New Bounds on Quantum Sample Complexity of Measurement Classes

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***Abstract*—This paper studies the sample complexity of learning in a quantum environment under a quantum counterpart of the well-known *probably approximately correct* (PAC) model. In this model, available are n randomly generated quantum states with classical labels for the training. The objective is to find a quantum measurement that with high probability predicts the labels of unseen samples correctly. The model is *agnostic* as the labeling law and the quantum states are unknown to the learner. It subsumes well-studied problems such as state discrimination, quantum property testing, and even classical PAC. Moreover, it abides by quantum mechanical laws such as no-cloning, state collapse, and measurement incompatibility. Such properties prohibit sample reuse and, thus, raise unique challenges for learning in quantum settings. We propose a new learning algorithm called shadow quantum risk minimizer and derive upper bounds on the sample complexity of several quantum concept classes. Particularly, we prove that the sample complexity of any quantum concept class $\mathcal{C}$ grows with $\mathcal{O}\Big(\frac{1}{\epsilon^2}\log\frac{|\mathcal{C}^*|}{\delta}\Big)$, where $\mathcal{C}^*$ is the set of extreme points of the convex closure of $\mathcal{C}$. Hence, in the worst case, the bound grows with the logarithm of the size of the concept class. This is a significant improvements compared to prior works.**

I. Introduction

Quantum learning is one of the leading applications of quantum computing both for classical and quantum problems. While some models suggest quantum-enhancements of classical learning by mapping data into input quantum states [1]–[6], quantum computers (QCs) have a far greater capability to learn patterns from inherently quantum data. This is possible by directly operating on quantum states of physical systems (e.g., photons or states of matter) or their qubit representations [7]–[14]. Learning from quantum data has been studied extensively in recent literature in the context of diverse applications, including condensed matter for phase-of-matter detection [7], [15], ground-state search [8], [9], [16], entanglement detection [10], [11], [17]–[20], and theoretical chemistry [12]–[14], [21], [22].

The focus of this paper is on the fundamental limits of quantum learning, particularly the quantum sample complexity as a measure of the hardness of training a model or tuning a quantum device. In classical learning theory, limits of learning has been studied for decades under the well-known PAC framework [23], [24]. In this work, we study a quantum counterpart of this problem under the *quantum probably approximately correct* (QPAC) framework [25].

Several models for quantum learning have been introduced and studied [26]–[29]. A survey on this topic is provided in [30]. In *quantum state discrimination*, the objective is to distinguish an unknown quantum state ρ from another (known or unknown) state using *measurements* on multiple samples [27], [29], [31]–[36]. In another model, introduced by Bshouty and Jackson [28], one is interested in solving a classical PAC problem using a quantum oracle that outputs identical copies of an associated superposition state [28], [37]–[40].

QPAC is a recent framework that subsumes several models such as state discrimination, quantum property testing, quantum state classification and classical PAC. It consists of a set of n labeled quantum states $(\rho_i, y_i)_{i=1}^n$ as the training samples. The samples are randomly generated independent and identically distributed (i.i.d.) and according to an unknown but fixed probability distribution. There is no structural assumption about the states ρ_i, the labeling y_i, and the underlying distribution. Here, predictors are quantum measurements applied to the quantum states. Thus, one seeks a model training procedure for finding a quantum measurement to minimize the prediction loss. The objective is to obtain a loss that is close to the optimal loss within a library of predictors (a.k.a concept class). Quantum sample complexity is, then, the minimum number of samples to guarantee such requirement for all quantum states, labeling, and the underlying distributions.

Therefore, QPAC is a stronger requirement than the above models, as it is a distribution-free and state-free condition. It is also stronger than PAC, as PAC is only distribution-free. Moreover, QPAC abides by quantum mechanical laws such as no-cloning, state collapse, and measurement incompatibility. Such properties prohibit sample reuse and, thus, raise new challenges for learning in quantum settings. Moreover, quantum models are significantly richer than classical models. Hence, given the fragility of quantum samples, the strictness of QPAC, and the richness of quantum models, one expects that quantum sample complexity to be significant, if not exponentially, greater than the classical one.

