Efficient Learning of Non-Interacting Fermion Distributions

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Abstract

We give an efficient classical algorithm that recovers the distribution of a non-interacting fermion state over the computational basis. For a system of \( n \) non-interacting fermions and \( m \) modes, we show that \( O(m^2 n^4 \log(m/\delta)/\varepsilon^4) \) samples and \( O(m^4 n^4 \log(m/\delta)/\varepsilon^4) \) time are sufficient to learn the original distribution to total variation distance \( \varepsilon \) with probability \( 1 - \delta \). Our algorithm empirically estimates the one- and two-mode correlations and uses them to reconstruct a succinct description of the entire distribution efficiently.

1 Introduction

Identical particles come in two types: bosons and fermions. Each particle can be in certain modes (e.g., states or positions). For a system of \( n \) identical particles, a configuration of the system is described by specifying how many particles are in each of \( m \) modes. Bosons are particles where multiple occupancy of a mode is allowed, whereas fermions are particles where multiple occupancy is forbidden; that is, two or more fermions cannot occupy the same mode at once (this is the Pauli exclusion principle). It follows that a system of \( n \) fermions and \( m \) modes has \( \binom{m}{n} \) possible configurations; we denote the set of possible configurations by \( \Lambda_{m,n} \).

Our main result is an efficient algorithm (both in sample complexity and time complexity) for learning a non-interacting fermion distribution, which is a probability distribution over configurations in \( \Lambda_{m,n} \). Even though a non-interacting fermion distribution can have exponentially large support, we show how to exploit its structure to output a succinct description of the distribution efficiently. A non-interacting fermion distribution can be completely specified by an \( m \times n \) matrix \( A \), where the probability of observing an outcome \( S \in \Lambda_{m,n} \) corresponds to the squared absolute value of the determinant of an \( n \times n \) submatrix of \( A \). As such, we say the non-interacting fermion distribution \( \mathcal{D}_A \) is induced by the matrix \( A \). Given samples \( S_1, \ldots, S_N \) from such a distribution \( \mathcal{D}_A \), our polynomial-time algorithm outputs an \( m \times n \) matrix \( \hat{A} \) that induces a distribution \( \mathcal{D}_{\hat{A}} \). We prove that a polynomial number of samples is enough for \( \mathcal{D}_A \) and \( \mathcal{D}_{\hat{A}} \) to be \( \varepsilon \)-close in total variation distance. The key ingredient of the algorithm is a subroutine called “triangulation,” which iteratively finds the rows of the matrix \( \hat{A} \). We show how triangulation can be reduced to solving systems of linear equations.

![Theorem 1.1. Let \( \mathcal{D}_A \) be a non-interacting fermion distribution. Given \( O(m^2 n^4 \log(m/\delta)/\varepsilon^4) \) samples from \( \mathcal{D}_A \), there exists a classical algorithm that runs in \( O(m^4 n^4 \log(m/\delta)/\varepsilon^4) \) time and outputs a matrix \( \hat{A} \) that induces a non-interacting fermion distribution \( \mathcal{D}_{\hat{A}} \), such that the total variation distance between \( \mathcal{D}_A \) and \( \mathcal{D}_{\hat{A}} \) is at most \( \varepsilon \) with probability at least \( 1 - \delta \).]

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1.1 Related Work

Previous work showed how to simulate non-interacting fermions efficiently. In 2002, Valiant [Val02] introduced a class of quantum circuits called matchgate circuits and showed that they can be simulated classically in polynomial time. Soon after, Terhal and DiVincenzo [TD02] (see also Knill [Knill01]) showed that evolutions of non-interacting fermions give rise to unitary matchgate circuits. (See also [AA14][Appendix 13] for a simpler and faster simulation algorithm.) Thus, the contribution of this paper is to complement these classical simulation results with a classical learnability result.

