Small quantum computers and large classical data sets

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Abstract

We introduce hybrid classical-quantum algorithms for problems involving a large classical data set \( X \) and a space of models \( Y \) such that a quantum computer has superposition access to \( Y \) but not \( X \). These algorithms use data reduction techniques to construct a weighted subset of \( X \) called a coreset that yields approximately the same loss for each model. The coreset can be constructed by the classical computer alone, or via an interactive protocol in which the outputs of the quantum computer are used to help decide which elements of \( X \) to use. By using the quantum computer to perform Grover search or rejection sampling, this yields quantum speedups for maximum likelihood estimation, Bayesian inference and saddle-point optimization. Concrete applications include k-means clustering, logistical regression, zero-sum games and boosting.

1 Introduction

What can a quantum computer do with a large classical data set? At first glance it would seem that the costs of loading the data into the quantum computer would overwhelm any possible quantum speedup. And how can Grover’s algorithm be used for practical problems? While the original title of Grover’s paper \[34\] is “A fast quantum mechanical algorithm for database search,” its applications so far have mostly been to exploring combinatorial search spaces. Similar questions apply to other quantum optimization algorithms, such as the adiabatic algorithm \[26\], quantum walks \[43\], and the QAOA \[23\].

Existing quantum algorithms for optimization and machine learning are often less complete than their classical counterparts because they do not use realistic models of their input data \[1\]. One way to view this is that they are meant to be subroutines in larger “end-to-end” algorithms that will provide the data in the needed format. However, there has been relatively little research on these more complete algorithms and their development has often been nontrivial. Indeed, the trivial methods of turning large classical datasets into either quantum oracles or quantum states are so expensive as to negate any possible quantum advantage. As a result, even Grover’s algorithm has not yet been successfully applied to speed up any natural machine learning task, despite being arguably the simplest, most widely known, and most widely applicable quantum algorithm.

One proposal is to use a “quantum RAM,” typically meaning a large classical memory which can be queried in superposition \[32, 31\]. This enables powerful quantum algorithms to be used, often with provable speedups. However, current classical computing or data storage hardware does not function as quantum RAM, and near-term hardware plans by leading groups using trapped
ions, superconductors, or photons on chips do not involve quantum RAM. Also, building a large quantum RAM may run into many of the same challenges that occur in building a large universal quantum computer [4].

At first glance it seems that quantum advantage requires problems with small input sizes. If the input size is \( n \) then it is hard to avoid expending effort proportional to \( n \) even before the computation starts, in order to acquire, store and load the input. Even alternate models such as property testing or streaming can typically mitigate only some of these. Similar issues apply to large outputs. For problems that can be solved on classical computers in time \( \tilde{O}(n) \), it would seem that there is little scope for quantum advantage. For this reason, proposals for quantum advantage usually involve problems where the best known classical runtime scales rapidly with the input size, perhaps exponentially.

At the same time, many tasks in classical computing, such as machine learning, are evolving towards the use of increasingly large data sets, for which a runtime of even \( O(n^2) \) can be infeasible. How can quantum computers be of use in this setting?

This paper will explore the ability of small quantum computers to work together with large classical computers to analyze large data sets. We will work in a regime where our input size is \( n \), the classical computer runs in time nearly linear in \( n \), and we do not use any unconventional access models for the quantum computer. Since qubits are likely to always remain more expensive than bits, this hybrid classical-quantum model should be relevant even when quantum computers with millions or billions of qubits are available.

The key principle will be data reduction. We will approximate a data set \( X = \{x_1, \ldots, x_n\} \) with a much smaller subset \( X' \) (called a “coreset”) along with a weight function \( w : X' \rightarrow \mathbb{R}_{\geq 0} \) such that \( X', w \) can adequately substitute for \( X \) in solving problems of interest. This can be achieved either by a classical computer alone, or a classical computer together with a quantum computer. Then a hard optimization problem can be solved on the quantum computer using the reduced data set \( X' \).

Data reduction can be useful for any quantum optimization algorithm for which computing the objective function requires examining a large data set. We illustrate its benefits with a representative example in Section 1.1 before giving an informal overview of our algorithms and their benefits in Section 1.2 and discussing input data models in Section 1.3. The rest of the paper spells out the results more formally, beginning with formal descriptions of the problem setting in Section 2 and the previously developed algorithms in Section 3 and proceeding to describe our algorithms in detail in Section 4. There are several relevant related algorithms, such as variational quantum algorithms and stochastic gradient descent, and we compare our approach with these in Section 5 before concluding in Section 6.

1.1 Motivating example: minimizing empirical loss with Grover.

Suppose we are given a set of data points \( X \), a set of models \( Y \), and a loss function \( f : X \times Y \rightarrow \mathbb{R} \). Our goal is to compute

\[
\arg \min_{y \in Y} \sum_{x \in X} f(x, y),
\]

i.e. to choose the model which minimizes the empirical loss. It is important to emphasize the form of the input: \( X \) is an explicit data set \( x_1, \ldots, x_n \); \( Y \) is a set that may be large or infinite but has a succinct description, e.g. \( Y \) might be the set of all ways of choosing a mixture of up to \( k \) Gaussians in \( \mathbb{R}^d \); \( f \) is given as an explicit and short algorithm.
To apply Grover’s algorithm (technically the Dürr-Høyer algorithm for minimizing a black-box function [22]) will require $O(\sqrt{|Y|})$ evaluations of $F(y) := \sum_{x \in X} f(x, y)$. However, each evaluation of $F$ requires iterating over the entire data set $X$. This takes time $O(|X|)$ if we assume for simplicity that $f$ can be computed in time $O(1)$. The crucial feature of this problem is that the set $Y$ can be accessed in superposition, so that we can obtain the quadratic Grover speedup in searching over it, but $X$ is a classical data set which cannot be queried in this way. Thus we could not use quantum algorithms such those for approximate counting [11] to speed up the evaluation of $F(y)$. As a result, the classical runtime of $O(|X|)$ turns into a quantum runtime of $O(|X| \cdot \sqrt{|Y|})$. If $|X|$ is comparable to $|Y|$, then this erodes much of the savings from Grover’s algorithm.

Instead we will use a coreset $X'$ (with weight function $w$) and replace $F(y)$ with its approximation $F_w(y) := \sum_{x \in X'} w(x)f(x, y)$. This results in a hybrid classical-quantum algorithm for the overall problem. A classical computer needs to examine the original data set $X$ in order to calculate $X'$ and then a quantum computer can minimize $F_w$ in time $O(\sqrt{|Y||X'|})$. If $|X'| \ll |X|$ then this yields a nearly quadratic speedup, and if $\min_y F_w(y) \approx \min_y F(y)$ then this provides a good approximation to the original problem. Coresets satisfying both of these properties are known in a large number of cases, as we discuss below in Sections 3.3 and 4.

In some cases (see Section 4) the size of $X'$ will depend only on the level of approximation desired and not on the size of the original data set $X$. When this happens, the classical or quantum runtime will not depend on the product of $|X|$ and $|Y|^1$ or $\frac{1}{2}$, but instead on (roughly) their sum. Coresets speed up both classical and quantum algorithms, but they increase the relative quantum speedup by reducing the time spent on tasks where there is no known quantum advantage.

1.2 More general uses of coresets

There are three main directions in which this basic example can be modified.

- The Dürr-Høyer minimization algorithm could be replaced by any other quantum algorithm for minimizing functions, such as adiabatic optimization or QAOA. In almost any such algorithm, either $F(y)$ or its gradients will need to be evaluated, and the cost of doing so will scale linearly with $|X|$ (see Section 3.1 for details). Thus, using a coreset can provide significant savings. We explore these more in Algorithms 1 and 1.1 in Section 4.

