Clifford Circuits can be Properly PAC Learned if and only if $\text{RP} = \text{NP}$

Daniel Liang

Department of Computer Science
University of Texas at Austin

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Abstract

Given a dataset of input states, measurements, and probabilities, is it possible to efficiently predict the measurement probabilities associated with a quantum circuit? Recent work of Caro and Datta [19] studied the problem of PAC learning quantum circuits in an information theoretic sense, leaving open questions of computational efficiency. In particular, one candidate class of circuits for which an efficient learner might have been possible was that of Clifford circuits, since the corresponding set of states generated by such circuits, called stabilizer states, are known to be efficiently PAC learnable [37]. Here we provide a negative result, showing that proper learning of CNOT circuits is hard for classical learners unless $\text{RP} = \text{NP}$. As the classical analogue and subset of Clifford circuits, this naturally leads to a hardness result for Clifford circuits as well. Additionally, we show that if $\text{RP} = \text{NP}$ then there would exist efficient proper learning algorithms for CNOT and Clifford circuits. By similar arguments, we also find that an efficient proper quantum learner for such circuits exists if and only if $\text{NP} \subseteq \text{RQP}$.

1 Introduction

The goal of efficient learning of quantum states and the circuits that act on them, is to be able to predict the outcome of various measurements with some degree of accuracy. For example, given a quantum state $\rho$ and a two-outcome measurement $M$ can we predict the probability that the measurement accepts?

Naively, one can try and learn everything there is to know about the system, a technique known as tomography with versions for quantum states [27, 35, 36] and quantum processes [4, 21]. However, this requires exponential time in the number of qubits due to information theoretic reasons related to the exponential dimension of the system. This exponential bound remains when trying to find a state close in trace distance as shown by a combination of Flammia et al. [24] and Holevo’s bound. To address this, one can choose to restrict the type of information one wanted to learn, which led to the ideas of shadow tomography [2] and classical shadows [28]. By only needing to predict the value of $M$ observables $\{O_i\}$ one is able to use only a number of measurements that is polynomial in the number of qubits and polylogarithmic in $M$. In a similar vein, Aaronson [1] proposed the idea of PAC
learning quantum states, which is the idea of learning relative to some distribution over measurements, but only being given samples from that distribution as well (see Section 2.5 for details).

An alternative direction was to restrict the class of objects being learned on, but allow one to choose what kind of measurements are taken. Montanaro [34] was able to learn stabilizer states and later Low [33] learned an unknown Clifford circuit. Lai and Cheng [32] built on these results in the case of actually recovering the circuit, as well as limited learning in the presence of a small amount of non-Clifford gates. Stabilizer states and Clifford circuits are of particular interest to the quantum information community because many of our quantum communication protocols and well known quantum query algorithms [10–12, 14, 25, 39] utilize these states and circuits. Gottesman and Knill [26] (with improvements by Aaronson and Gottesman [3]) were also able to give an efficient classical simulation of these objects, showing these class of objects to seemingly be much simpler than the set of all quantum states or circuits. Combined with the fact that stabilizer states are good approximations to Haar random states [31, 41], we get a set of circuits and states that are highly quantum with many interesting uses, but still have enough exploitable structure to be classically simulable, making them a prime candidate for learning.

Rocchetto [37] was able to combine the ideas of PAC learning with the structure provided by restricting to stabilizer states to give an efficient PAC algorithm for learning stabilizer states. In particular, the algorithm given was a proper learner, in that the hypothesis state was required to also be a stabilizer state, rather than something that is non-stabilizer but acts close to stabilizer and with low error. Caro and Datta [19] extended the ideas of PAC learning to quantum circuits, giving an analogous generalization theorem to Aaronson [1]. As such, an open problem was whether or not Clifford circuits could be efficiently PAC learned in an analogous way to stabilizer states. To that extent, we show in this paper that an efficient proper learner for Clifford circuits exists if and only if $\text{RP} = \text{NP}$. Here, we are given inputs of the form $(\rho, \frac{I^{\otimes n} + P}{2})$ for some stabilizer state $\rho$, Pauli matrix $P$ with labels $\text{Tr}\left[\frac{I^{\otimes n} + P}{2}C\rho C^\dagger\right]$ corresponding to an unknown Clifford circuit $C$ and asked to predict future labels. Furthermore, this is true even just for a learner of a subset of Clifford circuits called CNOT circuits. This subset essentially restricts to the set of Clifford circuits that map computational basis states to other computational basis states and these circuits are highly related to the complexity class $\oplus L$ (see Section 2.4). Note however that we slightly alter the definition of PAC learning a quantum circuit from that of Caro and Datta [19] to a setting we find more comparable to Aaronson [1]’s original PAC learning result for quantum states. In the setting introduced by Caro and Datta, the measurements were limited to being rank 1 projectors with product structure, rather than the rank $2^{n-1}$ projectors we use in our proof.

One can also imagine that the learning algorithm has access to a quantum computer. Since there exists problems like factoring [38] for which we have an efficient quantum algorithm but not an efficient classical algorithm, this learner may be able to efficiently learn more expressive concept classes. We also give results for this setting by relating $\text{NP}$ to $\text{RQP}$ the quantum analogue of $\text{RP}$. We now informally state our main theorems regarding CNOT and Clifford circuits.

**Theorem 1.1.** There exists an efficient randomized proper PAC learner for CNOT circuits
if and only if $RP = NP$. Furthermore, an efficient quantum proper PAC learner for CNOT circuits exists if and only if $NP \subseteq RQP$.

**Corollary 1.2.** There exists an efficient randomized proper PAC learner for Clifford circuits if and only if $RP = NP$. Furthermore, an efficient quantum proper PAC learner for Clifford circuits exists if and only if $NP \subseteq RQP$.

We prove this by first realizing that finding a CNOT circuit with zero training error requires finding a full rank matrix in an affine subspace of matrices under matrix addition (so as to differentiate from a coset of a matrix group using matrix multiplication). This is known as the Nonsingularity problem [17] and is NP-Complete. While this may seem like a backwards reduction, it turns out that the set of matrix affine subspaces used to show that Nonsingularity can solve 3SAT are a subset of the ones needed to learn CNOT circuits with zero training error. Thus, there exist a set of samples such that a CNOT circuit with zero training error exists if and only if the SAT instance is satisfiable. Finding such a CNOT circuit is what is known as the search version of the consistency problem and in turn the decision version of the consistency problem is also NP-Complete.

To show that an efficient proper learner for CNOT circuits implies $RP = NP$, let $S$ be some sample from the decision version of the consistency problem for CNOT circuits. Using the uniform distribution over each element in $S$, we will sample every element of $S$ with high probability given enough queries. Thus we are able to show that an efficient learner would necessarily also solve the consistency problem with high enough probability to create a solution in $RP$.

To show that $RP = NP$ implies an efficient learner, we utilize search-to-decision reductions for NP-complete problems to get an efficient algorithm for the search problem of minimizing training error. We can treat this search algorithm as our means of generating such a hypothesis circuit $C$ with low training error. By the generalization theorem provided by Caro and Datta [19], assuming we have enough samples this $C$ will properly generalize and have low true error, thus completing the proof. The quantum forms of the proof essentially come for free by replacing $RP$ with $RQP$ everywhere and using learners capable of doing quantum computation.

### 1.1 Related Work

We note that we are dealing with the problem of classically PAC learning a classical function (i.e. classical labels) derived from a quantum system. This is as opposed to quantum PAC learning of a classical function as in Arunachalam and de Wolf [5, 6], Arunachalam et al. [7, 9] where instead of a distribution over samples we receive access to copies of a quantum state. This state results in the same distribution classically when measured in the computational basis but can be measured in other basis to get different results. There is also the attempt to directly learn a quantum process with quantum labels, as in Caro [18], Chung and Lin [22]. Here, they do not choose to measure the output state, and have samples of the form $(\rho, \mathcal{M}(\rho))$ for quantum process $\mathcal{M}$. Other related quantum learning works, some of which are outside the PAC model, include Cheng et al. [20], Low [33], Yoganathan [40].
2 Preliminaries

2.1 Quantum States and Circuits

A quantum state \( \rho \) on \( n \) qubits is a \( 2^n \times 2^n \) PSD matrix with trace 1. If the matrix is rank 1 then we refer to \( \rho \) being a pure state, since it can be decomposed as \( \rho = |\psi\rangle \langle \psi| \) where \( |\psi\rangle \) is a \( 2^n \)-dimensional column vector with norm 1 and \( \langle \psi| \) is its complex conjugate. A two-outcome measurement \( E \) is then a projector such that \( E^2 = E \) such that the probability of a ‘1’ outcome is \( \text{Tr}[E \rho] \) and the probability of a ‘0’ outcome is \( 1 - \text{Tr}[E \rho] \), leaving the expectation value as simply \( \text{Tr}[E \rho] \).

