Quantum gradient descent for linear systems and least squares

Iordanis Kerenidis ∗ Anupam Prakash †

May 2, 2017

Abstract

Quantum Machine Learning is an exciting new area that was initiated by the breakthrough quantum algorithm of Harrow, Hassidim, Lloyd [10] for solving linear systems of equations and has since seen many interesting developments [13, 14, 15, 11]. In this work, we start by providing a quantum linear system solver that outperforms the current ones for large families of matrices and provides exponential savings for any low-rank (even dense) matrix. Our algorithm uses an improved procedure for Singular Value Estimation which can be used to perform efficiently linear algebra operations, including matrix inversion and multiplication.

Then, we provide the first quantum method for performing gradient descent for cases where the gradient is an affine function. Performing τ steps of the quantum gradient descent requires time $O(\tau C_S)$, where $C_S$ is the cost of performing quantumly one step of the gradient descent, which can be exponentially smaller than the cost of performing the step classically. We provide two applications of our quantum gradient descent algorithm: first, for solving positive semidefinite linear systems, and, second, for performing stochastic gradient descent for the weighted least squares problem.

∗ CNRS, IRIF, Université Paris Diderot, Paris, France and Centre for Quantum Technologies, National University of Singapore, Singapore. Email: jkeren@irif.fr.
† Centre for Quantum Technologies and School of Physical and Mathematical Sciences, Nanyang Technological University, Singapore. Email: aprakash@ntu.edu.sg.
1 Introduction

Quantum Machine Learning is an area that has seen a flurry of new developments in recent years. It was initiated by the breakthrough algorithm of Harrow, Hassidim, Lloyd [10], that takes as input a system of linear equations which is sparse and well-conditioned, and in time polylogarithmic in the system’s dimension outputs the solution vector as a quantum state. In other words, given a matrix $A$ and a vector $b$, it outputs the quantum state $|A^{-1}b\rangle$ corresponding to the solution. Note that this algorithm does not explicitly output the classical solution, nevertheless, the quantum state enables one to sample from the solution vector or perform some interesting computation on it. This is a powerful algorithm and has been very influential in recent times, where several works obtained quantum algorithms for machine learning problems based on similar assumptions [15, 18, 14]. The review [1] further discusses these developments and the underlying assumptions. More recently, we also provided a new application to competitive recommendation systems [11], where the quantum algorithm can provide a good recommendation to a user in time polylogarithmic in the dimension of the system and polynomial in the rank which is much smaller than the dimension, unlike classical recommendation systems that require time linear in the dimension. In all these examples, the power of quantum information comes from quantum routines that can implement efficiently some linear algebra operations, such as matrix multiplication, inversion or projection.

A classical linear system solver is a very powerful tool in machine learning, since it can be leveraged to solve optimization problems using iterative methods. Such iterative methods are very versatile and most optimization problems can be solved using first order iterative methods like gradient descent or second order methods like Newton’s method and the interior point algorithms for linear and semidefinite programs. Each step of an iterative method involves a gradient computation or the inversion of a positive semidefinite Hessian matrix, but these methods allow us to solve a large number of problems that do not have a closed form solution and thus cannot be solved using linear systems alone.

If we look a little more closely at these iterative methods, we see that they start with a random initial state $\theta_0$ that is updated iteratively according to a rule of the form $\theta_{t+1} = \theta_t + \alpha r_t$. The first thing to notice is that in many cases, these updates can be implemented using linear algebra operations such as matrix multiplication and inversion.

This raises the question of whether, in a similar manner, the quantum linear system solvers can be leveraged to solve more general optimization problems via iterative methods. However, there are some obvious obstacles towards realizing a general quantum iterative method. Most importantly, the quantum routines for matrix multiplication and inversion only output a quantum state that corresponds to the classical solution vector and not the classical vector itself. Hence, if at any step during the iterative method the quantum procedure fails, one needs to start from the very beginning of the algorithm. Another main problem, is that the current quantum linear systems solvers only work for sparse matrices. Even though one may argue that in some practical settings the data is indeed sparse, there is no reason to believe that the matrix multiplications necessary for the updates in the iterative methods will be sparse.

Let us discuss some related work: in [19] the authors develop quantum algorithms for gradient descent and Newton’s methods for polynomial optimization problems, but the proposed methods can be used only for a logarithmic number of steps. More precisely, the running time of the quantum algorithm presented depends exponentially on the necessary number of steps. While in some cases the gradient descent may converge fast, it is clear that the running time of a general quantum gradient descent method should scale at most polynomially with the number of steps.
Quantum speedups for semidefinite programs were obtained in [4] using Gibbs sampling and the multiplicative update method, while developing a quantum interior point method is stated as an open problem there.

1.1 Our results

In this work we make significant progress on both the challenges described above. We start by designing an improved quantum linear systems solver and then use it to define an efficient quantum iterative method for implementing gradient descent with affine update rules. Last, we show how to use our iterative method for solving linear systems and for performing stochastic gradient descent for the weighted least squares problem.

1.1.1 An improved quantum linear systems solver

First, we provide a quantum linear system solver that outperforms the current ones for large families of matrices and provides exponential savings for any low-rank (even dense) matrix, where by low-rank we mean that the rank is poly-logarithmic in the dimensions.

Let us remark that the running time of the HHL algorithm is $\tilde{O}(s(A)^2 \kappa(A)^2 / \epsilon)$ where $s(A)$ and $\kappa(A)$ are the sparsity and the condition number of the matrix $A$, $\epsilon$ the error parameter, and we hide factors logarithmic in the dimension of the matrix. Subsequent works have improved the running time of the HHL algorithm to linear in both $s(A)$ and $\kappa(A)$ and the precision dependence to $\log(1/\epsilon)$ [2, 7]. In the case of dense matrices, these algorithms run in time linear to the dimension of the matrix.

Our quantum linear systems solver runs in time that, instead of the sparsity, depends on the matrix parameter $\mu(A)$ which is always smaller than the Frobenius norm of the matrix, $\|A\|_F$, and also smaller than $s_1(A)$, the maximum $\ell_1$ norm of a row of the matrix $A$.

**Result 1 (Theorem 4.6).** There exists a quantum algorithm that given access to a matrix $A$ and a vector $b$, outputs a quantum state $|z\rangle$, such that $\|z - |A^{-1}b\rangle\| \leq \delta$, with running time $\tilde{O}(\kappa^2(A)\mu(A)/\delta)$. 

Let us compare with the HHL algorithm under the same assumptions [9] that the eigenvalues of $A$ lie in the interval $[1/\kappa, 1]$. Note, that for the Frobenius norm we have $\|A\|_F = (\sum_i \sigma_i^2)^{1/2} \leq \sqrt{rk}(A)$. Hence, our algorithm achieves an exponential speedup even for dense matrices whose rank is poly-logarithmic in the matrix dimensions. Moreover, while for general dense matrices the sparsity is $\Omega(n)$, we have $\mu(A) \leq \|A\|_F \leq \sqrt{n}$ and thus we have a worst case quadratic speedup over the HHL algorithm. Moreover, for the same normalization as in [7], we have that $s_1(A) \leq s(A)$ for all matrices $A$, hence we improve on the linear system solver in [7], whose running time depends on $s(A)$. For example, real-valued matrices with most entries close to zero and a few entries per row close to 1, e.g. small perturbations of permutation matrices, will have $s(A) = \Omega(n)$, $\|A\|_F = \Omega(\sqrt{n})$, while $s_1(A)$ will be $O(1)$ for small enough perturbations. Last, the parameter $\mu(A) = \Omega(\sqrt{n})$ for some matrices, meaning that our algorithm does not provide exponential savings for all matrices.

We believe that one can improve the dependence on $\kappa(A)$ to linear and the dependence on the error to $\log(1/\delta)$ using the techniques in [2, 7]. In this work, we focus on achieving a dependence on $\mu(A)$ instead of the sparsity of the matrix.

The main technical tool is an improved quantum walk based algorithm for performing singular value estimation (SVE). In other words, we are given a matrix $A = \sum_i \sigma_i u_i v_i^T$ where $\sigma_i$ are the singular values and $(u_i, v_i)$ are the singular vectors, and a vector $b$, which we can see as a
superposition of the singular vectors of the matrix $A$, i.e. $|b⟩ = \sum_i \beta_i |v_i⟩$, and the goal is to coherently estimate the corresponding singular values, i.e. perform the mapping

$$|b⟩ = \sum_i \beta_i |v_i⟩ \xrightarrow{SVE} \sum_i \beta_i |v_i⟩ |\tilde{σ}_i⟩,$$

such that $\tilde{σ}_i$ is a good estimation for $σ_i$. The relation between quantum walks and singular values has been well known in the literature, for example see [20, 6]. Here, we use an approach similar to [11] and a better tailored analysis of the quantum walk in order to achieve the improvements in running time, and prove the following result

**Result 2** (Theorem 4.5). **Given access to a matrix $A$, there exists a quantum algorithm that performs Singular Value Estimation for $A$ to precision $δ$ in time $\overline{O}(\mu(A)/δ)$.**

The SVE procedure can be used to perform a number of different linear algebra operations. For example, solving a linear system reduces to performing the SVE, then applying a conditional rotation by an angle proportional to the inverse of each singular value, and performing the SVE again to erase the singular value estimation. Namely, the following operation is performed

$$\sum_i \beta_i |v_i⟩ |\tilde{σ}_i⟩ |0⟩ \rightarrow \sum_i \beta_i |v_i⟩ |0⟩ \left( \frac{σ_{\text{min}}}{σ_i} |0⟩ + \sqrt{1 - \frac{σ_{\text{min}}^2}{σ_i^2}} |1⟩ \right)$$

Note that conditioned on the last register being $|0⟩$, one gets a good approximation to the desired output $|A^{-1}b⟩ = \sum_i \frac{\beta_i}{σ_i} |v_i⟩$. To complete the analysis of the linear system solver, we take the appropriate error in the SVE estimation (which turns out to be $O(1/κ(A))$) and perform amplitude amplification to increase the probability of the desired state by repeating the procedure $O(κ(A))$ times, which gives the running time stated in Result 1.

Note, that there is nothing special about multiplying with $A^{-1}$, one can as easily multiply with the matrix $A$, by again performing the SVE procedure and then performing a conditional rotation by an angle proportional to $\tilde{σ}_i$ instead of its inverse. This way, one gets an algorithm for matrix multiplication with the same guarantee and running time.

One important remark here is that the main quantum ingredient is the possibility, given a singular vector of a matrix $A$ (or a coherent superposition thereof), to estimate the corresponding singular value (also coherently). This is basically what the well-known phase estimation procedure does for a unitary matrix. Once we know how to do this then one can perform many different linear algebra operations, including multiplying by the inverse of the matrix (as in the linear systems solvers), multiplying with the matrix or a power of the matrix (as we will need for the iterative method), or even project a vector in some eigenspace of the matrix (as we used in [11]).

### 1.1.2 Quantum iterative methods

In our second main result, we provide a new framework for performing first order quantum iterative methods, or quantum gradient descent, for cases where the gradient is an affine function. This includes the case of positive semidefinite linear systems and regularized weighted least squares problems. Before explaining our quantum iterative method, we provide some details about classical iterative methods that are necessary for our description.
Classical iterative methods for empirical risk minimization. We define more precisely classical iterative methods in the framework of empirical risk minimization. In this framework we are given \( m \) examples from a training set \( (x_i, y_i) \) where variables \( x_i \in \mathbb{R}^n \) and outcome \( y_i \in \mathbb{R} \). The model is parametrized by \( \theta \in \mathbb{R}^n \) and is obtained by minimizing the following objective function,

\[
F(\theta) = \frac{1}{m} \sum_{i \in [m]} \ell(\theta, x_i, y_i) + R(\theta).
\]

The loss function \( \ell(\theta, x_i, y_i) \) assigns a penalty when the model does not predict the outcome \( y_i \) well for example \( (x_i, y_i) \) while the regularization term \( R(\theta) \) penalizes models with high complexity. We refer to \[3\] for a classical overview of empirical risk minimization.

The first order iterative method for problems described by this framework is called gradient descent. The algorithm starts with some \( \theta_0 \in \mathbb{R}^n \), and for \( \tau \) steps updates this point via the following update rule:

\[
\theta_{t+1} = \theta_t + \alpha \nabla F(\theta_t)
\]

In the end, it outputs \( \theta_\tau \) which is guaranteed to be close to the solution for sufficiently large \( \tau \). The running time of this method is \( \tau C_S \), where \( C_S \) is the cost of a single step, in other words it is the cost of the update. The cost can be much higher than the number of steps for high dimensional problems.

