Quantum-inspired classical algorithms for principal component analysis and supervised clustering

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We describe classical analogues to Lloyd et al.'s quantum algorithms for principal component analysis and nearest-centroid clustering. We introduce a classical algorithm model that assumes we can efficiently perform ℓ^2 -norm samples of input data, a natural analogue to quantum algorithms assuming efficient state preparation. In this model, our classical algorithms run in time polylogarithmic in input size, matching the runtime of the quantum algorithms with only polynomial slowdown. These algorithms indicate that their corresponding problems do not yield exponential quantum speedups.

INTRODUCTION

Quantum machine learning (QML) has shown great promise towards yielding new exponential quantum speedups in machine learning ever since the pioneering linear systems algorithm of Harrow, Hassidim, and Lloyd [1]. Since ML routines often push real-world limits of computing power, an exponential improvement to algorithm speed would allow for machine learning systems with vastly greater capabilities. While we have found many fast QML subroutines for machine learning problems since HHL [2–6], researchers have struggled to prove that these subroutines can be used to achieve an exponentially faster algorithm for a classical machine learning problem even in the strongest input and output models [7]. A recent work of the author [8] suggests a surprising reason why: even our best QML algorithms, with issues with input and output models resolved, fail to achieve exponential speedups. This previous work constructs a classical algorithm matching, up to polynomial slowdown, a corresponding quantum algorithm for recommendation systems [9], which was previously believed to be one of the best candidates for an exponential speedup in machine learning [10]. In light of this result, we need to question our intuitions and reconsider one of the guiding questions of the field: when is quantum linear algebra exponentially faster than classical linear algebra?

The main challenge in answering this question is not in finding fast classical algorithms, as one might expect. Rather, most QML algorithms are *incomparable* to classical algorithms, since they take quantum states as input and output quantum states: we don't even know an analogous classical model of computation where we can search for similar classical algorithms. The quantum recommendation system is unique in that it has a classical input (QRAM) and classical output (a sample from a vector in the computational basis), allowing for rigorous comparisons with classical algorithms.

In our previous work we suggest an idea for developing classical analogues to QML algorithms beyond this exceptional case [8]:

When QML algorithms are compared to classical ML algorithms in the context of finding speedups, any state preparation assumptions in the QML model should be matched with ℓ^2 -norm sampling assumptions in the classical ML model.

In this work, we implement this idea by formalizing a particular notion of ℓ^2 -norm sampling assumption, which we call sample and query access. We can get sample and query access to data under typical state preparation assumptions, so fast classical algorithms in this model are strong barriers to their QML counterparts admitting exponential speedups. To support that the resulting model is the right notion to consider, we use it to dequantize two more well-known QML algorithms, quantum principal component analysis [11] and quantum supervised clustering [12]. That is, we give classical algorithms that, with classical sample and query access assumptions replacing quantum state preparation assumptions, match the bounds and runtime of the corresponding quantum algorithms up to polynomial slowdown. This disproves the claims in these QML papers that their algorithms give exponential speedups. Surprisingly, we do so using only the classical toolkit originally applied to the recommendation systems problem, demonstrating the power of this model in analyzing QML algorithms.

Notation. $[n] := \{1, \ldots, n\}$. Consider a vector $x \in \mathbb{C}^n$ and matrix $A \in \mathbb{C}^{m \times n}$. $A_{i,*}$ and $A_{*,i}$ will refer to A's ith row and column, respectively. $\|x\|$, $\|A\|_F$, and $\|A\|$ will refer to ℓ^2 , Frobenius, and spectral norm, respectively. $|x\rangle := \frac{1}{\|x\|} \sum_{i=1}^n x_i |i\rangle$ and $|A\rangle := \frac{1}{\|A\|_F} \sum_{i=1}^m \|A_{i,*}\| |i\rangle |A_{i,*}\rangle$. $A = \sum_{i=1}^{\min m, n} \sigma_i u_i v_i^{\dagger}$ is A's singular value decomposition, where $u_i \in \mathbb{C}^m$, $v_i \in \mathbb{C}^n$, $\sigma_i \in \mathbb{R}$, $\{u_i\}$ and $\{v_i\}$ are sets of orthonormal vectors, and $\sigma_1 \geq \sigma_2 \geq \cdots \geq \sigma_{\min m, n} \geq 0$. $A_{\sigma} := \sum_{\sigma_i \geq \sigma} \sigma_i u_i v_i^{\dagger}$ and $A_k := \sum_{i=1}^k \sigma_i u_i v_i^{\dagger}$ denote low-rank approximations to A. We assume basic arithmetic operations take unit time, and $\tilde{O}(f) := O(f \log f)$.

THE DEQUANTIZATION MODEL

QML algorithms typically work in the model where state preparation of input is efficient and a quantum state (or an expectation of it) is output. In particular, given a data point $x \in \mathbb{C}^n$ as input, we assume we can prepare copies of $|x\rangle$. For m input data points as a matrix $A \in \mathbb{C}^{m \times n}$, we additionally assume efficient preparation of $|A\rangle$, to preserve relative scale. When these states are prepared from classical data, we typically require access to the data and normalization factors. This inspires the classical input model for our quantum-inspired algorithms, where we assume such access, and instead of preparing states, we can prepare measurements of these states.

Definition. We have O(T)-time sample and query access to $x \in \mathbb{C}^n$ (notated $\mathrm{SQ}(x)$) if, in O(T) time, we can query an index $i \in [n]$ for its entry x_i ; produce an independent measurement of $|x\rangle$ in the computational basis; and query for ||x||. If we can only query for an upper bound on the norm $\tilde{x} \in [||x||, (1+\nu)||x||)$, then we denote this by $\mathrm{SQ}^{\nu}(x)$. For $A \in \mathbb{C}^{m \times n}$, sample and query access to A (notated $\mathrm{SQ}(A)$) is $\mathrm{SQ}(A_{1,*},\ldots,A_{n,*})$ along with $\mathrm{SQ}(\tilde{A})$ where \tilde{A} is the vector of row norms, i.e. $\tilde{A}_i := ||A_{i,*}||$.

Sample and query access will be our classical analogue to quantum state preparation. This makes sense. As we noted previously [8], QML algorithms shouldn't rely on fast state preparation as the "source" of an exponential speedup: the algorithm itself should create the speedup. So, our classical model should be able to assume that fast measurements of input states are possible.