A quantum process is how one evolves a quantum state, and therefore it must preserve the trace 1 and the PSD condition. We will be primarily interested in quantum circuits, which are the subset of quantum processes that map pure states only to other pure states. These are constrained to be unitary operations, such that after acting on \( \rho \) with the circuit \( C \), the state that we are left with is \( C \rho C^\dagger \) where \( C^\dagger \) is the complex conjugate of \( C \).

2.2 Paulis and Stabilizer States/Groups

We will start by giving the following matrices, known as the Pauli matrices.

\[
I = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \quad X = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad Y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad Z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}
\]

Noting that these are all unitaries that act on a single qubit, we can generalize to \( n \) qubits.

Definition 2.1. Let \( P_n = \{ \pm 1, \pm i \} \times \{ I, X, Y, Z \}^{\otimes n} \) be the matrix group consisting all \( n \)-qubit Paulis with phase \( \pm 1 \) or \( \pm i \).

We’ll also introduce some shorthand notation:

Definition 2.2. Let \( X_i \) and \( Z_i \) be the Pauli acting only on the \( i \)-th qubit with \( X \) or \( Z \) respectively and the identity matrix on all other qubits.

Definition 2.3. For \( v \in \{0,1\}^n \), let \( X^v = \prod_{i=1}^n X_i^{v_i} \) and \( Z^v = \prod_{i=1}^n Z_i^{v_i} \).

Note that \( Z^v \cdot Z^w = Z^{v+w} \), assuming the dimensions of \( v \) and \( w \) match. It is easy to see that \( v \neq w \) also implies that \( Z^v \neq Z^w \).

A stabilizer state \( \rho \) is any state that can be written as \( \frac{1}{2^n} \sum_{g \in G} g \), where \( G \) is an abelian subgroup \( G \subseteq P_n \setminus \{ -I^{\otimes n} \} \) without the negative identity. \( G \) is known as the stabilizer group of \( \rho \). As it turns out, if \( G \) is order \( 2^n \) then \( \rho \) will be a pure state. This leads to the alternative (and more popular definition) where \( \rho = |\psi\rangle \langle \psi| \), is the unique state that is stabilized by \( G \). That is, for all \( g \in G \), \( g |\psi\rangle = |\psi\rangle \). This definition shows why \( -I^{\otimes n} \) isn’t allowed to be in \( G \), since \( -I^{\otimes n} \) stabilizes nothing. It also shows why one must restrict the entries of \( G \) to only have real phase.

Proposition 2.4. Any abelian subgroup of \( G \subseteq P_n \setminus \{ -I^{\otimes n} \} \) cannot contain any Paulis with an imaginary phase

Proof. Given a Pauli with an imaginary phase, it’s square would be equal to \( -I^{\otimes n} \), making the group not closed. This is a contradiction.
One of the reasons stabilizer states are so important is this bijection between the stabilizer group of a stabilizer state and the state itself; by simply knowing the generators of the state one can easily reconstruct the state. And since there are at most $n$ generators, if one can efficiently write down the generators themselves then there is a polynomial size representation of a stabilizer state. We now show how one can write down any member of a stabilizer group as follows. Given, $P \in \mathbb{P}_n$ with real phase such that $P = \pm \bigotimes_i P_i$, define a function $N : \mathbb{P} \rightarrow \{0,1\}^2$ for each qubit $N(I) = 00$, $N(X) = 10$, $N(Z) = 11$, and concatenate to make $N(P) = (N(P_1), N(P_2), \ldots, N(P_n))$. Additionally, have an extra bit for the sign for whether the sign is $-1$ or $1$. This results in a $2^n + 1$ bit string for each generator, so writing down a stabilizer state requires only $O(n^2)$ bits to write down classically.

### 2.3 Clifford Circuits

**Definition 2.5.** A **Clifford circuit** is a unitary $U$ such that $U\mathbb{P}_n U^\dagger = \mathbb{P}_n$, while ignoring global phase on the unitary. More formally, consider the normalizer $N(\mathbb{P}_n) = \{U \in U(2^n) \mid U\mathbb{P}_n U^\dagger = \mathbb{P}_n\}$, and let $\mathcal{C}_n = N(\mathbb{P}_n)/U(1)$ be the **Clifford group**.

More informally, a Clifford circuit maps stabilizer states to other stabilizer states.

**Lemma 2.6.** Aaronson and Gottesman [3] Any Clifford circuit has an equivalent Clifford circuit with $O(n^2)$ gates and parallel depth $O(\log n)$.

Like stabilizer states, generators are an important part of how we deal with Clifford circuits. If we consider how a Clifford circuit $U$ acts on the canonical generators of $\mathbb{P}_n$, we find that

$$UX_j U^\dagger = (-1)^{p_j} \prod_{i=1}^n X_i^{\alpha_{ij}} Z_i^{\beta_{ij}} \quad UZ_j U^\dagger = (-1)^{q_j} \prod_{i=1}^n X_i^{\gamma_{ij}} Z_i^{\theta_{ij}}. \quad (1)$$

A Clifford circuit can then be encoded as a $(2n+1) \times 2n$ boolean matrix where column $2j-1$ is equal to $(\alpha_{1j}, \beta_{1j}, \ldots, \alpha_{nj}, \beta_{nj}, p_j)$ and column $2j$ is equal to $(\gamma_{1j}, \theta_{1j}, \ldots, \gamma_{nj}, \theta_{nj}, q_j)$. However, because commutation relations are preserved, not all possible values of $\alpha, \beta, \gamma, \theta$ are allowed (the $p$ and $q$ values can be arbitrary). This leads us to the idea of symplectic matrices.

**Definition 2.7.** A **symplectic matrix** over $\mathbb{F}_2^{2n}$ is a $2n \times 2n$ matrix $S$ with entries in $\mathbb{F}_2$ such that

$$S^T \Lambda(n) S = \Lambda(n) \equiv \bigoplus_{i=1}^n \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}. \quad (2)$$

These matrices form the symplectic group $\text{Sp}(2n, \mathbb{F}_2)$.

The symplectic matrices preserve the symplectic inner product $\omega(v, w) = v^T \Lambda(n) w$ on $\mathbb{F}_2^{2n}$. It turns out that if we consider the submatrix defined by the first $2n$ rows of our potential encoding of a clifford circuit, a necessary and sufficient condition to preserving the commutation relations of the generators is for this submatrix to be symplectic, as...
\{X_i\} \cup \{Z_i\} form what is known a symplectic basis. Formally, $C_n/P_n \cong \text{Sp}(2n, \mathbb{F}_2)$, where the Pauli in the divisor determines the $p$ and $q$ values.

### 2.4 CNOT circuits and $\oplus L$

It is a well known fact that every Clifford circuit can be generated using only $H$, $P$, and CNOT gates as defined below:

$$H = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} \quad P = \begin{pmatrix} 1 & 0 \\ 0 & i \end{pmatrix} \quad \text{CNOT} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix}$$

(3)

We note that $X = HP^2H$. If we restrict to the subset of circuits that are generated by only $X$ and CNOT, we get what are known as CNOT circuits [3], which are a clear subset of Clifford circuits.

**Definition 2.8** (Aaronson and Gottesman [3]). The complexity class $\oplus L$ is the class of problems that reduce to simulating a polynomial-size CNOT circuit.

A perhaps more familiar definition for complexity theorists is the class of problems that are solvable by a nondeterministic logarithmic-space Turing machine that accepts if and only if the total number of accepting paths is odd.

Let us now consider the set of all Clifford circuit that map computational basis states to other computational basis states, thereby stabilizing the subgroup $\{\pm 1\} \times \{I, Z\}^{\otimes n}$. Very briefly, we will call these classical Clifford circuits as we will now prove that they are largely equivalent to CNOT circuits.

**Proposition 2.9.** Let $C$ be an arbitrary classical Clifford circuit. It can be efficiently generated using solely $X$, $Z$, and CNOT gates. Moreover, it’s effect on the computational basis states can be entirely simulated using only $X$ and CNOT.