More broadly, quantum state tomography is the task of constructing a classical description of a $d$-dimensional quantum mixed state, given copies of the state. The optimal number of copies for quantum state tomography is known to be $\Theta(d^2)$ due to Haah et al. [HHJ+17] and O’Donnell and Wright [OW16].

The classical analogue of state tomography is discrete distribution learning: recover a discrete probability distribution $D$ over a known support of size $d$, given samples from the distribution. It is known that learning $D$ requires $\Theta(d)$ samples [DL01]. This setting most closely resembles ours, since we only use independent measurements in the computational basis.

Different models for learning properties of mixed states $\rho$ have been studied. For example, Aaronson [Aar07] showed that such states are learnable under the Probably Approximately Correct (PAC) model, using training sequences of length only logarithmic in the Hilbert space dimension. Since all our samples come from the same distribution, and our goal is simply to learn that distribution, we have no need for the PAC framework.

Rocchetto [Roc18] showed that the class of stabilizer states is efficiently PAC-learnable, while Montanaro [Mon17] showed that stabilizer states are efficiently learnable using measurements in the Bell basis. With this work, non-interacting fermion states join stabilizer states as two of the only classes of quantum states for which we know computationally efficient learning algorithms.

1.2 Main Ideas

A non-interacting fermion distribution $D_A$ is supported by the elements of $\Lambda_{m,n}$ and can be described by an $m \times n$ column-orthonormal matrix $A \in \mathbb{C}^{m \times n}$ ($m \geq n$). Formally, $\Lambda_{m,n}$ is the set of all lists $S = (s_1, \ldots, s_m)$ such that $s_i \in \{0,1\}$ and $\sum_{i \in [m]} s_i = n$. For each element $S = (s_1, \ldots, s_m) \in \Lambda_{m,n}$, let $A_S$ be the $n \times n$ submatrix obtained by removing row $i$ of $A$ if $s_i = 0$. Then, $D_A$ is defined by

$$\text{Pr}_{S \sim D_A} [S] = |\text{det}(A_S)|^2.$$

Our goal is to produce a matrix $\hat{A}$ such that $|\text{det}(\hat{A}_S)|^2$ is close to $|\text{det}(A_S)|^2$ for all $S \in \Lambda_{m,n}$, given samples from $D_A$.

Let $n_i$ be 1 if the $i$th mode is occupied and 0 if not, and let $E[n_i] = p_i$. Let $n_{ij} = n_i n_j$ be 1 if the $i$th and $j$th modes are both occupied and 0 if not, and let $E[n_{ij}] = p_{ij}$. Our algorithm begins by empirically estimating each $p_i$ and $p_{ij}$ to accuracy $\pm \gamma$ with probability at least $1 - \delta$. It is easy to show that $O((\log(m/d)/\gamma^2)$ samples suffice to achieve this.$\dagger$

The main point of our work is that the empirical estimates, which we denote by $\hat{p}_i$ and $\hat{p}_{ij}$, are enough to reconstruct a succinct description of the non-interacting fermion distribution. At a high level, how is this reconstruction done? First, observe that the square of the $\ell_2$-norm of the $i$th
\[\text{In the language of quantum mechanics, } n_i\text{ and } n_{ij}\text{ are the one- and two-mode number operators, respectively. We use computational basis measurement outcomes to empirically estimate the expectation values of } n_i\text{ and } n_{ij}\text{ with respect to an unknown non-interacting fermion state.}\]
row of $A$ is the probability that the $i$th mode is occupied, i.e., $\|v_i\|^2 = p_i$, where $v_i$ is the $i$th row. Therefore, $\hat{p}_i$ is an estimate of $\|v_i\|^2$. Second, one can compute $|\det(A_S)|^2$ given only the $\ell_2$-norms of the rows of $A_S$ and the angles between each pair of rows. To see this, recall that $|\det(A_S)|^2$ is the square of the volume of a parallelootope (the $n$-dimensional generalization of a parallelepiped) formed by the rows of $A_S$, and the volume depends only on the $\ell_2$-norm of each row and the angles between them. Finally, observe that

