## Learning from

## quantum experiments

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## Motivation

- One of the central goals of science is to learn how the physical world operates.
- By performing experiments, humans can receive information about the physical world, and process information to form predictive models.


Examples of scientific disciplines


A cartoon depiction of learning

## Motivation

- To accelerate and automate scientific development, it is important to understand how to design better algorithms to learn from experiments.
- A burgeoning field in Ol considers the task of learning from quantum experiments.


Examples of scientific disciplines


A cartoon depiction of learning

## Outline

- Basic setting and examples
- Key ideas:

Part I — Designing good learning algorithms
Part II — Proving no good learning algorithms exist

- Outlook and open questions



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- Basic setting and examples
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## Basic setting

- There is an unknown quantum object (states, processes, entire phase diagram, ...).
- Learn that object from experiments. So it becomes (approximately) known.


Unknown quantum object

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- Learn that object from experiments. So it becomes (approximately) known.
- How many experiments are needed? (Sample and query complexity)


Unknown quantum object

## Overview



Goal: Provide a learning-theoretic foundation for various applications

## Example 1: Quantum state tomography

- There is an unknown $n$-qubit quantum state described by $\rho \in \mathbb{C}^{2^{n} \times 2^{n}}$.
- Learn a classical description $\hat{\rho}$ by performing measurements on copies of $\rho$.
- After learning, we want $\hat{\rho} \approx \rho$ under trace norm $\|\cdot\|_{1}$.


## Motivations:

- The most basic quantum learning problem


Unknown quantum state

## References:

[1] Leonhardt, Ulf. "Quantum-state tomography and discrete Wigner function." Physical review letters 74.21 (1995): 4101
[2] Gross, David, et al. "Quantum state tomography via compressed sensing." Physical review letters 105.15 (2010): 150401.
[3] O'Donnell, Ryan, and John Wright. "Efficient quantum
tomography." Proceedings of the forty-eighth annual ACM symposium on Theory of Computing. 2016.
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## Motivations:

- The most basic quantum learning problem
- Benchmark quantum systems


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> Complexity is exponential in $n$

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- 2nd most basic quantum learning problem


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[1] Aaronson, Scott. "Shadow tomography of quantum states." SIAM Journal on Computing 49.5 (2019): STOC18-368.
[2] Bădescu, Costin, and Ryan O'Donnell. "Improved quantum data
analysis." Proceedings of the 53rd Annual ACM SIGACT Symposium on Theory of Computing. 2021.
[3] Huang, Hsin-Yuan, Richard Kueng, and John Preskill. "Predicting many properties of a quantum system from very few measurements. " Nature Physics 16.10 (2020): 1050-1057. [4] Cotler, Jordan, and Frank Wilczek. "Quantum overlapping tomography." Physical review letters 124.10 (2020): 100401.

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- Benchmark quantum systems w/ good scaling in $n$
- A basic primitive in hybrid quantum/classical algorithms


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Complexity is linear or independent in $n$

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## Example 3: Pauli channel tomography

- There is an unknown $n$-qubit Pauli channel $\mathscr{P}$.
- Learn $\hat{\mathscr{P}}$ by preparing input states, evolving under $\mathscr{P}$, and measuring output states.
- After learning, we want $\hat{\mathscr{P}} \approx \mathscr{P}$ under diamond norm.


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## Motivations:

- Characterize quantum noise
- Useful for quantum error correction, error mitigation


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[1] Flammia, Steven T., and Joel J. Wallman. "Efficient estimation of Pauli channels." ACM Transactions on Quantum Computing 1.1 (2020): 1-32. [2] Harper, Robin, Steven T. Flammia, and Joel J. Wallman. "Efficient learning of quantum noise. " Nature Physics 16.12 (2020): 1184-1188. [3] Flammia, Steven T., and Ryan O'Donnell. "Pauli error estimation via Population Recovery." Quantum 5 (2021): 549. [4] Chen, Senrui, et al. "Quantum advantages for pauli channel estimation." Physical Review A 105.3 (2022): 032435.