**Proof.** Let us first consider what happens to a computational basis state by acted upon by $C$. Referencing Eq. (1), the $\gamma_{ij}$ must be 0 for all $i$ and $j$, and we will essentially ignore $\alpha_{ij}$, $\beta_{ij}$, and $p_j$ for now leaving us with $\theta_{ij}$ and $q_j$. Let us now view the $\theta_{ij}$ as a $n \times n$ matrix $\Theta$ over $\mathbb{F}_2$. Since every member of $\text{Sp}(2n, \mathbb{F}_2)$ is full rank, $\Theta$ must also be full rank. As an example, since the identity circuit is also a classical Clifford circuit, the resulting $\Theta$ is the $n \times n$ identity matrix. We note that a CNOT from qubit $i$ to qubit $j$ performs the rowsum operation of adding row $i$ to row $j$. Thus it is possible to efficiently construct a circuit with matching $\Theta$ using rowsum operations via CNOT gates. To get a matching $q_j$, one can simply apply an $X$ gate at the beginning of each qubit that has $q_j = 1$, since $XZX = -Z$, and the following CNOT gates will not itself introduce any negative phases. From here, we have already proved the *moreover* statement.

To prove the full result, we return to the $\alpha_{ij}$ and $\beta_{ij}$. We will show that there exists a single unique solution. Similar to $\Theta$ we will define the corresponding $n \times n$ matrices $A$ and $B$ for the $\alpha_{ij}$ and $\beta_{ij}$ respectively. Based on Eq. (2), to form a symplectic basis we find that $A^T \Theta = I$ and $A^T B = 0$, since $\gamma_{ij} = 0$. Clearly $A^T = \Theta^{-1}$, which is guaranteed to exist,
and $B = 0$ since $A$ will also be full rank. To match the $p_j$ values we simply place $Z$ gates in front of the qubits where $p_j = 1$, similar to the $X$ gates for $q_j$.

Another way of viewing this is that CNOT circuits are the set of all Clifford circuits with $\gamma_{ij} = 0$ and $p_j = 0$ for all $i$ and $j$. Using the moreover part, CNOT circuits can realize any valid full rank $\Theta$.

2.5 PAC Learning

The goal of PAC learning is to learn a function relative to a certain distribution of inputs, rather than in an absolute sense. Let’s say we want to learn an arbitrary $f$ from some concept class $C$. If a hypothesis function $h$ matches the true function $f$ on many of the high probability inputs, then we can say that we have *approximately learned* $f$. If we can do this with high probability for arbitrary $f$, then we *probably approximately* (PAC) learned $C$.

Definition 2.10. Let $C$ be a set of functions $f : \chi \rightarrow [0, 1]$. We say that $C$ is $(\epsilon, \delta)$-PAC-learnable if there exists a learner that, when given samples of the form $(x, f(x))$ for $x \sim D$ for arbitrary $f$ and unknown distribution $D$, outputs with probability at least $1 - \delta$ a hypothesis $h$ with error satisfying

$$\mathbb{E}_{x \sim D}[(f(x) - h(x))^2] \leq \epsilon.$$

The number of samples used is referred to as the sample complexity, and we refer to the learner being *efficient* if it can compute $h$ in polynomial time.

From here, one can define two types of learning, based on where $h$ comes from. If $h$ is allowed to be any function that meets the PAC constraints, we refer to this as **improper learning**. If instead $h \in C$, we get what is known as **proper learning**, which will be the focus of this paper. With proper learning, we can then begin to talk about the consistency problem formally.

Definition 2.11. Let $S$ be a set of labeled samples such that $|S| < s$. Let $\text{CONSISTENT SEARCH}(C, s)$ be the problem of finding a function $h \in C$ that is *consistent* with all of $S$ (i.e., for all $(x, f(x)) \in S$, $f(x) = h(x)$) if such an $h$ exists, otherwise reject.

Intuitively, given a set of samples the best one can really hope to do is find such an $h$ that gets zero training error and hope that the true error for $h$ is also low. This leads to the idea of *generalization*, which aims to show that if for all $(x, f(x)) \in S$, $|h(x) - f(x)| \leq \alpha$ and $|S| > m$ for suitable $m$ implies

$$\mathbb{E}_{x \sim D}[(f(x) - h(x))^2] \leq \epsilon$$

with high probability. In terms of computational efficiency, this effectively reduces the problem of proper learning to the consistency problem, or an approximation of the consistency problem depending on the value of $\alpha$. It also bounds the sample complexity to be at most $m$, since solving the consistency problem without computational constraints is always doable in this realizable setting. We will see a formal statement of a generalization theorem in Section 3.
One can also define the decision version of the consistency problem, which is deciding if there even exists an \( h \in \mathcal{C} \) that is consistent with all of \( S \). We show that the existence of efficient learning algorithms can imply efficient one-sided error algorithms for the decision version of the consistency problem.

**Definition 2.12.** Let \( \text{ConsistentDecide}(\mathcal{C}, s) \) be decision version of the consistency problem for \( \mathcal{C} \) using at most \( s \) samples.

**Proposition 2.13.** An efficient randomized \((\epsilon < \frac{\alpha^2}{s^2}, \delta < \frac{1}{2} + \frac{1}{2s^2})\) proper learning algorithm implies \( \text{ConsistentDecide}(\mathcal{C}, s) \in \text{RP} \) where \( \alpha = \inf_{x \in \chi, f(x) \neq g(x)} |f(x) - g(x)| \) is the minimum non-zero error any hypothesis function can make on a single input.

**Proof.** For every set of samples \( S \) such that \(|S| \leq s\), we can define the \( D_S \) to be the uniform distribution over all \( x \in \chi \) such that \((x, f(x)) \in S\). By coupon collector, if we draw \( O(s \log s) \) many samples then with probability at least \( 1 - \frac{1}{s} \) we will have drawn every item from \( S \). Now imagine that there exists some hypothesis \( h \in \mathcal{C} \) that is not consistent with \( S \). Then our error must be at least \( \frac{\alpha^2}{s^2} \) by the definition of \( \alpha \).

Now assume we have some efficient randomized \((\epsilon, \delta)\) proper learning algorithm for \( \epsilon < \frac{\alpha^2}{s^2} \) and \( \delta < \frac{1}{2} + \frac{1}{2s^2} \). When running the learner on an arbitrary \( D_S \), it will see samples \( S \) with probability at least \( 1 - \frac{1}{s} \). To get error less than \( \frac{\alpha^2}{s^2} \) the learner must then be able to solve the search version consistency problem with probability \( p \) such that \( \frac{1}{s} + (1 - \frac{1}{s})p \geq 1 - \delta \). Solving for \( p \) we find \( p \geq \frac{1}{2} \) on accepting instances.

This gives rise to the following algorithm in \( \text{RP} \) for solving \( \text{ConsistentDecide}(\mathcal{C}, s) \). Given samples \( S \) with \(|S| \leq s\), we can run our learning algorithm and pretend that \( S \) is what we sampled from \( D_S \) to get hypothesis \( h \). If \( h \) is consistent with \( S \) then accept, otherwise reject. On an accepting instance \( h \) will be consistent with probability at least \( \frac{1}{2} \) while on rejecting instances it will never be consistent so the algorithm will always reject.

Informally, it can be possible to go the other way and show that an efficient algorithm for \( \text{ConsistentDecide}(\mathcal{C}, s) \) implies an efficient proper learner for \( \mathcal{C} \). Namely, if a search-to-decision reduction exists for the consistency problem on \( \mathcal{C} \) and a generalization theorem exists for the learning problem on \( \mathcal{C} \) then we can also expect to show that an efficient algorithm for the decision problem would imply an efficient proper learner for \( \mathcal{C} \). Of particular interest will be \( \text{NP} \)-complete problems, which always admit search-to-decision reductions [29].

### 3 PAC Learning Quantum Circuits

Aaronson [1] was the first to try and apply the ideas of PAC learning to that of learning quantum states by giving a generalization theorem for quantum states. Here \( \chi \) is the set of all two-outcome measurements and \( \mathcal{C} \) the set of quantum states with samples of the form \((E, \text{Tr}[E\rho])\). We stress that with this result and the proceeding result, the information is assumed to be classical in nature\(^2\). Caro and Datta [19] then gave a similar generalization

\(^1\)We abuse notation to signify that \( \epsilon \) is a value less than \( \frac{\alpha^2}{s^2} \) and likewise for \( \delta < \frac{1}{2s^2} \).