Indeed, for typical instantiations of state preparation oracles, we can get efficient sample and query access to input. For example, given input in QRAM [13], we can get log-dimension-time sample and query access to input [8, Proposition 3.2]. Similarly, sparse and close-to-uniform vectors can be prepared efficiently, and correspondingly admit efficient sample and query access (details in appendix). So, in usual QML settings, sample and query assumptions are easier to satisfy than state preparation assumptions, at least for the forseeable future.

This leads to a model based on SQ access that we codify with the informal definition of "dequantization". This is the sense in which we dequantized the quantum recommendation system in prior work [9].

Definition. We say we dequantize a quantum protocol S: O(T)-time state preparation of $|\phi_1\rangle, \ldots, |\phi_c\rangle \to |\psi\rangle$ if we describe a classical algorithm of the form $\mathcal{C}_S: O(T)$ -time $\mathrm{SQ}(\phi_1,\ldots,\phi_c) \to \mathrm{SQ}^{\nu}(\psi)$ with similar guarantees to S up to polynomial slowdown.

THREE SUBROUTINES

Now, we present the three protocols from our previous work [8] rephrased in our access model (details in

appendix). The first can be seen as a dequantized swap test, and follows from a standard sampling strategy.

Algorithm 1 Inner product estimation

Input: O(T)-time $SQ^{\nu}(x) \in \mathbb{C}^n$, $Q(y) \in \mathbb{C}^n$ Output: an estimate of $\langle x|y \rangle$

- 1: Let $s = 54 \frac{1}{\epsilon^2} \log \frac{2}{\delta}$
- 2: Collect measurements i_1, \ldots, i_s from $|x\rangle$
- 3: Let $z_j = x_{i_j}^{\dagger} y_{i_j} \frac{\|x\|^2}{|x_{i_j}|^2}$ for all $j \in [s]$ $\triangleright \mathbb{E}[z_j] = \langle x|y \rangle$
- 4: Separate the z_j 's into $6\log\frac{2}{\delta}$ buckets of size $\frac{9}{\varepsilon^2}$, and take the mean of each bucket
- 5: Output the (component-wise) median of the means

Proposition 1 ([8, Proposition 4.2]). For $x, y \in \mathbb{C}^n$, given $\mathrm{SQ}^{\nu}(x)$ and $\mathrm{Q}(y)$, Algorithm 1 outputs an estimate of $\langle x|y\rangle$ to $(\varepsilon + \nu)\|x\|\|y\|$ error with probability $\geq 1 - \delta$ in time $O(\frac{T}{\varepsilon^2}\log\frac{1}{\delta})$.

For this protocol, quantum algorithms can achieve a quadratic speedup via amplitude estimation, but certainly not an exponential speedup: this insight will suffice to dequantize supervised clustering. The second protocol uses rejection sampling to dequantize the swap test over a subset of qubits: getting $|Vw\rangle$ via $\langle V| (|w\rangle \otimes I)$.

Algorithm 2 Matrix-vector sample and query access

Input: O(T)-time $SQ(V^{\dagger}) \in \mathbb{C}^{k \times n}$, $Q(w) \in \mathbb{C}^k$ Output: $SQ^{\nu}(Vw)$

- 1: function RejectionSample($\mathrm{SQ}(V^\dagger)$, $\mathrm{Q}(w)$)
- 2: Sample $i \in [k]$ proportional to $|w_i|^2 ||V_{*,i}||^2$
- 3: Sample $s \in [n]$ from $V_{*,i}$
- 4: Compute $r_s = (Vw)_s^2/(k\sum_{j=1}^k (V_{sj}w_j)^2)$
- 5: Output s with probability r_s (success); otherwise, output \varnothing (failure)
- 6: end function
- 7: Query: output $(Vw)_s$
- 8: Sample: run RejectionSample until success (outputting s) or $kC(V,w)\log\frac{1}{\delta}$ failures (outputting \varnothing)
- 9: NORM(ν): Let p be the fraction of successes from running RejectionSample $\frac{k}{\nu^2}C(V,w)\log\frac{1}{\delta}$ times; output $pk\sum_{i=1}^k|w_i|^2\|V_{*,i}\|^2$

Proposition 2 ([8, Proposition 4.3]). For $V \in \mathbb{C}^{n \times k}$, $w \in \mathbb{C}^k$, given $\mathrm{SQ}(V^{\dagger})$ and $\mathrm{Q}(w)$, Algorithm 2 simulates $\mathrm{SQ}^{\nu}(Vw)$ where the time to query is O(Tk), sample is $O(Tk^2C(V,w)\log\frac{1}{\delta})$, and query norm is $O(Tk^2C(V,w)\frac{1}{\nu^2}\log\frac{1}{\delta})$. Here, δ is the desired failure probability and $C(V,w) = \sum \|w_iV_{*,i}\|^2/\|Vw\|^2$.

Quantum algorithms achieve a speedup here when k is large and C(V, w) is small, such as when V is a high-dimensional unitary, confirming our intuition. Alternatively, V could be low-rank and large in the direction of w; in that case, we can find this direction classically via the following method for finding low-rank approximations.

Algorithm 3 Low-rank approximation

Input: O(T)-time $\mathrm{SQ}(A) \in \mathbb{R}^{m \times n}, \, \sigma, \, \varepsilon, \, \delta$ Output: $\mathrm{SQ}(S) \in \mathbb{C}^{\ell \times n}, \, \mathrm{Q}(\hat{U}) \in \mathbb{C}^{q \times \ell}, \, \mathrm{Q}(\hat{\Sigma}) \in \mathbb{C}^{\ell \times \ell}$

- 1: Set $K = ||A||_F^2/\sigma^2$ and $q = \Theta\left(\frac{K^4}{\varepsilon^2}\log(\frac{1}{\delta})\right)$
- 2: Sample rows i_1, \ldots, i_q from \tilde{A} and define $S \in \mathbb{R}^{q \times n}$ such that $S_{r,*} := A_{i_r,*} \frac{\|A\|_F}{\sqrt{q} \|A_{i_r,*}\|}$
- 3: Sample columns j_1, \ldots, j_q from \mathcal{F} , where \mathcal{F} denotes the distribution given by sampling a uniform $r \sim [q]$, then sampling c from S_r .
- 4: Let $W \in \mathbb{C}^{q \times q}$ be the normalized submatrix $W_{*,c} := \frac{S_{*,j_c}}{q\mathcal{F}(j_c)}$
- 5: Compute the left singular vectors of W $\hat{u}^{(1)}, \ldots, \hat{u}^{(\ell)}$ that correspond to singular values $\hat{\sigma}^{(1)}, \ldots, \hat{\sigma}^{(\ell)}$ larger than σ
- 6: Output SQ(S), $\hat{U} \in \mathbb{R}^{q \times \ell}$ the matrix with columns $\hat{u}^{(i)}$, and $\hat{\Sigma} \in \mathbb{R}^{\ell \times \ell}$ the diagonal matrix with entries $\hat{\sigma}^{(i)}$.