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Complexity varies under additional assumptions

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[1] Flammia, Steven T., and Joel J. Wallman. "Efficient estimation of Pauli channels." ACM Transactions on Quantum Computing 1.1 (2020): 1-32. [2] Harper, Robin, Steven T. Flammia, and Joel J. Wallman. "Efficient learning of quantum noise. " Nature Physics 16.12 (2020): 1184-1188. [3] Flammia, Steven T., and Ryan O'Donnell. "Pauli error estimation via Population Recovery." Quantum 5 (2021): 549. [4] Chen, Senrui, et al. "Quantum advantages for pauli channel estimation." Physical Review A 105.3 (2022): 032435.

## Example 4: Predicting ground states

- There is an unknown $f(x)$ mapping parameter $x$ to the ground state of $H(x)$.
- Learn $\hat{f}$ by preparing ground states under different $x^{\prime}$ s, and measuring the states.
- After learning, we want $\hat{f}(x) \approx f(x)$ for most of $x$.


Unknown phase diagram

## References:

[1] Carleo, Giuseppe, and Matthias Troyer. "Solving the quantum manybody problem with artificial neural networks." Science 355.6325 (2017): 602-606.
[2] Gilmer, Justin, et al. "Neural message passing for quantum chemistry." International conference on machine learning. PMLR, 2017. [3] Qiao, Zhuoran, et al. "OrbNet: Deep learning for quantum chemistry using symmetry-adapted atomic-orbital features." The Journal of chemical physics 153.12 (2020): 124111.
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## Motivations:

- Machine learning for quantum chemistry/physics
- Speed up computation with ML


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## Type your problem here

- Almost all problems contain some aspects about learning an unknown object.



## More problems

- What quantum circuits/algorithms can we learn? (OML \& VQA)
- What aspects of an unknown quantum machine is learnable? (Benchmarking \& Noise)
- How to learn a good quantum sensor given an unknown quantum machine? (Sensing)
- Can a learning algorithm discover "new physics"? (ML for physics)
- The list goes on ...



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## Key Ideas

- Part I focuses on upper bounds (how to design good learning algorithms).
- Part II focuses on lower bounds (how to show that no good algorithms exist).


> Part II


## Key Ideas

Algorithmic side: randomized experiments + data processing
Analysis side: geometric analysis + concentration inequality


## A dive into shadow tomography

Algorithmic side: randomized experiments + data processing Analysis side: geometric analysis + concentration inequality

Recall the task of shadow tomography:

- There is an unknown $n$-qubit quantum state described by $\rho \in \mathbb{C}^{2^{n} \times 2^{n}}$.
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## A dive into shadow tomography

Randomized experiment:

- Sample a random Clifford $U_{i}$ to rotate the quantum state $\rho$.
- Measure the state in the computational basis $\left|b_{i}\right\rangle \in\{0,1\}^{n}$.



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Data processing:

- Construct $\hat{\rho}_{i}=\left[\left(2^{n}+1\right) U_{i}^{\dagger}\left|b_{i} X b_{i}\right| U_{i}-I\right]$ for each experiment.



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Geometric analysis:

- The geometry of Clifford unitary says $\mathbb{E}\left[\operatorname{Tr}(O \hat{\rho})_{i}\right]=\operatorname{Tr}(O \rho)$ and $\operatorname{Var}\left[\operatorname{Tr}\left(O \hat{\rho}_{i}\right)\right] \leq 3 \operatorname{Tr}\left(O^{2}\right)$.


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Concentration bound:

- For $O_{1}, \ldots, O_{M}$ with $\operatorname{Tr}\left(O^{2}\right)=\mathcal{O}(1)$, we can predict $\operatorname{Tr}\left(O_{i} \rho\right)$ after $\mathcal{O}(\log (M))$ measurements.


## A dive into shadow tomography

Theorem (Huang et al.; 2020)

1. Given $B, \epsilon>0$, the procedure learns a classical representation of an unknown quantum state $\rho$ from

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N=\mathcal{O}\left(B \log (M) / \epsilon^{2}\right) \text { measurements. }
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2. Subsequently, given any $O_{1}, \ldots, O_{M}$ with $B \geq \max \left\|O_{i}\right\|_{2}^{2}$, the procedure can use the classical representation to predict $\hat{o}_{1}, \ldots, \hat{o}_{M}$, where $\left|\hat{o}_{i}-\operatorname{tr}\left(O_{i} \rho\right)\right|<\epsilon$, for all $i$.