A basic example of an optimization problem in the above form is that of solving the linear system \( Ax = b \) for a positive semidefinite matrix \( A \). The solution to the linear system is the unique minimum for the loss function \( F(\theta) = \theta^T A \theta - \theta^T b \) and can be computed using the gradient descent update. In addition, several well known classical algorithms for regression and classification problems can be expressed in the empirical loss minimization framework.

Regression problems correspond to the setting where the outcome \( y \in \mathbb{R} \) is real valued, the predicted value for \( y_i \) is \( \theta^T x \). The linear regression or least squares problem corresponds to the loss function \( F(\theta) = \frac{1}{m} \sum_{i \in [m]} (\theta^T x_i - y_i)^2 \), a least squares model thus minimizes the average squared prediction error over the dataset. The \( \ell_2 \)-regularized least squares or ridge regression problem and the \( \ell_1 \)-regularized least squares or Lasso regression use the regularization term \( R(\theta) \) to be \( \lambda \| \theta \|_2^2 \) and \( \lambda \| \theta \|_1 \) respectively and are of considerable importance in machine learning, see for example \[17\].

Classification problems correspond to the setting where the outcomes \( y_i \) are discrete valued. Many well known classification algorithms including logistic regression, support vector machines and perceptron algorithms correspond to different choices of loss functions for the empirical loss minimization framework and can thus be solved using first order methods.

One important subclass of the empirical loss minimization framework is when the gradient is an affine function, as for the linear systems, least squares and ridge regression problems. In these cases, the iterative method starts with some \( \theta_0 \) and updates this point via an update rule of the form for \( t \geq 0 \),

\[
\theta_{t+1} = \theta_t + \alpha r_t
\]

where \( \alpha \) is some scalar that denotes the step size and \( r_t \) is an affine function \( L \) (that depends on the data) of the current solution \( \theta_t \), i.e. \( r_t = L(\theta_t) = A \theta_t + c \). It is easy to see that this also implies that \( \tau_{t+1} = S(r_t) \) for a linear operator \( S \). Indeed,

\[
r_{t+1} = L(\theta_{t+1}) = L(\theta_t + \alpha r_t) = A(\theta_t + \alpha r_t) + c = r_t + \alpha A r_t = S(r_t)
\]
The final state of a linear update iterative method can be written hence as

$$
\theta_\tau = \theta_0 + \alpha \sum_{t=0}^{\tau-1} r_t = \theta_0 + \alpha L(\theta_0) + \alpha \sum_{t=1}^{\tau-1} S^t(r_0).
$$

(1)

where $S^t$ is the operator that applies $S$ for $t$ time steps and $S^0$ is the identity operator.

We are slightly going to change notation in order to make the presentation clearer. We rename $\theta_0$ as $r_0$, which means that $r_0$ is renamed as $L(r_0)$. This way, we have

$$
\theta_\tau = r_0 + \alpha L(r_0) + \alpha \sum_{t=1}^{\tau-1} S^t(L(r_0)) = r_0 + \alpha \sum_{t=1}^{\tau} S^{t-1}(L(r_0)).
$$

Without loss of generality we assume that the initial point has unit norm, i.e. $\|r_0\| = 1$.

**A quantum gradient descent algorithm with affine updates** We are now ready to explain the main ideas of the quantum algorithm for performing the above iterative method. Let us make things simpler for this exposition by looking at the case where we take $r_0 = 0$ and $\alpha = 1$, meaning we just want to output the state $|\theta_\tau\rangle = \sum_t r_t$. We only make this assumption here for conveying clearly the main ideas and not in the rest of the paper where we address the most general case.

Imagine that there was a procedure that performs the following mapping perfectly

$$
|t\rangle |\theta_t\rangle \rightarrow |t+1\rangle |\theta_{t+1}\rangle
$$

Then, our task would be easy, since applying this unitary $\tau$ times would provide us with the desired state $|\theta_\tau\rangle$. Alas, this is not the case, or at least we do not know how to achieve it. Notice for example that the mapping $\theta_t$ to $\theta_{t+1}$ is not a unitary transformation and in fact the norm of $\theta_{t+1}$ could be larger than the one of $\theta_t$. Even so, imagine one could in fact perform this mapping with some “probability” (meaning mapping $\theta_t$ to some state $(\beta |\theta_{t+1}\rangle |0\rangle + \sqrt{1-\beta^2} |G\rangle |1\rangle$), for some garbage state $G$). The main issue is that one cannot amplify this amplitude, since the state $|\theta_{t+1}\rangle$ is unknown, being the intermediate step of the iterative method, and in the quantum case we only have a single copy of this state. Hence, the issue with the iterative method is that one needs to perform $\tau$ sequential steps, where each one may have some constant probability of success without the possibility of amplifying this probability. In the end, the probability of getting the desired state is unfortunately proportional to the product of the success probabilities for each step, which drops exponentially with the number of steps $\tau$. This is also the reason previous attempts for a quantum gradient descent algorithm break down after a logarithmic number of steps.

Here we manage to overcome this obstacle in the following way.

The first idea is to deal with the vectors $r_t$ instead of the $\theta_t$’s, since in this case, we know that the norm of $r_{t+1}$ is smaller than the norm of $r_t$. Our goal would be to find a unitary mapping that, in some sense, maps $r_t$ to $r_{t+1}$. Again, there is the problem that the norms are not equal, but in this case, since the norm of $r_{t+1}$ is smaller, we can possibly make it into a unitary mapping by adding some garbage state. Indeed, we define the quantum step of the quantum iterative method via the following unitary

$$
|t\rangle ||r_t\rangle \rightarrow |t+1\rangle (||r_{t+1}\rangle |0\rangle + |G\rangle |1\rangle),
$$

6
where the norm of the garbage state is such that the norm of the right hand side is equal to \( \| r_t \| \).

Note that the above vectors are not unit norm but \( V \) is still length preserving. We write it in this way to mimic the mapping of the unnormalized vectors \( r_t \rightarrow r_{t+1} \). Since we are dealing with linear updates, the above transformation is basically a matrix multiplication and we use our SVE procedure to perform it with high accuracy.

The second idea is noticing that our goal now is not to obtain the final state \( r_\tau \), but the sum of all the vectors \( \sum_t r_t \). Let us see how to construct this efficiently. Given a procedure for performing one step of the iterative method as above, we design another procedure \( U \) that given as input a time \( t \) and the initial state \( r_0 \) can map \( r_0 \) to \( r_t \). We do this by basically applying the unitary \( V \) \( t \) times, conditioned on the first register. In other words, we can perform the mapping

\[
|t, r_0\rangle \xrightarrow{U} |t\rangle (\|r_t\| |r_t\rangle |0\rangle + |G\rangle |1\rangle).
\]

Note that if the cost of \( V \) is \( C_V \), then naively, the cost of \( U \) will be \( \tau C_V \) by applying \( V \) sequentially. We will actually see that in fact we can implement \( C_U \) in time \( O(C_V + \log \tau) \).

We are now ready for the last step of the algorithm that consists in starting with a superposition of time steps from 0 to \( \tau \) and applying \( U \), in order to get a superposition of the form

\[
\frac{1}{\sqrt{\tau}} \sum_t |t\rangle |r_0\rangle \rightarrow \frac{1}{\sqrt{\tau}} \sum_t |t\rangle (\|r_t\| |r_t\rangle |0\rangle + |G\rangle |1\rangle).
\]

Then, we can “erase” the time register by performing a Hadamard on the first register and accepting the result when the first register is 0. In other words, we are having a state of the form

\[
\frac{1}{\tau} \sum_t \|r_t\| |r_t\rangle |0\rangle + |G\rangle |1\rangle
\]

Using Amplitude Amplification, we can get the desired state \( \frac{1}{\sqrt{\tau}} \sum_t \|r_t\| |r_t\rangle \), in overall time \( O(\frac{1}{\|r_\tau\|}) \) times the cost of applying the unitary \( U \), and since in our applications \( \|\theta \| = \Omega(1) \) we get the efficient quantum gradient descent algorithm.

**Result 3 (Section 3.3)**. *Given a unitary \( V \) that approximately applies one step of the iterative method in time \( C_V \), there exists a quantum algorithm that performs \( \tau \) steps of the iterative method and outputs a state close to \( \theta \), in time at most \( O(\tau C_V) \).*

Our running time is quadratic in the number of steps the classical iterative method needs to take in order to get close to a solution, times the cost of taking one step of the iterative method, i.e. quantumly implementing the update rule. The updates are performed using SVE and the update cost can be exponentially smaller in the quantum case. Hence we can get quantum algorithms with vastly improved performance, for cases where the number of steps of the classical iterative method is not too large compared to the update cost, such as linear systems and least squares.

Let us remark that our algorithm does not try to create all the intermediate states \( \theta_t \) of the iterative method, which we do not know how to achieve with non-negligible probability for large \( \tau \). Instead, we first see that the final state \( \theta_\tau \) is equal to the sum of all the update states \( r_t \) and then we try to create the sum of these states in the way we described above: we first go to a superposition of all time steps from 0 to \( \tau \) and then conditioned on the time being \( t \) we apply coherently \( t \) updates to the initial state \( r_0 \) in order to create a sort of “history” quantum state. This is reminiscent of
the “history” states in Kitaev’s proof of the QMA-completeness of the Local Hamiltonian problem [13]. Last, erasing the register that keeps the time can be done in time linear in the number of time steps, which is still efficient.

Finally, we note that in all these quantum machine learning algorithms, one needs to use a classical data structure for the input (which can be seen as a matrix or set of vectors) so that the quantum algorithm be able to efficiently create superpositions of rows of the input matrix or of the vectors. While in many cases one just assumes this ability, here, we also rigorously describe such a classical data structure with efficient update and retrieval time that extends the proposals in [8, 11] and allows to efficiently create the necessary quantum superpositions, as we want our application to be end-to-end in the sense of [1].

1.1.3 Applications of quantum gradient descent

We provide two applications of our quantum gradient descent method.

Positive semidefinite linear systems First, we use it for solving positive semidefinite linear systems, namely, given a positive semidefinite matrix $A$ and a vector $b$, output a state close to $|A^{-1}b\rangle$. Of course, linear systems can be solved directly as we have seen, but we provide the analysis and running time of our gradient descent algorithm in order to compare the two methods. Also, we will see below that in many cases, gradient descent is preferable in practice than direct methods.

The error analysis shows that the number of steps we need to perform in order to get $\delta$ close to the solution of the linear system is roughly $O(\kappa(A) \log(1/\delta))$, while in order to keep the error of the final state small, we need to perform the SVE for $I - \alpha A$ (which can be performed using SVE for $A$) with precision $\frac{\delta}{\kappa(A)}$, which then takes time $O(\kappa(A)^2 \mu(A)/\delta)$. Let $A|b$ denote the matrix with row $b$ added to $A$. Overall, we have

Result 4 (Theorem 5.1). Given positive semidefinite matrix $A$ and vector $b$ stored in memory, there is an iterative quantum algorithm that outputs a state $|z\rangle$ such that $|||z\rangle - |A^{-1}b\rangle|| \leq 2\delta$ with expected running time $\tilde{O}(\frac{\kappa(A)^2 \mu(A)|b|}{\delta^2})$.

Note that the running time has an extra factor $\kappa(A)$ compared to the direct method we described, while again the algorithm depends linearly on the parameter $\mu(A)$ which is smaller than the sparsity.

Stochastic gradient descent for weighted least squares Our second application is to the weighted least squares problem. For this problem, we are given a matrix $X$ of examples and a corresponding vector $y$ of labels, as well as a vector $w$ of weights, and the goal is to find $\theta$ that minimizes the squared loss $\sum_i w_i (y_i - x_i^T \theta)^2$.

One can provide a closed form solution, which is given by

$$\theta = (X^TWX)^{-1}X^TWy$$

and thus the problem a priori can also be solved using a direct method. Quantum algorithms for unweighted least squares problems with a polynomial dependence on sparsity using the direct method were described in [21]. There are two ways in which we extend this work, first using our improved SVE algorithm we can perform matrix multiplication and inversion efficiently for a larger class of matrices and can also solve the weighted version of the problem. We thus extend the results
on efficient quantum algorithms for this problem which has numerous applications in science and engineering.

More importantly, we are able to implement an iterative stochastic gradient method for this problem which has many advantages in practical settings (see for example [3] for a more detailed discussion). In fact, the least squares problem is used in practice for regression or data fitting, where in many cases this data comes from internet traffic, social networks, or scientific experiments. There, the data matrix is extremely skewed in shape since the number of data points is order of magnitudes larger than the dimension of the data points. Therefore, it is too expensive to perform any linear algebra operation using the entire data set and moreover due to redundancy in the data, the gradient can be estimated efficiently over small batches.