At a high level, Algorithm 3 finds the large singular vectors of A by reducing its dimension down to W, whose SVD we can compute quickly. Then, $S, \hat{U}, \hat{\Sigma}$ define approximate large singular vectors \hat{V} (described below); our low-rank approximation D is A projected onto their span. Note that we can achieve O(T)-time $\mathrm{SQ}(S)$ because all rows are normalized, and rows of S are simply rows of S. Thus, sampling from S is a uniform sample from S and sampling from S is sampling from a row of S.

Proposition 3 ([8, Theorem 4.4], adapted from Frieze et al. [14]). Suppose we are given O(T)-time $SQ(A) \in \mathbb{C}^{n \times d}$, a singular value threshold σ , and an error parameter $\varepsilon \in (0, \sqrt{\sigma/\|A\|_F}/4]$. Denote $K := \|A\|_F^2/\sigma^2$. Then in

$$O\Big(\frac{K^{12}}{\varepsilon^6}\log^3\frac{1}{\delta} + T\frac{K^8}{\varepsilon^4}\log^2\frac{1}{\delta}\Big)$$

time, Algorithm 3 outputs O(T)-time $SQ(S) \in \mathbb{C}^{q \times n}$ and $\hat{U} \in \mathbb{C}^{q \times \ell}, \hat{\Sigma} \in \mathbb{R}^{\ell \times \ell}$ (for $\ell = \Theta(\frac{K^4}{\varepsilon^2} \log \frac{1}{\delta})$) implicitly describing a low-rank approximation to $A, D := A\hat{V}\hat{V}^{\dagger}$ with $\hat{V} := S^{\dagger}\hat{U}\Sigma^{-1}$ (notice rank $D \leq \ell$).

This description satisfies the following with probability $\geq 1 - \delta$: (a) $\sigma_{\ell} \geq \sigma - \varepsilon \|A\|_F$ and $\sigma_{\ell+1} < \sigma + \varepsilon \|A\|_F$; (b) $\|A - D\|_F^2 \leq \|A - A_{\ell}\|_F^2 + \varepsilon \|A\|_F^2$; (c) $\sum_{i=1}^{\ell} |\hat{\sigma}_i^2 - \sigma_i^2| \leq \varepsilon \|A\|_F^2/K^{1.5}$; (d) $\|\hat{V} - \Lambda\|_F \leq \varepsilon$ for some Λ with orthonormal columns and the same image as \hat{V} .

Intuitively, (a) shows that ℓ is the right place to truncate up to ε error, (b) is the low-rank approximation guarantee, (c) shows that our singular values are approximately correct, and (d) shows that our singular vectors are approximately orthonormal.

NEAREST-CENTROID CLASSIFICATION

Lloyd, Mohseni, and Rebentrost's quantum algorithm for clustering estimates the distance of a data point to the centroid of a cluster of points [12]. The paper claims that this quantum algorithm gives an exponential speedup over

classical algorithms. We dequantize Lloyd et al's quantum supervised clustering algorithm [12] with only quadratic slowdown. While this quantum algorithm is elementary and appears to have no "inherently quantum" steps, a formal proof demonstrating lack of exponential speedup appears to have eluded researchers. Classical algorithms by Aaronson [7] for uniform input and Wiebe et al. [15, Section 7] for sparse input and random input (which is close-to-uniform with high probability) dequantize this algorithm in restricted settings. We are the first to give a general classical algorithm for this problem.

Problem 4 (Centroid distance). Suppose we are given access to $V \in \mathbb{C}^{n \times d}$ and $u \in \mathbb{C}^d$. Estimate $\|u - \frac{1}{n}\vec{1}V\|^2$ to ε additive error with probability $\geq 1 - \delta$.

Note that we are treating vectors as rows, with $\vec{1}$ the vector of ones. Let \bar{u} and \bar{V} be the row-normalized versions of u and V, respectively. Both classical and quantum algorithms argue about $M \in \mathbb{R}^{(n+1)\times d}$ and $w \in \mathbb{R}^{n+1}$ instead of u and V, where

$$M := \begin{bmatrix} \bar{u} \\ \frac{1}{\sqrt{n}} \bar{V} \end{bmatrix}$$
 and $w := \begin{bmatrix} \|u\| & -\frac{1}{\sqrt{n}} \tilde{V} \end{bmatrix}$.

Because $wM = u - \frac{1}{n}\vec{1}V$, we wish to estimate $||wM||^2 = wMM^{\dagger}w^{\dagger}$. Let $Z := ||w||^2 = ||u||^2 + \frac{1}{n}||V||_F^2$ be an "average norm" parameter appearing in our algorithms.

Theorem 5 (Quantum Nearest-Centroid [12]). Suppose that, in O(T) time, we can (1) determine ||u|| and $||V||_F$; or (2) prepare a state $|u\rangle, |V_1\rangle, \ldots, |V_n\rangle$, or $|\tilde{V}\rangle$. Then we can solve Problem 4 in $O(T^{\underline{Z}}_{\varepsilon} \log \frac{1}{\delta})$ time.