This paper presents a new bound on quantum sample complexity which is rather surprising. We show that with sophisticated algorithms the quantum sample complexity could potentially be comparable to the classical one. We introduce a novel algorithm called *quantum shadow risk minimization* (QSRM).

In classical learning *empirical risk minimization* (ERM) is a brute-force search in a given concept class $\mathcal{C}$ to minimize the empirical loss. With that ERM is an *agnostic* PAC learner as long as the training samples are a good representation of the true distribution which is guaranteed if the sample size is $n = O(\log|\mathcal{C}|)$ [41]. Extending this algorithm to quantum is not straightforward. One could naively propose the same technique to compute the empirical risk of each quantum predictor and chose the one with the minimum risk. However, the no-cloning and measurement incompatibility make this approach prohibitive. Essentially, the training samples will be distorted each time we measure the empirical risk of a predictor. If we use that naively, then we might need fresh samples for each predictor. That gives a sample complexity that grows with the size of the class $n = O(|\mathcal{C}|)$. There have been multiple attempts [25], [42]. [25] introduced an algorithm that measures the risk of compatible predictors together and hence obtained a better bound that grows with $O(\log|\mathcal{C}|)$ in fully compatible scenarios to $O(|\mathcal{C}|)$ in the worst case scenario with fully incompatible class. This is clearly larger than classical. Whether one can reduce the bound remains the question.

Contributions: We propose a new approach called QSRM to measure the empirical risk of the predictors in the class. that substantially improves the quantum sample complexity. Particularly, we prove that the quantum sample complexity of any measurement concept class $\mathcal{C}$ grows with $\mathcal{O}\left(\frac{1}{\epsilon^2}\log\frac{|\mathcal{C}^*|}{\delta}\right)$, where $\mathcal{C}^*$ is the set of extreme points generating $\mathcal{C}$. Hence, in the worst case, the bound grows with $O(\log|\mathcal{C}|)$ if $\mathcal{C}$ is finite. Interestingly, the bound can be much lower than $\log|\mathcal{C}|$. This is surprising especially since sample duplication is prohibited and measurement incompatibility would lead to an exponentially larger sample complexity with standard methods. We derive these bounds by proposing a quantum algorithm that tackles the issue of measurement incompatibility.

II. Model Formulation

Notations: For shorthand, denote $[d]$ as $\{1, 2, ..., d\}$. For any $d \in \mathbb{N}$, let H_d be the Hilbert space of d-qubits with $\dim = 2^d$. The identity operator on H_d is denoted by I_d. As usual, a quantum state is defined as a *density operator*; that is a Hermitian, unit-trace, and non-negative linear operator. A quantum measurement $\mathcal{M}$ is a positive operator-valued measure (POVM) represented by a set of operators $\mathcal{M} := \{M_v, v \in \mathcal{V}\}$, where $\mathcal{V}$ is theset of possible outcomes, $M_v \geq 0$ for any $v \in \mathcal{V}$, and $\sum_{v\in\mathcal{V}} M_v = I_d$. For an operator A, denote $\|A\|_1 = \mathrm{tr}\{|A|\}$ as the trace norm, and $\|A\|_2 = \sqrt{\mathrm{tr}\{A^\dagger A\}}$ as the Hilbert–Schmidt norm.

A. Quantum Learning Model

Before presenting the main results, we formally define our quantum learning model. In this model [25], the objective is to distinguish between multiple groups of unknown quantum states without prior knowledge about the states. Available is only a training set of quantum states with a classical label determining their group index. We seek an agnostic procedure that given enough samples learns the labeling law. The model is defined more precisely as follows.