For these reasons, in practice the gradient is estimated over randomly sampled batches of the training set, an approach which is called stochastic gradient descent. This way, the stochastic gradient descent avoids having to perform linear algebra operations on huge matrices, which would be the case if we were to solve the problem directly or use the usual gradient descent.

Our quantum iterative method can also be used to perform stochastic gradient descent for the above problems, hence considerably reducing the requirements compared to an algorithm that provides a direct solution. This works in a manner similar to the classical setting, the data is split randomly into batches and for each step of the iterative method one considers only one batch of data in order to compute the gradient and perform the linear update. Our quantum gradient descent algorithm can be readily adapted to this setting.

The main technical difference between the quantum iterative method for linear systems and that for the least squares problem, is that in the second case, one needs to perform a matrix inversion and multiplication by a matrix which is not a priori stored in memory. More precisely, we have in memory the matrix \(X\), the diagonal matrix \(W\) and a vector \(y\) and we need to perform matrix multiplication with the matrix \((X^T WX)^{-1}\) and also for creating the vector \(X^T Wy\). We show how to do this efficiently and get the following algorithm, where \(\sqrt{WX}\) is the matrix obtained by adding row \(y\) to \(\sqrt{WX}\).

**Result 5 (Theorem 5.2).** Given access to a semidefinite matrix \(X\), a diagonal weight matrix \(W\) and a vector \(y\) there is a quantum gradient descent algorithm that outputs a state \(|z\rangle\) such that 
\[
\| |z\rangle - |(X^T WX)^{-1} X^T Wy\rangle \| \leq 2\delta
\]
with expected running time \(\tilde{O}(\kappa(X^T WX)^3 \mu(\sqrt{WX}y)^2)\).

Let us remark that while linear updates capture a significant class of iterative methods, a generalization to non-linear update functions would imply the ability to perform a much larger family of algorithms of interest to machine learning, as discussed in section 1.1.2. Also note that it is straightforward to generalize the weighted least squares algorithm to include \(\ell_2\) regularization. Machine learning algorithms on the other hand often use \(\ell_1\) regularization and in some case \(\ell_p\) regularization for \(p \in [1, 2]\). It would be interesting to find a quantum algorithm for \(\ell_p\) regularization for \(p \neq 2\).

The paper is organised as follow: In Section 2, we provide some linear algebra definitions and some basic quantum procedures that we will be using in our algorithms. In Section 3, we define the quantum gradient descent method and analyse its correctness and running time. In Section 4, we provide the improved SVE procedure and show how to use it to directly solve linear systems of equations and how to perform the linear update of the quantum gradient descent method. Last, in Section 5, we provide two applications of our quantum gradient descent method to linear systems and weighted least squares.
2 Preliminaries

2.1 Linear algebra

The set \{1, 2, \cdots, n\} is denoted by \([n]\), the standard basis vectors in \(\mathbb{R}^n\) are denoted by \(e_i, i \in [n]\). For a vector \(x \in \mathbb{R}^n\) we denote the \(\ell_p\) norm as \(\|x\|_p = (\sum_i x_i^p)^{1/p}\). The Euclidean norm \(\|x\|_2\) is denoted as \(\|x\|\). The rank of a matrix is denoted as \(\text{rank}(A)\). A matrix is positive semidefinite if it is symmetric and has non negative eigenvalues, the notation \(A \succeq 0\) indicates that \(A\) is a psd matrix.

The singular value decomposition of a symmetric matrix \(A\) symmetric and has non negative eigenvalues, the notation \(A \succeq 0\) indicates that \(A\) is a psd matrix. The singular value decomposition of a symmetric matrix \(A \in \mathbb{R}^{n \times n}\) is written as \(A = \sum_i \lambda_i v_i v_i^T\) where \(\lambda_i \geq 0\) are the eigenvalues and \(v_i\) are the corresponding eigenvectors.

The singular value decomposition of \(A \in \mathbb{R}^{m \times n}\) is written as \(A = \sum_i \sigma_i u_i v_i^T\) where \(\sigma_i\) are the singular values and \((u_i, v_i)\) are the singular vectors. The Frobenius norm \(\|A\|_F^2 = \sum_{ij} A_{ij}^2 = \sum_i \sigma_i^2\), where \(\sigma_i\) are the singular values. The spectral norm \(\|A\| = \sigma_{\max}\), the largest singular value. The condition number \(\kappa(A) = \sigma_{\max}/\sigma_{\min}\).

The \(i\)-th row of matrix \(A \in \mathbb{R}^{m \times n}\) is denoted as \(a_i\) and the \(j\)-th column is denoted as \(a^j\). The \(\circ\) operator denotes the Hadamard product, that is \(A = P \circ Q\) implies that \(A_{ij} = P_{ij} Q_{ij}\) for \(i \in [m], j \in [n]\). For a matrix \(A \in \mathbb{R}^{m \times n}\), the maximum \(\ell_p\) of the row vectors is denoted \(s_p(A) := \max_{i \in [m]} \|a_i\|_p\), the maximum \(\ell_p\) norm of the column vectors is \(s_p(A^T)\). The sparsity \(s(A)\) is the maximum number of non-zero entries in a row of \(A\).

The \(\tilde{O}\) notation is used to suppress factors poly-logarithmic in vector or matrix dimensions, that is it \(O(f(n)\text{polylog}(mn))\) is written as \(\tilde{O}(f(n))\).

2.2 Quantum Algorithms

We will use phase estimation and variants of amplitude amplification that we recall below. The time required to implement a unitary operator \(U\) will be denoted by \(T(U)\).

**Theorem 2.1.** [Phase estimation, [12]] Let \(U\) be a unitary operator with eigenvectors \(|v_j\rangle\) and eigenvalues \(e^{\theta_j}\) for \(\theta_j \in [-\pi, \pi]\). There exists a quantum algorithm with running time \(O(T(U) \log n/\epsilon)\) that transforms \(|\phi\rangle = \sum_{j \in [n]} \alpha_j |v_j\rangle \rightarrow \sum_{j \in [n]} \alpha_j |v_j\rangle |\theta_j\rangle\) such that \(|\theta_j - \tilde{\theta}_j| \leq \epsilon\) for all \(j \in [n]\) with probability at least \(1 - 1/\text{poly}(n)\).

We state a version of amplitude amplification and estimation below, more precise statements can be found in [5].

**Theorem 2.2.** [Amplitude amplification and estimation, [5]] If there is unitary operator \(U\) such that \(U|0^t\rangle = |\phi\rangle = \sin(\theta) |x, 0\rangle + \cos(\theta) |G, 0^t\rangle\) then \(\sin^2(\theta)\) can be estimated to additive error \(\epsilon\sin^2(\theta)\) in time \(O(\frac{T(U)}{\epsilon \sin(\theta)})\) and \(|x\rangle\) can be generated in expected time \(O(\frac{T(U)}{\epsilon \sin(\theta)})\).

Last we provide a simple claim that shows that if two unnormalized vectors are close to each other, then their normalized versions are also relatively close.

**Claim 2.3.** Let \(\theta\) be the angle between \(\phi, \tilde{\phi}\) and assume that \(\theta < \pi/2\). Then, \(\|\phi - \tilde{\phi}\| \leq \epsilon\) implies \(\|\phi\| = \|\tilde{\phi}\|\) implies \(\|\phi - \tilde{\phi}\| \leq \frac{\epsilon}{\|\phi\|}\).

**Proof.** We bound the \(\ell_2\) distance \(\|\phi - |\tilde{\phi}\rangle\|\) using the following argument. Let \(\theta\) be the angle between \(\phi, \tilde{\phi}\). For the unnormalized vectors we have \(\|\phi - \tilde{\phi}\| \leq \epsilon\), and assuming that \(\theta < \pi/2\) we
have $\epsilon \geq \|\phi\| \sin(\theta)$. The distance between the normalized states can thus be bounded as,

$$
\|\langle \phi | - |\tilde{\phi}\rangle\|^2 = (2\sin(\theta/2))^2 \leq 2\sin^2(\theta) \leq \frac{2\epsilon^2}{\|\phi\|^2}
$$

(2)

2.3 The access model for quantum machine learning applications

Quantum algorithms for linear algebra require quantum access to the matrices being manipulated, and most prior research in the literature works in the model of oracle access to the matrix entries, that is quantum queries of the form $|i,j,0\rangle \rightarrow |i,j,a_{ij}\rangle$ are allowed. Such an access model can be particularly helpful in cases where the matrix is structured so that $a_{ij}$ is a simple function of $(i,j)$, for example it can be used to represent well structured matrices of even exponential size.

The matrices that arise in machine learning applications do not have such structure, since they arise from empirical datasets and are represented by a list of entries $(i,j,a_{ij})$. There is no succinct way to compute $a_{ij}$ from $i,j$ and thus even to implement the quantum queries of the form $|i,j,0\rangle \rightarrow |i,j,a_{ij}\rangle$, an implicit data structure must be stored in memory. In the machine learning setting, there is no a priori reason to restrict ourselves to the model with black box access to matrix entries, in particular we can modify the data structure storing the matrix if it provides an algorithmic speedup. We also note that prior work on lower bounds has been in the model with quantum access to the matrix entries and does not apply to the setting where one has quantum access to a different data structure instead.

In our work, we make the data structure explicit and ensure that it has poly-logarithmic insertion and update times, which is the best that one could hope for. Our access model is particularly useful for data that is acquired over time and in settings where it is important that the new elements can be efficiently added to the data structure. In such settings it would be prohibitive to make $poly(m,n)$ time preprocessing after the entire matrix has been stored or each time a new element comes into the data structure. For these reasons, we believe that our access model is well suited for quantum machine learning applications.

3 The Quantum Gradient Descent algorithm

In this section we provide the definition of a quantum step of the quantum gradient descent in the case of a linear update rule and then describe the full quantum procedure that performs the quantum iterative method.

3.1 The quantum step

We assume that the classical iterative method has an update rule such that

$$
\theta_\tau = r_0 + \alpha \sum_{t=1}^{\tau} S^{t-1}(L(r_0)).
$$

for an affine operator $L$, a linear, contracting operator $S$, and a random initial vector $r_0$ with $\|r_0\| = 1$. This is the case, for example, for solving linear systems or least squares.
First we define the notion of an approximate quantum step of the quantum iterative method. Let us denote by \( \tau \) the number of steps of the classical iterative algorithm, and let \( \tau + 1 = 2^\ell \) (if not just increase \( \tau \) to the next power of 2).

**Definition 3.1.** The \((\epsilon, \delta)\)-approximate quantum step algorithm is a unitary \( V \) such that for any \( 1 \leq t \leq \tau - 1 \),

\[
V : |0\rangle |r_0\rangle |0\rangle \rightarrow |1\rangle \left( \alpha \|\tilde{L}(r_0)\| |\tilde{L}(r_0)\rangle |0\rangle + |G_1\rangle |1\rangle \right)
\]
\[
: |t\rangle |r_t\rangle |r_t\rangle |0\rangle \rightarrow |t + 1\rangle \left( \|\tilde{S}(r_t)\| |\tilde{S}(r_t)\rangle |0\rangle + |G_{t+1}\rangle |1\rangle \right),
\]

where \( |G_{t+1}\rangle \) is an unnormalised garbage state, \( \tilde{S} \) is an approximation to the linear, contractive operator \( S : r_t \rightarrow r_{t+1} \), \( \tilde{L} \) is an approximation to the affine, contractive operator \( L : r_0 \rightarrow r_1 \), in the sense that with probability \( \geq 1 - \delta \), it holds that for any \( r_t \), \( \|S(r_t) - \tilde{S}(r_t)\| \leq \epsilon \) and also \( \|L(r_0) - \tilde{L}(r_0)\| \leq \epsilon \).

Notice that \( \|\tilde{L}(r_0)\| \) might be larger than 1, but by taking \( \alpha \) a small constant we have \( \alpha \|\tilde{L}(r_0)\| \leq 1 \). The way we defined \( V \), it is norm preserving but the vectors we wrote down are not unit. We can of course do that by dividing both parts with \( \|r_t\| \). We prefer this notation in order to resemble more the classical mapping of the unnormalised vectors \( r_t \rightarrow r_{t+1} \). We can define the following procedure \( U \) similar to the ideal case.