The quantum algorithm proceeds by constructing the states $|M\rangle$ and $|w\rangle$, then performing a swap test to get $|wM\rangle$. The swap test succeeds with probability $\frac{1}{Z}wMM^{\dagger}w^{\dagger}$, so we can run amplitude amplification to get an estimate up to ε error with $O(\frac{1}{\varepsilon}\log\frac{1}{\delta})$ overhead. The quadratic speedup from amplitude amplification is the only speedup that this algorithm achieves:

Theorem 6 (Classical Nearest-Centroid). Suppose we are given O(T)-time $\mathrm{SQ}(V) \in \mathbb{C}^{n \times d}$ and $\mathrm{SQ}(u) \in \mathbb{C}^d$. Then Algorithm 4 outputs a solution to Problem 4 in $O(T^{\frac{Z^2}{\varepsilon^2}}\log\frac{1}{\delta})$ time.

Proof. First, notice that we have O(T)-time SQ(M) and Q(w): M's rows are rescaled vectors that we have sample and query access to; and $\tilde{M} := [1 \frac{1}{\sqrt{n}} \cdots \frac{1}{\sqrt{n}}]$, so we have $SQ(\tilde{M})$ trivially; and w's entries can be queried using our given access. Next, use that $wMM^{\dagger}w^{\dagger} = \langle a|b\rangle$ for a,b the flattened tensors

$$a := \sum_{i=1}^{d} \sum_{j=1}^{n+1} \sum_{k=1}^{n+1} M_{ji} \| M_{k,*} \| |i\rangle |j\rangle |k\rangle = M \otimes \tilde{M}; \quad (1)$$

$$b := \sum_{i=1}^{d} \sum_{j=1}^{n+1} \sum_{k=1}^{n+1} \frac{w_j w_k M_{ki}}{\|M_{k,*}\|} |i\rangle |j\rangle |k\rangle.$$
 (2)

Given O(T)-time SQ(M) and Q(w), we have O(T)-time SQ(a) and Q(b): namely, we can sample from a by sampling j and k from M, and then sampling i from $M_{i,*}$. Thus, we can apply Proposition 1 to estimate $w^T M^T M w$ to $\varepsilon(4Z)$ error with probability $1-\delta$ in $O(T\frac{1}{\varepsilon^2}\log\frac{1}{\delta})$ time, using that $||a|| = ||M||_F^2 = 4$ and $||b|| = ||w||^2 = Z$. Rescaling ε by 4Z gives the desired result.

Algorithm 4 Classical Supervised Clustering

Input: O(T)-time $SQ(V_1, \ldots, V_n, u)$

Output: An estimate of $\lambda = \|u - \frac{1}{n}V\vec{1}\|^2$

- 1: Achieve O(T)-time SQ(a), Q(b) for a, b as in (1), (2)
- 2: Run Algorithm 1 to estimate $\langle a|b\rangle$ to ε error and output the result

PRINCIPAL COMPONENT ANALYSIS

We now dequantize Lloyd, Mohseni, and Rebentrost's quantum principal component analysis (QPCA) algorithm [11], an influential early example of QML [16, 17]. While the paper describes a more general strategy for Hamiltonian simulation of density matrices, their central claim is an exponential speedup in an immediate application: producing quantum states corresponding to the top principal components of a low-rank dataset [11].

The setup for the problem is as follows: suppose we are given a matrix $A \in \mathbb{R}^{n \times d}$ whose rows correspond to data in a dataset. We will find the principal eigenvectors and eigenvalues of $A^{\dagger}A$; when A is a mean zero dataset, this corresponds to the top principal components.

Problem 7 (Principal component analysis). Suppose we are given access to $A \in \mathbb{C}^{n \times d}$, σ , k, and η with the guarantee that, for $i \in [k]$, $\sigma_i \ge \sigma$ and $\sigma_i^2 - \sigma_{i+1}^2 \ge \eta ||A||_F^2$. With probability $\geq 1 - \delta$ output estimates to $\sigma_1^2, \ldots, \sigma_k^2$ accurate up to $\varepsilon_{\sigma} ||A||_F^2$ additive error $(\varepsilon_{\sigma} < \eta)$ and access to v_1, \ldots, v_k accurate up to ε_v additive ℓ^2 -norm error.

Denote $||A||_F^2/\sigma^2$ by K. Lloyd et al. get the following:

Theorem 8. Given $||A||_F$ and the ability to prepare copies of $|A\rangle$ in O(T) time, a quantum algorithm can output the desired estimates for Problem $7 \hat{\sigma}_1^2, \ldots, \hat{\sigma}_k^2$ and $|\hat{v}_1\rangle, \ldots, |\hat{v}_k\rangle$ in $\tilde{O}(TK\min(\varepsilon_{\sigma}, \delta)^{-3})$ time.

Later results [9, 18, Theorems 5.2, 27] improve the runtime here to $\tilde{O}(T\frac{\|A\|_F^2}{\sigma^2}\varepsilon_\sigma^{-1}\operatorname{polylog}(nd/\delta))$ when A is given in QRAM and QRAM's procedures can be inverted. To avoid this additional assumption, we compare to the original QPCA result.

All of these algorithms follow the same high-level idea: use Hamiltonian simulation to perform phase estimation. By applying phase estimation to the second set of qubits in $|A\rangle$, which has density matrix $\frac{1}{\|A\|_{2}^{2}}A^{\dagger}A$, we see a singular vector $|v_i\rangle$ with probability proportional to its singular

value σ_i^2 . As we assume our eigenvalues have an $\eta \|A\|_F^2$ gap, the precise eigenvector $|v_i\rangle$ sampled can be identified by the eigenvalue estimate. Then, by computing enough samples, we can learn all of the eigenvalues of at least σ^2 and get the corresponding states with only $O(\|A\|_F^2/\sigma^2)$ overhead, giving Theorem 8 (full proof in appendix).

Note that we crucially use the assumptions in Problem 7 for our QML algorithm: without guarantee on the gap or that $\sigma_i \geq \sigma$, finding the top k singular vectors would be intractable, even with samples of $|v_i\rangle$'s.

In the classical setting, our low-rank approximation Algorithm 3 outputs a description of approximate singular values and vectors. From this description, we get $\hat{\sigma}_i$'s directly and \hat{v}_i 's described as a small linear combination of rows of S. So, by Proposition 2, we can get $SQ^{\nu}(\hat{v}_i)$. This high-level idea is similar to that of the quantuminspired recommendation system [8], but showing that $\hat{v}_i \approx v_i$ requires a novel analysis.