- The form of (1) could be substantially changed. A small change would be to minimize $F(y) := r(y) + \sum_x f(x, y)$, where $r(y)$ is a regularizer, perhaps intended to favor simpler models. A bigger change would be to perform Bayesian inference. As we will discuss below, Bayesian inference can be described as sampling from a distribution $\pi(y) \propto \exp(F(y))$. Here too quantum algorithms can achieve roughly quadratic speedups provably, and heuristic algorithms have been proposed which may have better performance (see section 3.2). In each case, quantum speedups are not known for iterating over $X$, and so reducing the size of $X$ would increase the relative quantum speedup. One benefit of sampling over optimization is that the samples output by the quantum computer could be used by the classical computer to adaptively augment the coreset. This idea is explored in Algorithms 2 and 2.1 of Section 4.

- The coreset can be built iteratively using interaction between the classical and quantum processors. First the classical computer produces a coreset $X'_1$ which the quantum computer uses to produce output $y_1$. Then $y_1$ is used by the classical computer to produce a new coreset $X'_2$, which the quantum computer uses to produce output $y_2$, and so on for $r$ rounds. The
final answer could either be \( y_r \) or some average of \( y_1, \ldots, y_r \). See Algorithm 3 in Section 4 for details.

The common theme in these algorithms is that there is an outer loop involving \( Y \) and an inner loop involving \( X \). This outer loop could involve iterating over all elements of \( Y \), performing a Grover-style search, using adiabatic optimization, or other classical or quantum algorithms. Suppose that in general this outer loop requires \( \tau_{\text{outer}}(Y) \) iterations (e.g. \(|Y|\) for classical brute-force search, \( \sqrt{|Y|} \) for Grover, and so on). Then if the inner loop sums over all of \( X \), the overall algorithm will require \( O(|X|\tau_{\text{outer}}(Y)) \) evaluations of \( f \). Suppose we have a coreset \( X' \) that can be constructed in time \( \tau_{\text{core}}(X) \). Then our total (classical + quantum) run-time becomes

\[
O(\tau_{\text{core}}(X) + |X'|\tau_{\text{outer}}(Y)).
\]

Assume that \( \tau_{\text{core}}(X) \) scales roughly with \(|X|\) while \(|X'|\) is roughly independent of \(|X|\) and is determined instead by the complexity of the model and the desired accuracy. Then we have again replaced a run-time that scales as the product of \(|X|\) and \( \tau_{\text{outer}}(Y) \) with one that scales roughly as their sum. If the run-time is dominated by the complexity of searching over \( Y \) then this will increase the relative quantum speedup.

We illustrate this point with a plot. Suppose for simplicity that \(|X| = n\), \(|X'| = O(1)\), \( \tau_{\text{core}}(X) = n^\alpha \), and \( \tau_{\text{outer}}(Y) = n^\beta \), for some constants \( \alpha, \beta > 0 \). Assume as well that the quantum speedup is quadratic (e.g. based on Grover) so that \( \tau_{\text{quantum}}(Y) = n^{\beta/2} \). We can summarize the effects of both coresets and classical-vs-quantum computing as follows.

| Using coreset? | No | Yes |
|---------------|----|-----|
| Classical     | \( n^{1+\beta} \) | \( n^\alpha + O(n^\beta) \) |
| Quantum       | \( n^{1+\beta/2} \) | \( n^\alpha \) classical and \( O(n^{\beta/2}) \) quantum |

In the lower-right box, the algorithm uses both classical and quantum resources, since the classical computer constructs the coreset in time \( n^\alpha \) and the quantum computer performs the optimization in time \( O(n^{\beta/2}) \). The situation is similar if we replace a simple coreset with an iterative construction.

To define the speedup, we say that if the classical and quantum runtimes are \( T_{cl}, T_q \) respectively then the speedup is \( \log(T_{cl})/\log(T_q) \). Thus “1” means no speedup, “2” is the Grover speedup, \( \infty \) would mean a superpolynomial (e.g. exponential) speedup and \(< 1 \) would mean a slowdown. Suppose that \( \alpha = 1 \), since this is often achievable (as we discuss below). The resulting quantum speedups as a function of \( \beta \) are illustrated in Fig. 1.

### 1.3 Data model

An important departure of this work from much of the quantum machine learning literature is in the choice of input data model. This seemingly mundane issue turns out to be crucial to understanding the utility of many quantum algorithms and in this section we will broadly review the role of different data models in quantum algorithms.

Existing quantum algorithms have used several different input models. The Standard model is a string of bits \( x = (x_1, \ldots, x_n) \) which could be thought of as either as labeling a standard basis
Figure 1: Classical and quantum runtime exponents, as well as speedup, as a function of $\beta$. Assume that $\alpha = 1$.

state $|x\rangle$ that is an input to a quantum circuit, or as input to a classical computer which generates a quantum circuit $C_x$ which is applied to a fixed input. The former interpretation is the standard theoretical model of quantum circuits, while the latter is closer to how quantum computers would be likely to function in practice. Another important model is the Oracle model in which the quantum computer is given access to a unitary $O$ such that $O|i, a\rangle = |i, a \oplus x_i\rangle$. This would arise most naturally if we are given a (classical or quantum) circuit that can compute $x_i$ given input $i$. Other uniquely quantum models exist as well. In the Quantum Data model, the input is given as an arbitrary $n$-qubit quantum state $|\psi\rangle$. Another model is the Quantum Oracle, meaning black-box access to an $n$-qubit unitary $U$.

All of these models have been widely used in the quantum algorithms literature. Prominent examples of algorithms using each model are summarized in Table 1.

Many papers on quantum machine learning [8] use the Oracle (or quantum RAM [32, 31]) model or the Quantum Data model. These models are closely related because states of the form $2^{-n/2} \sum_{x \in \{0,1\}^n} e^{i \phi_x} |x\rangle$ can be prepared easily using an oracle for $\phi_x$ and even general states $\sum_x \alpha_x |x\rangle$ can be prepared fairly efficiently using an oracle for $\alpha_x$ as long as $2^{-n/2} \sum_x |\alpha_x| \approx 1$. Current experimental plans for quantum computing do not correspond to this model and some discussions of the difficulties of quantum RAM can be found in [4,11,17]. Moreover, even under optimistic assumptions about quantum RAM, a data set of size $N$ will have cost scaling at least with $N$: both a “classical” cost in acquiring and storing the data, and “quantum” cost in pieces of hardware that can interact with qubits without decohering them. But once we have $O(N)$ pieces of quantum hardware, we might use other algorithmic approaches, such as parallelism; see [35] for a discussion in a related context.

Some algorithms use multiple data models. For example, Hamiltonian simulation and the linear systems solver may use oracles to specify entries of the matrices, or these could be specified explicitly as sums of Paulis or creation/annihilation operators. The recent quantum LP and SDP algorithms [10, 9, 57, 16, 56] use a combination of oracles and quantum data, and [56] also has an algorithm for the Quantum Oracle model.

The input model in this paper can be thought of as a hybrid between the standard and oracle
| Input Model          | Definition                                                                 | Examples                                                                 |
|---------------------|---------------------------------------------------------------------------|--------------------------------------------------------------------------|
| Standard            | $x = (x_1, \ldots, x_n) \in \{0, 1\}^n$                                   | Factoring and other number theory problems. 3-SAT and combinatorial optimization. variational quantum eigensolver |
| Oracle              | $O |i, a\rangle = |i, a + x_i\rangle$                                                   | OR (Grover search), max, approximate counting NAND tree, collision, [graph] property testing hidden subgroup problem, welded trees |
| Quantum Data        | given state $|\psi\rangle$                                               | quantum Fourier transform SWAP test, Schur transform, state tomography Hamiltonian simulation, linear systems solver learning with quantum examples |
| Quantum Oracle      | given access to unitary $U$ and controlled unitary $C_U$                  | phase estimation. quantum sensing and process tomography qubitization and singular value transform |

Table 1: Examples of algorithms using each input model. In the Quantum Data model we sometimes assume instead the ability to perform $V$ and $V^\dagger$ for some unitary satisfying $V |0\rangle = |\psi\rangle$. In the Quantum Oracle model the controlled unitary $C_U$ is of the form $\sum_{t=0}^{T-1} |t\rangle \langle t| \otimes U^t$. Here we can take $T = 2$ in some cases or can take $T$ to be exponentially large in other cases; see [5] for discussion.

models. We are given inputs $X = \{x_1, \ldots, x_n\}$ explicitly, say as records on a hard drive. Here the $x_i$ are typically not bits but belong to some alphabet $X$. We are also given oracle access to a function $f : X \times Y \mapsto \mathbb{R}$. Here $Y$ is either the set $[m] := \{1, 2, \ldots, m\}$, or some other set that can be bijectively and efficiently mapped to $[m]$. For this model to be realistic, $f$ should be easy to compute.