Let $\mathcal{Y}$ denote the labeling set and $\mathcal{H}$ be the underlying Hilbert space[1]. Each time, a sample $(|\phi\rangle_i, y_i), i \in [n]$ is randomly generated according to an unknown but fixed probability distribution D. A predictor is a quantum measurement $\mathcal{M} := \{M_{\hat{y}} : \hat{y} \in \mathcal{Y}\}$ that acts on the quantum states and outputs $\hat{y} \in \mathcal{Y}$ as the predicted label. Note that, unlike classical learning, the predicted label is random even for a fixed input. From Born's rule, $\hat{y}_i$ is generated randomly with probability $\langle\phi_i|M_{\hat{y}_i}|\phi_i\rangle$. The prediction loss is determined via a loss function $l : \mathcal{Y}\times\mathcal{Y} \to [0,\infty)$. The risk of a predictor $\mathcal{M}$ is computed by randomly generating a test sample $(|\phi\rangle_{test}, y_{test})$ according to D and measuring $|\phi\rangle_{test}$ with $\mathcal{M}$ to get $\hat{y}_{test}$. Hence, from Born's rule, the generalization (expected) loss is calculated as $L_D(\mathcal{M}) = \mathbb{E}[l(Y,\hat{Y})]$, where the expectation is taken over the sample's distribution D and the distribution of $\hat{Y}$.

Remark 1. *The generalization can be written compactly in terms of the density operators. Let ρ_y be a mixed state (density operator) representing the overall state of the system under label y. We can view ρ_y is the state averaged under the condition that the label is y. Then, the generalization loss of $\mathcal{M}$ is given by*

$$L_D(\mathcal{M}) = \sum_{y\in\mathcal{Y}}\sum_{\hat{y}\in\mathcal{Y}} D_Y(y)l(y,\hat{y})\,\mathrm{tr}\{M_{\hat{y}}\rho_y\}. \tag{1}$$

The problem in the binary case is simplified. The following is an example of this setting.

Example 1. *As an example, consider a simple setting where there are only three types of states $|\psi_j\rangle, j = 0, 1, 2$ with label set $\mathcal{Y} = \{0, 1\}$. Each labeled sample is either of the four possibilities: $(|\psi_0\rangle, 0), (|\psi_1\rangle, 1), (|\psi_2\rangle, 0)$, and $(|\psi_2\rangle, 1)$ with probabilities $p_{0,0}, p_{1,1}, p_{2,0}$, and $p_{2,1}$, respectively. Hence, the label of $|\psi_2\rangle$ is probabilistic. Also consider the 0-1 loss $l(y, \hat{y}) := \mathbb{1}_{\{y\neq\hat{y}\}}$. Then, the generalization loss of a measurement $\mathcal{M} = \{M_0, M_1\}$ is given by $L_{0\text{-}1}(\mathcal{M}) = p_{0,0}\langle\psi_0|M_1|\psi_0\rangle + p_{1,1}\langle\psi_1|M_0|\psi_1\rangle + p_{2,0}\langle\psi_2|M_0|\psi_2\rangle + p_{2,1}\langle\psi_2|M_0|\psi_2\rangle$. Hence, the corresponding density operators are $\rho_0 = p_{0,0}|\psi_0\rangle\langle\psi_0| + p_{2,0}|\psi_2\rangle\langle\psi_2|$, and $\rho_0 = p_{1,1}|\psi_1\rangle\langle\psi_1| + p_{2,1}|\psi_2\rangle\langle\psi_2|$.*

The generalization loss is compared to the optimal value within a concept class which is a collection $\mathcal{C}$ of quantum predictor measurements. With this setup, a quantum learning algorithm processes the training samples and finds a predictor $\mathcal{M}$ which may or may not belong to $\mathcal{C}$. Let opt be the minimum loss among all the predictors in $\mathcal{C}$. We are interested in algorithms that without any knowledge of the sample's description, the labeling, and D, output a predictor whose loss is close to opt.