\(^2\)While the astute reader may note that representation of the measurements and states may be impossible to efficiently classically encode simply due to the dimension, for the case of Clifford/CNOT circuits later this will not be an issue.
algorithm but for quantum circuits, where the goal is to learn
\[
\left\{ f(x, y) = |\langle x|U|y \rangle|^2 \mid U \in \mathcal{U}_{\Delta, \Gamma}(d^n) \right\}
\]  
(4)
such that \(\mathcal{U}_{\Delta, \Gamma}(d^n)\) is the set of all unitaries on \(n\) qudits formed by two qudit gates of depth at most \(\Delta\) and size at most \(\Gamma\). In their proof the measurements were rank 1 projections with tensor product structure. We present a modified version of their result to allow arbitrary rank measurements with an informal proof sketch explaining why our modification works:

**Theorem 3.1.** Caro and Datta [19] Let \(X\) be the set of quantum states on \(n\) qudits, and let \(Y\) be the set of all projectors on \(n\) qudits. Let \(U^*\) be a quantum circuit of 2-qudit quantum unitaries with size \(\Gamma\) and depth \(\Delta\). Let \(\mathcal{D}\) be a probability distribution on \(X \times Y\) unknown to the learner. Let
\[
S = \left\{ \left( (x^{(i)}, y^{(i)}), \text{Tr}\left[ y^{(i)} U^* x^{(i)} U^*_\dagger \right] \right) \right\}_{i=1}^m
\]
be a corresponding training data drawn i.i.d according to \(\mathcal{D}\). Let \(\delta, \epsilon, \alpha, \beta \in (0, 1)\). Then, training data of size
\[
m = \mathcal{O}\left( \frac{1}{\epsilon} \left( \Delta \Gamma^2 \log \Delta \log^2 \left( \frac{\Delta \Gamma^2 \log(\Gamma)}{(\beta - \alpha)\epsilon} \right) + \log \frac{1}{\delta} \right) \right)^3
\]
suffice to guarantee that, with probability \(\geq 1 - \delta\) with regard to choice of the training data, any quantum circuit \(U\) of size \(\Gamma\) and depth \(\Delta\) that satisfies
\[
\left| \text{Tr}\left[ y^{(i)} U^* x^{(i)} U^*_\dagger \right] - \text{Tr}\left[ y^{(i)} U x^{(i)} U^*_\dagger \right] \right| \leq \alpha \quad \forall 1 \leq i \leq m
\]
also satisfies
\[
\mathbb{E}_{(x,y) \sim \mathcal{D}} \left[ \left( \text{Tr}\left[ y^{(i)} U^* x^{(i)} U^*_\dagger \right] - \text{Tr}\left[ y^{(i)} U x^{(i)} U^*_\dagger \right] \right)^2 \right] \leq (1 - \epsilon) \beta^2 + \epsilon
\]

**Proof.** The Caro and Datta results shows that with regard to rank 1 projectors \(|y\rangle\langle y|\), the trace \(\text{Tr}\left[ |y\rangle\langle y| \cdot U|x\rangle\langle x| U^*_\dagger \right]\) can be described as a polynomial over the entries of \(U\) with bounded degree \(d\). Because every rank \(r\) projector \(E\) is simply the sum of \(r\) rank 1 projectors, linearity of the trace tells us that the resulting trace \(\text{Tr}\left[ E \cdot U|x\rangle\langle x| U^*_\dagger \right]\) is the linear combination of \(r\) polynomials with bounded degree. Thus we are again left with a polynomial bounded by the same degree \(d\). \qed

Now that we have a formal statement of a generalization theorem, we can also formalize the ideas at the end of Section 2.5 and expand on them.

**Lemma 3.2.** Let \(\mathcal{C}\) be a subset of 2-qudit quantum unitaries with size \(\Gamma\) and depth \(\Delta\) and let
\[
m = \mathcal{O}\left( \frac{1}{\epsilon} \left( \Delta d^4 \Gamma^2 \log \Delta \log^2 \left( \frac{\Delta d^4 \Gamma^2 \log(\Gamma)}{\beta \epsilon} \right) + \log \frac{1}{\delta} \right) \right)
\]

\footnote{A similar thing can be done with \(n\) qudit quantum processes, by simply changing the \(d^4\) to \(d^8\) in both the product and the logarithm due to the increase in the free parameters of a quantum process on \(n\) qudits versus a unitary.}
be the parameter from Theorem 3.1. If $\text{ConsistentDecide}(C, s)$ for $s > m$ is NP-Complete then an NP-oracle can be used to efficiently $((1 - \epsilon)\beta^2 + \epsilon, \delta)$ proper learn $C$.

**Proof.** Because search-to-decision reductions exist for all NP-Complete problems [29], an oracle for $\text{ConsistentDecide}(C, s)$ can be used to efficiently solve $\text{ConsistentSearch}(C, s)$. Let us run our algorithm for $\text{ConsistentSearch}(C, s)$ on a sample $S$ such that $s \geq |S| \geq m$. We now have a $U$ such that

$$\left| \text{Tr}\left[y^{(i)}U_s x^{(i)}U_s^\dagger\right] - \text{Tr}\left[y^{(i)}U x^{(i)}U^\dagger\right] \right| = 0 \quad \forall 1 \leq i \leq m$$

and so by Theorem 3.1

$$E_{(x, y) \sim D} \left[ (\text{Tr}\left[y^{(i)}U_s x^{(i)}U_s^\dagger\right] - \text{Tr}\left[y^{(i)}U x^{(i)}U^\dagger\right])^2 \right] \leq (1 - \epsilon)\beta^2 + \epsilon.$$

Naturally, any other oracle for an NP-Complete problem can also be used since they all reduce to one another, thus completing the proof.

**Corollary 3.3.** Let $C$ be a subset of 2-qudit quantum unitaries with size $\Gamma$ and depth $\Delta$ and let

$$m = \mathcal{O}\left(\frac{1}{\epsilon} \left( \Delta d^4 \Gamma^2 \log \Delta \log^2 \left( \frac{\Delta d^4 \Gamma^2 \log(\Gamma)}{\beta \epsilon} \right) + \log \frac{1}{\delta} \right) \right)$$

be the parameter from Theorem 3.1. If $\text{ConsistentDecide}(C, s)$ for $s > m$ is NP-Complete and $\text{RP} = \text{NP}$ then an RP-oracle can be used to efficiently $((1 - \epsilon)\beta^2 + \epsilon, \frac{\delta}{c})$ proper learn $C$ for arbitrary $c = \mathcal{O}(1)$.

**Proof.** If $\text{NP} \subseteq \text{RP}$ then there must exist an efficient one-sided error randomized algorithm $A$ for $\text{ConsistentDecide}(C, s)$. With probability at least $\frac{1}{2}$ if we query $A$ it will output the same thing NP-oracle on YES instances. We can efficiently boost our success probability such that the probability that the algorithm fails to perfectly match the NP-oracle on the at most poly$(n)$ queries to the oracle is less than $\frac{1}{c}$ for $c = \mathcal{O}(1)$, resulting in algorithm $A'$.

By Lemma 3.2 if we had an NP-oracle there would then exist an efficient $(\epsilon, \delta)$ proper learner for $C$ when given at least

$$m = \mathcal{O}\left(\frac{1}{\epsilon} n^4 \log n \log \log n \log^2 \left( \frac{n \log^2 n}{\epsilon} \right) + \frac{1}{\delta} \right)$$

samples. Naturally, this reduction can only use poly$(n)$ calls to the NP-oracle, so with probability at least $1 - \frac{1}{c}$ our queries from $A'$ will be correct. The total probability that the learner outputs a bad hypothesis is at most $\frac{\delta}{c}$. Thus we have an efficient $((1 - \epsilon)\beta^2 + \epsilon, \frac{\delta}{c})$ proper learner for $C$. \hfill \square

## 4 PAC Learning applied to Clifford Circuits

Because of the works of Rocchetto [37] and Lai and Cheng [32], Clifford circuits are a prime candidate for an efficiently PAC-learnable class of circuits. Additionally, due to Lemma 2.6 one could hope to use Lemma 3.2 with $d = 2$, $\Delta = \mathcal{O}(\log n)$, and $\Gamma = \mathcal{O}(n^2)$ in the same way the main theorem from Aaronson [1] was invoked for learning stabilizer states.
Noting that each Pauli matrix is Hermitian, a very natural way to measure a stabilizer state is in a product basis where we measure each qubit with respect to a Pauli.