A concrete example of this model is $k$-means clustering in some metric space $X$ with distance function $\text{dist}(\cdot, \cdot)$, e.g. $\mathbb{R}^d$ with Euclidean norm. We are given points $x_1, \ldots, x_n \in X$ and are looking for cluster centers $y_1, \ldots, y_k \in X$. Given $x \in X$ and $y = (y_1, \ldots, y_k) \in (\mathbb{R}^k)^d$ the loss is

$$f(x, y) = \min_{i \in [k]} \text{dist}(x, y_i)^\rho.$$  

(3)

Here $\rho = 2$ for $k$-means clustering, $\rho = 1$ for $k$-median clustering, and other values of $\rho > 0$ can be chosen to tune the relative importance of outliers. If dist is easy to compute (e.g. the Euclidean norm) then $f$ is easy to compute as well, and so the oracle assumption is reasonable. The set $Y$ here is just the set of points $X$, made finite by considering only points on a discrete grid within some bounding box. Such a simple set is easy to map bijectively to $[m]$ for some large integer $m$. Finally, the most natural way to expect the input $x_1, \ldots, x_n$ for a clustering problem is as data on a classical storage medium.

The hybrid model in this paper works naturally with classical data stored in the same form that would be used for classical algorithms. There is only a minor way in which current quantum computing hardware does not meet its requirements, which is that pulse generators are often slow to
reprogram. This makes it easy to repeatedly run the same quantum algorithm but more expensive to modify the gate set either between iterations or during a single run of the quantum computer. However, this latency will have to be improved much more to meet the requirements of fault-tolerant quantum computing. It also appears to be a limitation that is not fundamental but rather applies to current off-the-shelf technology which was originally designed for other tasks.

This paper is not the only one with optimization algorithms that run on current models of hybrid classical/quantum computers. There has been a recent explosion of interest in variational quantum algorithms, such as those for ground states of Hamiltonians [48], constraint satisfaction problems [23, 24], learning [27, 46, 54] and other tasks. These algorithms have the advantage of running on near-term hardware [25] with modest requirements for gates, connectivity and qubits. They also make use of a classical computer to run an algorithm such as gradient descent in the outer loop while the quantum computer is used to evaluate the cost function or its gradients in the inner loop. In this way, variational algorithms make use of the longer memory lifetime of the classical computer. By contrast, our algorithms also use the larger storage of the classical computer. Depending on the computational cost of constructing the coreset, our algorithms may also use many more gates from the classical computer. We return to this comparison in Section 5.1 after describing our algorithms.

2 Problem setting

The algorithms introduced in this paper involve a choice of computational tasks, of quantum optimization or sampling subroutines and of classical data reduction subroutines. In this section we formally describe these computational tasks and review the quantum and classical subroutines that we will make use of.

Common assumptions and notation. In each task, we are given sets $X, Y$ with $|X| = n$ and $|Y| = m$, along with a function $f : X \times Y \mapsto \mathbb{R}$, or a function $f : \mathcal{X} \times Y \mapsto \mathbb{R}$ for some $\mathcal{X} \supseteq X$. The set $X = \{x_1, \ldots, x_n\}$ is stored in classical memory (say a hard drive) while the elements of $Y$ can be implicitly described. In other words, there is a bijection $\varphi : [m] \mapsto Y$ such that $\varphi, \varphi^{-1}$ are both efficiently computable. For simplicity, we could also assume that $Y = [m]$. We assume that a classical algorithm for computing $f$ is known, and our results will be most relevant when its runtime is small.

Tasks This paper focuses on three tasks arising in data analysis.

Maximum a posteriori estimation (MAP) Suppose further we are given an easily computable function $r : Y \mapsto \mathbb{R}$. Define the log-likelihood function

$$F(y) := r(y) + \sum_{x \in X} f(x, y)$$

(4)

The goal is to compute

$$\arg \max_{y \in Y} F(y)$$

(5)

To connect this rather general optimization question to MLE, we make the following interpretations. Define $p(x|y) := \exp(f(x, y))/Z_x$ to be the probability of observing data point $x$ given a
model $y$, and $\pi_{\text{prior}}(y) := \exp(r(y))/Z_0$ to be the prior distribution. Here $\{Z_x\}_{x \in X}, Z_0$ are normalization factors that do not need to be known to the algorithm. (Note that this interpretation, especially with nonzero $r(y)$, is typically referred to as MAP, or maximum a posteriori estimation.)

Technically we do not need an underlying probabilistic model. If $f(x, y)$ is the loss that model $y$ incurs from data point $x$, then $[5]$ corresponds to empirical loss minimization. An example is clustering, where the loss is a function only of the distance to the nearest cluster center.

**Bayesian inference**  Given a prior distribution $\pi_0(y)$, define the posterior distribution

$$
\pi(y) = \frac{\exp(\sum_{x \in X} f(x, y))}{\sum_{y' \in Y} \pi_0(y') \exp(\sum_{x \in X} f(x, y'))} = \frac{\exp(F(y))}{Z}.
$$

(6)

The second equality uses the definitions of $F, r, Z$ from the MLE task. The goal here is to sample from $\pi_{\text{posterior}}(y)$.

**Saddle-point optimization.** The above two problems can be thought of as taking the max of a sum and sampling from a distribution defined by a sum. A third task is to take the max of a min (or a min of a max), a problem sometimes known as saddle-point optimization. We describe a version of the problem where the max and min are taken over probability distributions.

Let $\Delta(S)$ denote the set of probability distributions over a set $S$. A typical saddle-point optimization problem is to compute

$$
\max_{\theta_Y \in \Delta(Y)} \min_{x \in X} \sum_y \theta_y f(x, y) = \min_{\theta_X \in \Delta(X)} \max_{y \in Y} \sum_x \theta_x f(x, y)
$$

(7)

The equality here is due to von Neumann’s minimax theorem. We could equivalently write $\max_{\theta_Y \in \Delta(Y)} \min_{\theta_X \in \Delta(X)}$ or $\min_{\theta_X \in \Delta(X)} \max_{\theta_Y \in \Delta(Y)}$. As in the previous problems, $X$ is a set of records in a classical data set and $Y$ is a set that can be searched by a quantum computer. This task has several interpretations.

- **Computing a Nash equilibrium of a zero-sum game.** One player’s strategies are specified on a hard drive (the set $X$) and the other have an implicit description (the set $Y$).

- **Linear programming.** Each $x \in X$ is a linear constraint and we search over the set $\Delta(Y)$ for a point satisfying these constraints.

- **Approximate MLE.** Here we let $\Delta(Y)$ be our set of models and we approximate the sum over $x$ in MLE with the minimum in saddle-point optimization. This could be appropriate if the quality of a model were determined by its worst point.

This problem can also be generalized to the case where $f$ is a concave function of $y$. In this case, there are a wide number of applications described by Clarkson [18]. We discuss a range of additional applications in Section 4.

### 3 Known algorithms

The new algorithms in this paper are fairly simple combinations of existing classical algorithms for data reduction and quantum algorithms for optimization and sampling. In this section we will review these algorithms.
3.1 Quantum optimization algorithms.

We will consider a few quantum subroutines for the problem of maximizing $F(y)$. These can be seen as quantum analogues of brute-force search and of simulated annealing.