Definition 1 (QPAC)**.** *A quantum learning algorithm agnostically QPAC learns a measurement class $\mathcal{C}$ if there exists*

[1]For presentation simplicity, we assume $\mathcal{Y}$ is finite and $\mathcal{H}$ is finite-dimensional.

a function $n_{\mathcal{C}} : (0,1)^2 \mapsto \mathbb{N}$ *such that for every* $\epsilon, \delta \in [0, 1]$ *and given* $n > n_{\mathcal{C}}(\epsilon, \delta)$ *samples drawn i.i.d. according to any probability distributions* D *and any unknown states* $|\phi\rangle_i, i \in [n]$*, the algorithm outputs, with probability of at least* $(1-\delta)$*, a measurement whose loss is less than* $\mathsf{opt}_{\mathcal{C}} = \inf_{\mathcal{M}\in\mathcal{C}} L_D(\mathcal{M}) + \epsilon$.[2]

Consequently, the quantum sample complexity of a concept class $\mathcal{C}$ is the minimum of $n_{\mathcal{C}}$ for which there exists a QPAC learning algorithm.

Note that the state discrimination problem is a special case in which samples are identical and are either of two *a priori* known states. Also, note that QPAC also subsumes classical PAC as classical samples can be embedded into pure and orthogonal states, and functions can be considered as a special form of quantum measurements. Therefore, QPAC is a stronger requirement than PAC and other methods. It is a *agnostic*, distribution-free and state-free condition; whereas PAC is only distribution-free. In addition, principles such as the no-cloning and state collapse after measurements, indicate that quantum samples are more fragile than classical ones.

B. Related Works on QERM

It is known that classical ERM PAC learns any (classical) finite concept class $\mathcal{C}$ with sample complexity that scales with $\mathcal{O}\Big(\frac{1}{\epsilon^2}\log\frac{|\mathcal{C}|}{\delta}\Big)$. In quantum settings, there have been various attempts in developing counterparts of ERM algorithm. Due to the no-cloning theorem, the straightforward quantum extension of ERM results in a sample complexity of $\mathcal{O}\Big(\frac{|\mathcal{C}|}{\epsilon^2}\log\frac{1}{\delta}\Big)$, see [25] for more details. This is problematic as the sample complexity grows linearly with the size of the concept class.

In [25], a new ERM-type algorithm is introduced to improve this bound. The new bound depends on the measurement *incompatibility* structure of the concept class. Incompatible measurements cannot be measured simultaneously (for more details see [43]). On one extreme, all the measurements in the concept class are mutually compatible; on another extreme, there is no pair of compatible measurements. Based on this, an improved bound on sample complexity is as follows.

Remark 2 ([25])**.** *Quantum sample complexity of any finite concept class* $\mathcal{C}$ *is upper bounded as*

$$n_{\mathcal{C}}(\epsilon,\delta) \leq \min_{\mathcal{C}_r \text{Comp. partition}} \sum_{r=1}^{m} \Big\lceil \frac{8}{\epsilon^2}\log\frac{2m|\mathcal{C}_r|}{\delta}\Big\rceil,$$

where the minimization is taken over all compatibility partitioning of $\mathcal{C}$*. This bound ranges from* $\mathcal{O}\Big(\frac{1}{\epsilon^2}\log\frac{|\mathcal{C}|}{\delta}\Big)$*, for fully compatible class, to* $\mathcal{O}\Big(\frac{|\mathcal{C}|}{\epsilon^2}\log\frac{1}{\delta}\Big)$ *for fully incompatible class.*

In [42], this result was extended to infinite concept classes through an ϵ-netting argument. In this paper, we propose a new quantum ERM that substantially improves the above bounds to one that, in the worst case, grows with $\mathcal{O}\Big(\frac{1}{\epsilon^2}\log\frac{|\mathcal{C}|}{\delta}\Big)$ even for fully incompatible concept classes.

[2]Naturally, we are interested in efficient learning with $n_{\mathcal{C}}$ being at most polynomial in ϵ, δ and $\dim(\mathcal{H})$.

III. Main Results

In this section, we present the main results of the paper. We first, start with studying the convex closure of the concept class.