**Claim 3.2.** Given access to the \((\epsilon, \delta)\)-approximate quantum step algorithm \( V \) (with running time \( C_V \)), there exists a quantum procedure \( U \) with running time at most \( O(\tau C_V) \), such that for any \( t \in [\tau] \),

\[
U : |0\rangle |0\rangle |0\rangle |r_0\rangle |0\rangle \rightarrow |0\rangle |0\rangle |0\rangle |r_0\rangle |0\rangle
\]
\[
: |t\rangle |0\rangle |0\rangle |r_0\rangle |0\rangle \rightarrow |t\rangle |0\rangle \left( \alpha \|\tilde{S}^{t-1}(L(r_0))\| |t\rangle \|\tilde{S}^{t-1}(L(r_0))\rangle |0\rangle + |G_t\rangle |1\rangle \right),
\]

where \( |G_t\rangle \) is an unnormalised garbage state, and with probability at least \( (1 - t\delta) \) it holds that \( \|\tilde{S}^{t-1}(L(r_0)) - \tilde{S}^{t-1}(L(r_0))\| \leq t\epsilon \).

Note that out of the five registers used for the iterative method, registers 1 and 3 store the time step, 4 stores the quantum state for the iterative method while 2 and 5 are control qubits or flags.

**Proof.** We define the operator \( W \) on four registers, such that if the control register is 0, then it applies a \( V \) on the other three registers and then a CNOT to copy the last register into the control register. If the control register is 1, then it does nothing. Namely

\[
W : |0\rangle |0\rangle |r_0\rangle |0\rangle \rightarrow |0\rangle |1\rangle \alpha \|\tilde{L}(r_0)\| |\tilde{L}(r_0)\rangle |0\rangle + |1\rangle |1\rangle \left( G_1 \right) |1\rangle
\]
\[
: |t\rangle |t\rangle |r_t\rangle |r_t\rangle |0\rangle \rightarrow |t\rangle |t + 1\rangle \left( \|\tilde{S}(r_t)\| |\tilde{S}(r_t)\rangle |0\rangle + |1\rangle |t + 1\rangle \left( |G_{t+1}\rangle |1\rangle \right), \quad t \in [1, \tau - 1]
\]
\[
: |1\rangle |t\rangle |b\rangle |1\rangle \rightarrow |1\rangle |t\rangle |b\rangle |1\rangle \quad t \in [0, \tau - 1]
\]

We define the following procedure \( U \) that acts as Identity for \( t = 0 \) and for \( t \in [\tau - 1] \) it does
the following:

\[
|t\rangle |0\rangle |0\rangle |r_0\rangle |0\rangle \xrightarrow{W^t} |t\rangle W^t |0\rangle |0\rangle |r_0\rangle |0\rangle \\
= |t\rangle |0\rangle |t\rangle \alpha \| \tilde{S}^{t-1}(\tilde{L}(r_0))\| \| \tilde{S}^{t-1}(\tilde{L}(r_0))\| |0\rangle + |t\rangle |1\rangle \sum_{i=1}^{t} |i\rangle |G_i\rangle |1\rangle \\
\xrightarrow{CNOT_{5,2}} |t\rangle |0\rangle \left( \alpha \| \tilde{S}^{t-1}(\tilde{L}(r_0))\| \| \tilde{S}^{t-1}(\tilde{L}(r_0))\| |0\rangle + |G_i\rangle |1\rangle \right)
\]

The equality on line 2 follows from the definition of \( W \). We prove the properties by induction on \( t \). For \( t = 1 \) we use the definition of the quantum step \( V \) and the property holds. Assume it holds for \( t - 1 \), i.e. with probability \( 1 - (t - 1)\delta \) we have \( \| S^{t-2}(L(r_0)) - \tilde{S}^{t-2}(\tilde{L}(r_0))\| \leq (t - 1)\epsilon \).

Then, we have

\[
\| S^{t-1}(L(r_0)) - \tilde{S}^{t-1}(\tilde{L}(r_0))\| \leq \| S(S^{t-2}(L(r_0))) - S(\tilde{S}^{t-2}(\tilde{L}(r_0)))\| + \| S(\tilde{S}^{t-2}(\tilde{L}(r_0))) - \tilde{S}(\tilde{S}^{t-2}(\tilde{L}(r_0)))\| \\
\leq \| S^{t-2}(L(r_0)) - \tilde{S}^{t-2}(\tilde{L}(r_0))\| + \| S(\tilde{S}^{t-2}(\tilde{L}(r_0))) - \tilde{S}(\tilde{S}^{t-2}(\tilde{L}(r_0)))\|
\]

where we used the fact that \( S \) is contractive. Also, by definition of the iterative step, with probability \( (1 - \delta) \) we have \( \| S(\tilde{S}^{t-2}(\tilde{L}(r_0))) - \tilde{S}(\tilde{S}^{t-2}(\tilde{L}(r_0)))\| \leq \epsilon \) and with probability \( 1 - (t - 1)\delta \), by induction hypothesis, we have \( \| S^{t-2}(L(r_0)) - \tilde{S}^{t-2}(\tilde{L}(r_0))\| \leq (t - 1)\epsilon \). Hence overall, with probability at least \( 1 - t\delta \), we have

\[
\| S^{t-1}(L(r_0)) - \tilde{S}^{t-1}(\tilde{L}(r_0))\| \leq t\epsilon.
\]

\[\square\]

### 3.2 The Quantum Iterative Method algorithm: general case

Again, we use Amplitude Amplification to optimize the running time of our method. The main part is the efficient construction of the necessary unitary \( Q \).

**The Quantum Iterative Method** Use Amplitude Amplification and Estimation with unitary \( Q \)

\[
Q : |0\rangle^\ell \rightarrow \frac{1}{T} \left| \tilde{\theta}_\tau \right\rangle |0\rangle + |G\rangle |0\rangle^\perp
\]

to output \( |\tilde{\theta}_\tau\rangle \) and \( \| \tilde{\theta}_\tau \| \).

**The unitary** \( Q : |0\rangle^\ell \rightarrow \frac{1}{T} \left| \tilde{\theta}_\tau \right\rangle |0\rangle + |G\rangle |0\rangle^\perp \)

1. Create the state \( \frac{1}{\sqrt{T + 1}} \sum_{t=0}^{T} |t\rangle |0\rangle |0\rangle |r_0\rangle |0\rangle \)
2. Apply the unitary procedure \( U \) and trace out the second register to get

\[
\frac{1}{\sqrt{T + 1}} |0\rangle |0\rangle |r_0\rangle |0\rangle + \frac{1}{\sqrt{T + 1}} \sum_{t=1}^{T} |t\rangle \left( \alpha \| \tilde{S}^{t-1}(\tilde{L}(r_0))\| \| \tilde{S}^{t-1}(\tilde{L}(r_0))\| |0\rangle + |G_t\rangle |1\rangle \right)
\]
3. Conditioned on the last register being 0, perform a $CNOT_{1,2}$ to erase the second copy of $t$ and then by exchanging the place of the second and third register we get
\[
\frac{1}{\sqrt{\tau + 1}} |0\rangle| r_0\rangle |0\rangle + \frac{1}{\sqrt{\tau + 1}} \sum_{t=1}^{\tau} |t\rangle \left( \alpha \|S^{t-1}(\tilde{L}(r_0))\| |\tilde{S}^{t-1}(\tilde{L}(r_0))\rangle |0\rangle + |G'_t\rangle |1\rangle \right)
\]

4. Conditioned on the last register being 0 perform a Hadamard on the first register and then by exchanging the place of the first and second register we get
\[
\frac{1}{\tau + 1} \sum_{y=0}^{\tau} \left( |r_0\rangle + \alpha \sum_{t=1}^{\tau} (-1)^y t \|S^{t-1}(\tilde{L}(r_0))\| |\tilde{S}^{t-1}(\tilde{L}(r_0))\rangle \right) |y\rangle |0\rangle |0\rangle + |G''\rangle |1\rangle =
\]
\[
\frac{\|\tilde{\theta}_r\|}{\tau + 1} \left( \frac{1}{\|\tilde{\theta}_r\|} \left( |r_0\rangle + \alpha \sum_{t=1}^{\tau} \|S^{t-1}(\tilde{L}(r_0))\| |\tilde{S}^{t-1}(\tilde{L}(r_0))\rangle \right) \right) |0\rangle |0\rangle |0\rangle + |G\rangle (|0\rangle |0\rangle |0\rangle)^{\perp} =
\]
\[
\frac{1}{T} |\tilde{\theta}_r\rangle |0\rangle + |G\rangle |0\rangle^{\perp}
\]
with $|\tilde{\theta}_r\rangle = \frac{1}{\|\tilde{\theta}_r\|} \left( |r_0\rangle + \alpha \sum_{t=1}^{\tau} \|S^{t-1}(\tilde{L}(r_0))\| |\tilde{S}^{t-1}(\tilde{L}(r_0))\rangle \right)$ and $T = \frac{\tau + 1}{\|\tilde{\theta}_r\|}$.

3.3 Analysis

3.3.1 Correctness

We just need to calculate how close the final state of our algorithm is to the correct state $|\theta_r\rangle = \frac{1}{\|\theta_r\|} \left( |r_0\rangle + \alpha \sum_{t=1}^{\tau} \|S^{t-1}(L(r_0))\| |S^{t-1}(L(r_0))\rangle \right)$.

We first look at the non-normalised distance and have
\[
\|\theta_r - \tilde{\theta}_r\| \leq \alpha \sum_{t=1}^{\tau} \|S^{t-1}(L(r_0)) - \tilde{S}^{t-1}(\tilde{L}(r_0))\| \leq \alpha \sum_{t=1}^{\tau} t\epsilon \leq \alpha \tau^2 \epsilon
\]

Then by Claim 2.3 we have
\[
\|\|\theta_r\| - |\tilde{\theta}_r\|\| \leq \frac{\sqrt{2\alpha \tau^2 \epsilon}}{\|\theta_r\|}.
\]

For the norms, Amplitude Estimation will output the norm $\|\tilde{\theta}_r\|$ within any constant error (by increasing the running time by a constant factor) and note that $\|\tilde{\theta}_r\|$ is $(\alpha \tau^2 \epsilon)$-close to $\|\theta_r\|$. Hence by taking $\epsilon = O\left(\frac{1}{\sqrt{\tau}}\right)$ appropriately small, the approximation of the norm can be made to have some small constant error.

We note that in the applications we will consider, $\|\theta_r\|$ is at least $\Omega(1)$ and at most $O(\tau)$ and $\alpha = O(1)$. Hence, again, by taking $\epsilon = O\left(\frac{1}{\sqrt{\tau}}\right)$ appropriately small, we can make this distance less than some small constant.
3.3.2 Running time

The expected running time is the expected running time of the Amplitude Amplification (which is the same as for Amplitude Estimation for constant error), which is \( T \) times the cost of implementing the unitary \( Q \), which is \( O(C_U + \log \tau) \). Overall, the expected running time is \( O(T(C_U + \log \tau)) \).

As we said, in our applications we will have \( \| \theta \| = \Omega(1) \), which also implies that \( \| \theta \| - \alpha \tau^2 \epsilon = \Omega(1) \) for appropriately small \( \epsilon \). Hence, the running time for the applications will be \( O(\tau(C_U + \log \tau)) \). In the worst case, \( C_U \) could be at most \( \tau C_V \), but we will see that in fact in many cases we can implement \( U \) with basically the same cost as \( V \) (i.e. \( C_U = O(C_V + \log \tau) \)) and hence get an overall running time \( O(\tau(C_U + \log \tau)) \), the proof is given in Section 4.4.

4 Improved quantum algorithms for matrix multiplication and linear systems

In sections 4.1 and 4.2 we generalize the data structure and quantum algorithm used for singular value estimation in [11] obtaining an improvement in the running time for several classes of matrices. We use the improved singular value estimation algorithm for solving quantum linear systems and quantum matrix multiplication in section 4.3. Finally, in section 4.4 we show how to implement a single step of the quantum iterative method described in section 4.

4.1 The data structure

We first define normalized states and then describe a data structure that enables efficient preparation normalized states corresponding to the rows/columns of a matrix.

**Definition 4.1.** The normalized vector state corresponding to vector \( x \in \mathbb{R}^n \) and \( M \in \mathbb{R} \) such that \( \| x \|_2^2 \leq M \) is the quantum state \( |\bar{x}\rangle = \frac{1}{\sqrt{M}} \sum_{i \in [n]} x_i |i\rangle + (M - \| x \|_2^2)^{1/2} |n + 1\rangle \).

We work in a computational model where the entries of the matrix \( A \) arrive in an online manner and are stored in a classical data structure, where a quantum algorithm has quantum access. This is the normal quantum query model, used for example for Grover’s algorithm. The insertion and update times for the data structure are poly-logarithmic per entry. The time required to construct the data structure is \( O(w \log^2 mn) \) where \( w \) is the number of non-zero entries in \( A \). We have the following theorem.