**Grover/Durr-Høyer [34, 22].** This can find the maximum using $O(\sqrt{m})$ evaluations of $F$.

**Adiabatic optimization [26].** Suppose for simplicity that $m$ is a power of 2, and define the Hamiltonians

$$H(s) = (1-s)H_0 + sH_F$$

$$H_0 = -\sum_{i=1}^{\log(m)} \sigma_x^i, \quad H_F = -\sum_y F(y) |y\rangle \langle y|.$$  

The algorithm starts with all qubits in the $|+\rangle$ state and evolves under $H(s)$ with $s$ gradually changing from 0 to 1. (Many variations of this basic idea have also been proposed including running quickly and/or at variable speeds, starting in different states, replacing $H_0$, using more complicated paths, running at nonzero temperature and/or using noisy hardware.) In general this algorithm can be thought of as a heuristic since sharp bounds are usually not known on its runtime, or on the minimum spectral gap. The presence of the diag($F$) term means that running $H(s)$ for time $T$ generally requires $O(T)$ evaluations of $F$, a point originally made in [26, Section 5] and later improved by modern Hamiltonian simulation algorithms such as [45].

**Quantum Approximate Optimization Algorithm (QAOA) [23, 24].** The algorithm is parametrized by a positive integer $p$. The algorithm has a classical outer loop which searches over parameters $\theta_1, \ldots, \theta_{2p}$ and an inner loop which measures $H_F$ on the state

$$e^{i\theta_2 H_0} e^{i\theta_1 H_F} \ldots e^{i\theta_2 H_0} e^{i\theta_1 H_F} |+\rangle \otimes \log m,$$

where $H_0, H_F$ are defined in eq. (8). In the limit $p \to \infty$, this includes adiabatic optimization as a special case. Indeed an adiabatic-like schedule could be used as a starting point for the search over $\theta$. The parameter $p$ is analogous to the $T$ in the adiabatic algorithm and likewise the inner loop of QAOA uses $O(p)$ evaluations of $F$.

**Quantum Quench [38].** A variant of the above two algorithms simply performs $\exp(i(\alpha H_0 + \beta H_F))$ for some appropriately chosen real numbers $\alpha, \beta$.

A common theme for each algorithm is that their cost is dominated by evaluations of $F$. The number of evaluation differs, as does the probability of finding an optimal or near-optimal choice of $y$.

3.2 Sampling algorithms

We also consider quantum algorithms for the task of sampling from the distribution $\pi(y) = \exp(F(y))/Z$, given the ability to calculate $F(y)$. Here $Z = \sum_y \exp(F(y))$ does not have to be known to the algorithm. We will assume that $F(y) \leq 0$ for all $y$. Otherwise we can assume we know an upper bound $F_{\max} \geq F(y)$ for all $y$ and can replace $F(y)$ with $F(y) - F_{\max}$. 


**Rejection sampling.** Choose \( y \) uniformly at random from \([m]\) and accept with probability \( \exp(F(y)) \), so that the overall acceptance probability is \( Z/m \). On a classical computer, this requires on average \( m/Z \) repetitions to produce a sample from \( \pi \), while a quantum computer can produce a sample from \( \pi \) using \( \sqrt{m/Z} \) evaluations of \( F \).

If we start with \( y \) drawn instead from the distribution \( \pi_0 \) then the acceptance probability is instead \( \frac{\exp(F(y))}{Z_0 \pi_0(y)} \), where \( Z' \geq \max_y \frac{\exp(F(y))}{\pi_0(y)} \). The average acceptance probability is then \( Z/Z' \). This means \( O(\sqrt{Z'/Z}) \) evaluations of \( F \). Here we need to assume that \( \sqrt{\pi_0} = \sum_y \sqrt{\pi_0(y)} |y \rangle \) can be efficiently prepared. More details can be found in \[47\], including optimal schemes for approximate or exact rejection sampling.

**Decohering quantum walks \[50, 51\].** The classical Metropolis walk fixes some \( d \)-regular graph on \( Y \) and has transition probability \( W_{y,y'} = \exp(\min(0,F(y) - F(y'))) \) of moving from \( y' \) to \( y \). Iterating \( W \) on a classical computer will converge to \( \pi \), although with a mixing time that is often hard to characterize. On a quantum computer we can alternate between applying \( e^{iWt} \) and measuring. This strategy is conjectured to mix quadratically faster than the classical approach, but this has been proven only in special cases.

**Quantum simulated annealing.** For \( \beta \in [0,1] \), define the distribution \( \pi_\beta(y) = \exp(\beta F(y))/Z_\beta \) where \( Z_\beta = \sum_y \exp(\beta F(y)) \). Suppose that the Metropolis walk on \( \pi_\beta \) has spectral gap \( \geq g \) for all \( \beta \). Then \[60\] shows how to sample from \( \pi \) in time \( \tilde{O}(g^{-1/2} \max_y |F(y)|) \). This was recently improved in \[37\] to \( \tilde{O}(g^{-1/2} \sqrt{\log(Z_0/Z)})) \).

### 3.3 Data reduction (coreset) techniques

The above quantum algorithms can be directly applied to the first two tasks: optimization algorithms for MLE and sampling algorithms for Bayesian inference. (Later we will see that either type of algorithm also can apply to saddle-point optimization.) However, in each case the runtime is dominated by evaluations of \( F(y) \) for superpositions of values \( y \). In general these evaluations require an inner loop that iterates over the entire set \( X \), requiring time \( O(n) \). As discussed in Section 1, this reduces the achievable quantum speedup. To address this, we will use classical algorithms for data reduction, which we review here.

**Coreset definition.** Given a data set \( X \), a coreset is a pair \((X', w)\) with \( X' \subseteq X \) and \( w : X \rightarrow \mathbb{R}_{\geq 0} \) a weight function. We can take \( X' := \text{supp}(w) \) so that \( w \) alone is enough to define the coreset, and \(|X'| = ||w||_0 \). Define \( F_w \) by

\[
F_w(y) = r(y) + \sum_{x \in X'} w(x) f(x,y),
\]  

(10)

with \( r(x), f(x,y) \) defined as above. We say that \((X', w)\) (or simply \( w \)) is an \( \epsilon \)-coreset if

\[
|F(y) - F_w(y)| \leq \epsilon |F(y)|, \quad \forall y \in Y.
\]  

(11)

For MLE, using an \( \epsilon \)-coreset means that the best likelihood based on the coreset is within a \( 1 + \epsilon \) multiplicative factor of the true optimum. For Bayesian inference, the probabilities obtained will be within a multiplicative factor of \( e^{\epsilon |F(y)|} \) of the true probabilities, which means that highly unlikely
events remain fairly unlikely even with a coreset. Stronger guarantees on the posterior mean and variance can also be obtained by using a more application-specific metric \[40\].

We now review several methods for constructing coresets.

**Importance sampling.** A standard approach to constructing coresets is importance sampling. The idea here is to estimate the “importance” of each element \(x \in X\) by an easy-to-compute function \(s(x) \geq 0\). Let \(s_{\text{tot}} = \sum_x s(x)\). Then each element in \(X'\) is chosen by independently choosing element \(x\) with probability \(s(x)/s_{\text{tot}}\). We repeat this \(k\) times, so \(|X'| = k\), possibly taking \(X'\) to be a multiset. To make the resulting estimator unbiased, we choose \(w(x) = \frac{n}{k} \frac{s_{\text{tot}}}{s(x)}\).

This leaves open the question of how we choose the importance weights. One approach is by estimating the “sensitivity” of each point \(x \in X\), defined as

\[
\sigma(x) := \max_{y \in Y} \frac{|f(x, y)|}{|F(y)|}.
\]  

(12)

While directly computing even a single \(\sigma(x)\) seems to already require a sum over \(x\) within a max over \(y\), it suffices to use any \(s(x)\) satisfying \(s(x) \geq \sigma(x)\), and in this way we can reduce the cost of computing \(s(x)\). However, the coreset size will depend on \(s_{\text{tot}}\) and not directly on the \(\sigma(x)\).

To state this result formally we also need to define the dimension of the query space (following Definition 4.5 of \[12\] and building on VC dimension \[59\]).