$$p_{ij} = p_ip_j \sin^2(\theta_{ij}) = \|v_i\|^2 \|v_j\|^2 \sin^2(\theta_{ij}),$$

which is the square of the area of the base (formed by $v_i$ and $v_j$) of an $n$-dimensional parallelootope. This relation allows us to compute estimates of the pairwise angles of the rows of $A$, which we denote by $\hat{\theta}_{ij}$. Thus, to construct $\hat{A}$, which can be any matrix that is equivalent to $A$ up to some global rotation, it suffices to find $m$ $n$-dimensional vectors whose lengths and pairwise angles match our estimates $\hat{p}_i$ and $\hat{\theta}_{ij}$. Finding these $m$ vectors reduces to solving $m$ systems of linear equations, as we explain in detail in Section 2.

The technical part is to understand how far $D_{\hat{A}}$ is from $D_A$ in total variation distance, given the initial noise in our estimates. To do this, we adapt an error analysis of Arkhipov [Ark15] from non-interacting bosons to non-interacting fermions. In Section 3 we show that the total variation distance between $D_{\hat{A}}$ and $D_A$ is at most $n\sqrt{m\gamma}$. Therefore, the total variation distance will be $\varepsilon$-close if we estimate each $p_i$ and $p_{ij}$ to accuracy $\pm \varepsilon^2/mn^2$.

1.3 Notation

We use the following notation. $\{1, \ldots, n\} := [n]$, and $\binom{[n]}{2} := \{(i, j) \in [n]^2 \mid i < j\}$. Let $A \in \mathbb{C}^{n \times n}$ and $v \in \mathbb{C}^n$. Then, $\|v\|_2 = (\sum_{i \in [n]} |v_i|^2)^{1/2}$ is the $\ell_2$-norm, and $\|A\|_{\text{op}} := \sup_{\|v\|_2 = 1} \|Av\|_2$ is the operator norm.

We also use some distance measures in the error analysis. Let $P = \{p_x\}_x$ and $Q = \{q_x\}_x$ be discrete probability distributions. Then, $d_{\text{TV}}(P, Q) := \frac{1}{2} \sum_x |p_x - q_x| = \frac{1}{2} \|P - Q\|_1$ is the total variation distance. Let $|\psi\rangle$ and $|\phi\rangle$ be quantum pure states. Then, $F(\psi, \phi) = |\langle \psi | \phi \rangle|^2$ is the fidelity, and $D_{\text{tr}}(\psi, \phi) = \sqrt{1 - F(\psi, \phi)}$ is the trace distance. Occasionally, we drop Dirac notation for brevity.

2 Learning Algorithm

In this section, we state our algorithm which, given samples from a non-interacting fermion distribution $D_A$, outputs a matrix $\hat{A}$ that induces a distribution $D_{\hat{A}}$. The algorithm has three phases: empirical estimation, triangulation, and matrix generation. In the empirical estimation phase, we empirically estimate the one- and two-mode correlations and use them to estimate the pairwise angles of the rows of $A$. In the triangulation phase, we find $m$ $n$-dimensional vectors $\hat{v}_1, \ldots, \hat{v}_m$ that satisfy the constraints imposed by the empirical estimates. Finally, in the matrix generation phase, we output the $m \times n$ matrix generated by taking $\hat{v}_1, \ldots, \hat{v}_m$ to be rows of the matrix.
Algorithm 1 Efficient learning of non-interacting fermion distributions

Input: $N$ samples from $\mathcal{D}_A$, denoted by $\{S_1, \ldots, S_N\}$ where $S_i = (s_{i,1}, \ldots, s_{i,m}) \in \Lambda_{m,n}$.
Output: an $m \times n$ matrix $\hat{A}$