Let $\bar{\mathcal{C}}$ denote the convex closure (envelope) of $\mathcal{C}$. When $\mathcal{C}$ is finite, then $\bar{\mathcal{C}}$ is the set of all POVMs that can be written as a convex combination of measurements in $\mathcal{C}$. More precisely, POVMs of the form $\bar{\mathcal{M}} = \{\bar{M}_{\hat{y}}, \hat{y} \in \mathcal{Y}\}$ such that

$$\bar{M}_{\hat{y}} = \sum_{j=1}^{k} \alpha_j M^j_{\hat{y}}, \quad \forall \hat{y} \in \mathcal{Y},$$

where each $\mathcal{M}^j = \Big\{M^j_{\hat{y}}, \hat{y} \in \mathcal{Y}\Big\}$ belongs to $\mathcal{C}$, and $\alpha_j \in [0, 1]$ with $\sum_j \alpha_j = 1$.

Theorem 1. *Suppose* ℓ *is a bounded loss function and* $\mathcal{C}$ *is a measurement class with finite extreme points. Then, QSRM (Algorithm 1) agnostically QPAC learns* $\mathcal{C}$ *with quantum sample complexity bounded as*

$$n_{\mathcal{C}}(\epsilon,\delta) \leq \mathcal{O}\Big(\frac{1}{\epsilon^2}\log\frac{|\mathcal{C}^*|}{\delta}\Big),$$

where $\mathcal{C}^*$ *is the set of extreme points of convex closure of* $\mathcal{C}$*.*

Note that $|\mathcal{C}^*| \leq |\mathcal{C}|$. Even when $\mathcal{C}$ is infinite $\mathcal{C}^*$ can be finite. Hence an interesting distinction compared to the classical is observed. When $\mathcal{C}$ is finite, then the bound in theorem scales at most with $\mathcal{O}\Big(\frac{1}{\epsilon^2}\log\frac{|\mathcal{C}|}{\delta}\Big)$. Interestingly, in other scenarios where $|\mathcal{C}^*| \ll |\mathcal{C}|$ the bound is significantly lower. However, even though the Hilbert space is finite-dimensional and $\mathcal{Y}$ is finite, there could be infinitely many extreme points in $\bar{\mathcal{C}}$. In that case, an ϵ-netting argument will give a bound on the sample complexity.

IV. Algorithm and Analysis

In this section, we present our quantum learning algorithm called quantum shadow risk minimization (QSRM). Further, we propose a concentration analysis and prove the main theorem.

A. Measuring the Empirical Loss

We start with defining the loss measurement for each predictor $\mathcal{M}$. Without loss of generality, assume $l : \mathcal{Y}\times\mathcal{Y} \mapsto [0, 1]$. Let $\mathcal{Z}$ be the image set of l. Since $\mathcal{Y}$ is a finite set, then so is $\mathcal{Z}$. With that, the loss observable for any predictor $\mathcal{M} := \{M_{\hat{y}} : \hat{y} \in \mathcal{Y}\}$ is given by $\mathcal{L}_M := \{L^M_z : z \in \mathcal{Z}\}$, where

$$L^M_z = \sum_{y,\hat{y}\in\mathcal{Y}} \mathbb{1}_{\{l(y,\hat{y})=z\}} M_{\hat{y}} \otimes |y\rangle\langle y|, \qquad \forall z \in \mathcal{Z}. \tag{2}$$

Therefore, the loss of $\mathcal{M}$ for predicting y from a given ρ_x is obtained by applying $\mathcal{L}_M$ on $\rho_x \otimes |y\rangle\langle y|$. The result is a random variable $Z = \ell(y, \hat{Y})$ taking values from $\mathcal{Z}$ as in (2). With this formulation the expected loss of $\mathcal{M}$ equals to

$$L_D(\mathcal{M}) = \langle \mathcal{L}_M \rangle_{\rho_{XY}}$$

Moreover, a realization of the empirical loss of $\mathcal{M}$ over the samples is

$$L_{\mathcal{S}_n}(\mathcal{M}) \triangleq \frac{1}{n}\sum_i z(i),$$

where $z(i)$ is the outcome of the measurement $\mathcal{L}_M$ on the ith sample. Note that, unlike classical learning, even for fixed samples the empirical loss is not fixed. From Born's law, one can calculate the probability of each realization of the empirical loss.