Algorithm 5 Principal Component Analysis

Input: $SQ(A) \in \mathbb{C}^{n \times d}$, σ, k, η as in Problem 7

- **Output:** $\hat{\sigma}_i$ and \hat{v}_i for $i \in [k]$ as in Problem 7 1: Set $\varepsilon \leftarrow \min(\varepsilon_{\sigma}K^{1.5}, \varepsilon_v^2 \eta, \frac{1}{4}K^{-1/2})$ and $\sigma' \leftarrow \sigma \varepsilon ||A||_F$
- 2: Run Algorithm 3 with parameters σ' , ε , and δ/k to find a low-rank approximation described by $SQ(S) \in \mathbb{C}^{q \times n}$, $\hat{U} \in \mathbb{C}^{q \times \ell}, \, \hat{\Sigma} \in \mathbb{C}^{\ell \times \ell}$
- 3: For $i \in [k]$, let $\hat{\sigma}_i := \hat{\Sigma}_{ii}$, $\hat{v}_i := S^{\dagger} \hat{U}_{*,i} / \hat{\Sigma}_{ii}$ 4: Output $\hat{\sigma}_i^2$ and $SQ^{\nu}(\hat{v}_i)$; sample and query access follows from Algorithm 2 with matrix S^{\dagger} and vector $\hat{U}^{(i)}/\hat{\Sigma}_{ii}$.

Theorem 9. Given O(T)-time $SQ(A) \in \mathbb{C}^{n \times d}$, with $\varepsilon_{\sigma}, \varepsilon_{v}, \delta \in (0, 0.01)$, Algorithm 5 outputs the desired estimates for Problem 7 $\hat{\sigma}_1, \ldots, \hat{\sigma}_k$ and $O(T\frac{K^9}{\varepsilon^4} \log^3(\frac{k}{\delta}))$ -time $SQ^{0.01}(\hat{v}_1, \ldots, \hat{v}_k)$ in $O(\frac{K^{12}}{\varepsilon^6} \log^3(\frac{k}{\delta}) + T\frac{K^8}{\varepsilon^4} \log^2(\frac{k}{\delta}))$ time, where $\varepsilon = \min(\varepsilon_{\sigma} K^{1.5}, \varepsilon_v^2 \eta, \frac{1}{4} K^{-1/2})$.

Under the non-degeneracy condition $\eta \leq \frac{1}{4}K^{-1/2}$, this runtime is $\tilde{O}(T\frac{K^{12}}{\varepsilon_{\phi}^6\varepsilon_{v}^{12}}\log^3(\frac{1}{\delta}))$. While the classical runtime depends on ε_v , note that a quantum algorithm must also incur this error term to learn about v_i from copies of $|v_i\rangle$. For example, computing entries or expectations of v_i given copies of $|v_i\rangle$ requires poly $(\frac{1}{\varepsilon_n})$ or poly(n) time.

Proof. First, consider runtime. From Proposition 3, using that $\sigma' > 3\sigma/4$, we have that the runtime of Algorithm 5 is correct. Further, for our \hat{v}_i 's, applying Algorithm 2 gives the desired runtimes, since

$$\begin{split} C(S^{\dagger}, \hat{U}_{*,i}/\hat{\Sigma}_{ii}) &= \frac{\sum_{j} \|S_{j,*}\|^{2} (\hat{U}_{ji}/\hat{\Sigma}_{ii})^{2}}{\|\hat{v}_{i}\|^{2}} \\ &\leq \frac{\|S\|_{F}^{2} \|\hat{U}_{*,i}\|^{2}}{\hat{\Sigma}_{ii}^{2} \|\hat{v}_{i}\|^{2}} &= \frac{\|A\|_{F}^{2}}{\hat{\Sigma}_{ii}^{2} \|\hat{v}_{i}\|^{2}} \leq \frac{\|A\|_{F}^{2}}{\sigma^{2}(1-\varepsilon)} = O(K). \end{split}$$

where we used Cauchy-Schwarz, that $||S||_F^2 = ||A||_F^2$, $\|\hat{U}_{*,i}\| = 1, \ \hat{\Sigma}_{ii} \geq \sigma$, and Proposition 3(d).

For correctness: by 3(a), $\sigma_{\ell+1} < \sigma$, so $\ell \ge k$, and Step 3 of Algorithm 5 is well-defined. Further, by 3(c), we can bound $\hat{\sigma}_i$ error $|\hat{\sigma}_i^2 - \sigma_i^2| \le \varepsilon ||A||_F^2 / K^{1.5} \le \varepsilon_\sigma ||A||_F^2$.

Showing that $||v_i - \hat{v}_i|| \leq \varepsilon_{\sigma}$ requires controlling each \hat{v}_i individually. However, a priori, the 3(b) bound, even with $\varepsilon = 0$, only implies that $\{\hat{v}_i\}$ span the same subspace as $\{v_i\}$. So, we consider the rank-r approximation formed by using only $\hat{v}_1, \ldots, \hat{v}_r$, for $r \in [k]$. The 3(b) bound for all r approximations give the desired bounds: using the gap assumption, the first \hat{v}_r to deviate from v_r will violate the bound for that rank approximation. A full proof of this fact is in the appendix.

DISCUSSION

Related and follow-up work The closest prior work is a classical randomized linear algebra algorithm for Hamiltonian simulation [19]. This work requires sampling assumptions similar to sampling and query access and gets qualitatively similar bounds and runtimes, but lacks the conceptual step of formalizing the model key to our dequantization results. Algorithm 3 of Frieze et al. [14] is one result among an extensive classical sketching literature [20, 21]; while we are a part of this literature to some extent, since our quantum-inspired model is weaker than typical classical settings, we are forced to use nonstandard techniques, marking a significant departure from that body of work. Since this work, numerous follow-ups have cemented the significance of the sample and query access model introduced here [22–26]. These algorithms use fundamentally the same techniques to dequantize a wide swathe of low-rank quantum machine learning.

Concluding thoughts We have introduced the sample and query access assumption as a classical analogue to the QML state preparation assumption and demonstrated two examples where, in this classical model, we can dequantize QML algorithms with ease. This model shows promise: we believe continuing to explore the capabailities and limitations of this model is a fruitful direction for driving QML research moving forward. We hope these algorithms serve as helpful references when dequantizing other quantum machine learning algorithms.