Empirical estimation
1: for $i = 1, \ldots, m$ do
2: Set $\hat{p}_i = \frac{1}{N} \sum_{a=1}^{N} s_{a,i}$
3: for $(i, j) \in \binom{[m]}{2}$ do
4: Set $\hat{p}_{ij} = \frac{1}{N} \sum_{a=1}^{N} s_{a,i} \cdot s_{a,j}$
5: Set $\hat{\theta}_{ij} = \sin^{-1} \sqrt{\hat{p}_{ij}/(\hat{p}_i \hat{p}_j)}$

Triangulation
6: for $j = 1, \ldots, m$ do
7: Find a vector $\hat{v}_j \in \mathbb{R}^n$ s.t. $\|\hat{v}_j\|_2^2 = \hat{p}_j$ and the angle between $\hat{v}_i$ and $\hat{v}_j$ is $\hat{\theta}_{ij}$ for all $i \in [j - 1]$

Matrix generation
8: Let $\hat{A}$ be the $m \times n$ matrix obtained by taking $\hat{v}_1, \ldots, \hat{v}_m$ as row vectors
9: return $\hat{A}$

In total, our algorithm estimates $\binom{m}{2} + m$ parameters that are on the interval $[0, 1]$ to an additive error $\gamma$ with probability at least $1 - \delta$. It is easy to show that the optimal sample complexity for this is $N = O(\log(m/\delta)/\gamma^2)$ and that it is achieved with the empirical estimator. In the next section, we show that if $\gamma = \varepsilon^2/mn^2$, then the total variation distance between $\mathcal{D}_A$ and $\hat{\mathcal{D}}_A$ is at most $\varepsilon$. The sample complexity is then $N = O(m^2n^4\log(m/\delta)/\varepsilon^4)$. Note that we can compute estimates of the one- and two-mode correlations via fast rectangular matrix multiplication in $O(Nm^{\omega-1})$ time, where $\omega$ is the matrix multiplication constant [BCS13]. However, we still must compute each $\hat{\theta}_{ij}$, which adds a factor of $m^2$ to the running time, so the running time for the empirical estimation phase is $O(Nm^2) = O(m^4n^4\log(m/\delta)/\varepsilon^4)$.

In the triangulation phase, we are solving a feasibility problem, i.e., finding any vector that satisfies some constraints, which can be done in polynomial time. Specifically, given vectors $\hat{v}_1, \ldots, \hat{v}_{j-1}$, we want to solve the following:

\[
\text{find } \hat{v}_j \in \mathbb{R}^n \\
\text{subject to } \|\hat{v}_j\|_2^2 = \hat{p}_j \\
\langle \hat{v}_i, \hat{v}_j \rangle = \|\hat{v}_i\|_2\|\hat{v}_j\|_2 \cos \hat{\theta}_{ij}, \quad \forall i \in [j - 1].
\]

Let $B$ be the $(j-1) \times n$ matrix obtained by taking $\hat{v}_1, \ldots, \hat{v}_{j-1}$ as rows, let $x \in \mathbb{R}^n$ be unknown, and let $b$ be the $(j-1)$-dimensional column vector whose entries are $b_i = \|\hat{v}_i\|_2\|\hat{v}_j\|_2 \cos \hat{\theta}_{ij}$. The above feasibility problem reduces to solving the system of linear equations $Bx = b$ and then re-scaling $x$ such that $\|x\|_2^2 = \hat{p}_j$. When $j - 1 < n$, the system of linear equations is underdetermined; when $j - 1 = n$ the system is perfectly determined; and when $j - 1 > n$ the system is overdetermined. However, in all cases we are guaranteed to find a solution because at least one solution exists (i.e., the set of vectors that induces the distribution that matches our samples). Solving each system reduces to bringing the matrix $B$ into row echelon form, which, for an $r \times c$ matrix ($r > c$) can be done in $O(rc^{\omega-1})$ time (see Section 16.5 of [BCS13]), where $\omega$ is the matrix multiplication constant. Thus, triangulation runs in $O(m^2n^{\omega-1})$ time.
3 Error Analysis

In this section, we show that if we estimate the one- and two-mode correlations up to an additive error $\gamma$, then the total variation distance between $D_A$ and $D_A'$ is at most $n \sqrt{m \gamma}$. This implies that if $\gamma = \sqrt{2}/mn^2$, then the total variation distance between $D_A$ and $D_A'$ is at most $\varepsilon$.