B. Joint Estimation of Empirical Loss

The main challenge in the quantum setting is to measure the empirical loss for all the measurements in the class. This however is impossible due to the no-cloning and measurement incompatibility. The loss measurements $\mathcal{L}_M$ might be incompatible for different $\mathcal{M} \in \mathcal{C}$ — hence impossible to be measured simultaneously. In [25] it was proposed to partition $\mathcal{C}$ into mutually compatible subsets. With that approach bounds on the sample complexity were introduced. Unfortunately, in the worst-case scenario, the bounds could grow with $|\mathcal{C}|$. In what follows, we introduce a new approach that, in the worst-case, grows with $\log|\mathcal{C}|$.

Our approach is inspired by Shadow Tomography [44], [45] that is applied to identical copies of quantum states. To the best of our knowledge, this is the first work on applying such a technique to a learning context. Moreover, we consider an extension of it to randomly generated states; rather than identical copies. we perform the following procedure for each sample $(\rho_i, y_i), i \in [n]$. In what followed, we explain our approach.

First, we generate a unitary operator U_i randomly and uniformly from the space of all unitary operators on the underlying Hilbert space $\mathcal{H}$. We rotate ρ_i by applying U_i resulting the state $U_i^\dagger \rho_i U_i$. Let $\{|j\rangle, j = 1, 2, ..., \dim_{\mathcal{H}}\}$ be a basis on $\mathcal{H}$. We measure the rotated state on this basis. From Born's rule the probability of getting the output j is $P_j = \langle j|U_i^\dagger \rho_i U_i|j\rangle$. Suppose the outcome for the ith sample is $j_i \in [\dim_{\mathcal{H}}]$. Then, the following state is prepared

$$\omega_i = U_i\,|j_i\rangle\langle j_i|\,U_i^\dagger.$$

As a result, the expected state ω_i over the measurement randomness (P_j) and the choice of unitary U_i equals to

$$\Gamma[\rho_i] := \mathbb{E}_U\Big[\sum_{j\in[\dim_{\mathcal{H}}]} \langle j|U^\dagger\rho_i U|j\rangle\;\; U\,|j\rangle\langle j|\,U^\dagger\Big]. \tag{3}$$

Remark 3. *Γ is a linear mapping on $\mathcal{B}(\mathcal{H})$ with its inverse, denoted as Γ^{-1}, also a linear mapping.*

Given this definition, we apply Γ^{-1} on ω_i resulting in the following final state

$$\hat{\rho}_i := \Gamma^{-1}\big[U_i\,|j_i\rangle\langle j_i|\,U_i^\dagger\big]. \tag{4}$$

This state is the "shadow" of ρ_i. Since j_i is classical, we can create multiple copies of $\hat{\rho}_i$. Particularly, we create one copy for each $\mathcal{M} \in \mathcal{C}^*$, measure it by the measurement, and calculate the incurred loss $l(y_i, \hat{y}_i)$. Let $\hat{Z}_{i,\ell}$ be (random) loss values on the ith shadow for the ℓth measurement in $\mathcal{C}^*$ that is $\mathcal{M}_\ell = \{M_{\ell,\hat{y}} : \hat{y} \in \mathcal{Y}\}$. Then,

$$\mathbb{E}[\hat{Z}_{i,\ell}] = \sum_{\hat{y}_i\in\mathcal{Y}} l(y_i, \hat{y}_i)\,\mathrm{tr}\{M_{\ell,\hat{y}_i}\hat{\rho}_i\}.$$

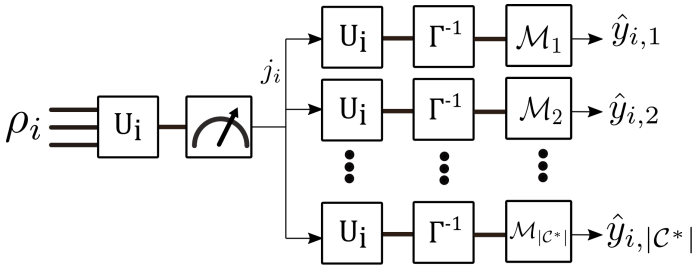

Fig. 1. The process for estimating the empirical loss of each measurement.