**Definition 4.1.** If $P \in \mathcal{P}_n$ is a Pauli operator, then the two-outcome measurement associated with $P$ is $I^{\otimes n} + P^2$, and is referred to as a Pauli measurement.

**Definition 4.2.** Let the problem of PAC learning Clifford circuits with respect to Pauli measurements be defined as follows. Let $C$ be an unknown Clifford circuit and let $D$ be an unknown joint distribution over both stabilizer states and Pauli measurements. Finally, let samples to $C$ be given as $(\rho, E, \text{Tr}[EC\rho C^\dagger])$ where $\rho, E \sim D$ are a stabilizer state and Pauli measurement jointly drawn from $D$ and represented as classical bit strings using the stabilizer formalism. The goal is then to learn the measurements $\text{Tr}[EC\rho C^\dagger]$ up to error $\epsilon$ under the distribution $D$.

A critical part of Rocchetto [37] was noting that the measurement results with Pauli measurements could only have three distinct values:

**Lemma 4.3.** Let $E_P = I^{\otimes n} + P^2$ be a Pauli measurement associated to a Pauli operator $P \in \mathcal{P}_n$ and $\rho$ be an $n$-qubit stabiliser state. Then $\text{Tr}[E_P C\rho C^\dagger]$ can only take on the values $\{0, \frac{1}{2}, 1\}$, and:

\[
\begin{align*}
\text{Tr}[E_P C\rho C^\dagger] = 1 & \text{ iff } P \text{ is a stabilizer of } C\rho C^\dagger; \\
\text{Tr}[E_P C\rho C^\dagger] = 1/2 & \text{ iff neither } P \text{ nor } -P \text{ is a stabilizer of } C\rho C^\dagger; \\
\text{Tr}[E_P C\rho C^\dagger] = 0 & \text{ iff } -P \text{ is a stabilizer of } C\rho C^\dagger.
\end{align*}
\]

Now let $S$ be the stabilizer group of $\rho$. From this, we can gather that if $\text{Tr}[E_P C\rho C^\dagger] = 1$ then $C^\dagger PC \in S$, and if $\text{Tr}[E_P C\rho C^\dagger] = 0$ then $C^\dagger PC \in -S$ where $S = \{-G \mid G \in S\}$. Finally, if $\text{Tr}[E_P C\rho C^\dagger] = \frac{1}{2}$ then $C^\dagger PC$ is in the complement of $S \cup -S$. If the measurement $E_P$ appears multiple times, we can gather further information. For instance, have

\[S = \left\{ (\rho_i, E^P, \text{Tr}[E^P C\rho_i C^\dagger]) \right\}\]

be the set of all samples such that $E^P$ is the measurement taken and let $S_i$ be the stabilizer group of each $\rho_i$. Based on each $\text{Tr}[E^P C\rho_i C^\dagger]$ we know that $C^\dagger PC$ must lie in some set $H_i$, and thus must lie in $\bigcap_i H_i$. To actually be a Clifford circuit, we must also add the constraint that $C^\dagger PC \neq I^{\otimes n}$, giving us

\[C^\dagger PC \subset \left( \bigcap_i H_i \right) \setminus \{I^{\otimes n}\} \]

The problem of finding a Clifford circuit with zero training error then reduces to the search problem of finding a set of $\alpha, \beta, \gamma, \theta, p, q$ from Eq. (1) representing a $C^\dagger$ that is consistent with all of these constraints while remaining symplectic according to Eq. (2). Let $\mathcal{C}$ be the set of Clifford circuits. We will call this problem $\text{CLIFFORDSEARCH}(s) = \text{CONSISTENTSEARCH}(\mathcal{C}, s)$. Due to Gottesman-Knill [3, 26] showing that Clifford circuits are classically simulable, the act of verifying that we have a circuit that has zero training error is
efficient meaning that the decision version $\text{CliffordDecide}(s) = \text{ConsistentDecide}(C, s)$ of the problem is in $\text{NP}$:

**Proposition 4.4.** The decision problem, $\text{CliffordDecide}(\text{poly}(n))$, of deciding if there exists a Clifford circuit consistent with polynomially sized sample $S$ is in $\text{NP}$.

**Proof.** Given a set of $\alpha, \beta, \gamma, \theta, p, q$, it easy to check that the $\gamma, \theta, p, q$ form a symplectic matrix by checking with respect to $\Lambda(n)$. Checking that they are consistent with the samples in $S$ can be done by iterating through $S$ since the trace can be computed efficiently using Gottesman-Knill. Knowing this, we find that $\text{CliffordSearch}(\text{poly}(n)) \in \text{FNP}$. This property extends to analogous problems for CNOT circuits $\text{CNOTSearch}(\text{poly}(n))$ and $\text{CNOTDecide}(\text{poly}(n))$, since one can also efficiently verify that $\gamma_{ij} = 0$ and $p_j = 0$ for all $i$ and $j$.

**5 Generating Samples with Certain Constraints**

We will now show how we can use samples from PAC learning to generate certain kinds of constraints. It will suffice to only consider CNOT circuits with computational basis state measurements and measurements of the form $\{I, Z\} \otimes^n$. The net effect of this is that from a PAC learning standpoint, for unknown CNOT circuit $C$ we only need to figure a set of $C^\dagger Z_i C$ that is consistent with the samples as described in Section 4. Since we will never be tested on a measurement with some component of $X_i$ involved, this is equivalent to finding the $\theta_{ij}$ and $q_j$ values from Eq. (1) of $C^\dagger$. We will again choose to view the $\theta_{ij}$ as the matrix $\Theta$, such that $\Theta$ must be full rank.

**Definition 5.1.** Given a set of abelian generators $\{P_i\}$, let

$$\rho(P_1, P_2, \ldots, P_n) = \frac{1}{2^n} \sum_{P \in \text{Span}(\{P_i\})} P$$

be the stabilizer state that is formed from that stabilizer group.

**Lemma 5.2.** Let $C$ be a CNOT circuit on $n$ qubits and have $v + \text{Span}(w) \subset \{0, 1\}^n$ be a one-dimensional affine subspace of column vectors such that $v \neq w$ and $w, v \neq 0$. Given an arbitrary pauli $P$ there exists a set of $n$ samples that constrains $C^\dagger PC$ to only have consistent solutions lying in $Z^v \cdot \text{Span}(Z^w)$. Furthermore, these samples can be efficiently generated.

**Proof.** Let $(v, w, v_3, \cdots, v_n)$ be an arbitrary basis for $\{0, 1\}^n$ containing $v$ and $w$. This can be done using $O(n)$ samples in expectation. Recalling Definition 2.3, let us start by creating the sample

$$\left(\left(\rho(Z^v, Z^w, Z^{v_3}, Z^{v_4}, \ldots, Z^{v_n}), \frac{I^\otimes n + P}{2}\right), 1\right),$$

which limits $C^\dagger PC$ to be in $\{I, Z\} \otimes^n$ with positive phase.
We can create the set of samples:

\[
\left( \left( \rho(Z^v, Z^w, -Z^{v_3}, Z^{v_4}, \ldots, Z^{v_n}), \frac{I^\otimes n + P}{2} \right), 1 \right),
\left( \left( \rho(Z^v, Z^w, Z^{v_3}, -Z^{v_4}, \ldots, Z^{v_n}), \frac{I^\otimes n + P}{2} \right), 1 \right),
\vdots
\left( \left( \rho(Z^v, Z^w, Z^{v_3}, Z^{v_4}, \ldots, -Z^{v_n}), \frac{I^\otimes n + P}{2} \right), 1 \right).
\]

By construction \(C^\dagger PC\) cannot have any component of \(Z^{v_3}\) because of the first sample of this set, nor any \(Z^{v_i}\) for \(i > 3\) due to the remaining samples. This leaves \(C^\dagger PC\) to be one of \(Z^v, Z^w,\) or \(Z^v + w\) (since it cannot be identity). To remedy this, we can introduce the final sample:

\[
\left( \left( \rho(-Z^v, Z^w, Z^{v_3}, Z^{v_4}, \ldots Z^{v_n}), \frac{I^\otimes n + P}{2} \right), 0 \right),
\]

which then eliminates \(Z^w\) (and identity, due to the negative sign). The total number of samples is \(n\) and the whole process takes polynomial in \(n\) time.

