Learning from quantum experiments

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Motivation

- One of the central goals of science is to learn how the physical world operates.
- process information to form predictive models.



Examples of scientific disciplines

• By performing experiments, humans can receive information about the physical world, and



A cartoon depiction of learning

Motivation

- design better algorithms to learn from experiments.
- A burgeoning field in QI considers the task of learning from quantum experiments.



Examples of scientific disciplines

• To accelerate and automate scientific development, it is important to understand how to



A cartoon depiction of learning

- Basic setting and examples
- Key ideas: Part I — Designing good learning algorithms
- Outlook and open questions



Outline

Part II — Proving no good learning algorithms exist

Basic setting and examples

• Key ideas: Part I — Designing good learning algorithms

Outlook and open questions



Outline

Part II — Proving no good learning algorithms exist

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



Unknown quantum object

Basic setting

- There is an unknown quantum object (states, processes, entire phase diagram, ...).
- Learn that object from experiments. So it becomes (approximately) known.
- How many experiments are needed? (Sample and query complexity)



Unknown quantum object

Basic setting

Quantum benchmarking



Quantum sensing

Learning from quantum experiments

Goal: Provide a learning-theoretic foundation for various applications

Overview

Machine learning for physics

Noise characterization

Variational quantum algorithms

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 ρ .
- 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.

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



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Motivations:

- The most basic quantum learning problem
- Benchmark quantum systems



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Unknown quantum state

Complexity is exponential in n

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References:

[1] Aaronson, Scott. "Shadow tomography of quantum states." SIAM Journal on Computing 49.5 (2019): STOC18-368.

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Motivations:

• 2nd most basic quantum learning problem



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Motivations:

- 2nd most basic quantum learning problem
- Benchmark quantum systems w/ good scaling in *n*



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



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Unknown quantum state

Complexity is linear or independent in *n*

References:

[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.



Example 3: Pauli channel tomography

- There is an unknown *n*-qubit Pauli channel \mathcal{P} .
- After learning, we want $\hat{\mathscr{P}} \approx \mathscr{P}$ under diamond norm.



• Learn $\hat{\mathscr{P}}$ by preparing input states, evolving under \mathscr{P} , and measuring output states.

Unknown Pauli channel

References:

[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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Motivations:

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



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Unknown Pauli channel

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Complexity varies under additional assumptions

References:

[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).
- After learning, we want $\hat{f}(x) \approx f(x)$ for most of x.



Unknown phase diagram

• Learn \hat{f} by preparing ground states under different x's, and measuring the states.

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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Unknown phase diagram

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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? (QML & 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 ...



Basic setting and examples

• Key ideas: Part I — Designing good learning algorithms

Outlook and open questions



Outline

Part II — Proving no good learning algorithms exist

• Basic setting and examples

• Key ideas: Part I — Designing good learning algorithms Part II — Proving no good learning algorithms exist

Outlook and open questions



Outline

- 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 I



Key Ideas



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

Part I



Key Ideas





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 $\rho \in \mathbb{C}^{2^n \times 2^n}$.
- Learn $\hat{\rho}$ by performing measurements on copies of ρ .
- After learning, we want $Tr(O\hat{\rho}) \approx Tr(O\rho)$ for observables $O_1, ..., O_M$.





Randomized experiment:

- Sample a random Clifford U_i to rotate the quantum state ρ .
- Measure the state in the computational basis $|b_i\rangle \in \{0,1\}^n$.

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Data processing:

• Construct
$$\hat{\rho}_i = \left[(2^n + 1) U_i^{\dagger} | b_i \rangle \langle b_i | U_i - L_i^{\dagger} \rangle \right]$$

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Geometric analysis:

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Geometric analysis:

Concentration bound:

I for each experiment.



• For O_1, \ldots, O_M with $Tr(O^2) = O(1)$, we can predict $Tr(O_i\rho)$ after $O(\log(M))$ measurements.





Theorem (Huang et al.; 2020)

- 1. Given $B, \epsilon > 0$, the procedure learns a classical representation of an unknown quantum state ρ from $N = \mathcal{O}(B \log(M)/\epsilon^2)$ measurements. the procedure can use the classical representation to predict $\hat{o}_1, \ldots, \hat{o}_M$, where $|\hat{o}_i - \operatorname{tr}(O_i\rho)| < \epsilon$, for all *i*.
- 2. Subsequently, given any O_1, \ldots, O_M with $B \ge \max \|O_i\|_2^2$,

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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Application: Quantum fidelity $|\psi\rangle\langle\psi|$



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Other applications

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

- 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].

References:

[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.

References:

[1] Chen, Sitan, et al. "Exponential separations between Foundations of Computer Science (FOCS). IEEE, 2022.
[2] Anshu, Anurag, Zeph Landau, and Yunchao Liu. "Dis
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• Basic setting and examples

• Key ideas: Part I — Designing good learning algorithms Part II — Proving no good learning algorithms exist

Outlook and open questions



Outline

- Basic setting and examples
- Key ideas: Part I — Designing good learning algorithms
- Outlook and open questions



Outline

Part II — Proving no good learning algorithms exist

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

Part I



Key Ideas

Mostly focus on **Conventional Experiments**





Conventional Experiments

What scientists currently do in the lab

Classical Memory



Receive, process, and store classical information

Receiving

¢ · · · · · |

Physical Measurements



Classical Computation

Processina



Quantum-enhanced Experiments

What future experiments could be like

Quantum Memory



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Storing

Receive, process, and store quantum information



Transduce from quantum sensors





Processing



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

Part |



Key Ideas



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

Related framework has been considered in [Bubeck, Chen, Li, FOCS'20], [Huang, Kueng, Preskill, PRL'21], [Aharonov, Cotler, Qi, '21]







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storing data from all POVM

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Store in quantum memory



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Quantum memory storing all copies of ρ

Process all quantum data with quantum computation

Predict properties of the physical system ρ





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



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

Theorem

quantum agent only need $\mathcal{O}(n)$ experiments to predict all 4^n observables.

Classical agent needs $\Omega(2^n)$ experiments to predict observable from the set, but

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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 ρ is a classical distribution over product states (no entanglement!).



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- We consider a graphical representation for the memory state of the classical agent.









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Probability distribution (bottom layer) sufficiently different \equiv Classical agent can distinguish ρ_A and ρ_B





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Probability distribution (bottom layer) sufficiently different \equiv Classical agent can distinguish ρ_A and ρ_B More experiments done \equiv Deeper the tree \equiv More distinct the distribution





Many-vs-one distinguishing task

a corresponding distinguishing task.



Partially-revealed many-versus-one distinguishing task

If the classical agent succeeds in the prediction task, then he/she must succeeds in





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Other examples

Current proof techniques vary rather substantially for different tasks.

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

References:

[1] Anshu, Anurag, Zeph Landau, and Yunchao Liu. "Distributed quantum inner product estimation." arXiv preprint arXiv:2111.03273 (2021).

[2] Chen, Sitan, et al. "Tight Bounds for State Tomography with Incoherent Measurements." arXiv preprint *arXiv:2206.05265* (2022)

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- Basic setting and examples
- Key ideas: Part I — Designing good learning algorithms
- Outlook and open questions



Outline

Part II — Proving no good learning algorithms exist

- Basic setting and examples
- Key ideas: Part I — Designing good learning algorithms
- Outlook and open questions



Outline

Part II — Proving no good learning algorithms exist

Quantum benchmarking

Quantum machine learning

Quantum sensing

Outlook

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



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

Quantum benchmarking

Quantum machine learning

Quantum sensing

Outlook


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?