This process is demonstrated in Figure 1. Then, we repeat this process for each sample, to obtain $\hat{\rho}_i$ and then $\hat{z}_{i,\ell}$ for $i \in [n]$ and $\ell \in [|\mathcal{C}^*|]$. Lastly, we compute the following as the estimate of the empirical loss for each $\mathcal{M} \in \mathcal{C}^*$:

$$\hat{L}(\mathcal{M}_\ell) := \frac{1}{n}\sum_{i=1}^{n} \hat{z}_{i,\ell}. \tag{5}$$

Note that $\hat{L}$ is different from $L_{\mathcal{S}_n}$ as it is based on the shadows $\hat{\rho}_i, i \in [n]$. In what follows, we provide the analysis for this estimation.

Lemma 1. *$\hat{\rho}_i$ is an unbiased estimate of ρ_i, that is $\mathbb{E}_{U_i,J_i}[\hat{\rho}_i] = \rho_i$, where the expectation is taken over the rotation U and measurement randomness.*

Proof. By linearity of Γ^{-1}, taking the expectation of $\hat{\rho}_i$ over the choice of U_i and the randomness of J_i gives

$$\mathbb{E}_{\sim(U_i,J_i)}[\hat{\rho}_i] = \Gamma^{-1}\Big[\mathbb{E}\Big[U_i\,|J_i\rangle\langle J_i|\,U_i^\dagger\Big]\Big].$$

The expectation term equals to

$$\mathbb{E}_U\Big[\sum_{j\in[\dim_{\mathcal{H}}]} \langle j|U^\dagger\rho_i U|j\rangle\;\; U\,|j\rangle\langle j|\,U^\dagger\Big] = \Gamma[\rho_i],$$

where the last equality is from (3). Hence, the expectation of $\hat{\rho}_i$ equals to $\Gamma^{-1}[\Gamma[\rho_i]] = \rho_i$, as desired. □

Lemma 2. *The estimation $\hat{L}(\mathcal{M})$ is an unbiased estimate of $L_D(\mathcal{M})$, that is $\mathbb{E}[\hat{L}(\mathcal{M})] = L_D(\mathcal{M})$, where the expectation is taken over all sources of randomness including the training samples.*

Proof. By taking the expectation, from Lemma 1 we obtain the following chain of equalities:

$$\begin{aligned}\mathbb{E}[\hat{L}(\mathcal{M})] &= \frac{1}{n}\sum_i \mathbb{E}_{(\hat{\rho}_i,y_i)}[\langle \mathcal{L}_M\rangle_{\hat{\rho}_i\otimes|y_i\rangle\langle y_i|}] \\ &= \frac{1}{n}\sum_i \langle \mathcal{L}_M\rangle_{\mathbb{E}_{(\hat{\rho}_i,y_i)}[\hat{\rho}_i\otimes|y_i\rangle\langle y_i|]} \\ &= \frac{1}{n}\sum_i \langle \mathcal{L}_M\rangle_{\rho_{XY}} \\ &= L_D(\mathcal{M}).\end{aligned}$$

where we used the linearity of the expectation and the fact that the average $\langle\mathcal{N}\rangle_\sigma$ of any observable $\mathcal{N}$ over any state σ is linear in σ. □

C. Proof of Theorem 1

We start with the following lemma:

Lemma 3. *Let $\bar{\mathcal{C}}$ be the convex closure of $\mathcal{C}$ and $\mathcal{C}^*$ be the set of all extreme points of $\bar{\mathcal{C}}$. Then, $\mathsf{opt}_{\mathcal{C}} = \mathsf{opt}_{\bar{\mathcal{C}}} = \inf_{\mathcal{M}\in\mathcal{C}^*} L_D(\mathcal{M})$.*