We can easily extend this to the 0-dimensional case by simply treating \(w\) as \(v_2\), using an extra sample to remove the last dimension. More importantly, let’s say we’ve constrained \(C^\dagger Zx\) to lie in \(Z^v \cdot \text{Span}(Z^w)\). The effect of this on \(\Theta\) is that if we sum the columns \(i\) where \(x_i = 1\) then the sum must lie in \(v + \text{Span}(w)\).

**Corollary 5.3.** Let

\[v + \text{Span}(w) = \left[ \begin{array}{cccc} v_1 & v_2 & \ldots & v_k \end{array} \right] + \text{Span} \left( \left[ \begin{array}{cccc} w_1 & w_2 & \ldots & w_k \end{array} \right] \right)\]

be a one-dimensional affine subspace of \(n \times k\) matrices over \(\{0, 1\}\) such that for all \(i\), \(v_i \neq w_i\) and \(v_i, w_i \neq 0\). Finally, let \(\Theta'\) be an arbitrary \(n \times k\) submatrix of \(\Theta\). Then there exists a set of \(kn + k - 1\) samples that constrain \(\Theta'\) to only have consistent solutions lying in \(v + \text{Span}(w)\) for CNOT circuit \(C\). Furthermore these samples can be efficiently generated.

**Proof.** WLOG, we will let the set of \(k\) different columns we choose for \(\Theta'\) to be columns 1 through \(k\). We will use induction on \(k\) to prove this corollary, with the base case covered by Lemma 5.2. Now let us assume that we have samples that constrain columns 2 through \(k\) to lie in

\[\left[ \begin{array}{cccc} v_2 & v_3 & \ldots & v_k \end{array} \right] + \text{Span} \left( \left[ \begin{array}{cccc} w_2 & w_3 & \ldots & w_k \end{array} \right] \right)\]

The goal will be to generate constraints such that if column 2 is \(v_2\) then column 1 must be \(v_1\). Otherwise, if column 2 is \(v_2 + w_2\) then column 1 is constrained to be \(v_1 + w_1\). To start us off, Lemma 5.2 lets us constrain column 1 to lie in \(v_1 + \text{Span}(w_1)\). We can then use
Lemma 5.2 again to constrain the sum of columns 1 and 2 to lie in \( v_1 + v_2 + \text{Span}(w_1 + w_2) \). If we focus on columns 1 and 2, the solutions to this specific constraint lie in an affine subspace that starts with either

\[
\begin{bmatrix}
  v_1 + v_2 \\
  \vdots \\
  0
\end{bmatrix}
\quad \text{or} \quad
\begin{bmatrix}
  v_1 + w_1 + v_2 + w_2 \\
  \vdots \\
  0
\end{bmatrix}
\]

and then adds the same vector to both columns. To lie in the intersection of the solutions we already have, we will need to set column 2 to either be \( v_2 \) or \( v_2 + w_2 \) such that the whole set of columns from 2 to \( k \) lies in either

\[
\begin{bmatrix}
  v_2 & v_3 & \ldots & v_k
\end{bmatrix}
\quad \text{or} \quad
\begin{bmatrix}
  v_2 + w_2 & v_3 + w_3 & \ldots & v_k + w_k
\end{bmatrix}
\]

as described before. The only way to get to the first value is to add

\[
\begin{bmatrix}
  v_2 \\
  v_2
\end{bmatrix}
\]

to either starting point to get

\[
\begin{bmatrix}
  v_1 & v_2 \\
  v_1 & v_2 \\
\end{bmatrix}
\quad \text{and} \quad
\begin{bmatrix}
  v_1 + w_1 + w_2 & v_2 \\
  v_1 + w_1 + w_2 & v_2
\end{bmatrix}
\]

respectively. Examining the constraints on the first column, \( v_1 + w_1 + w_2 \neq v_1 + w_1 \) since \( w_2 \neq 0 \) so if the second column is \( v_2 \) then the first column must be \( v_1 \) as desired.

To get to \( v_2 + w_2 \) as the value in the second column we instead need to add

\[
\begin{bmatrix}
  v_2 + w_2 & v_2 + w_2
\end{bmatrix}
\]

to either starting points to get

\[
\begin{bmatrix}
  v_1 + w_2 & v_2 + w_2 \\
  v_1 + w_2 & v_2 + w_2
\end{bmatrix}
\quad \text{and} \quad
\begin{bmatrix}
  v_1 + w_1 & v_2 + w_2 \\
  v_1 + w_1 & v_2 + w_2
\end{bmatrix}
\]

respectively. Again, \( v_1 + w_2 \neq v_1 \) because \( w_2 \neq 0 \). Thus if the second column is \( v_2 + w_2 \) then the first column must be \( v_1 + w_1 \).

Collectively, we achieve our goal of constraining the entire solution to lie in \( v + \text{Span}(w) \). We used \( n \) samples at the first step and \( n + 1 \) for every inductive step after, giving us a total number of samples of \( (n + 1)(k - 1) + n = kn + k - 1 \). Since each step was efficient than the whole process takes polynomial in \( n \) time to generate all of the samples. \( \square \)
| Formula $F$       | The series-parallel $s$-$t$ graph $G_F$ with edge withs |
|------------------|--------------------------------------------------------|
| Constant $c$     | $s \xrightarrow{c} 1 \xrightarrow{} t$               |
| Variable $x$    | $s \xrightarrow{x} 1 \xrightarrow{} t$               |
| $F = F_1 \cdot F_2$ | $s = s_1 \xrightarrow{} G_{F_1} \xrightarrow{} G_{F_2} \xrightarrow{} t = t_2$ |
| $F = F_1 + F_2$ | $s = s_1 = s_2 \xrightarrow{} G_{F_1} \xrightarrow{} G_{F_2} \xrightarrow{} t = t_1 = t_2$ |

Figure 1: Inductive Construction from Formula to Graph

6 On the NP-Completeness of NonSingularity

**Definition 6.1.** Given matrices $M_0, M_1, \ldots, M_k$ over some field $\mathbb{F}$, **NonSingularity** is the problem of deciding if there exists $\alpha_1, \alpha_2, \ldots, \alpha_k$ such that $M_0 + \sum_i \alpha_i M_i$ results in a non-singular matrix.

**Theorem 6.2** (Buss et al. [17]). **NonSingularity** over $\mathbb{F}_2$ is **NP-Complete**.

The high level idea of the proof is to first reduce a 3SAT instance over variables $\{x_i\}$ to solving an arithmetic formula $F$. The formula is then turned into a weighted directed graph whose adjacency matrix $M(x)$ has a determinant that is equal to the formula $F$, where $M(x)$ has entries from $\{0, 1\} \cup \{x_i\}$, and can thus be viewed as an affine subspace over $\mathbb{F}_2^{(|F|+2) \times (|F|+2)}$.

While we will not prove the correctness of this statement, we will want to ascertain exactly what kind of $M_i$ are formed through the reduction. We now describe the construction of the graph (see Fig. 1 and Fig. 2 for relevant illustrations):

- For each atomic formula $F'$, create vertices $s$ and $t$. 

15
\[ F : x_1(x_2 + x_3) + x_3 \cdot x_4 \]

Figure 2: Example of constructing the adjacency matrix with a specific determinant
For each constant $c$ create a unique node $v_c$ with a path from $s$ to $v_c$ with weight $c$ and a path from $v_c$ to $t$ with weight 1.

For each variable $x_i$ create a unique node $v_{x_i}$ with a path from $s$ to $v_{x_i}$ with weight $x_i$ and a path from $v_{x_i}$ to $t$ with weight 1.

- For multiplication of $F_i$ and $F_j$, place the graphs of $F_i$ and $F_j$ in series.
- For addition of $F_i$ and $F_j$, place the graphs of $F_i$ and $F_j$ in parallel.
- Once all of this is done, create a path of weight 1 from the global $t$ vertex to the global $s$ vertex.
- Create self loops at every vertex besides the global $s$ vertex.