Based on these results, our belief is that QML algorithms that are *not* BQP-complete are highly susceptible to dequantization using the approaches we outline here, with only polynomial slowdown. We, therefore, urge caution when claiming exponential speedups over classical algorithms. Nevertheless, BQP-complete problems/algorithms, such as sparse matrix inversion [1] and quantum Boltzmann machine training [27], are still unlikely to be dequantized in full.

Two fundamental questions remain. First, can we reduce the polynomial gap between quantum-inspired algorithms and QML algorithms? Super-quadratic speedups, particularly provable ones, are still theoretically inter-

esting and give hope for use of QML in practice. Second, are quantum-inspired algorithms fast and practical compared to other classical algorithms? The quantum-inspired model is not designed for standard classical computation, but ideas from QML could still provide some insights in restricted practical settings. Both positive and negative answers to these questions are meaningful and help us clear the current uncertainty about the nature of QML speedups.

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Motivating sample and query access

In this section, we demonstrate how typical input models where efficient state preparation oracles are possible also admit efficient sample and query access to input.

QRAM. Quantum random access memory is a proposal to implement state preparation of an n-dimensional quantum state in time polynomial in $\log n$ through the use of a clever data structure and parallelization [7, 10, 13, 28]. If the same input is reused or dynamically updated [9], using QRAM for QML can amortize the cost of data loading, removing the input bottleneck of these algorithms in certain cost models. In our previous work [8, 3.1, 3.2], we noted that this gives sample and query access to input as well.

Grover-Rudolph state preparation. Suppose we have an efficient way to apply an integration function on the state $x \in \mathbb{C}^n$ we wish to prepare: $\Im(s,t) = \sum_{i=s}^t |x_i|^2$. Then, Grover-Rudolph state preparation [29] can perform the rotations done in a QRAM protocol without issues with parallelization, only assuming the ability to query entries of x in superposition.

Given an efficient integration oracle, we can also gain sample and query access to x: because all of the nodes of a QRAM can be expressed as an integral of x over some interval, we can simply perform that sample and query access protocol, replacing calls to the data structure with calls to the integration oracle. If integrating takes O(T) time, this gives $O(T \log n)$ -time SQ(x), the equivalent result to the quantum setting.

Sparsity. When $x \in \mathbb{C}^n$ has only s nonzero entries, and we know their locations, we can prepare $|x\rangle$ in $O(s \log n)$ gates. We can also get SQ(x) by querying all of the

nonzero entries to compute the corresponding distribution for sampling and norm in O(s) time.

Uniformity. When entries of x are close to uniform, the corresponding state can be prepared given the ability to query x in superposition. Classically, samples and norm estimates can be found quickly using rejection sampling: sample $i \in [n]$ uniformly at random, and choose it with probability $\frac{n|x_i|^2}{C||x||^2}$, where C is chosen so that $C \ge \max_{i \in n} \frac{n|x_i|^2}{||x||^2}$.

Generic state preparation. Finally, we can generically convert a state preparation procedure to sample and query access: given input vectors $x \in \mathbb{C}^n$ classically, norms ||x||, and a quantum procedure to create copies of $|x\rangle$, we can get SQ(x) by measuring $|x\rangle$ in the computational basis. This could be useful when preparing $|x\rangle$ is feasible, but a full QRAM algorithm is impractical due to the space and time overhead inherent to current QRAM proposals (e.g. from storing magic states or error-correcting).

Analysis of three subroutines

Proof of Proposition 1. We analyze Algorithm 1. Computing the z_i 's, means, and medians all take linear time, so the runtime is dominated by the collection of samples, as desired.

As for correctness, first notice that the z_j 's satisfy that $\mathbb{E}[z_j] = \langle x|y \rangle$ and $\mathrm{Var}[z_j] \leq \|x\|^2 \|y\|^2$. Taking the mean of $\frac{9}{\varepsilon^2}$ copies of z_j reduces the variance to $\varepsilon^2 \|x\|^2 \|y\|^2/9$, so by Chebyshev's inequality, the probability that the mean is $\frac{\varepsilon}{\sqrt{2}} \|x\| \|y\|$ -far from $\langle x|y \rangle$ is $\leq \frac{9}{2}$. Next, we treat the real and imaginary components of the means separately, and take the median of the means component-wise. The median of $6 \log \frac{2}{\delta}$ these means is $\frac{\varepsilon}{\sqrt{2}} \|x\| \|y\|$ -far from $\langle x|y \rangle$ in the real axis only if at least half of the means are that far in; a Chernoff bound shows that this happens with probability $\leq \frac{\delta}{2}$. We combine the two components to get the desired correctness property.

Proof of Proposition 2. We analyze Algorithm 2. We use the following easy-to-verify facts about the function RE-JECTIONSAMPLE: (1) $r_s \leq 1$ by Cauchy-Schwarz, so the protocol is well-defined; (2) conditioned on success, s is a measurement from $|Vw\rangle$; (3) the function succeeds with probability $(kC(V, w))^{-1}$; (4) running it takes O(Tk) time

QUERY clearly has the stated properties. (2) implies that SAMPLE is correct if it succeeds, (3) implies that it has the stated failure probability, and (4) implies the stated runtime. (3) implies that NORM is correct (by a Chernoff bound), and (4) implies the stated runtime.

Proof of Proposition 3. Because the only difference between Algorithm 3 and ModFKV from previous work [8] are the different choice of ε , this result mostly follows directly from previous work. The algorithm and runtime

are given in Section 4; (a) follows from Lemma $4.5(\heartsuit)$; (b) follows from Lemma $4.5(\diamondsuit)$; (d) follows from Proposition 4.6. For (c), we know that

$$||A^{\dagger}A - S^{\dagger}S||_F, ||SS^{\dagger} - CC^{\dagger}||_F \le ||A||_F^2/\sqrt{q} = \varepsilon\sigma^2/K.$$