Proof. Note that $L_D(\mathcal{M})$ is linear, and hence convex, in $\mathcal{M}$. This is due to the linearity of the trace and the definition of the loss given in (1). As a result, given that $\mathcal{C}\subseteq\bar{\mathcal{C}}$ and that

$$\mathsf{opt}_{\bar{\mathcal{C}}} = \inf_{\mathcal{M}\in\bar{\mathcal{C}}} L_D(\mathcal{M})$$

then $\mathsf{opt}_{\bar{\mathcal{C}}} = \mathsf{opt}_{\mathcal{C}}$. Moreover, since the above expression is a convex optimization, then the optimal values occur at the extreme points of $\bar{\mathcal{C}}$. Hence the proof is complete. □

This result implies that QPAC learning of $\mathcal{C}$ is reduced to its extreme points $\mathcal{C}^*$. Given Lemma 2, the theorem follows by a large deviation analysis. From McDiarmid's inequality:

$$\begin{aligned}\mathbb{P}\Big\{\max_{\mathcal{M}\in\mathcal{C}^*}\big|\hat{L}(\mathcal{M}) - L_D(\mathcal{M})\big| \geq \epsilon\Big\} \\ \leq 2|\mathcal{C}^*|\exp\Big\{-\frac{2n\epsilon^2}{(b-a)^2}\Big\},\end{aligned}$$

where $b = \max l(y,\hat{y})$ and $a = \min l(y,\hat{y})$. Equating the right-hand side to δ, we obtain the following bound on the estimation error:

$$\max_{\mathcal{M}\in\mathcal{C}^*}\big|\hat{L}(\mathcal{M}) - L_D(\mathcal{M})\big| = \mathcal{O}\left(\sqrt{\frac{1}{n}\log\left(\frac{|\mathcal{C}^*|}{\delta}\right)}\right). \quad (6)$$

Now, let $\widehat{\mathcal{M}}$ and $\mathcal{M}^*$ be the measurements minimizing the $\hat{L}$ and L_D, respectively. Then, from (6), with probability $(1-\delta)$ the following chain of inequalities hold:

$$\begin{aligned}L_D(\widehat{\mathcal{M}}) &\leq \hat{L}(\widehat{\mathcal{M}}) + \frac{\epsilon}{2} \\ &\leq \hat{L}(\mathcal{M}^*) + \frac{\epsilon}{2} \leq L_D(\mathcal{M}^*) + \epsilon.\end{aligned}$$

The left-hand side is the loss of the selected predictor by QSRM (Algorithm 1, and the right-hand side equals $\mathsf{opt}_{\mathcal{C}} + \epsilon$ and hence the proof is complete.

Algorithm 1: QSRM

Input: $\mathcal{C}^*$ of the concept class and n training samples.

for $i = 1$ **to** n **do**
- Generate a unitary U_i randomly.
- Apply U_i on ρ_i as in Figure 1.
- Measure along $\{|j\rangle, j\in[\dim_{\mathcal{H}}]\}$ to get j_i.
- **for** $\ell = 1$ **to** $|\mathcal{C}^*|$ **do**
  - Prepare the state $\hat{\rho}_i$ as in (4).
  - Measure $\hat{\rho}_i$ by $\mathcal{M}_\ell$ to get $\hat{y}_{i,\ell}$.
  - Calculate the incurred loss $z_{i,\ell} = l(y_i,\hat{y}_{i,\ell})$.

Compute the estimated empirical loss for each measurement as $\hat{L}(\mathcal{M}_\ell) = \frac{1}{n}\sum_i \hat{z}_{i,\ell}$.

return $\hat{\mathcal{M}}$ as the measurement with the minimum $\hat{L}$.

Conclusion

This paper studies the learning of quantum measurement classes. It introduces a novel quantum algorithm called QSRM for learning quantum concept classes. Using this algorithm, a new upper bound on the quantum sample complexity is derived. It is shown that the quantum sample complexity grows at most with he logarithm of the size of the extreme points of the convex closure of the concept class. This is a significant improvement over prior results. The approach is based on a novel method to estimate the empirical loss of the concept class via creating random shadows of the training samples. With that QSRM algorithm can perform risk minimization while abiding to no-cloning, state collapse, and measurement incompatibility.

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