Let $M$ be the resulting adjacency matrix of this graph. For every entry that is a constant, we can assign that to $M_0$. Then for each variable $x_i$, we can set $M_i$ to be the matrix that is zero everywhere except where $x_i$ appears in $M$. As an example, for a matrix

$$M(x) = \begin{pmatrix} x_1 & 1 \\ x_2 & x_1 \end{pmatrix}$$

we can describe it using $M(x) = M_0 + x_1M_1 + x_2M_2$ where

$$M_0 = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} \quad M_1 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \quad M_2 = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}$$

**Corollary 6.3.** **NonSingularity** over $\mathbb{F}_2$ is still NP-Complete if one only considers $M_1, M_2, \ldots, M_n$ that are non-zero on disjoint columns. That is, no two $M_i$ $M_j$ exist such that column $k$ are both non-zero for arbitrary $k$. In addition, if we restrict to the non-zero columns of a particular $M_i$ for $i > 0$ then

$$M_0 + \text{Span}(M_i) = \left[ \begin{array}{cccc} | & | & | & | \\ v_1 & v_2 & \ldots & v_k \end{array} \right] + \text{Span}\left( \left[ \begin{array}{cccc} | & | & | & | \\ w_1 & w_2 & \ldots & v_k \end{array} \right] \right)$$

such that for all $j$, $v_j \neq w_j$ and $v_j, w_j \neq 0$. We will call this the **Simplified NonSingularity** problem.

**Proof.** Rather than reduce the general problem to this problem, we merely show that the reduction from 3SAT naturally leads to instances of this specific problem. Let $G$ be the graph produced by the reduction from 3SAT with adjacency matrix $M(x)$. We first need to show that from the construction of $G$, the resulting $M(x)$ has at most one variable appears in each column such that the $M_i$ act on disjoint columns for $i > 0$. If $M(x)_{ij} = 1$ if and only if there exists an edge from vertex $i$ to vertex $j$, then we require that no more than one variable-weighted edge can direct to any particular vertex in $G$.

By the construction given above, we see that every instance of a variable will connect to it’s own unique vertex, with no other variable possibly connected to it. This conversely means no more than one variable weighted edge can connect to any particular vertex. For variable $x_i$ with $i > 0$, the matrix $M_i$ will then be nonzero for the columns of the adjacency
matrix associated with these vertices receiving the edges with weight $x_i$. Since none of these vertices will receive both $x_i$ and some $x_j$, then the $M_i$ will be nonzero for disjoint columns. Furthermore, since the weight of an edge will never be $x_i + 1$, then we ensure that if we restrict to the non-zero columns of a particular $M_i$ for $i > 0$ then

$$M_0 + \text{Span}(M_i) = \begin{bmatrix} v_1 & v_2 & \cdots & v_k \\ | & | & \cdots & | \\ w_1 & w_2 & \cdots & w_k \end{bmatrix} + \text{Span} \left( \begin{bmatrix} | & | & \cdots & | \\ w_1 & w_2 & \cdots & w_k \end{bmatrix} \right)$$

such that for all $j$, $v_j \neq w_j$ and $w_j \neq 0$.

Finally, to ensure that $v_j \neq 0$, we note that each vertex besides $s$ receives a self loop with weight 1. $s$ instead receives an edge from $t$ with weight 1. These self loops and the edge from $t$ to $s$ ensures that each column of $M_0$ has at least entry with 1 in it such that the $v_j \neq 0$.

7 PAC Learning CNOT Circuits and NP

Lemma 7.1. The decision problem, CNOTDecide($\binom{n+1}{n}$), of deciding whether or not there exists a CNOT circuit consistent with at most $(n+1)n$ samples is NP-Complete.

Proof. By Corollary 6.3, if one can determine if an affine subspace of a certain constrained set of matrices contains a full rank matrix then one can solve all of NP. Looking at each individual $M_i$ for $i > 0$, they are all non-zero on disjoint columns. If we restrict to the non-zero columns of a particular $M_i$ for $i > 0$, we find that if we consider the space $M_0 + \text{Span}(M_i)$, that $M_0$ and $M_i$ meet the requirements for Corollary 5.3. Since the $M_i$ act on disjoint columns, if we apply Corollary 5.3 for each $M_i$ then we have efficiently created a set of samples $S$ that restricts those columns of $\Theta$, the matrix form of $\theta_{ij}$ values, to lie in $M_0 + \text{Span}(\{M_i\})$. To fix the columns not touched by the $M_i$, it is not hard to show that the ideas of Lemma 5.2 can also create a 0-dimensional affine space over these columns, thereby setting the whole matrix to lie in $M_0 + \text{Span}(\{M_i\})$. Altogether, we are able to use Lemma 5.2 and Corollary 5.3 to set $\Theta$ to lie in $M(x)$ from SIMPLIFIED NONSINGULARITY. Since Proposition 2.9 ensures us that CNOT circuits can instantiate any realizable $\Theta$, there will exist a CNOT circuit consistent with $S$ if and only if $M(x)$ is an accepting instance. This shows CNOTDecide($\binom{n+1}{n}$) is NP-Hard. Combined with Proposition 4.4 we find that CNOTDecide($\binom{n+1}{n}$) to be NP-Complete. \qed

Since CNOTDecide($\binom{n+1}{n}$) $\subset$ CNOTDecide(poly($n$)) then CNOTDecide(poly($n$)) is also NP-Hard.

Theorem 7.2 (Formal Statement of Theorem 1.1). There exists an efficient randomized $(\epsilon, \delta)$ proper PAC learner for CNOT circuits with arbitrary $\epsilon$ and $\delta$ as arbitrary $\frac{1}{\text{poly}(n)}$ values if and only if RP = NP. Furthermore, an efficient quantum $(\epsilon, \delta)$ proper PAC learner for CNOT circuits with arbitrary $\epsilon$ and $\delta$ as arbitrary $\frac{1}{\text{poly}(n)}$ values exists if and only if NP $\subseteq$ RQP.

Proof. We will start by proving the NP $\subseteq$ RP version for classical randomized learners. The quantum version will follow trivially by replacing the learner with a quantum algorithm and
therefore RP with RQP. The only change then is that NP \subseteq RQP does not necessarily imply NP = RQP like it does with RP.

Because CNOT circuits with classical inputs and measurements only has labels 0 and 1, the smallest non-zero error is 1. By Proposition 2.13 with \( \alpha = 1 \), an efficient

\[
\left( \epsilon < \frac{1}{(n+1)^2 \cdot 2^2}, \delta < \frac{1}{2} + \frac{1}{2(n+1)n} \right)^4
\]

randomized proper learner for CNOT circuits will imply CNOTDecide((n + 1)n) \in RP. Since CNOTDecide((n + 1)n) is NP-Complete by Lemma 7.1, efficient randomized learners for CNOT circuits with arbitrary \( \epsilon = \frac{1}{\text{poly}(n)} \) and \( \delta = \frac{1}{\text{poly}(n)} \) are only possible if NP \subseteq RP.

Conversely, by Corollary 3.3 with \( \beta = \frac{1}{2} \), \( d = 2 \), \( \epsilon = \frac{4\epsilon' - 1}{\alpha} \), \( \delta = \alpha \delta' \), \( \Delta = O(\log n) \) and \( \Gamma = O(n^2) \) if NP \subseteq RP then there must exist an efficient \((\epsilon', \delta')\) proper learner for CNOT circuits as long as the number of samples \( m \) is polynomial in \( n \). For arbitrary \( \epsilon' = \frac{1}{\text{poly}(n)} \) and \( \delta' = \frac{1}{\text{poly}(n)} \) our required number of samples becomes

\[
m = O\left( \frac{1}{\epsilon} \left( \frac{\Delta d^4 \Gamma^2 \log \Delta \log^2 \left( \frac{\Delta d^4 \Gamma^2 \log \Gamma}{\beta \epsilon} \right)}{\beta \epsilon} \right) + \log \frac{1}{\epsilon \delta} \right) = O(\text{poly}(n))
\]

This is sufficiently small as desired, completing the proof. \( \square \)

Corollary 7.3 (Formal Statement of Corollary 1.2). There exists an efficient randomized \((\epsilon, \delta)\) proper PAC learner for Clifford circuits with arbitrary \( \epsilon \) and \( \delta \) as arbitrary \( \frac{1}{\text{poly}(n)} \) values if and only if RP = NP. Furthermore, an efficient quantum \((\epsilon, \delta)\) proper PAC learner for Clifford circuits with arbitrary \( \epsilon \) and \( \delta \) as arbitrary \( \frac{1}{\text{poly}(n)} \) values exists if and only if NP \subseteq RQP.