This is stated in the proof of [8, Proposition 4.6]; no factor of $\log(1/\delta)$ appears because it is used to amplify the probability of this equation being true. Let $\sigma_{M,i}$ denote the singular values of M, respectively. By applying the Hoffman-Wielandt inequality to both, we get that

$$\sqrt{\sum |\sigma_{A,i}^{2} - \sigma_{S,i}^{2}|^{2}}, \sqrt{\sum |\sigma_{S,i}^{2} - \sigma_{C,i}^{2}|^{2}} \leq \varepsilon ||A||_{F}^{2}/K^{2}.$$
so
$$\sum_{i=1}^{k} |\sigma_{A,i}^{2} - \sigma_{C,i}^{2}| \leq \sqrt{k} \left(\sum_{i=1}^{k} |\sigma_{A,i}^{2} - \sigma_{C,i}^{2}|^{2}\right)^{1/2}$$

$$\leq \sqrt{k} \left(\sum |\sigma_{A,i}^{2} - \sigma_{C,i}^{2}|^{2}\right)^{1/2}$$

$$< \sqrt{k}\varepsilon ||A||_{F}^{2}/K^{2} < \varepsilon ||A||_{F}^{2}/K^{1.5}.$$

Proof of Theorem 8

We use Prakash's analysis of Lloyd et al's QPCA result:

Proposition (3.2.1 [28]). Given the ability to prepare states with density matrix ρ in T time, Lloyd et al's PCA algorithm [11] runs in time $\tilde{O}(T\min(\varepsilon_{\sigma},\delta)^{-3})$ where $T(\rho)$ is the time to prepare ρ and returns a sample $(|v\rangle,\bar{\lambda})$ with $\Pr[|v\rangle = |v_j\rangle] = \lambda_j$ and $\bar{\lambda} \in \lambda_j \pm \varepsilon_{\sigma}/4$ with probability at least $1 - \delta$.

Because we can prepare $|A\rangle$ in O(T) time, we can also prepare ρ with density matrix $\frac{1}{\|A\|_F^2}A^\dagger A$ in O(T) time, since this is the state of the second set of qubits of $|A\rangle$. So, we can get a sample $(|v\rangle,\bar{\lambda})$ in $O(T\min(\varepsilon_\sigma,\delta)^{-3})$ time. The eigenvectors and eigenvalues of ρ are v_i and σ_i^2 , respectively, from the SVD of A.

Notice that this result isn't particularly useful if A is not low-rank: if ρ is high-dimensional, we would expect that λ_j 's are around O(1/n), and if we wanted to distinguish individual eigenvectors, we would also have that $\varepsilon_{\sigma} = O(1/n)$, ruining any exponential speedup.

However, in the setting given by Problem 7, we know that the first k eigenvectors have size $\geq \sigma^2$, and because we estimate our λ_i 's to $\varepsilon_{\sigma}/4$ error, we can identify an eigenvector by its eigenvalue estimate. For each $i \in [k]$, $|v_i\rangle$ appears with probability $\geq \sigma^2/\|A\|_F^2$, so we see it in $\|A\|_F^2/\sigma^2\log\frac{1}{\delta}$ samples with probability $\geq 1-\delta$. By union bound, we can find $|v_i\rangle$ and their corresponding eigenvalue estimates for all k with $O(\|A\|_F^2/\sigma^2\log\frac{k}{\delta})$ samples. The eigenvectors are exactly correct and the eigenvalues have $\varepsilon_{\sigma}\|A\|_F^2$ error, as desired: so, this is the desired output. The runtime is the time to output $O(\|A\|_F^2/\sigma^2\log\frac{k}{\delta})$ samples.

Proof that $||v_i - \hat{v}_i|| \leq \varepsilon_v$ for Theorem 9

Proof. Let \hat{V}_r denote \hat{V} truncated to its first r columns. Observe that for all $r \leq \ell$, $\|A - A\hat{V}_r\hat{V}_r^{\dagger}\|_F^2 \leq \|A - A_r\|_F^2 + \varepsilon \|A\|_F^2$ holds with probability $\geq 1 - \delta$. This holds for $r = \ell$ by Proposition 3(b), so suppose $r < \ell$. We can imagine that our run of Algorithm 3 is equivalent to simultaneous runs with different singular value thresholds $\gamma_r := \frac{1}{2}(\sigma_r + \sigma_{r+1})$, the only differences being that we truncate to threshold σ instead of γ_r , and q is larger. Truncating to γ_r is equivalent to truncating at the rth singular value, since $\hat{\sigma}_r > \gamma_r > \hat{\sigma}_{r+1}$:

$$|\hat{\sigma}_{i} - \sigma_{i}| \leq \frac{1}{\sigma} |\hat{\sigma}_{i}^{2} - \sigma_{i}^{2}| \leq \frac{1}{\sigma} \sum_{i=1}^{\ell} |\hat{\sigma}_{i}^{2} - \sigma_{i}^{2}| \leq \frac{\eta}{10} ||A||_{F};$$

$$|\sigma_{i} - \gamma_{i}| = \frac{1}{2} |\sigma_{i} - \sigma_{i+1}| \geq \frac{1}{4 ||A||_{F}} |\sigma_{i}^{2} - \sigma_{i+1}^{2}| \geq \frac{\eta}{4} ||A||_{F}.$$

So, $\hat{\sigma}_r \geq \sigma_r - \frac{\eta}{10} \|A\|_F > \sigma_r - \frac{\eta}{4} \|A\|_F \geq \gamma_r$, and similarly for the other side. Increasing q is equivalent to decreasing ε , so for our truncated $\hat{V}_{[r]}$'s, the guarantees from Proposition 3 hold. Namely, 3(b) holds as desired. By choosing failure probability δ/k , we can guarantee, with probability $\geq 1 - \delta$, $\|A - A\hat{V}_r\hat{V}_r^{\dagger}\|_F^2 \leq \|A - A_r\|_F^2 + \varepsilon \|A\|_F^2$ holds for all $r \in [k]$.