For example:

- $M=10^{6}, B=1$, then naively we need $10^{6} / \epsilon^{2}$ measurements.
- This theorem shows that we only need $6 \log (10) / \epsilon^{2}$ measurements.

Furthermore, we don't need to know $O_{1}, \ldots, O_{M}$ in advance.

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Small for low-rank observables
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Application: Quantum fidelity $|\psi\rangle\langle\psi|$

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Depends on randomized experiments
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Furthermore, we don't need to know $O_{1}, \ldots, O_{M}$ in advance.

## Other applications

Algorithmic side: randomized experiments + data processing
Analysis side: geometric analysis + concentration inequality

## References:

- Cross platform verification [1, 2]
- Characterizing topological order [3, 4]
- Probing entanglement entropy $[5,6]$
- Diagnosing quantum chaos [7]
- Learning quantum noise $[8,9]$

See more examples in the review [10].
[1] Elben, Andreas, et al. "Cross-platform verification of intermediate scale quantum devices." Physical review letters 124.1 (2020): 010504 [2] Anshu, Anurag, Zeph Landau, and Yunchao Liu. "Distributed quantum inner product estimation." arXiv preprint arXiv:2111.03273 (2021).
[3] Elben, Andreas, et al. "Many-body topological invariants from randomized measurements in synthetic quantum matter." Science advances 6.15 (2020)
[4] Huang, Hsin-Yuan, et al. "Provably efficient machine learning for quantum many-body problems." arXiv preprint arXiv:2106.12627 (2021).
[5] Brydges, Tiff, et al. "Probing Rényi entanglement entropy via randomized measurements." Science 364.6437 (2019): 260-263.
[6] Elben, Andreas, et al. "Mixed-state entanglement from local randomized
measurements." Physical Review Letters 125.20 (2020): 200501.
[7] Vermersch, Benoît, et al. "Probing scrambling using statistical correlations between randomized measurements." Physical Review X 9.2 (2019): 021061.
[8] Flammia, Steven T., and Joel J. Wallman. "Efficient estimation of Pauli channels." ACM Transactions on Quantum Computing 1.1 (2020): 1-32.
[9] Helsen, Jonas, et al. "Estimating gate-set properties from random sequences. " arXiv preprint arXiv:2110.13178 (2021).
[10] Elben, Andreas, et al. "The randomized measurement toolbox." arXiv preprint arXiv:2203.11374 (2022)

## Why randomized experiments?

A. In many cases, they are asymptotically optimal! Adaptively choosing experiments based on new information seems better, but often don't [1, 2, 3].
B. Randomization turns bad scenarios into low-probability events.
C. If information is distributed evenly, random sampling quickly converges.

[^1]
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## Key Ideas

- Part II focuses on lower bounds (showing no good algorithms exist).


Part II


## Conventional Experiments

What scientists currently do in the lab
Receive, process, and store classical information


## Quantum-enhanced Experiments

What future experiments could be like
Receive, process, and store quantum information


## Key Ideas

- Proving lower bounds for conventional experiments (classical agents) helps us understand the potential quantum advantage in learning from experiments.


## Part I

Part II


## Mathematical Framework

- We consider a simple task of learning about an unknown physical system $\rho$ (density matrix).
- Assume that a physical source that could generate a single copy of $\rho$ at a time.



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Perform
POVM measurement

Obtain classical data


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Perform
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Store the
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Perform
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Process the classical data And pick next measurement


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Process the classical data And pick next measurement

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## Mathematical Framework

- We consider a simple task of learning about an unknown physical system $\rho$ (density matrix).
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Classical memory storing data from all POVM

Process all classical data


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888 Quantum-enhanced experiments


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888 Quantum-enhanced experiments


## Mathematical Framework

- Main difference:

Having quantum memory for entangling quantum information from past and future experiments.

- We can then analyze the possible protocols/algorithms to study their learning ability.

Algorithms without quantum memory


Algorithms with quantum memory


## Quantum advantage in predicting properties

- The classical/quantum agent learns a classical model of the $n$-qubit state $\rho$.
- Subsequently, one can use the classical model to predict $|\operatorname{Tr}(P \rho)|$ for an observable $P$ chosen from $\{I, X, Y, Z\}^{\otimes n}$.