\textbf{Proof.} Since CNOT circuits are also a form of Clifford circuits, CNOTDecide((n + 1)n) \subseteq CliffordDecide((n + 1)n), and so CliffordDecide((n + 1)n) is also NP-Complete. The proof of Theorem 7.2 continues but with \( \alpha = \frac{1}{2} \) instead due to Lemma 4.3. This leads to slightly different constants, but the proof ideas all follow without major change. \( \square \)

8 Discussion and open problems

In this work, we prove a negative result in proper learning of one of the best candidates for efficient PAC learning of quantum circuits. However, it should be noted that in many cases there exist improper learners even in the case where proper learning is NP-Hard, such as 2-clause CNF [15, 16]. This immediately leaves the problem of whether or not an improper learner exists for Clifford circuits. One way of showing hardness would be to leverage cryptographic hardness such as in Arunachalam et al. [8], Kharitonov [30]. Another approach would be to assume the hardness of random k-DNF, such as the work of Daniely and Shalev-Shwartz [23]. For upper bounds, the work of Caro and Datta [19] can also be used to get agnostic generalization results, providing a possible pathway to answering research questions in that direction.

\footnote{We again abuse notation to signify that \( \epsilon \) is a value less than \( \frac{1}{(n+1)^2 \cdot 2^2} \) and likewise for \( \delta < \frac{n^2 + n + 1}{2n^2 + 2n} \).}
We also note that a single output bit of a CNOT circuit is simply an XOR, which is easy to learn efficiently if there is no noise. However, because we are dealing with reversible computation each output bit has to be a linearly independent XOR such that each input bit is recoverable. Finding a CNOT circuit that matches a single XOR function $f$ can be done by sampling expected $O(n)$ random XOR until we get $n$ linearly independent XOR with one of them being $f$ (see Appendix A.1). Thus, the entire difficulty of proper learning CNOT circuits is this linear independence of the output bits. As such, even though $\text{AC}^0 \subseteq \text{TC}^0 \subseteq \text{NC}^1 \subseteq \mathbb{L} \subseteq \mathbb{⊕L}$ with the lower classes having improper hardness results based on cryptographic hardness [30], one cannot directly give an improper learning result for CNOT circuits despite the fact that simulating CNOT circuits is complete for $\mathbb{⊕L}$.

As noted previously, our PAC learning framework is slightly different from that of Caro and Datta [19], in that we use Pauli matrices, rather than rank 1 projectors as measurements. To the author’s knowledge, there exists no proof showing that one framework is necessarily harder than the other. The author also do not see an obvious way of proving an analogous hardness theorem in the specific framework of Caro and Datta [19] for Clifford or CNOT circuits.

Finally, with everything from the input states to the circuits involved being classical, it is entirely possible to prove the technical results about CNOT circuits only talking about bit strings and parity functions. Namely, one can replace the entire problem with samples of the form $(x, s, s^TCx \mod 2)$ where $(x, s) \sim D$ are $n$-bit strings and $C$ is a CNOT circuit. Since the stabilizer group of a computational basis state always lies in $\{±1\} \times \{I, Z\}^{⊗n}$, we can uniquely define it by the subgroup that has positive phase. This is equivalent to the orthogonal complement of $x$, which is the subspace $W_x = \{x \in \{0, 1\}^n \mid w \cdot x = 0\}$. From there, a sample of the form $(x, s, 0)$ simply says that $Cx \in W_s$, and one can get an analogous proof by copying the lemmas and theorems in Section 5 and Section 7. However, this proof isn’t anymore intuitive than the one given using stabilizer groups, and in fact is probably less intuitive to the average reader due to the lack of established formalism from stabilizers and paulis. It would be interesting if a more intuitive purely classical proof could be made to show hardness of learning CNOT circuits under this model.

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A Special Cases with Efficient Proper Learners

Despite the results given, there still exist situations where it is possible to efficiently proper learn Clifford circuits and CNOT circuits. We give brief proof sketches of some of them here.

A.1 CNOT Circuits for a distribution with support over a single measurement

Let us try to learn CNOT circuits with regard to a distribution $\mathcal{D}$ such that there exists some Pauli $P \in \{I,Z\}^\otimes n$ with $P_{\rho,E}\sim \mathcal{D}[E = \frac{I^\otimes n + P}{2}] = 1$. Because we are dealing with CNOT circuit the labels will always be 0 and 1 so by Lemma 4.3 each label will tell us an affine subspace that $C^\dagger PC$ lies in. We can efficiently compute the intersection of this using Gaussian elimination with the generators to find a $P'$ that is consistent with all of the labels. From there, let $P, Q_2, Q_3, \ldots, Q_n$ be a set of Paulis whose span is $\{I,Z\}^\otimes n$. Let $P', Q_2', Q_3', \ldots, Q'_n$ also be a set of Paulis whose span is $\{I,Z\}^\otimes n$. It is clear that if we define our CNOT circuit such that $C^\dagger PC = P'$ and $C^\dagger Q_iC = Q'_i$ then we have a valid CNOT
circuit. Efficiently finding such \( \{ Q_i \} \) and \( \{ Q'_i \} \) only takes \( \mathcal{O}(n) \) expected samples of random Paulis in \( \{ I, Z \}^\otimes n \) and so can be done efficiently. From there we appeal to Theorem 3.1 and we are done.

### A.2 Clifford circuits with the uniform distribution over Pauli measurements

We note that if the distribution \( D \) entails the measurements being uniform over the Paulis then the problem is trivially easy to properly learn with \( \epsilon < \frac{1}{\exp(n)} \) and \( \delta = 0 \) by just outputting a random Clifford circuit. This is because the probability that a random Pauli is in a given state’s stabilizer group is \( \frac{2^n}{4^n} \) so we will almost always see the label \( \frac{1}{2} \) regardless of the hypothesis circuit we choose.

### A.3 CNOT Circuits with the uniform distribution over \( \{ I, Z \}^\otimes n \)

Let \( \Theta \) and \( Q \) be the matrix/vector forms of \( \theta_{ij} \) and \( q_j \) values from Eq. (1). We note that if we have enough independent samples that \( \Theta \oplus Q \) is confined to a \( \mathcal{O}(\log n) \) dimensional affine subspace then we can simply iterate through all possible \( \Theta \) and \( Q \) combinations to find one with a non-singular \( \Theta \) in \( \text{poly}(n) \) time. Let’s say that we’ve restricted \( \Theta \oplus Q \) to lie in a \( d \) dimensional affine subspace. Let \( M' \) be the true value of \( \Theta \), and let \( M \neq M' \) be another arbitrary matrix. Likewise let \( x' \) be the true value of \( Q \) and \( x \) some arbitrary vector. Now let \( Z^w \in \{ I, Z \}^\otimes n \) be a Pauli selected uniformly at random, and \( \rho = |v\rangle \langle v| \) a uniformly random computational basis state. The pair \( M \) and \( x \) will give the same label as the true label on the input \( (\rho, I^\otimes n + Z^w) \) if and only if

\[
(v^T(M + M') + x^T + (x')^T)w = 0 \mod 2.
\]

Because \( w \) is uniform random, as long as \( v^T(M + M') + x^T + (x')^T \) is not the zero vector over \( \mathbb{F}_2 \) then this will only be 0 at most half the time. Since at least one of \( M \neq M' \) or \( x \neq x' \) is true, then \( (M + M')^Tv = x + x' \) will only be true with probability at most \( \frac{1}{2} \) as well. So the probability that any arbitrary \( M \) and \( x \) have different labels is at least \( \frac{1}{4} \). Thus with \( \mathcal{O}(n) \) expected samples uniformly drawn from arbitrary basis states and \( Z^w \) we will have constrained our system to something we can bruteforce to find a full rank \( \Theta \) and corresponding \( q_j \) values that is consistent with all samples. From there apply Theorem 3.1 to generalize with zero training error as long as the samples is also at least the parameter \( m \) from the theorem statement.

### A.4 Clifford Circuits for a distribution with support over a single state

In the converse of an earlier situation, let us try to learn Clifford circuits with regard to a distribution \( D \) such that there exists some stabilizer state \( \sigma \) with \( \mathbb{P}_{(\rho, E) \sim D}[\rho = \sigma] = 1 \). This situation effectively reduces to that of Rocchetto [37]. If we run that algorithm we will find a state \( \sigma' \) that is consistent with all of the labels. Let \( \{ g_i \} \) be the generators of \( \sigma \) and \( \{ g'_i \} \) the generators of \( \sigma' \). If we let \( Cg_iC^\dagger = g'_i \) we define the first part of a Clifford circuit that maps \( \sigma \) to \( \sigma' \) as desired. We can then run the algorithm from Berg [13] to fill in the remainder of the Clifford circuit. Appealing to Theorem 3.1 once again completes the proof.