**Theorem 4.2.** Let \( A \in \mathbb{R}^{m \times n} \) and \( M = \max_{i \in [m]} \| a_i \|_2^2 \). There is an algorithm that given a list of matrix entries \((i,j,a_{ij})\) of length \( w \), creates a data structure of size \( O(w \log mn) \) in time \( O(w \log^2 mn) \) such that a quantum algorithm with quantum access to the data structure can implement the following unitary in time \( O(\log(mn)) \).

\[
U |i, 0|^{\log(n+1)}\rangle = |i\rangle \frac{1}{\sqrt{M}} \left( \sum_{j \in [n]} a_{ij} |j\rangle + (M - \| a_i \|_2^2)^{1/2} |n + 1\rangle \right)
\] (3)

**Proof.** The data structure maintains an array of \( m \) binary trees \( B_i, i \in [m] \) one for each row of the matrix. The leaf node \( j \) of tree \( B_i \), if present, stores \((a_i^2, \text{sign}(a_{ij}))\). An internal node \( u \) stores the sum of the values of the leaf nodes in the subtree rooted at \( u \). In addition, there is an extra node
$M$ that, at any instant of time stores the maximum row norm $M = \max_{i \in [m]} \|a_i\|^2$ for the matrix $A$ currently stored in the data structure.

The data structure is initially empty and the value stored in node $M$ is 0. We next describe the update when entry $(i, j, a_{ij})$ is added to the data structure and then the procedure for implementing the unitary $U$ in (3) using the data structure.

The algorithm on receiving entry $(a_{ij}, i, j)$ creates the leaf node $j$ in tree $B_i$ if not present and updates it otherwise. Then, it creates or updates the value of all nodes in the path between the leaf and the root of the tree. The update requires time $O(\log^2 mn)$ as at most $O(\log n)$ nodes on the path from node $j$ to the root in the tree $B_i$ are updated and each update requires time $O(\log mn)$ to find the address of the node being updated. At the end of each update the root of $B_i$ stores the squared norm $\|a_i\|^2$ for the vector stored in $B_i$. The algorithm compares $M$ with $\|a_i\|^2$ and updates the maximum if $\|a_i\|^2 > M$, this additional step requires time $O(\log n)$.

The time needed to construct the data structure is $O(w \log^2 mn)$ as there are $w$ updates each taking $O(\log^2 mn)$ time, and the space required is $O(w \log mn)$. After the data structure has been created the value stored in $M = \max_{i \in [m]} \|a_i\|^2$. In order to implement $U$ we first perform a controlled rotation using the values at $M$ and the root of $B_i$ and tag the part of the superposition with value $|n + 1\rangle$,

$$|i, 0^{\log(n+1)}\rangle \rightarrow |i\rangle \frac{1}{\sqrt{M}} (\|a_i\| |0^{\log(n+1)}\rangle |0\rangle + (M - \|a_i\|^2)^{1/2} |n + 1\rangle |1\rangle) \quad (4)$$

We then proceed similarly to the construction in [11]. Let $B_{i,k}$ be the value of an internal node $k$ of tree $B_i$ at depth $t$. We apply a series of conditional rotations to the second register, conditioned on the first register being $|i\rangle$, the first $t$-qubits of the second register being $|k\rangle$ and the tag qubit being $|0\rangle$, the rotation applied is:

$$|i\rangle |k\rangle |0\rangle \rightarrow |i\rangle |k\rangle \frac{1}{\sqrt{B_{i,k}}} (\sqrt{B_{i,2k}} |0\rangle + \sqrt{B_{i,2k+1}} |1\rangle)$$

We take positive square roots except for the leaf nodes where the sign of the square root is the same as $\text{sign}(a_{ij})$ of the entry stored at the leaf node. The tag qubit is uncomputed after all the conditional rotations have been performed by mapping $|n + 1\rangle |1\rangle$ to $|n + 1\rangle |0\rangle$.

Correctness follows since conditioned on the tag qubit being $|0\rangle$ the conditional rotations produce the state $\sqrt{\frac{1}{M\|a_i\|}} \sum_j a_{ij} |j\rangle$ and the amplitude for the tagged part is $\sqrt{(M - \|a_i\|^2)/M}$ matching the amplitudes in equation (3). The time for implementing $U$ is $\tilde{O}(\log mn)$ as the number of quantum queries to the data structure is $O(\log mn)$ and each query takes poly-logarithmic time.

\section{Improved Singular Value Estimation}

We first recall the notion of singular value estimation,

\textbf{Definition 4.3.} Let $A = \sum_i \sigma_i u_i v_i^\dagger$ be the singular value decomposition for matrix $A \in \mathbb{R}^{m \times n}$. A quantum algorithm estimates the singular values of $A$ with precision $\delta$ if it transforms $\sum_i \beta_i |v_i\rangle \rightarrow \sum_i \beta_i |v_i\rangle |\sigma_i\rangle$ where $|\sigma_i - \sigma_i| \leq \delta$ for all $i \in [n]$ with probability $1 - 1/poly(n)$.

The theorem below provides a generalized quantum walk algorithm for singular value estimation. It extends the SVE algorithm from [11] and the quantum walk algorithms used for linear systems, for example [7].
Theorem 4.4. Let \( A \in \mathbb{R}^{m \times n} \) be a matrix and suppose there exist \( P, Q \in \mathbb{R}^{m \times n} \) and \( \mu > 0 \) such that \( \| p_i \|_2 \leq 1 \forall i \in [m], \| q^j \|_2 \leq 1 \forall j \in [n] \) and
\[
A/\mu = P \circ Q.
\] (5)

If unitaries \( U : |i\rangle |0[^{\log(n+1)}]\rangle \rightarrow |i\rangle |\bar{p}_i\rangle \) and \( V : |0[^{\log(m+1)}]\rangle |j\rangle \rightarrow |\bar{p}^j\rangle |j\rangle \) can be implemented in time \( \tilde{O}(\log(mn)) \) then there is a quantum algorithm that estimates the singular values of \( A \) with precision \( \delta \) in time \( \tilde{O}(\mu/\delta) \).

Proof. Let \( \bar{P}, \bar{Q} \in \mathbb{R}^{(m+1) \times (n+1)} \) be matrices with rows and columns respectively equal to the normalized states \( \bar{p}_i, \bar{p}^j \) for \( i \in [m], j \in [n] \) and an additional row or column \( \bar{p}_{m+1} = e_{m+1}, \bar{p}^{n+1} = e_{n+1} \). Let \( \overline{A} = \begin{pmatrix} A & 0 \\ 0 & \mu \end{pmatrix} \) be an extension of \( A \) of size \( (m+1) \times (n+1) \) so that the factorization \( \overline{A}/\mu = \bar{P} \circ \bar{Q} \) holds. The singular value decomposition of \( \overline{A} \) is \( \sum_i \sigma_i \bar{u}_i \bar{v}_i^t + \mu e_{m+1} e_{n+1} \) where \( \sigma_i \) are singular values for \( A \) and the singular vectors \( \bar{u}_i, \bar{v}_i \) are obtained by appending an additional 0 coordinate to the singular vectors \( u_i, v_i \) of \( A \).

The operators \( \bar{P} \in \mathbb{R}^{(m+1)(n+1) \times (m+1)}, \bar{Q} \in \mathbb{R}^{(m+1)(n+1) \times (n+1)} \) are defined as follows,
\[
\bar{P} |i\rangle = |i\rangle |\bar{p}_i\rangle, \quad \bar{Q} |j\rangle = |\bar{p}^j\rangle |j\rangle.
\] (6)

The columns of \( \bar{P}, \bar{Q} \) are orthogonal unit vectors so we have \( \bar{P}^t \bar{P} = I_{m+1} \) and \( \bar{Q}^t \bar{Q} = I_{n+1} \). Multiplication by \( \bar{P}, \bar{Q} \) can be implemented efficiently using the unitaries \( U, V \) in the theorem statement, we illustrate below for multiplication by \( \bar{P} \).

\[
|z\rangle \rightarrow |z, 0[^{\log(n+1)}]\rangle \xrightarrow{\bar{U}} \sum_{i \in [n+1]} z_i |i, \bar{p}_i\rangle = |ar{P}z\rangle
\] (7)

The unitary \( \bar{U} \) acts as \( U \) conditioned on \( 0 \leq i \leq m \) and maps \( |0[^{\log(n+1)}]\rangle \rightarrow |e_{n+1}\rangle \) for \( i = m+1 \). Multiplication by \( Q \) can be implemented similarly using \( \bar{V} \), thus the reflections \( 2\bar{P} \bar{P}^t - I \) and \( 2\bar{Q} \bar{Q}^t - I \) can be performed in time \( \tilde{O}(\log(mn)) \).

Finally, the factorization \( \bar{P}^t \bar{Q} = \overline{A}/\mu \) implies that the unitary \( W = (2\bar{P} \bar{P}^t - I)(2\bar{Q} \bar{Q}^t - I) \) has eigenspaces \( \text{Span}(\bar{P} \bar{u}_i, \bar{Q} \bar{v}_i) \) with eigenvalues \( e^{\theta_i} \), such that \( \cos(\theta_i/2) = \sigma_i/\mu \) and hence phase estimation for \( W \) on \( |\bar{Q} \bar{v}_i\rangle \) recovers an estimate of \( \sigma_i \) up to additive error \( \delta \) in time \( \tilde{O}(\mu/\delta) \).

\[ \square \]

Theorem 4.4 holds for any choice of \( P, Q \) such that \( A/\mu = P \circ Q \) provided the unitaries \( U \) and \( V \) can be implemented efficiently in time \( \tilde{O}(\log mn) \), that is if the normalized states corresponding to the rows of \( P \) and the columns of \( Q \) can be prepared efficiently. We show that the data structure in Theorem 4.2 allows us to implement \( U, V \) for the following choice of \( P \) and \( Q \).

\[
p_{ij} = \frac{a_{ij}^p}{\max \|a_i\|_{2p}}, \quad q_{ij} = \frac{a_{ij}^{1-p}}{\max \|a^j\|_{2(1-p)}}
\] (8)

Indeed, in order to implement the unitaries \( U \) and \( V \) corresponding to this choice of \( P, Q \), we create two copies of the data structure in Theorem 5.2 that respectively store the rows and the columns of \( A \). Given entry \((i, j, a_{ij})\) instead of \( a_{ij} \), we store \( a_{ij}^p \) and \( a_{ij}^{1-p} \) in the two data structures. Then, Theorem 5.2 implies that the unitaries \( U, V \) can be implemented efficiently.
We therefore obtain quantum algorithms for singular value estimation that are parametrized by $p \in [0, 1]$. The normalization factors are $\mu_p(A) = \sqrt{s_{2p}(A)s_{2(1-p)}(A^t)}$, where we denote by $s_p(A) := \max_{i \in [m]} \|a_i\|^p$ the maximum $\ell_p$ of the row vectors, and by $s_p(A^T)$ the maximum $\ell_p$ norm of the column vectors. Note that the SVE algorithm \[11\] corresponds to the choice $p_{ij} = \frac{a_{ij}}{\|a_i\|}$ and $q_{ij} = \frac{\|a_i\|}{\|A\|_F}$ and has $\mu(A) = \|A\|_F$.

**Theorem 4.5.** Let $A \in \mathbb{R}^{m \times n}$ be stored in the data structure of Theorem 4.2. There is a quantum algorithm that performs singular value estimation for $A$ to precision $\delta$ in time $\tilde{O}(\mu(A)/\delta)$ where

$$\mu(A) = \min_{p \in [0, 1]} \left( \|A\|_F, \sqrt{s_{2p}(A)s_{2(1-p)}(A^t)} \right).$$

Note that the optimal value of $p$ depends on the matrix $A$. One important case is when we consider a symmetric matrix $A$ and $p = 1/2$ and obtain $\mu(A) \leq s_1(A)$, showing that $\mu(A)$ is at most the maximum $\ell_1$-norm of the row vectors.

The generalized singular value estimation is stated next as Algorithm 4.1 using notation as in the proof of Theorem 4.4.

**Algorithm 4.1** Generalized quantum singular value estimation.

**Require:** $A \in \mathbb{R}^{m \times n}$, $x \in \mathbb{R}^n$, efficient implementation of unitaries $U, V$ in Theorem 4.4. Precision parameter $\epsilon > 0$.

