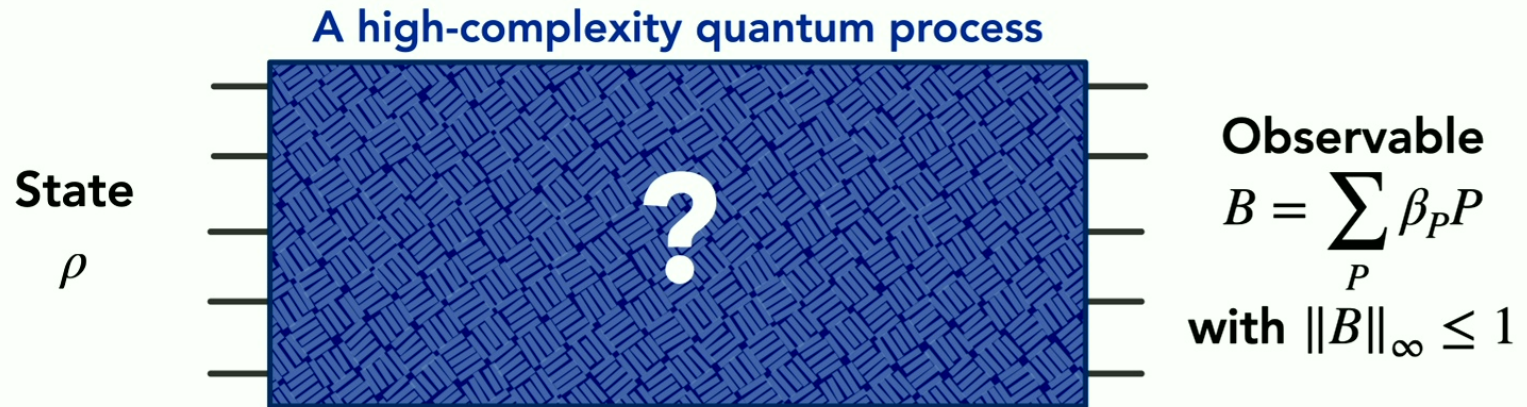
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for $\ell = 1, \dots, N$.

Predict $\text{Tr} \left(\hat{O}^{(\text{low})} \rho \right) \approx \text{Tr} (B \mathcal{E}(\rho))$