Our error analysis begins by repeating Arkhipov’s error analysis [Ark15] for the fermionic case. In fact, Arkhipov’s work relies only on properties of the homomorphism $\varphi$ that lifts $m \times m$ unitary transformations to $n$-boson unitary transformations (see [AA11]), and the same properties hold for $\varphi_f$, the homomorphism that lifts $m \times m$ unitary transformations to $n$-fermion unitary transformations. Therefore, we state some results below without proof, as the proofs are essentially identical to the proofs in [Ark15]. First, we define $\varphi_f$.

The homomorphism $\varphi_f$ can be defined in two ways: for any $m \times m$ unitary matrix $U$, $\varphi_f(U)$ is a unitary transformation on the Hilbert space of (1) non-interacting fermion states or (2) $m$-qubit states. In the latter case, the unitary transformation is a Hamming-weight-preserving matchgate. This follows directly from Terhal and DiVincenzo’s work [TD02], which shows the equivalence between these two cases. Specifically, for any $m \times m$ unitary matrix $U$, one way to define $\varphi_f$ is:

$$\langle S | \varphi_f(U) | T \rangle = \det(U_{S,T}),$$

for all $S = (s_1, \ldots, s_m), T = (t_1, \ldots, t_m) \in \Lambda_{m,n}$, where $U_{S,T}$ is the $n \times n$ submatrix obtained by removing row $i$ of $U$ if $s_i = 0$ and removing column $j$ of $U$ if $t_j = 0$.

**Claim 3.1** (Lemma 1 [Ark15]). Let $A$ and $B$ be unitary matrices. Their operator distance can be expressed in terms of eigenvalues $\{\lambda_i\}$ of $AB^{-1}$ as

$$\|A - B\|_{\text{op}} = \max_i |\lambda_i - 1|.$$

**Claim 3.2** (Lemma 2 [Ark15]). If an $m \times m$ unitary matrix $U$ has eigenvalues $(\lambda_1, \ldots, \lambda_m)$, then the eigenvalues of the $M \times M$ unitary $\varphi_f(U)$ are $\lambda_1^{\pi_1} \cdots \lambda_m^{\pi_m}$ for each $S \in \Lambda_{m,n}$.

Claims 3.1 and 3.2 can be combined to show that there is at most a factor of $n$ gap between the operator distance of the $n$-fermion unitary transformations and single-fermion unitary transformations.

**Lemma 3.3** (Theorem 3 [Ark15]). Let $\varphi_f$ be the homomorphism that takes an $m \times m$ unitary matrix $U$ acting on a single fermion and produces an $M \times M$ unitary matrix acting on $n$ identical fermions where $M = \binom{m}{n}$. Then,

$$\|\varphi_f(\hat{U}) - \varphi_f(U)\|_{\text{op}} \leq n\|\hat{U} - U\|_{\text{op}}.$$

For the remainder of this section, we will use the following notation. Let $|\Psi_0\rangle$ and $|\psi_0\rangle$ be some fixed $n$-fermion and single-fermion states, respectively. Then, for any $m \times m$ unitary matrices $U$ and $\hat{U}$, let $|\Psi\rangle := \varphi_f(U)|\Psi_0\rangle$ and $|\hat{\Psi}\rangle := \varphi_f(\hat{U})|\Psi_0\rangle$. Similarly, let $|\hat{\psi}\rangle := U|\psi_0\rangle$ and $|\hat{\psi}\rangle := \hat{U}|\psi_0\rangle$.