**Definition 1.** Given \(X, Y, f : X \times Y \mapsto \mathbb{R}_{\geq 0}, y \in Y\) and \(r \geq 0\), define the level set \(L(y, r) = \{x : f(x, y) \leq r\} \subseteq X\). The dimension of \((X, Y, f)\) is the smallest integer \(D\) such that for all \(S \subseteq X\),

\[
|\{L(y, r) : y \in Y, r \geq 0\}| \leq |S|^D.
\]  

(13)

For \(k\)-means/medians clustering in \(N\)-dimensional Euclidean space, we have \(D = O(kd)\), and for general metric spaces with \(n\) points we can bound \(D = O(k \log n)\), following the arguments in \[12\] Section 6.

**Theorem 2** (Thm 5.5 of \[12\]). Let \(X, Y, f, \sigma, s, s_{\text{tot}}, d\) be defined as above and choose a coreset \((X', w)\) of size \(k\) using the importance sampling procedure above. Suppose that

\[
k \geq c \frac{s_{\text{tot}}}{\epsilon^2} \left(d \log s_{\text{tot}} + \log \left(\frac{1}{\delta}\right)\right),
\]  

(14)

with \(c > 0\) a universal constant. Then with probability \(\geq 1 - \delta\), we have

\[
|F(y) - F_w(y)| \leq \epsilon |F(y)| \quad \forall y \in Y.
\]  

(15)

A review of the use of this technique with somewhat weaker bounds but a simpler exposition can be found in \[6\].

This framework has been used effectively for clustering problems \[28, 6, 12\] and for Bayesian inference \[39\]. It remains only to describe how to compute \(s(x)\) efficiently and to bound \(s_{\text{tot}}\). First a fast and crude approximation is constructed and used to estimate sensitivities. These estimates are then used to construct a coreset. Here the quality of the approximation determines how close \(s(x)\) is to \(\sigma(x)\) and thus determines the size of the coreset, but otherwise does not affect the quality of the final approximation. Finally a more careful (perhaps exhaustive) search for clusterings can be carried out on the coreset. Details including the resulting bounds on \(s_{\text{tot}}\) are described in more detail in Section 4.
Adaptive coresets. Proposals for adaptive coresets also exist in which \( X' \) is built up element by element \([15, 14, 18]\). There are many strategies for doing so, but a general theme is to solve the optimization problem on \( X' \) and use the solution to determine which points from \( X \) would be helpful to add next to \( X' \). One way to choose points for \( X' \) is to view \( w \) itself as the solution to an optimization problem, i.e. we would like to minimize the convex function

\[
L_{\text{core}}(w) := \max_y |F(y) - F_{w}(y)|,
\]

subject to \( \|w\|_1 = 1 \) and \( \|w\|_0 \leq k \) (if we want a coreset of size \( \leq k \)).

Approximately minimizing convex functions over sparse vectors in the simplex is a problem that naturally fits the Frank-Wolfe algorithm, also known as the conditional gradient algorithm \([29]\). Starting from an initial vector \( w_0 \), Frank-Wolfe constructs a series of iterates \( w_1, w_2, \ldots \) as follows. At step \( t \), find \( x = \text{arg min}(\nabla L_{\text{core}}(w_t))_x \), and then set \( w_{t+1} = (1 - \eta_t)w_t + \eta_t e_x \), where \( e_x \) is the vector with a 1 in position \( x \) and zeros elsewhere. In other words, find the best coordinate direction \( x \) in which to move and then take a step towards \( x \) of size \( \eta_t > 0 \). (This description is for optimizing within the probability simplex, but the algorithm can be defined for \( w \) constrained to any convex set, as described in \([29, 13]\).)

Here the \( \eta_t \) can be chosen according to a fixed schedule such as \( \eta_t = 1/\sqrt{t} \), by using known properties of \( L_{\text{core}}(w) \) such as smoothness and strong convexity, or adaptively, e.g. by using a line search. A key feature is that the \( t \)th iterate satisfies \( \|w\|_0 \leq t \), so we can obtain a coreset of size \( k \) by stopping after \( k \) iterations.

The problem with the above approach is that, as with computing sensitivities, the loss function \( L_{\text{core}}(w) \) takes as much time to compute as the original problem. Thus we will instead need to minimize some more efficiently computable proxy for \( L_{\text{core}}(w) \). Towards this end, interpret \( L_{\text{core}}(w) \) as the \( \infty \)-norm of the vector

\[
E_{\text{core}}(w) := \sum_y (F(y) - F_{w}(y))e_y \in \mathbb{R}^Y.
\]

We will consider two approaches, one suited to Bayesian inference and the other to saddle-point optimization.

Adaptive Hilbert coresets for Bayesian inference. Campbell and Broderick \([15, 14]\) replace \( L_{\text{core}}(w) \) with an appropriately weighted 2-norm of \( E_{\text{core}}(w) \), i.e. they fix an inner product \( \langle , \rangle \) on \( \mathbb{R}^Y \) and seek to minimize

\[
L_{\text{CB}} := \langle E_{\text{core}}(w), E_{\text{core}}(w) \rangle_{\text{CB}}
\]

One choice of inner product for the problem of Bayesian inference is

\[
\langle f, g \rangle_{\pi} := \sum_{y \in Y} \pi(y)f(y)g(y).
\]

Since it is inefficient to evaluate this exactly, we can instead use \( m \) samples \( y_1, \ldots, y_m \) from some approximation to \( \pi \) and define

\[
\langle f, g \rangle_{\tilde{\pi}} := m^{-1} \sum_{i \in [m]} f(y_i)g(y_i).
\]

This allows all computations to be carried out in an \( m \)-dimensional space, which can lead to significant savings. Explicitly we can define \( \Pi(f) = (f(y_1), \ldots, f(y_m)) \) so that \( \langle f, g \rangle_{\tilde{\pi}} = m^{-1}\langle \Pi(f), \Pi(g) \rangle \).
With this reduced space, it becomes efficient to compute the Frank-Wolfe updates. The algorithm needs to keep track of $\Pi(F)$ and $\Pi(F(w))$, which each take space $m$ and can be updated in time $|X|$ and $|X'| = \|w\|_0$ respectively. Finding the best $x$ to add to $X'$ requires computing $\langle F, f(x, \cdot) \rangle_{\tilde{\pi}}$ and $\langle F(w), f(x, \cdot) \rangle_{\tilde{\pi}}$ for each $x \in X$, where $f(x, \cdot) := \sum_y f(x, y)e_y$. Each of these inner products takes time $O(m)$ for a total cost of $O(|X|m)$. Adding a point to $X'$ also requires choosing its weight but the methods for doing this in [15, 14] also require time $O(|X|m)$.

**Adaptive coresets from zero-sum games.** Grigoriadis and Khachiyan [33] consider a slightly different problem in which our goal is instead to minimize

$$L_{SP} := \max_y F_w(y).$$

The notation $L_{SP}$ is used because this is a minimax or saddle-point optimization problem. Again, direct evaluation of $L_{SP}$ would be too expensive, so we resort to approximations. First, observe that $L_{SP} = \max_{v \in \Delta(Y)} \langle v, F(w) \rangle$. Then $\min_w L_{SP}$ is the minimax problem

$$\min_w \max_{v \in \Delta(Y)} \sum_{x,y} w(x)v(y)f(x,y)$$

(22)

corresponding to finding an equilibrium of a two-player zero-sum game. The idea of [33] is then to alternate steps of a stochastic version of Frank-Wolfe on each of $v$ and $w$. This has since been recognized as an example of the multiplicative weights update method [2] and even more generally, as Stochastic Saddle Point Mirror Descent (S-SP-MD) [13, Section 6.5]. In Section 4 we will see further applications of these generalizations.