1. Create $|x\rangle = \sum_{i \in [n]} \alpha_i |v_i\rangle$. Append a first register $|0^{\lceil\log(m+1)\rceil}\rangle$ and apply unitary $\tilde{V}$ to create the state $|\tilde{Q}x\rangle = \sum_i \alpha_i |\tilde{Q}v_i\rangle$.

2. Perform Phase Estimation with precision $2\epsilon > 0$ on input $|\tilde{Q}x\rangle$ for the unitary $W$ in Theorem 4.4.

3. Compute $\sigma_i = \cos(\tilde{\theta}_i/2)\mu(A)$ where $\tilde{\theta}_i$ is the estimate from Phase Estimation, and uncompute the output of the Phase Estimation to obtain $\sum_i \alpha_i |\tilde{Q}v_i, \sigma_i\rangle$.

4. Apply the inverse of $\tilde{V}$ to multiply the first register with the inverse of $\tilde{Q}$ and obtain $\sum_i \alpha_i |v_i\rangle |\sigma_i\rangle$.

### 4.3 Quantum matrix multiplication and linear systems

We provide algorithms for quantum linear systems and quantum matrix multiplication using the improved singular value estimation algorithm. We will see that once we perform singular value estimation for a matrix $A$, then multiplication with the matrix consists of a conditional rotation by an angle proportional to each singular value. Similarly, solving the linear system corresponding to the matrix $A$ is a multiplication with the inverse of $A$, in other words a conditional rotation by an angle proportional to the inverse of each singular value of $A$.

The two algorithms are therefore very similar. We will also extend our matrix multiplication algorithm, i.e. the application of a linear operator, to the case of an affine operator, namely, given matrix $A$ and vector $b$ in memory, the algorithm maps any state $|x\rangle$ to a state close to $|Ax + b\rangle$. Last, we discuss briefly the cases for which our algorithm improves upon the running time of existing quantum linear system solvers.
If \( A \in \mathbb{R}^{m \times n} \) is a rectangular matrix, then multiplication by \( A \) reduces to multiplication by the square symmetric matrix \( A' = \begin{pmatrix} 0 & A \\ A^t & 0 \end{pmatrix} \) as \( A'(0^m, x) = (Ax, 0) \). Therefore, without loss of generality we restrict our attention to symmetric matrices for the quantum matrix multiplication problem. Since, the matrix multiplication algorithm \ref{alg:matrix-multiplication} will be used for implementing a single step of the iterative method, and in that case we multiply by a positive semidefinite matrix \( A \) that is also contractive, we state the quantum matrix multiplication algorithm \ref{alg:matrix-multiplication} for such matrices. Note that linear systems for general symmetric matrices are not much harder than the case described in Algorithm \ref{alg:matrix-multiplication}.

**Algorithm 4.2** Quantum matrix multiplication/linear systems.

**Require:** Vector \( x = \sum_i \beta_i |v_i \rangle \in \mathbb{R}^n \) and matrix \( A \in \mathbb{R}^{n \times n} \) such that \( A \succeq 0 \) stored in the data structure, such that eigenvalues of \( A \) lie in \([1/\kappa, 1] \).

1. Perform singular value estimation with precision \( \epsilon_1 \) for \( \sum_i \beta_i |v_i \rangle \) to obtain \( \sum_i \beta_i |v_i \rangle | \lambda_i \rangle \).
2. Perform a conditional rotation and uncompute the SVE register to obtain the state:
   - (i) \( \sum_i \beta_i |v_i \rangle (\lambda_i |0 \rangle + \gamma |1 \rangle) \) for matrix multiplication.
   - (ii) \( \sum_i \beta_i |v_i \rangle (\frac{\lambda_i}{\lambda_i} |0 \rangle + \gamma |1 \rangle) \) for linear systems.
3. Perform Amplitude Amplification with the unitary \( V \) implementing steps 1 and 2, to obtain (i) \( |z \rangle = \sum_i \beta_i |\lambda_i \rangle |v_i \rangle \) or (ii) \( |z \rangle = \sum_i \beta_i |\lambda_i \rangle |v_i \rangle \).

Note that as in the analysis of the HHL algorithm \cite{HHL10}, the parameter \( \kappa \) does not have to be as big as the true condition number of \( A \). If \( \kappa \) is smaller, then it means that we invert only the well conditioned part of the matrix. In the appendix, we also provide an algorithm to normalize the matrix \( A \) such that \( \|A\| \leq 1 \). Let us analyze the correctness and running time of the above algorithm.

**Theorem 4.6.** Algorithm \ref{alg:matrix-multiplication} produces as output a state \( |z \rangle \) such that \( \|Ax - |z\rangle\| \leq \delta \) in expected time \( \tilde{O}(\frac{\kappa(A)\mu(A)}{\delta} \kappa(A)) \) for both matrix multiplication and linear systems.

**Proof.** We first analyze matrix multiplication. The unnormalized solution state is \( Ax = \sum_i \beta_i \lambda_i v_i \), while the unnormalized output of the algorithm is \( z = \sum_i (\lambda_i \pm \epsilon_i) \beta_i v_i \) for \( |\epsilon_i| \leq \epsilon_1 \). As the \( v_i \) are orthonormal, we have \( \|Ax - z\| \leq \epsilon_1 \|x\| \) and by Claim \ref{claim:svd-bound} we have \( \|Ax - |z\rangle\| \leq \sqrt{2\epsilon_1 \kappa(A)} \).

We next analyze linear systems. The unnormalized solution state is \( A^{-1}x = \sum_i \frac{\beta_i}{\lambda_i} v_i \). The unnormalized output is \( z = \sum_i \frac{\beta_i}{\lambda_i \pm \epsilon_i} v_i \) for \( |\epsilon_i| \leq \epsilon_1 \). We have the bound

\[
\|A^{-1}x - z\|^2 \leq \sum_i \beta_i^2 \left( \frac{1}{\lambda_i} \pm \frac{1}{\lambda_i} \right)^2 \leq \epsilon_1^2 \sum_i \frac{\beta_i^2}{\lambda_i^2 (\lambda_i - \epsilon_1)^2} \leq \frac{\epsilon_1^2 \kappa(A)^2 \|A^{-1}x\|^2}{(1 - \kappa(A)\epsilon_1)^2} \leq 4\epsilon_1^2 \kappa(A)^2 \|A^{-1}x\|^2
\]

\footnote{More precisely, the Singular Value Estimation procedure estimates the absolute value of the eigenvalues \( |\lambda_i| \) for a symmetric \( A \), and hence we also need to recover the sign of the lambda_i to perform matrix multiplication or to solve linear systems. The sign can be recovered by performing singular value estimation for the matrices \( A, A + \mu I \) and comparing the estimates \( |\lambda_i|, |\lambda_i + \mu| \). If \( \lambda_i \) is positive the second estimate is larger while if it is negative the first estimate is larger. Such a method for sign recovery was presented in \cite{BCW12} where it was used to construct a quantum linear system solver that corresponds to the case \( \mu(A) = \|A\|_F \).}
assuming that $\kappa(A)\epsilon_1 \leq 1/2$. Applying Claim 2.2 we obtain $\|A^{-1}x\| - |z|\| \leq 2\sqrt{2}\kappa(A)\epsilon_1$ for $\kappa(A)\epsilon_1 \leq 1/2$.

The running time bounds for the SVE in step 1 and 2 can be obtained by substituting the above error bounds for $\delta$. In addition, we perform Amplitude Amplification as in claim 2.2 with the unitary $V$ that represents the first two steps of the algorithm, this incurs on expectation a multiplicative overhead of $O(\kappa(A))$ over the cost of $V$.

Let us compare the new linear systems algorithm to the HHL algorithm. First, note that the quantum linear system problem is invariant under rescaling of $A$, thus we are free to choose a normalization for $A$. A quantum walk algorithm estimates the singular value $\sigma$ of a matrix by mapping the singular value to $\cos(\theta)$ for some $\theta \in [0, \pi]$ and then estimating $\cos(\theta)$. It is natural to use the normalization $\|A\| = 1$ as the eigenvalues being estimated have been scaled down to quantities in $[0, 1]$.

The HHL algorithm [10, 9] under the assumption that $A$ is a Hermitian matrix with eigenvalues in range $[-1, 1/\kappa] \cup [1/\kappa, 1]$ produces the state $|A^{-1}b\rangle$ and an estimate for $\|A^{-1}b\|$ in time $\tilde{O}(s^2(A)\kappa^2)$ where $s(A)$ is the number of non zero entries per row. Subsequent work has improved the running time to linear in both the condition number $\kappa(A)$ and the sparsity $s(A)$ [7, 2]. Our running time is quadratic on the condition number, like that of the HHL algorithm, we expect that the running time of our algorithm can also be improved to be linear on the condition number.

More importantly, instead of the sparsity $s(A)$ of the matrix, our running time depends on the parameter $\mu(A)$. On one hand, this factor is smaller than the Frobenius norm, for which we have $\|A\|_F = (\sum_i \sigma_i^2)^{1/2} \leq \sqrt{rk(A)}$. Hence, our algorithm 4.2 achieves an exponential speedup even for dense matrices whose rank is poly-logarithmic in the matrix dimensions. Moreover, for general dense matrices the sparsity is $\Omega(n)$, we have $\mu(A) \leq \|A\|_F \leq \sqrt{n}$ and thus we have a worst case quadratic speedup over the HHL algorithm.

In addition, the factor $\mu(A)$ is smaller than the maximum $\ell_1$-norm $s_1(A)$ which is always smaller than the maximum sparsity $s(A)$ when we take the normalization that $\|A\|_{max} = 1$, that is the entries of $A$ have absolute value at most 1. This is the normalization used in [7, 2], and we therefore also improve on the linear system solver in [7], whose running time depends on $s(A)$.

For example, real-valued matrices with most entries close to zero and a few entries close to 1, e.g. small perturbations of permutation matrices, will have $s(A) = \Omega(n)$, $\|A\|_F = \omega(\sqrt{n})$ but could have $s_1(A) = O(1)$ for small enough perturbations.

Last, there are also matrices with bounded spectral norm for which Algorithm 4.2 requires time $\Omega(\sqrt{n})$, for example consider a random sign matrix $A$ with $\|A\| = 1$. In this case, one can easily show that with high probability $\mu(A) = \Omega(\sqrt{n})$.

The optimal value $\mu(A) = \min_{\mu\{P \circ Q = A/\mu \mid \|p_i\|, \|q_i\| \leq 1\}}$ in Theorem 4.4 is the spectral norm of $|A|$ where $|A|$ is the matrix obtained by replacing entries of $A$ by their absolute values [10]. We recall that the matrix $A \in \mathbb{R}^{m \times n}$ has unique positive left and right eigenvectors, these eigenvectors are called the Perron-Frobenius eigenvectors and can be computed for example by iterating $x_{i+1} = Ax_i/\|Ax_i\|$. The optimal walk can be implemented efficiently if the coordinates of the Perron-Frobenius eigenvectors for $|A|$ are stored in memory prior to constructing the data structure. This is exactly the quantum walk that is also used in [6].

Hence, if one can precompute the Perron-Frobenius eigenvectors, for example if the matrix is stochastic it is the all ones vector, one can perform this optimal walk. However, the entries of the Perron-Frobenius eigenvector can not be computed in a single pass over a stream of the matrix entries, and hence the optimal walk can not be implemented in our model where we have quantum
access to a data structure built in linear time from a stream of matrix entries. We also note that the spectral norm of $|A|$ can be much larger than the spectral norm of $A$, for example for a random sign matrix with $\pm 1$ entries the spectral norm of $A$ is $\|A\| = O(\sqrt{n})$ but the spectral norm of $|A|$ is $\||A|| = n$. Thus there are two interesting questions about quantum linear system solvers, the first is to find the optimal quantum linear system algorithm given access to a data structure built from a stream of matrix entries and the second to find if there can exist more general quantum walk algorithms with $\mu(A) = \|A\|$, the latter is also stated as an open problem in [6].

4.4 The iterative step

We now show that the $(\epsilon,\delta)$-approximate quantum step for the iterative method in Definition 3.1 can be implemented using the quantum matrix multiplication algorithm presented above. The matrix $S$ for iterative methods corresponding to linear systems and least squares is of the form $S = I - \alpha A$ for a positive semidefinite matrix $A$. Further, we can assume that the matrix $A$ is stored in the data structure of Theorem 4.2 and that $S$ is positive semi-definite and contractive.

Proposition 4.7. The $(\epsilon,\delta)$-approximate quantum step for the iterative method with $S = I - \alpha A$ and $L(x) = b - Ax$ with $\|b\| = 1$, $\alpha \leq 1$, and for $A$ stored in the data structure of Theorem 4.2, can be implemented in time $O(\mu(A)b/\epsilon)$, where $A|b$ is the matrix $A$ to with an extra row equal to $b$.