The corollary below follows from Lemma 3.3.

**Corollary 3.4.** $\|\hat{\Psi} - \Psi\|_2 \leq n\|\hat{\psi} - \psi\|_2$.

**Proof.** $\|\hat{\Psi} - \Psi\|_2 = \|(|\varphi_f(\hat{U}) - \varphi_f(U)|\Psi_0\rangle\|_2 \leq n\|\hat{U} - U\|\psi_0\|_2 \leq n\|\hat{\psi} - \psi\|_2$.  

Since we do not care about the relative phases (i.e., we are only learning the distribution over the computational basis), we write $|\psi\rangle = \sum_{i \in [m]} \sqrt{p_i} |i\rangle$ and $|\hat{\psi}\rangle = \sum_{i \in [m]} \sqrt{\hat{p}_i} |i\rangle$, where for $i \in [m]$, $|i\rangle$ denotes which mode is occupied and $p_i, \hat{p}_i \in [0,1]$ such that $|\hat{p}_i - p_i| \leq \gamma$. Next, we upper bound the $\ell_2$-distance between the single-fermion states.
Claim 3.5. $\|\hat{\psi} - \psi\|_2 \leq \sqrt{m\gamma}$.

Proof. We need the following lower bound:

$$\sqrt{F(\hat{\psi}, \psi)} = \sum_{i \in [m]} \sqrt{p_i\hat{p}_i} \geq \sum_{i \in [m]} \sqrt{p_i(p_i - \gamma)}$$

$$= \sum_{i \in [m]} p_i\sqrt{1 - \gamma}$$

$$\geq \sum_{i \in [m]} p_i(1 - \gamma p_i)$$

$$= 1 - \frac{m\gamma}{2}.$$  

The second inequality follows from the fact that $(1 + x)^r \geq 1 + rx$ for every integer $r \geq 0$ and every real number $x \geq -1$ (Bernoulli's inequality). Then,

$$\|\hat{\psi} - \psi\|_2 = \sqrt{2 - 2\sqrt{F(\hat{\psi}, \psi)}}$$

$$\leq \sqrt{2 - 2(1 - \frac{m\gamma}{2})}$$

$$= \sqrt{m\gamma}.$$

Combining Corollary 3.4 and Claim 3.5 gives a bound on the total variation distance between the two distributions.

Theorem 3.6. $d_{TV}(D_{\hat{U}}, D_U) \leq n\sqrt{m\gamma}$.

Proof.

$$d_{TV}(D_{\hat{U}}, D_U) \leq D_{tr}(\hat{\Psi}, \Psi)$$

$$= \sqrt{1 - F(\hat{\Psi}, \Psi)}$$

$$\leq \|\hat{\Psi} - \Psi\|_2$$

$$\leq n\|\hat{\psi} - \psi\|_2$$

$$\leq n\sqrt{m\gamma}.$$

4 Open Problems

The most immediate directions for future work are improving the sample and time complexities of our algorithm, or giving conditional or unconditional lower bounds. Currently the best lower bound we know is that $\Omega(m/ \log m)$ samples are needed, just from an information-theoretic argument (each sample gives at most $n \log m$ bits of information and the distribution is characterized by $nm$ real
parameters). Recall that our algorithm requires $O(\log m/\gamma^2)$ samples to estimate the one- and two-mode correlations to accuracy $\pm \gamma$. The factor of $m^2 n^4$ in our final bound comes from the need to set $\gamma$ to $\varepsilon^2/m n^2$. Perhaps a more careful error analysis can lead to a better bound.

Beyond that, it could be interesting to generalize our algorithm (for example, to superpositions over different numbers of fermions, or fermionic circuits that take inputs), and to find other classes of quantum states that admit efficient learning algorithms (for example, perhaps low-entanglement states or the outputs of small-depth circuits).

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