The intuition for the algorithm of [33] comes from viewing $X$ and $Y$ as strategy sets for a game with payoff $-f(x,y)$ for the $X$ player and $f(x,y)$ for the $Y$ player. The algorithm samples a series of strategies $x_1, y_1, x_2, y_2, \ldots, x_t, y_t$, from distributions $w_1, v_1, \ldots, w_t, v_t$ respectively. These distributions are defined in a way that biases them towards responding well to the previous strategies of the other player.

$$w_t(x) = \frac{W_t(x)}{\sum_{x'} W_t(x')}$$

$$W_t(x) = \exp(-\eta_t(f(x, y_1) + \cdots + f(x, y_{t-1})))$$

$$v_t(y) = \frac{V_t(y)}{\sum_{y'} V_t(y')}$$

$$V_t(x) = \exp(\eta_t(f(x_1, y) + \cdots + f(x_t, y)))$$

Here the step size $\eta_t$ can be taken either to be a fixed $\epsilon/2$ following [33] or as $\sqrt{2/t}$ following [13]. If we set $\eta_t = \epsilon/2$ then [33] proved that the error will be $\leq \epsilon$ with probability $\geq 1/2$ after $t$ reaches $4\max_{x,y} f(x,y)^2 \log(mn)/\epsilon^2$. If we set $\eta_t = \sqrt{2/t}$ then a similar convergence guarantee holds [13], but without needing to fix in advance the number of rounds of the algorithm.

## 4 Algorithms

We are now ready to describe our new algorithms and performance guarantees. Each algorithm is designed for the hybrid quantum-classical setting described in Section 1.3.
tasks from Section 2 and uses as subroutines the quantum and classical algorithms from Section 3. Each algorithm is described both in full generality and for a specific representative example. The goal of this is to show the range of possibilities while also giving a self-contained presentation of applications.

**Algorithm 1 (general version)** Non-adaptive coresets for maximum a posteriori estimation.

**Inputs:** Data $X = \{x_1, \ldots, x_n\}$. This algorithm needs the user to specify a function $f$, a classical algorithm for generating a coreset (e.g. an approximation algorithm followed by importance sampling) and a quantum optimization algorithm (e.g. Grover, adiabatic, etc.)

**Output:** $y$, which is likely to be an exact or approximate solution to (5).

**Algorithm:**

1. Given input $X$, use the classical algorithm to construct a coreset $(X', w)$.
2. Run the quantum optimization algorithm on $(X', w)$.

This “algorithm” is more of a framework than a detailed algorithm. However, it can readily be adapted to hard and relevant optimization problems, such as the following example.

**Algorithm 1.1 (specific version)** Non-adaptive coresets for $k$-means clustering.

**Inputs:** Data points $x_1, \ldots, x_n \in \mathbb{R}^d$, a number of cluster centers $k$ and an accuracy parameter $\epsilon > 0$.

**Output:** Cluster centers $y_1, \ldots, y_k$ approximately minimizing

$$\sum_{i \in [n]} \min_{j \in [k]} \|x_i - y_j\|^2.$$

**Algorithm:**

1. Use the offline coreset algorithm of [12] to construct a coreset $(X', w)$ of size $m = O(\epsilon^{-2} k \log(k) \min(k/\epsilon, d))$.
2. Use Grover to search for the best clustering of $(X', w)$. To make the search space finite, we use [41] to reduce the search space to the $O(m dk)$ possible Voronoi partitions. Given such a partitioning, the cluster center is just the weighted center of those points.

The first step of the algorithm takes time $n \cdot \text{poly}(k, d, \epsilon^{-1})$ time on the classical computer, while the second step takes the quantum computer time $m^{dk/2} \cdot \text{poly}(m, k, d)$, since Grover’s algorithm requires $O(m^{dk/2})$ iterations and each inner loop requires time $\text{poly}(m, k, d)$. While classical computers of course could also make use of the coreset and achieve a runtime of $(n + m^{kd+O(1)}) \cdot \text{poly}(k, d, \epsilon^{-1})$, the resulting hybrid classical-quantum algorithm achieves nearly a quadratic speedup over the purely classical algorithm that also use coresets.

It is important to point out that Algorithm 1.1 is a significant specialization of Algorithm 1 and that many easy variants apply. For example, we could replace Grover’s algorithm with a heuristic such as the adiabatic algorithm or QAOA. Or we could replace the Euclidean $k$-means problem with a generalization known as M-estimators on metric spaces (see [12]) which can handle more general geometries, as well as having other properties, such as being robust to outliers.

Another large class of variants is to use non-adaptive coresets for the other computational tasks: Bayesian inference and saddle-point optimization. This application is fairly straightforward and we
will not explore it further in this paper.

However, there is a sense in which Algorithm 1 in all its flavors does not use the quantum computer in a very interesting way. Arguably the algorithm is mostly classical, with the quantum computer being used only after sophisticated classical algorithms have reduced the data set to a representative sample. Our remaining algorithms will instead use the quantum computer interactively.

**Algorithm 2 (general version)** Adaptive coresets for Bayesian inference.

**Inputs:** Data $x_1, \ldots, x_n$. A description of $\pi_0$, $f$ and a classical algorithm $A$ that takes as input $X$, a coreset $(X', w)$ and a set of samples $y_1, \ldots, y_k$ and outputs an updated coreset. A maximum coreset size $m$. A quantum algorithm $B$ for Bayesian inference.

**Output:** an approximate sample from $\pi_{\text{posterior}}$.

1: Initialize $(X', w)$ to be the empty set.
2: for $k \in \{1, \ldots, m\}$ do
3:   Use the quantum algorithm $B$ to sample $y_k$ according to the distribution
4:   \[ \pi(y_k) = \frac{\exp(F_{X',w}(y_k))}{Z_{X',w}}, \] (23)
5:   where $F_{X',w}$ is from (10) and $Z_{X',w} = \sum_y \exp(F_{X',w}(y))$.
6: end for
7: Use the classical algorithm $A$ to update the coreset $(X', w)$.
8: Output $y_m$.

In many cases the quantum algorithm could also return a q-sample at little or no extra cost. A q-sample from a distribution $\pi$ is defined to be the state
\[ \sum_y \sqrt{\pi(y)} |y\rangle. \] (24)

The idea of a q-sample was introduced in [2] and can have significant advantages over ordinary samples for some applications. In the examples given in Section 3.2, rejection sampling and quantum simulated annealing already return q-samples while decohering quantum walks do not.

Again we make Algorithm 2 concrete by specifying $A, B$ and other features of the problem. One representative example is logistic (or logit) regression. Here we are given a data set $\{(x_i, \ell_i)\}_{i \in [n]}$ consisting of points $x_i \in \mathbb{R}^d$ and labels $\ell_i \in \{-1, 1\}$. For convenience we assume that the first coordinate of each $x_i$ is equal to one, leaving $d - 1$ effective parameters. There is a parameter vector $y \in \mathbb{R}^d$ that we would like to sample from. (The reason sampling from the posterior might be preferable to MLE is that samples can yield additional information such as credible intervals.) Logistic regression models the probability of a label as
\[ p(\ell_i | x_i, y) = \frac{1}{1 + e^{-\ell_i \langle x_i, y \rangle}}, \] (25)
so that $f((x_i, \ell_i), y) = -\log(1 + e^{-\ell_i \langle x_i, y \rangle})$. For simplicity we can take our prior on $y$ to be $\mathcal{N}(0, I_d)$, i.e. $d$ independent Gaussians each with mean 0 and variance 1.
Algorithm 2.1 (specific version) Adaptive coresets for logistic regression.

**Inputs:** Data $\{(x_i, \ell_i)\}_{i \in [n]}$

**Output:** An approximate sample from $\pi_{\text{posterior}}$.

1: Initialize $(X', w)$ to be the empty set.
2: for $k \in \{1, \ldots, m\}$ do
3: Use quantum simulated annealing (see Section 3.2) to approximately sample $y_k$ according to the distribution
   $$\pi(y_k) = \frac{\exp(F_{X', w}(y_k))}{Z_{X', w}},$$
   where $F_{X', w}$ is from (10) and $Z_{X', w} = \sum_y \exp(F_{X', w}(y))$.
4: Use the GIGA algorithm (from Section 3.3) with the measure $\hat{\pi}$ which puts weight $1/k$ at each of the points $y_1, \ldots, y_k$. This yields a point to add to $X'$ and a prescription for updating the weights $w$.
5: end for
6: Output $y_m$.

The example of logistic regression was taken only for completeness, and we could have replaced it with any other cheap-to-evaluate model used in machine learning, such as restricted Boltzmann machines. In each case, the formal guarantees in [15, 14] depend on parameters that are often hard to rigorously bound, so this algorithm should be considered a heuristic. Empirically testing it on either classical or quantum hardware is left to future work.