Proof. We show how to implement the unitary $V$ in the iterative method,

$$V : |0\rangle |r_0\rangle |0\rangle \rightarrow |1\rangle \left( \alpha \|L(r_0)\| |\tilde{L}(r_0)\rangle |0\rangle + |G_1\rangle |1\rangle \right)$$

$$= |t\rangle \|r_t\| |r_t\rangle |0\rangle \rightarrow |t+1\rangle \left( \|\tilde{S}(r_t)\| |\tilde{S}(r_t)\rangle |0\rangle + |G_{t+1}\rangle |1\rangle \right),$$

where $|G_1\rangle , |G_{t+1}\rangle$ are unnormalised garbage states, such that with probability $\geq 1 - \delta$, it holds that $\|L(r_0) - \tilde{L}(r_0)\| \leq \epsilon$ and $\|S(r_t) - \tilde{S}(r_t)\| \leq \epsilon$. We first implement the linear part of $V$ that corresponds to $1 \leq t \leq \tau - 1$ and then the affine part corresponding to $t = 0$. We denote $r_t = \sum \beta_i |v_i\rangle$.

The linear part of $V$ is implemented by performing singular value estimation for $A$ and then using $\overline{\lambda}_i = (1 - \alpha \overline{\lambda}_i(A))$ as estimates for singular values of $S$,

$$|t\rangle \|r_t\| |r_t\rangle |0\rangle \equiv |t\rangle \sum \beta_i |v_i\rangle |0\rangle \rightarrow |t+1\rangle \sum \beta_i |v_i\rangle \left( \overline{\lambda}_i |0\rangle + \sqrt{1 - \overline{\lambda}_i^2} |1\rangle \right) \quad (9)$$

If the precision for singular value estimation is $\epsilon$ then the algorithm runs in time $O(\mu(A)/\epsilon)$. For bounding the difference of the norms we observe that $\|S(r_t) - \tilde{S}(r_t)\| \leq \|\sum \beta_i \tilde{\epsilon}_i v_i\| \leq \alpha \epsilon \leq \epsilon$ as all the errors $\epsilon_i \leq \epsilon$ if singular value estimation succeeds and $\|\beta\| \leq 1$. The procedure succeeds if the singular value estimation algorithm produces the correct estimates so $1 - \delta = 1 - 1/poly(n)$, that is $\delta$ can be taken to be $1/poly(n)$.

The affine part of $V$ is implemented as follows. Let $A_1 = \begin{pmatrix} -A & b \\ 0 & 0 \end{pmatrix}$ and $x_1 = (x, 1)$ so that $A_1 x_1 = (b - Ax, 0)$. Then we symmetrize $A_1$ by defining $A' = \begin{pmatrix} 0 & A_1 \\ A_1^t & 0 \end{pmatrix}$ and $x' = (0^{n+1}, x_1)$, and have $A' x' = (A_1 x_1, 0) = (b - Ax, 0)$. The columns of $A'$ are stored in the memory data structure so we can perform SVE for $A'$. We take $x = r_0$ and use the SVE algorithm for symmetric matrices.
on \(r_0'\) (where we add an extra factor \(\alpha\) in the conditional rotation) to map it to \(A'r_0' = (b - Ar_0, 0)\) as the last coordinates become 0. Denote \(r_0' = \sum \beta_i |v_i'\rangle\), where \(v_i'\) are the eigenvectors of \(A'\).

\[
\lvert 0 \rangle \parallel r_0' \parallel r_0' \rangle \equiv \lvert 0 \rangle \sum \beta_i |v_i' \rangle \lvert 0 \rangle \rightarrow \lvert 1 \rangle \sum \beta_i |v_i \rangle \left( \alpha \lambda_i(A') \lvert 0 \rangle + \sqrt{1 - \alpha^2 \lambda_i(A')^2} \lvert 1 \rangle \right)
\]

If the precision for singular value estimation is \(\epsilon\) then the algorithm runs in time \(\tilde{O}(\mu(A')/\epsilon)\) and the correctness analysis is the same as above. We next provide an upper bound for \(\mu(A')\). We have \(\|A'\|_F \leq 2\|A\|_F + 2\|b\|\), while \(s_1(A') \leq \max(s_1(A) + \|b\|_\infty, s_1(b))\). Let’s assume for simplicity that \(\|b\| = 1\), which is the case in our applications, then the upper bound is \(O(\mu(A|b)\) where \(A|b\) is a matrix obtained by adding an extra row \(b\) to \(A\).

Finally, let us see how to implement unitary \(U\) as defined in the quantum iterative method with cost \(O(C_V + \log \tau)\) which is asymptotically the same as the cost of \(V\). It is easy to see that the complexity of \(U\) is asymptotically upper bounded by the complexity of applying the unitary \(V^\tau\) on \(\lvert 0 \rangle \lvert r_0 \rangle \lvert 0 \rangle\). For this we first apply \(V\) once to get the affine transformation (with running time \(\tilde{O}(\mu(A|b)/\epsilon)\)), then we apply the SVE procedure on \(A\) to obtain estimates \(\lambda_i\) of the eigenvalues of \(S = (I - \alpha A)\) and then compute \(\lambda_i^{-1}\) (in time \(O(\log \tau)\)) as the estimates for the singular values of \(ST^{-1}\) for the conditional rotation. This gives us the desired unitary and the running time of the second part is \(\tilde{O}(\mu(A)/\epsilon + \log \tau)\). Hence, the overall running time is \(O(C_V + \log \tau)\).

## 5 Quantum iterative algorithms

### 5.1 Linear systems

Let \(A \succeq 0\) be a \(n \times n\) psd matrix and \(b\) a unit vector in \(\mathbb{R}^n\). We can assume \(b\) to be a unit vector as it is stored in memory and we know \(\|b\|\). The goal is to solve the linear system \(A\theta = b\). The quadratic form \(F(\theta) = \theta^T A \theta - b\theta\) is minimized at the solution to \(A\theta = b\). The classical iterative method starts with an arbitrary \(\theta_0\) and applies the following updates,

\[
\theta_{t+1} = \theta_t + \alpha(b - A\theta_t) = \theta_t + \alpha r_t
\]

where the step size \(\alpha\) will be specified later and the residuals \(r_t = b - A\theta_t\) for \(t \geq 0\). The residuals satisfy the recurrence \(r_{t+1} = b - A(\theta_t + \alpha r_t) = (I - \alpha A)r_t\) and the initial condition \(r_0 = (b - A\theta_0)\).

In order to be consistent with the normalization used in quantum linear systems, we assume that the eigenvalues of \(A\) lie within the interval \([1/\kappa, 1]\). The convergence analysis and the choice of the step size \(\alpha\) follow from the following argument that bounds the norm of the error. Let \(\theta^* = A^{-1}b\) be the optimal solution, the error \(e_t := \theta_t - \theta^*\) satisfies the recurrence \(e_{t+1} = (\theta_{t+1} - \theta^*) = \theta_t - \theta^* + \alpha(b - A\theta_t) = e_t + \alpha A(\theta^* - \theta_t) = (I - \alpha A)e_t\). After \(t\) steps of the iterative method we have,

\[
\|e_t\| = \|(I - \alpha A)^t e_0\| \leq (1 - \alpha/\kappa)^t \|e_0\|.
\]

The iterative method therefore converges to within error \(\epsilon\) to the optimal solution \(\theta^*\) in \(\tau = O(\kappa \log(\|e_0\|/\epsilon)/\alpha)\) iterations. The step size \(\alpha\) can be fixed to be a small constant say \(\alpha = 0.01\) and the starting point \(\theta_0\) chosen to be a unit vector so that \(\|e_0\| \leq \kappa\). With these choices the method converges to within error \(\epsilon\) of the optimal solution in \(O(\kappa \log(\kappa/\epsilon))\) steps.
In order to bound the running time of the iterative method we need that $\|\theta_\tau\| = \Omega(1)$ for $\tau = O(\kappa \log(\kappa/\epsilon))$. The solution $A^{-1}b$ to the linear system has norm at least 1 as $b$ is a unit vector and the eigenvalues of $A^{-1}$ are greater than 1. After $\tau$ steps we have $\|\theta_\tau - \theta^\star\| \leq \epsilon \Rightarrow \|\theta_\tau\| \geq \|\theta^\star\| - \epsilon \geq 1 - \epsilon$.

The $(\epsilon, \delta)$ approximate iterative step can be implemented in time $C_V = \tilde{O}(\mu(A)b)/\epsilon)$ by Proposition 4.7. Note also that in this case, the cost of implementing $V^t$ is the same as that of implementing $V$. This is because we do not have to apply $V$ sequentially $t$ times, but once the SVE has estimated the eigenvalues we can directly perform the conditional rotations by an angle proportional to the $\|\theta^\star\| - \epsilon$.

The analysis in section 3.3.2 and the fact that $\alpha, \|\tilde{\theta}_\tau\|$ are constants, shows that given an $(\epsilon, \delta)$ approximate step, the quantum iterative algorithm has error $\|\|\theta_\tau\| - \|\tilde{\theta}_\tau\|\| = O(\tau^2 \epsilon)$ and requires time $O(\tau C_U) = O(\tau C_V) = O(\tau \mu(A)b)/\epsilon)$. We take $\epsilon = O(\frac{\delta}{\tau})$ in order to have $\|\|\theta_\tau\| - \|\tilde{\theta}_\tau\|\| \leq \delta$ for some $\delta > 0$. Then, we can take $\tau = \kappa(A) \log \frac{\kappa(A)}{\delta} \mu(A)b)$ to have that $\|\|\theta_\tau\| - \|A^{-1}b\|\| \leq \delta$. Hence, we have the following theorem.

**Theorem 5.1.** Given positive semidefinite $A \in \mathbb{R}^{n \times n}, b \in \mathbb{R}^n$ stored in memory, there is an iterative quantum algorithm that outputs a state $|z\rangle$ such that $\| |z\rangle - |A^{-1}b\rangle \| \leq 2\delta$ with expected running time $O(\frac{\kappa(A)^3 \log^3 \frac{\kappa(A)}{\delta} \mu(A)b)}{\delta})$.

### 5.2 Weighted Least Squares

For the weighted least squares problem, we are given a matrix $X \in \mathbb{R}^{m \times n}$ and a vector $y \in \mathbb{R}^m$, as well as a vector $w \in \mathbb{R}^m$ of weights, and the goal is to find $\theta \in \mathbb{R}^n$ that minimizes the squared loss $\sum_{i \in [m]} w_i (y_i - x_i^T \theta)^2$. The closed form solution is given by,

$$\theta = (X^T W X)^{-1} X^T W y$$

and thus the problem can also be solved using a direct method. The iterative method for weighted least squares is a gradient descent algorithm with the update rule $\theta_{t+1} = \theta_t + \rho \sum_{i \in [m]} w_i (y_i - x_i^T \theta_t) x_i$, which in matrix form can be written as,

$$\theta_{t+1} = (I - \rho X^T W X) \theta_t + \rho X^T W y$$  \hspace{1cm} (10)

The update can also be written as $\theta_{t+1} = \theta_t + \rho r_t$ where $r_t = X^T W y - X^T W X \theta_t$. Note that these updates are analogous to the linear system updates in section 5.1 as $r_t = b - A \theta_t$ for $b = X^T W y$ and $A = X^T W X$. The step size $\rho$ is analogous to the $\alpha$ for the linear system and we assume the same scaling for $\alpha$ and $b$ as in the case of linear systems.

By the analysis of positive semidefinite linear system solvers in section 5.1 it follows that if we are able to implement the steps of the iterative method, the quantum iterative algorithm for weighted least squares has the following running time.

**Theorem 5.2.** Let semidefinite $X \in \mathbb{R}^{m \times n}, y \in \mathbb{R}^n, w \in \mathbb{R}^m$ stored in memory and define $W = \text{diag}(w)$, $A = X^T W X$ and $b = X^T W y$. There is an iterative quantum algorithm that outputs a state $|z\rangle$ such that $\| |z\rangle - |A^{-1}b\rangle \| \leq 2\delta$ with expected running time $O(\frac{\kappa(A)^3 \log^3 \frac{\kappa(A)}{\delta} \mu(\text{diag}(W) x y)}{\delta})$.