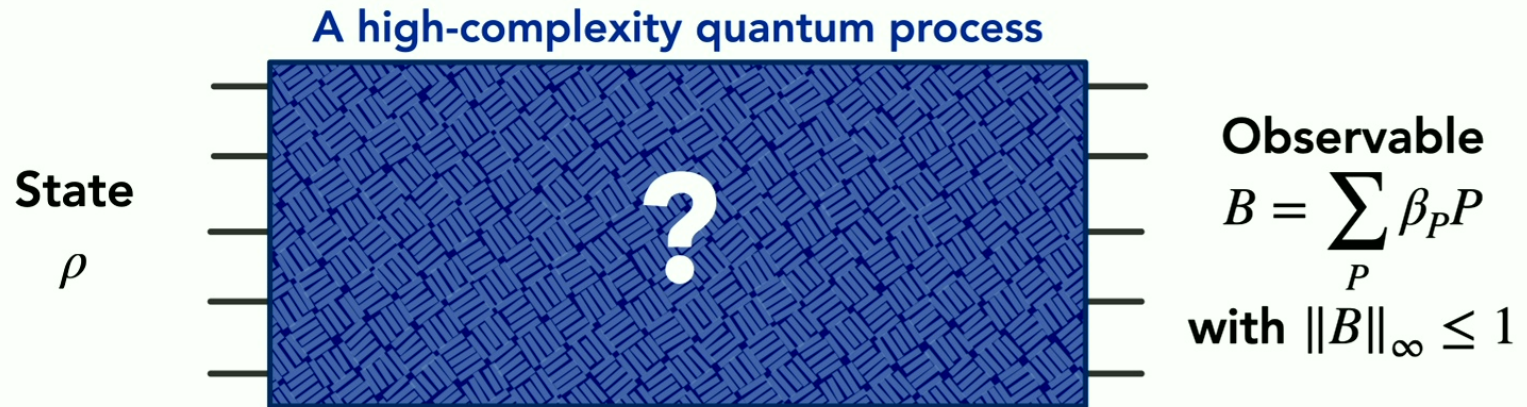
Surprising aspects of the ML algorithm

- We can learn to predict n -qubit exponential-size quantum circuits up to a const. relative error from only $\mathcal{O}(\log n)$ samples.
- The algorithm is computationally efficient (polynomial time for a const. relative error; quasi-polynomial time for a small error).

Surprising aspects of the ML algorithm

- We can learn to predict n -qubit exponential-size quantum circuits up to a const. relative error from only $\mathcal{O}(\log n)$ samples.
- The algorithm is computationally efficient (polynomial time for a const. relative error; quasi-polynomial time for a small error).
- After learning from product state inputs, the algorithm can predict entangled states.
- The entire algorithm can be run on a classical computer.

The ML algorithm



✱ Classical Dataset for $O = \mathcal{E}^\dagger(B)$

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Conclusion

- We give a computationally-efficient ML algorithm that can learn to predict the output of a quantum process with arbitrary complexity.
- Our results highlight the potential that ML models can predict outcomes of a complex quantum dynamics much faster than the process itself.

DALL-E impression of "Predicting quantum processes", "Optimizing quantum Hamiltonians", "Quantum Bohnenblust-Hille"



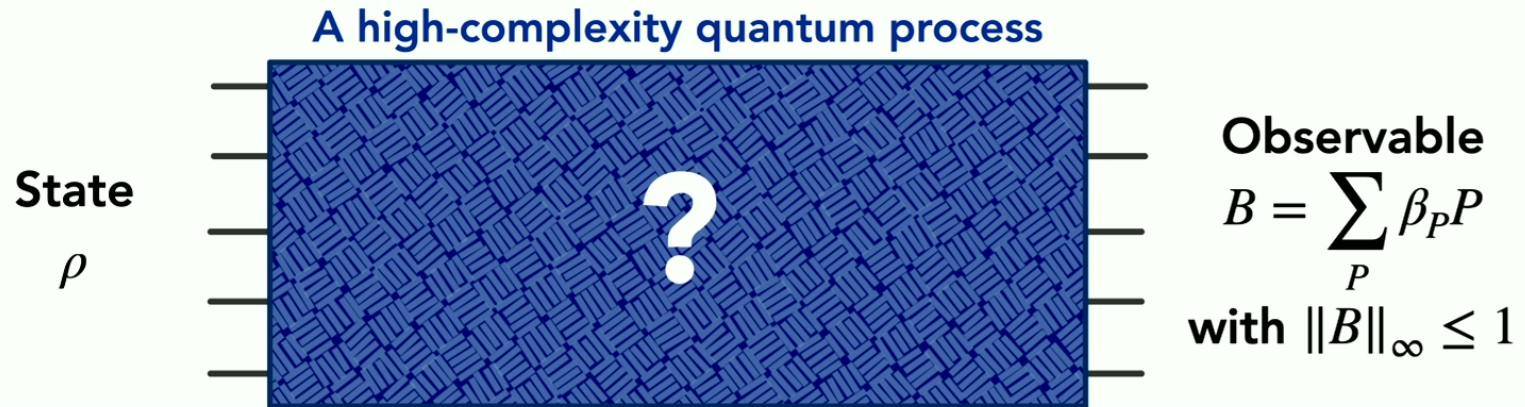
The Task

Given an n -qubit, k -local Hamiltonian $H = \sum_{|P| \leq k} \alpha_P P$.

Find a state $|\psi\rangle$ that maximizes or minimizes $\langle\psi|H|\psi\rangle$.

**We want a guarantee on $\langle\psi|H|\psi\rangle$
based on the description of $H = \sum_{|P| \leq k} \alpha_P P$**

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