Finally we will see an interactive algorithm with a rigorous performance guarantee. This will address the problem of saddle-point optimization, which we can think of as a zero-sum game with one player’s strategy set $X$ described by a classical database and the other player’s strategy set $Y$ accessible in superposition by a quantum computer.

Algorithm 3 (general version) Saddle-point optimization [7].

**Inputs:** A data set $X = \{x_1, \ldots, x_n\}$, accuracy parameter $\epsilon > 0$, and code for a function $f : X \times Y \mapsto [-1, 1]$.

**Output:** Distributions $\theta_Y, \theta_X$ approximately achieving the max or min (respectively) in (7).

1: Let $T = \lceil \log(|X| \cdot |Y|)/\epsilon^2 \rceil$.
2: for $t \in \{1, \ldots, T\}$ do
3: Use the classical computer to sample $x_t$ according to
   $$\Pr[x_t] \propto \exp\left(-\epsilon \sum_{s < t} f(x_s, y_s)\right).$$
4: Use a quantum sampling algorithm to sample $y_t$ according to
   $$\Pr[y_t] \propto \exp\left(\epsilon \sum_{s \leq t} f(x_s, y_t)\right).$$
5: end for
6: Let $\theta_X$ be the measure that places weight $1/T$ on each of $x_1, \ldots, x_T$.
7: Let $\theta_Y$ be the measure that places weight $1/T$ on each of $y_1, \ldots, y_T$.

According to [33], this algorithm yields an answer within $O(\epsilon)$ of the true value of (7).
appreciate its efficiency suppose we take ε to be constant. Then the classical algorithm sweeps through the entire dataset X only \( T = O(\log(|X| \cdot |Y|)) \) times (with an inner loop of time \( O(T) \)), and in any reasonable algorithm it would have to do this at least once. Likewise the quantum algorithm has an inner loop that takes time only \( O(T) \), and needs to generate only \( O(T) \) samples. For both the classical and the quantum runtime, we are within a factor of \( O(T^2) \) of the best possible time we could expect. (We note that while algorithms for this problem are known with nearly \( 1/\epsilon \) scaling \cite{20}, they do not have the sparsity properties of \cite{33} and so cannot be used here.) In general if we use a Grover-type algorithm for the quantum part (specifically rejection sampling; cf. Section 3.2), the run-time will be \( O(|X|T^2) \) for the classical computer and \( O(|Y|^{1/2}T^2) \) for the quantum computer.

For these algorithms to be useful we need \( |Y| \gg |X| \). Otherwise a classical computer could simulate the quantum computer in less time than it would take to read the dataset. In general if \( |Y| = |X|^2 \) we would expect the speedups plotted in Fig. 1.

Other recent work \cite{44} \cite{58} has also proposed quantum algorithms for zero-sum games, using a purely oracle data model. In this setting, they can also obtain a square-root speedup of the search over \( X \), yielding an overall runtime of \( \tilde{O}(\sqrt{|X|} + \sqrt{|Y|}) \). These works can be viewed as specializations of the SDP algorithms of \cite{10} \cite{9} \cite{57} \cite{16} \cite{56} that take advantage of the fact that they are working in the probability simplex.

Applications of Algorithm 3. While zero-sum games and saddle-point problems have widespread application (see e.g. \cite{21}), the challenge is finding a setting where the data model is natural. (Similar challenges apply of course to applying quantum algorithms with other non-standard data models such as linear systems solvers and the recent quantum algorithms for semidefinite programming and convex optimization.) Here are several possible examples that fit our desired data model.

3.1 Linear programming. The goal is to optimize over the \( m \)-dimensional probability simplex \( Y \) subject to a set of \( n \) constraints described by \( X \). Each point in \( X \) needs to be described by \( \ll m \) bits, and so should represent a succinct description of an \( m \)-dimensional vector.

3.2 \( \ell_1 \)-norm SVM (support vector machine). A further specialization of the linear programming is a nonlinear SVM. We are given a collection of labeled data points \( X \), a map \( \phi \) from \( X \) to a feature space \( Y \), and wish to select a feature vector \( f \in \Delta(Y) \) that will correctly classify all the points, meaning that \( \langle \phi(x), f \rangle \geq 0 \). This is the decision version of the problem, and the optimization version instead estimates \( \theta := \max_x \min_f \langle \phi(x), f \rangle \) up to additive error \( \epsilon \). If \( \theta < 0 \) then correct classification is impossible and if \( \theta > 0 \) then we call \( \theta \) the margin of the classifier. Because \( f \in \Delta(Y) \) we have \( \|f\|_1 = 1 \), and so we call this \( \ell_1 \) SVM, by contrast with the typical case where the feature vector has bounded 2-norm. The fact that \( f \geq 0 \) can be addressed by doubling the size of \( Y \) and replacing \( \phi(x) \) with \( \phi(x) \oplus -\phi(x) \). Applications of an \( \ell_1 \)-SVM to gene microarray data and text classification are described in \cite{30}, and in \cite{55} \( \ell_1 \)-SVMs are found to work well on both real and synthetic data.

3.3 Boosting \cite{18}. Suppose that \( X \) is a set of labeled data and \( Y \) is a set of classifiers (or “decision stumps”). We would like to choose a sparse convex combination of classifiers in \( Y \) such that no point in \( X \) has average error more than \( \epsilon \) higher than the optimal combination of classifiers.

3.4 Robust optimization \cite{7}. Suppose that \( X \) is a set of possible states of the world and \( Y \) is a set of possible strategies. We should think of \( X \) as a set on which we do not know the correct
probability distribution and so we would like to find a mixture of strategies that performs well on all elements of $X$. For example, let $Y$ be a set of investment options and let $X$ be historical data on asset prices. The goal is to find a distribution over assets whose returns are as large as possible on the entire historical record.

3.5 Security games. Suppose that $X$ is a set of targets and $Y$ is a set of defenses. The defender wants to allocate resources across different defense strategies in a way that the weakest target is still well-defended. This would make sense in defending a computer network where $X$ is the set of ways that an attacker can gain access (different accounts, machines, services, etc.) or in preventing credit-card fraud where $X$ is a historical database of past known fraudulent transactions. In this latter case, the minimax model is applicable because any profitable attack can be scaled up. More speculatively, the goal could be disease eradication (e.g. for polio), $X$ a set of known disease locations and $Y$ a set of eradication strategies. In each case, the solution corresponds to actual resources that are allocated and so it makes sense that this solution should be sparse.

3.6 Approximate Carathéodory in $\ell_\infty$ norm [15]. Let $X$ be a finite subset of $\mathbb{R}^m$. Carathéodory’s theorem states that any vector

It is tempting to attempt to apply Algorithm 3 to semidefinite programming where $Y$ is the space of trace-1 psd matrices and $X$ is a collection of succinctly described linear constraints. However, the algorithms used for this problem [10, 9, 57, 16, 56] all require some form of Grover search over $X$ for a constraint that is violated by a given state $\rho$. This does not appear compatible with an input model where $X$ is a classical dataset. By using oracle data models, the various quantum SDP solvers all work equally well for LPs and SDPs, but when $X$ is classical, LPs appear to be easier than SDPs.

For each algorithm the correctness guarantees follow essentially immediately from those of the various subroutines. In some cases, we may use heuristic algorithms for some of the subroutines, such as adiabatic optimization or the GIGA algorithm for coresets. In that case, the final algorithm would also be essentially a heuristic. It would have clear bounds on runtime (e.g. because the number of points in the coreset is chosen by the user) but without provable accuracy guarantees.

5 Comparison with other algorithms

How do the new algorithms presented in this paper compare with previous approaches to these problems, and to previous hybrid quantum-classical algorithms?

5.1 Comparison with variational algorithms

As discussed at the end of Section 1.3 variational algorithms use a classical outer loop to perform gradient descent on the circuit parameters of a quantum inner loop. These can be extremely general and in some cases amount to performing a local search over the set of all short circuits implementable in a particular hardware model. As a result, they often lack the provable guarantees of algorithms in this paper. On the other hand, they can be run on even very simple quantum computers and running them can teach us about what we might expect from future quantum hardware.