We now show how to implement the iterative step for the least squares problem, which is somewhat different from the case of linear systems as instead of the matrix $X^T W X$ and the vector $X^T W y$, the updated matrix is $X^T W X$ and the vector is $X^T W y$. In this case, the cost of implementing $X^T W X$ is $O(mn)$ and the cost of implementing $X^T W y$ is $O(mn)$. The total cost of implementing the iterative step is $O(mn) + O(mn) = O(mn)$. Therefore, the total running time of the quantum iterative algorithm for weighted least squares is $O(mn) + O(mn) = O(mn)$.
we have the matrix $X$ and the vectors $w$ and $y$ stored in memory. Nevertheless, the iterative step can be implemented in this setting as we show next.

Note that $A = B^T B$ where $B = \sqrt{W} X$, thus the eigenvalues of $A$ are the squared singular values of $B$, hence it suffices to perform the generalized SVE for $B$. We assume that the data structures for performing generalized SVE for $X$ have been created. The weights $w_i, i \in [m]$ are also stored in memory.

We maintain the variable $M_w$ that stores $\max_i w_i \|x_i\|^2$ and is updated whenever $w_i$ arrives or $\|x_i\|$ gets updated, that is if $M_w \leq w_i \|x_i\|^2$ then set $M_w = w_i \|x_i\|^2$. We replace $M \rightarrow M_w$ and $\|x_i\| \rightarrow \sqrt{w_i} \|x_i\|$ in the computation in equation (4) and follow the same steps in Theorem 4.2 to implement the unitary,

$$U' |i, 0[^{\log(n+1)}] = |i\rangle \frac{1}{\sqrt{M_w}} \left( \sum_{j \in [n]} \sqrt{w_{ij}} |j\rangle + (M_w - w_i \|x_i\|^2)^{1/2} |n+1\rangle \right)$$

Using $U', V$ instead of $U, V$ in Theorem 4.3 we can perform generalized SVE for $B = \sqrt{W} X$ in time $\mu(B)$. In order to multiply by $A$ for the iterative method, we perform generalized SVE for $B$ in equation (4) and then conditional rotation with factor $\alpha \sigma^2$.

Analogous to the above procedure one can also implement matrix multiplication for $B' = X^T W$. Note that the state $|b\rangle$ is not in the memory, so we can not do the first affine update used for linear systems (where we set $r_0 = b - A\theta_0$ for a random $\theta_0$). Instead we have $y$ and $X$ in memory, so we first do the affine step to create $(y - X\theta_0)$ and then multiply with the matrix $X^T W$,

$$b - A\theta_0 = X^T W y - X^T W X \theta_0 = X^T W (y - X\theta_0)$$

It is straightforward to add $\ell_2$ regularization to the weighted least squares problem. The loss function becomes $\sum_i w_i (y_i - \theta^T x_i)^2 + \lambda \|\theta\|^2$ and the update rule changes to $r_t = b - A\theta_t$ for $b = X^T W y$ and $A = X^T W X + \lambda I$. The algorithm therefore performs the generalized SVE for $X^T W X + \lambda I$ instead of $X^T W X$.

**Stochastic gradient descent for Weighted Least Squares:** It is prohibitive in practice to compute the gradient $\sum_{i \in [m]} w_i (y_i - \theta^T x_i) x_i$ by summing over the entire dataset when the dataset size is large. Moreover, due to redundancy in the dataset the gradient can be estimated by summing over randomly sampled batches. Stochastic gradient descent utilizes this fact in the classical setting to lower the cost of the updates. Stochastic gradient descent algorithms do not compute the gradient exactly, but estimate it over batches $\sum_{i \in S_j} w_i (y_i - \theta^T x_i) x_i$ obtained by randomly partitioning the dataset.

We could expect similar issues for the quantum case where a large dataset would require more memory capacity and controlled operations over a large number of qubits. Stochastic gradient descent therefore remains relevant for quantum iterative methods as well.

The stochastic gradient updates are defined for any choice of partition $\Pi = (S_1, S_2, \cdots, S_k)$. For a given partition $\Pi$ let $X_j$ be the the $|S_j| \times n$ matrix obtained by selecting the rows corresponding to $S_j$. Define $A_j = X_j^T W_j X_j$ where $W_j$ is the diagonal matrix of weights restricted to $S_j$. The residuals satisfy the recurrence $r_{t+1} = (I - \rho A_t') r_t$ where $t' = t \ mod \ k$ and the initial condition $r_0 = (b - A_1 \theta_0)$. All these updates can be implemented efficiently as the matrices $S_j$ are stored in memory. The running time will be linear in $\mu = \max_{i \in [k]} \mu(S_i)$. 

24
In the case of linear systems and least squares, the updates were of the form \( r_{t+1} = (I - \rho A) r_t \) for a fixed matrix \( A \), and hence we could apply simultaneously \( t \) steps of the update in one step and hence have that the running time is \( O(\tau C_V) \). In the stochastic gradient descent case, we have different matrices \( A_t \) for each time step which have different eigenbases. Therefore, we can only perform the linear updates sequentially, and hence the running time for the stochastic gradient descent is \( O(\tau^2 C_V) \) as opposed to \( O(\tau C_V) \) for the linear systems and weighted least squares.

Here, we provided two applications of our quantum gradient descent method, psd linear systems and stochastic gradient descent for weighted least squares. It would be interesting to find generalizations and further applications of the quantum gradient descent algorithm and to develop second order quantum iterative methods.

Acknowledgements:

IK was partially supported by projects ANR RDAM, ERC QCC and EU QAlgo. AP was supported by the Singapore National Research Foundation under NRF RF Award No. NRF-NRFF2013-13. We thank Robin Kothari for bringing reference [16] to our attention.

References

[1] S. Aaronson, “Read the fine print,” Nature Physics, vol. 11, no. 4, pp. 291–293, 2015.
[2] A. Ambainis, “Variable time amplitude amplification and quantum algorithms for linear algebra problems,” in STACS’12 (29th Symposium on Theoretical Aspects of Computer Science), vol. 14. LIPIcs, 2012, pp. 636–647.
[3] L. Bottou, F. E. Curtis, and J. Nocedal, “Optimization methods for large-scale machine learning,” arXiv preprint arXiv:1606.04838, 2016.
[4] F. G. Brandao and K. Svore, “Quantum speed-ups for semidefinite programming,” arXiv preprint arXiv:1609.05537, 2016.
[5] G. Brassard, P. Hoyer, M. Mosca, and A. Tapp, “Quantum amplitude amplification and estimation,” Contemporary Mathematics, vol. 305, pp. 53–74, 2002.
[6] A. M. Childs, “On the relationship between continuous-and discrete-time quantum walk,” Communications in Mathematical Physics, vol. 294, no. 2, pp. 581–603, 2010.
[7] A. M. Childs, R. Kothari, and R. D. Somma, “Quantum linear systems algorithm with exponentially improved dependence on precision,” arXiv preprint arXiv:1511.02306, 2015.
[8] L. Grover and T. Rudolph, “Creating superpositions that correspond to efficiently integrable probability distributions,” arXiv preprint quant-ph/0208112, 2002.
[9] A. W. Harrow, “Review of quantum algorithms for systems of linear equations,” arXiv preprint arXiv:1501.00008, 2014.
[10] A. W. Harrow, A. Hassidim, and S. Lloyd, “Quantum algorithm for linear systems of equations,” Physical review letters, vol. 103, no. 15, p. 150502, 2009.
A Spectral Norm Estimation

We assumed throughout the paper that the matrices $A$ are normalized such that the absolute value of the eigenvalues lie in the interval $[1/\kappa, 1]$. This is the same assumption as in [10]. We show here a simple quantum algorithm for estimating the spectral norm, which can be used to rescale matrices so that the assumption $\|A\| \leq 1$ is indeed valid. Note that $0 \leq \frac{\sigma_{\max}(A)}{\|A\|_F} \leq 1$. 

[11] I. Kerenidis and A. Prakash, “Quantum recommendation systems,” *Innovations in Theoretical Computer Science*, 2017.

[12] A. Y. Kitaev, “Quantum measurements and the abelian stabilizer problem,” *arXiv preprint quant-ph/9511026*, 1995.

[13] A. Y. Kitaev, A. Shen, and M. N. Vyalyi, *Classical and quantum computation*. American Mathematical Society Providence, 2002, vol. 47.

[14] S. Lloyd, M. Mohseni, and P. Rebentrost, “Quantum algorithms for supervised and unsupervised machine learning,” *arXiv preprint:1307.0411*, 2013.

[15] ——, “Quantum principal component analysis,” *Nature Physics*, vol. 10, no. 9, pp. 631–633, 2014.

[16] R. Mathias, “The spectral norm of a nonnegative matrix,” *Linear Algebra and its Applications*, vol. 139, pp. 269–284, 1990.

[17] K. P. Murphy, *Machine learning: a probabilistic perspective*. MIT press, 2012.

[18] P. Rebentrost, M. Mohseni, and S. Lloyd, “Quantum support vector machine for big data classification,” *Physical review letters*, vol. 113, no. 13, p. 130503, 2014.

[19] P. Rebentrost, M. Schuld, F. Petruccione, and S. Lloyd, “Quantum gradient descent and newton’s method for constrained polynomial optimization,” *arXiv preprint arXiv:1612.01789*, 2016.

[20] M. Szegedy, “Quantum speed-up of markov chain based algorithms,” in *Foundations of Computer Science, 2004. Proceedings. 45th Annual IEEE Symposium on*. IEEE, 2004, pp. 32–41.

[21] N. Wiebe, D. Braun, and S. Lloyd, “Quantum algorithm for data fitting,” *Physical review letters*, vol. 109, no. 5, p. 050505, 2012.

[22] L. Wossnig, Z. Zhao, and A. Prakash, “A quantum linear system algorithm for dense matrices.” *Arxiv preprint:1704.06174*, 2017.
Algorithm A.1 Spectral norm estimation.

Require: $A \in \mathbb{R}^{m \times n}$ stored in data structure in Theorem 4.2. Returns an estimate for $\eta := \sigma_{\max}(A)/\|A\|_F$ with additive error $\epsilon$.

1. Let $l = 0$ and $u = 1$ be upper and lower bounds for $\eta$, the estimate $\tau = (l + u)/2$ is refined using binary search in steps 2-5 over $O(\log 1/\epsilon)$ iterations.

2. Prepare $|\phi\rangle = \frac{1}{\|A\|_F} \sum_{i,j} a_{ij} |i,j\rangle = \frac{1}{\|A\|_F} \sum_{i,j} \sigma_i |u_i, v_i\rangle$ and perform SVE [11] with precision $\epsilon$ to obtain $\frac{1}{\|A\|_F} \sum_{i,j} \sigma_i |u_i, v_i, \sigma_i\rangle$. where $|\sigma_i - \sigma_i\rangle| \leq \epsilon$.

3. Append single qubit register $|R\rangle$ and set it to $|1\rangle$ if $\sigma_i \geq \tau$ and $|0\rangle$ otherwise. Uncompute the SVE output from step 2.

4. Perform amplitude estimation on $\sum_{i,j} \sigma_i |u_i, v_i, R\rangle$ conditioned on $R = 1$ to estimate $\sum_{i: \sigma_i \geq \tau} \sigma_i^2/\|A\|_F^2$ to relative error $(1 \pm \delta)$.

5. If estimate in step 4 is 0 then $u \rightarrow \tau$ else $l \rightarrow \tau$. Set $\tau = (u + l)/2$.

The following proposition proves correctness for Algorithm A.1 and bounds its running time.

**Proposition A.1.** Algorithm A.1 estimates $\eta$ to additive error $\epsilon$ in time $\tilde{O}(\log(1/\epsilon)/\epsilon \eta)$.

**Proof.** The running time for step 2 is $\tilde{O}(1/\epsilon)$ and that for the amplitude estimation in step 4 is $\tilde{O}(1/\epsilon \delta \eta)$ as the time $T(U) = \tilde{O}(1/\epsilon_1)$ and the amplitude being estimated is either 0 or at least $\eta^2$. We will see that $\delta$ can be chosen to be a small constant, the running time is $\tilde{O}(\log(1/\epsilon)/\epsilon \eta)$ as step 4 is repeated $\log(1/\epsilon)$ times.

For correctness, it suffices to show that if $|\tau - \eta| \geq \epsilon$ then the algorithm determines $sign(\tau - \eta)$ correctly. If $|\tau - \eta| \geq \epsilon$ then the amplitude $\sum_{i: \sigma_i \geq \tau} \sigma_i^2/\|A\|_F^2$ being estimated in step 4 is either 0 or at least $\eta^2$. Amplitude estimation yields a non-zero estimate in the interval $(1 \pm \delta)\eta$ for the latter case and thus the sign is determined correctly if $\delta$ is a small constant. \qed