Fix Λ as the isometry from Proposition 3(d) satisfying $\|\hat{V} - \Lambda\|_F \leq \varepsilon$. Now, consider a truncation \hat{V}_r for any $r \in [k]$, and notice that $\|\hat{V}_r - \Lambda_r\|_F \leq \varepsilon$.

$$||A - A\Lambda_r\Lambda_r^{\dagger}||_F^2 \le (||A - A\hat{V}_r\hat{V}_r^{\dagger}||_F + O(\varepsilon)||A||_F)^2$$

$$\le ||A - A\hat{V}_r\hat{V}_r^{\dagger}||_F^2 + O(\varepsilon)||A||_F^2$$

$$\le ||A - A_r||_F^2 + O(\varepsilon)||A||_F^2$$

Now, we rewrite the expression, heavily using that Λ_r and V_r (the matrix with columns v_1, \ldots, v_r from A's SVD) are isometries.

$$\begin{split} &O(\varepsilon)\|A\|_F^2 \\ &\geq \|A - A\Lambda_r\Lambda_r^{\dagger}\|_F^2 - \|A - A_r\|_F^2 \\ &= \|A\|_F^2 - \|A\Lambda_r\Lambda_r^{\dagger}\|_F^2 - (\|A\|_F^2 - \|A_r\|_F^2) \\ &= \|A_r\|_F^2 - \|A\Lambda_r\Lambda_r^{\dagger}\|_F^2 \\ &= \|A_r\|_F^2 - \|A\Lambda_r\Lambda_r^{\dagger}\|_F^2 \\ &= \sum_{i=1}^r \sigma_i^2 - \sum_{i=1}^{\min m,n} \sigma_i^2 \|\Lambda_r\Lambda_r^{\dagger}v_i\|^2 \\ &= \sum_{i=1}^r \sigma_i^2 (1 - \|\Lambda_r\Lambda_r^{\dagger}v_i\|^2) - \sum_{i=r+1}^{\min m,n} \sigma_i^2 \|\Lambda_r\Lambda_r^{\dagger}v_i\|^2 \\ &\geq \sigma_r^2 \sum_{i=1}^r (1 - \|\Lambda_r\Lambda_r^{\dagger}v_i\|^2) - \sigma_{r+1}^2 \sum_{i=r+1}^{\min m,n} \|\Lambda_r\Lambda_r^{\dagger}v_i\|^2 \\ &= \sigma_r^2 \|(I - \Lambda_r\Lambda_r^{\dagger})V_rV_r^{\dagger}\|_F^2 - \sigma_{r+1}^2 \|\Lambda_r\Lambda_r^{\dagger}(I - V_rV_r^{\dagger})\|_F^2 \\ &= \sigma_r^2 (r - \|\Lambda_r\Lambda_r^{\dagger}V_rV_r^{\dagger}\|_F^2) - \sigma_{r+1}^2 (r - \|\Lambda_r\Lambda_r^{\dagger}V_rV_r^{\dagger}\|_F^2) \\ &\geq \eta \|A\|_F^2 (r - \|\Lambda_r\Lambda_r^{\dagger}V_rV_r^{\dagger}\|_F^2) \end{split}$$

Here, we used the Pythagorean theorem ($\|A\Pi\|_F^2 + \|A(I - \Pi)\|_F^2 = \|A\|_F^2$ for Π an orthogonal projector), that $\|\Lambda\Lambda^{\dagger}v_i\|^2 \in [0,1]$, that $\|VM\|_F = \|M\|_F$ if V is an isometry, that Frobenius norm decomposes $\|M\|_F^2 = \sum \|M_{*,i}\|^2$, and the gap assumption from the PCA problem statement.

So, $\|\Lambda_r \Lambda_r^{\dagger} V_r V_r^{\dagger}\|_F^2 = \|\Lambda_r^{\dagger} V_r\|_F^2 \ge r - O(\varepsilon/\eta)$, and equivalently, $\|(V_r V_r^{\dagger} - I)\Lambda_r \Lambda_r^{\dagger}\|_F^2 = O(\varepsilon/\eta)$.

$$\begin{split} &\|v_r - \hat{v}_r\| \\ &\leq \|v_r - \Lambda_{*,r}\| + \|\Lambda_{*,r} - \hat{v}_r\| \\ &\leq \|v_r - \Lambda_{*,r}\| + \varepsilon \\ &\leq \|v_r - V_k V_k^{\dagger} \Lambda_{*,r}\| + \|V_k V_k^{\dagger} \Lambda_{*,r} - \Lambda_{*,r}\| + \varepsilon \\ &\leq \|v_r - V_k V_k^{\dagger} \Lambda_{*,r}\| + \|(V_k V_k^{\dagger} - I) \Lambda_k \Lambda_k^{\dagger}\|_F + \varepsilon \\ &\leq \|v_r - V_k V_k^{\dagger} \Lambda_{*,r}\| + O(\sqrt{\varepsilon/\eta}) \\ &= \sqrt{(v_r - V_k V_k^{\dagger} \Lambda_{*,r})^{\dagger} (v_r - V_k V_k^{\dagger} \Lambda_{*,r})} + O(\sqrt{\varepsilon/\eta}) \\ &\leq \sqrt{2 - 2\langle v_r, \Lambda_{*,r} \rangle} + O(\sqrt{\varepsilon/\eta}) \\ &= O(\sqrt{\varepsilon/\eta}) = O(\varepsilon_v) \end{split}$$

The last line follows from combining previously-seen inequalities: let $x_{i,j} = \langle v_i, \Lambda_{*,j} \rangle^2$. Then we can rewrite

$$\|\Lambda_s^{\dagger} V_s\|_F^2 \ge s - O(\varepsilon/\eta) \iff \sum_{i,j=1}^s x_{i,j} \ge s - O(\varepsilon/\eta);$$
$$\|\Lambda^{\dagger} v_i\|^2 \le 1 \iff \sum_{j=1}^k x_{i,j} \le 1;$$
$$\|(\Lambda_{*,j})^{\dagger} V_k\|^2 \le 1 \iff \sum_{i=1}^k x_{i,j} \le 1.$$

Now, consider taking a linear combination of these inequalities: add together the first inequality for s=r-1,r and subtract the second and third inequalities for $i,j\in[r-1]$.

$$\sum_{i,j=1}^{r-1} x_{i,j} + \sum_{i,j=1}^{r} x_{i,j} \ge 2r - 1 - O(\varepsilon/\eta)$$

$$- \sum_{i=1}^{r-1} \sum_{j=1}^{k} x_{i,j} \ge 1 - r$$

$$- \sum_{j=1}^{r-1} \sum_{i=1}^{k} x_{i,j} \ge 1 - r$$

$$\implies x_{rr} - \sum_{i=1}^{r-1} \sum_{j=r+1}^{k} (x_{i,j} + x_{j,i}) \ge 1 - O(\varepsilon/\eta)$$

So, $x_{rr} \geq 1 - O(\varepsilon/\eta)$, implying that $\langle v_r, \Lambda_{*,r} \rangle \geq 1 - O(\varepsilon/\eta)$.