While existing variational algorithms are not designed for a setting with a large classical dataset, there are some connections with the algorithms in this paper. Our algorithm 3 can be thought of as
running the Frank-Wolfe variant of mirror descent on the weight vector of the coreset. This makes the data-reduction approach closer to the variational algorithms that have recently become nearly synonymous with NISQ algorithms. However, there are two key features of our Algorithm 3 that are not suggested by the usual variational formulation: 1) the ansatz and the classical outer loop are structured carefully to present the quantum computer with a very limited subset of the overall data set, and; 2) the output of the quantum computer is usable for a form of stochastic mirror descent without any of the dimension dependence that is seen in general (e.g. [36]).

5.2 Comparison with stochastic gradient descent

Many of the problems with handling large datasets are also relevant to classical computers. For this reason, when training continuously parametrized models on large datasets, the standard classical algorithm is not gradient descent but stochastic gradient descent (SGD). One common version of SGD is to sample a single data point at a time and take a gradient step based on that point. We might imagine using this for the inner loop if the outer loop were, say, the Durr-Høyer minimization algorithm. One can also interpret between this form of SGD and the usual gradient descent with mini-batch gradient descent, which samples a set of \( k \ll n = |X| \) points at a time and uses these for gradient estimates. We use the term “SGD” to refer to this last approach.

Mini-batch gradient descent is most directly comparable to using a coreset of size \( k \). Traditionally, coresets are sampled using some form of importance sampling while mini-batches are often uniformly sampled. However, this is not necessary, and there have been proposals to use importance sampling also to construct mini-batches [19].

The essential difference between SGD and coresets is that coresets are sampled once and then used throughout the optimization, while SGD draws fresh samples for each gradient step. For classical gradient descent, this difference may not be important, or it may favor SGD. However, when used as a subroutine inside a Grover or Durr-Høyer search, the stochastic noise introduced by SGD can be harmful. Indeed, the Grover speedup is known to vanish when the oracle is stochastic and has a non-negligible chance of being replaced by the identity operator [49]. To see this, we briefly review an argument from [49]. Normally Grover search consists of a series of alternating reflections \( R_S R_O R_S R_O \cdots = (R_S R_O)^T \), where \( R_S \) reflects about the starting state and \( R_O \) is the oracle call. If a single \( R_O \) term is deleted, say in the \( j^{th} \) position, then this sequence becomes equivalent to \( (R_S R_O)^j (R_O R_S)^{T-j} \), using \( R_O^2 = I \). In other words, a single deletion reverses the order of all later rotations. If each \( R_S R_O \) rotates by an angle \( \theta \sim 1/T \) then \( R_O R_S \) rotates by \(-\theta\) and random deletions result in alternating between these two. Overall this random walk will take time \( \sim T^2 \) to rotate by an \( \Omega(1) \) angle, thus negating the Grover speedup. If the failure rate is \( \epsilon \ll 1 \) then we can view this as a random walk with step size \( 1/T\epsilon \), so the total time becomes \( T^2\epsilon \) (or \( T \), whichever is greater). Of course one may consider other strategies, but [49] prove that nothing asymptotically better is possible. This restriction applies only to stochastic oracles. If the oracle produces a coherent superposition of success and failure then the Grover speedup is possible [11], but in our setting that would require superposition access to the entire dataset.

Returning now to SGD vs coresets, we can see how SGD is equivalent to a fault Grover oracle by considering a simple toy model. Suppose we would like to estimate \( \max_{y \in [m]} F(y) \) with \( F(y) = \sum_{x \in [n]} f(x, y) \) and we are promised that each \( f(x, y) \in \{0, 1\} \) and that

\[
F(y) = \begin{cases} 
  n\epsilon & y = y_* \\
  0 & \text{otherwise}
\end{cases}
\] (29)
In other words, there is a subset of \( n\epsilon \) values of \( x \) for which \( f(x, y_\epsilon) = 1 \). For all other values of \( x, y \), we have \( f = 0 \).

If we use a coreset, then a set of size \( 1/\epsilon \) will have constant probability of hitting a good value of \( x \). We can then find \( y_\epsilon \) with constant probability in time \( \sim \sqrt{m}/\epsilon \).

Using SGD with a batch size of \( 1/\epsilon \) results in an estimator for \( F(y) \) with constant probability of success. This would result in time \( \sim m/\epsilon \) to find \( y_\epsilon \), which would be no better than in the classical case. If we were to stop early, say after \( \sqrt{m}/\epsilon \) iterations, then Grover would output a nearly uniformly random value of \( y \), yielding essentially no information. The only way to achieve the SGD speedup would be to increase the batch size to the point where the oracle had negligible probability of failure, i.e. to size \( \log(m)/\epsilon \). This would result in a runtime of \( \sqrt{m} \log(m)/\epsilon \).

This is an example of a more general problem. A subset of size \( k \), whether used as a coreset or a SGD minibatch, may be “bad” with probability \( \delta \). For coreset algorithms this means the overall algorithm fails with probability \( \delta \). For a Grover search using SGD, this means the overall algorithm fails with probability \( \sim \sqrt{|Y|} \delta \). (Other algorithms for searching over \( Y \), such as the adiabatic algorithm, may have a more complicated dependence on stochastic noise, and studying this difference is an important open question.) Coresets also fail more gracefully. In more complicated problems where the true max is not only 0 or 1 (as in our example), we can find the true maximum of \( F_w \) even for a nonoptimal choice of \( w \), while Grover with an SGD inner loop would return almost no information if run for too little time.

In classical optimization algorithms, SGD can also be improved by variance reduction techniques, such as [42]. However, these techniques do not seem obviously compatible with the hybrid approach in this paper. For example, [42] needs to occasionally calculate a full gradient, which in our terminology would take time \( O(mn) \).

Recently there has been enormous progress in our theoretical and practical understanding of more sophisticated variants of gradient descent [52], and it is an important open question to understand what potential these have for benefiting quantum algorithms.

6 Conclusion

This paper has a simple message. When quantum black-box optimization/sampling algorithms rely on computing a function in the inner loop, and that function involves a classical data set, we can use classical data-reduction techniques to reduce the effective size of this set. Without doing so, we could expect many quantum speedups to be significantly weakened, and Grover-type speedups would become effectively useless.

A more optimistic lesson from the paper is about how to design quantum algorithms for machine learning tasks. If we were to be as generous as possible to the power of quantum computers, we might hope that BQP=PSpace. Even in this case, we would still have the problem that near-term quantum computers will have a small number of qubits (say \( n \)) and because of decoherence will not able to run many gates (say \( T \)). (Note that even using FTQC, there is a poly log \( T \) overhead in the number of qubits, which will still present an effective upper limit on the number of gates.) Thus such a quantum computer could only handle \( O(T) \) pieces of classical data. Without good data-reduction techniques, fitting a model to a large data set would not obviously be sped up by a small quantum computer, even with the assumption that BQP=PSpace. Conversely, this optimistic assumption on the power of quantum computers could be a good place to look for new algorithms, since if quantum computers cannot help in this model, they will never be useful. The
current paper could be seen as an answer to the question of “suppose that the adiabatic algorithm worked as well as we could hope in every case; then how would we use it on practical problems?”

This work opens up many possible open problems. First, it would be useful to empirically test some of the many algorithms proposed here. While many coreset algorithms have been tested classically, they have generally not be tested in the regimes where quantum advantage would be expected.

Second, there are more general forms of data reduction that could be explored. One direction that is orthogonal to coresets would be to reduce the dimension of the data points. Here too it seems likely that adaptive schemes could improve on non-interactive algorithms.

Finally there are likely to be many more ways of developing hybrid classical-quantum algorithms with nontrivial interaction between the two devices. The field of quantum simulation already has many proposed quantum algorithms as well as many classical algorithms but there has been little research to date on useful mergers of the two. One promising approach in this direction is which speeds up Hamiltonian simulation by taking suitably weighted samples of the terms, although achieving this with a realistic input data model is still an open question.

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