## Theorem

Classical agent needs $\Omega\left(2^{n}\right)$ experiments to predict observable from the set, but quantum agent only need $\mathcal{O}(n)$ experiments to predict all $4^{n}$ observables.

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Uncertainty principle significantly hinders the learning ability of classical agent, but surprisingly not the ability of a quantum agent.

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Exponential quantum advantage is present even when the state $\rho$ is a classical distribution over product states (no entanglement!).

## Proof Sketch: Tree representation

- Consider the lower bound $\Omega\left(2^{n}\right)$ for classical agents; See [HKP21] for upper bound $\mathcal{O}(n)$.
- We consider a graphical representation for the memory state of the classical agent.



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- Consider the lower bound $\Omega\left(2^{n}\right)$ for classical agents; See [HKP21] for upper bound $\mathcal{O}(n)$.
- We consider a graphical representation for the memory state of the classical agent.


Probability distribution (bottom layer) sufficiently different $\equiv$ Classical agent can distinguish $\rho_{A}$ and $\rho_{B}$

## Proof Sketch: Tree representation

- Consider the lower bound $\Omega\left(2^{n}\right)$ for classical agents; See [HKP21] for upper bound $\mathcal{O}(n)$.
- We consider a graphical representation for the memory state of the classical agent.


Probability distribution (bottom layer) sufficiently different $\equiv$ Classical agent can distinguish $\rho_{A}$ and $\rho_{B}$ More experiments done $\equiv$ Deeper the tree $\equiv$ More distinct the distribution

## Many-vs-one distinguishing task

- If the classical agent succeeds in the prediction task, then he/she must succeeds in a corresponding distinguishing task.

Revealed to be $P_{A}$


Revealed to be $P_{B}$



Partially-revealed many-versus-one distinguishing task

## Quantum advantage in predicting properties

- The classical/quantum agent learns a classical model of the $n$-qubit state $\rho$.
- Subsequently, one can use the classical model to predict $|\operatorname{Tr}(P \rho)|$ for an observable $P$ chosen from $\{I, X, Y, Z\}^{\otimes n}$.


## Theorem

Classical agent needs $\Omega\left(2^{n}\right)$ experiments to predict observable from the set, but quantum agent only need $\mathcal{O}(n)$ experiments to predict all $4^{n}$ observables.

## Other examples

## Current proof techniques vary rather substantially for different tasks.

- Estimating $\operatorname{Tr}(\rho \sigma)$ [1]
- Quantum state tomography [2]
- Classifying symmetry [3]
- Quantum state certification [4]
- Quantum PCA [5]
- Learning Pauli channel [6]

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[1] Anshu, Anurag, Zeph Landau, and Yunchao Liu. "Distributed quantum inner product estimation." arXiv preprint arXiv:2111.03273 (2021).
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[3] Chen, Sitan, et al. "Exponential separations between learning with and without
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## Outline

- Basic setting and examples
- Key ideas:

Part I — Designing good learning algorithms
Part II — Proving no good learning algorithms exist

- Outlook and open questions



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- Basic setting and examples
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## Outlook

We know a little bit about what we can learn efficiently.


## Outlook

A lot of problems in these fields are yet to be studied rigorously.


## Open questions

- Can we perform shadow tomography on broader classes of observables computationally efficiently?
We only know how to do it efficiently for low-weight and Pauli observables.
- What classes of quantum dynamics/circuits are efficiently learnable? Many natural classes are either not efficiently learnable quantumly or efficiently learnable classically (e.g., local Hamiltonian evolution). Is there something in between?
- Could we efficiently learn if there are non-local quantum noise? Fault-tolerant quantum computers require local noise. Can we experimentally test this?


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    [4] Haah, Jeongwan, et al. "Sample-optimal tomography of quantum states." IEEE Transactions on Information Theory 63.9 (2017): 5628-5641.

[^1]:    References:
    [1] Chen, Sitan, et al. "Exponential separations between learning with and without quantum memory." 2021 IEEE 62nd Annual Symposium on Foundations of Computer Science (FOCS). IEEE, 2022.
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