Fast quantum learning with statistical guarantees

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Abstract

Within the framework of statistical learning theory it is possible to bound the minimum number of samples required by a learner to reach a target accuracy. We show that if the bound on the accuracy is taken into account, quantum machine learning algorithms—for which statistical guarantees are available—cannot achieve polylogarithmic runtimes in the input dimension. This calls for a careful revaluation of quantum speedups for learning problems, even in cases where quantum access to the data is naturally available.

1 Introduction

A wide class of quantum algorithms for learning problems exploit fast quantum linear algebra subroutines to achieve runtimes that are exponentially faster than their classical counterparts [Cil+18]. Examples of these algorithms are quantum support vector machines [RML14], quantum linear regression [WBL12; SSP16], and quantum least squares [KP17; CGJ18].

A careful analysis of these algorithms identified a number of caveats that limit their practical applicability such as the need for a strong form of quantum access to the input data, restrictions on structural properties of the data matrix (such as condition number or sparsity), and modes of access to the output [Aar15]. Furthermore, if one assumes that it is efficient to (classically) sample elements of the training data in a way proportional to their norm, then it is possible to show that classical algorithms are only polynomially slower (albeit the scaling of the quantum algorithms can be considerably better) [Tan18; CIW18; Chi+19a; GLT18; Chi+19b].

In this work we continue to investigate the limitations of quantum algorithms for learning problems. Our analysis focuses on the dependency on the size of the data set that is introduced when considering the statistical guarantees of the estimators. The key elements of our work are a series of well known results in statistical learning theory that show how the accuracy parameter of a supervised learning problem scales inverse polynomially with the number of samples in the training set. We leverage on these insights to show that quantum learning algorithms must have at least polynomial runtime in the dimension of the training data.

Our results are independent of the modes of access to the training data, that is, even if the data set is naturally stored in a quantum structure, quantum machine learning algorithms can have at most polynomial advantage over their classical variants.

We begin in Section 2 by reviewing key concepts and results in statistical learning theory. In Section 3 we discuss the main features of quantum algorithms for learning problems. In Section 4 we present our main result.
2 Statistical learning theory

Statistical learning theory quantifies the statistical resources required to solve a supervised learning problem. In this setting the goal is to find a model that fits well a set of training examples but that, more importantly, guarantees good prediction performance on new observations. This latter property, also known as generalisation capability of the learned model, is a key aspect separating machine learning from the standard optimisation literature. Indeed, while data fitting is often approached as an optimisation problem in practice, the focus of machine learning is to design statistical estimators able to ‘fit’ well future examples.

More formally, in supervised learning a learner receives a training set $S_n = \{(x_i, y_i), i = 1, \ldots, n\}$ i.i.d. sampled from an unknown probability distribution $\rho$ over the set $X \times Y$. $X$ is called the domain set and $Y$ the label set. The learning algorithm uses the labelled examples in $S_n$ to return a function $f$, known as hypothesis. The set of functions $\mathcal{H} = \{f : X \rightarrow Y\}$ that $A$ can output is called the hypothesis space.

The goal of supervised learning is to produce a hypothesis $f : X \rightarrow Y$ such that the expected risk or expected error

$$\mathcal{E}(f) := \mathbb{E}_\rho[\ell(y, f(x))]$$

is small with respect to a suitable loss function $\ell : Y \times Y \rightarrow \mathbb{R}$. Depending on whether the label set $Y$ is continuous or discrete the task is called regression (continuous) or classification (discrete). A common loss function for classification tasks where $Y = \{-1, 1\}$ is the $0-1$ loss $\ell_{0-1}(f(x), y) = 1_{f(x) \neq y}$. A common loss function for regression tasks where $Y = \mathbb{R}$ is the quadratic loss $\ell_{sq}(f(x), y) = (f(x) - y)^2$.

Because the distribution $\rho$ is unknown to the learner, it is not possible to compute the true risk. In machine learning one therefore uses the error on the training set, known as empirical risk,

$$\hat{\mathcal{E}}(f) := \frac{1}{n} \sum_{(x_i, y_i) \in T} \ell(y_i, f(x_i)),$$

as a proxy for the expected risk. Different machine learning frameworks have different prescriptions on how to choose the hypothesis $f$. The Empirical Risk Minimisation (ERM) framework prescribes to choose a hypothesis that minimises the empirical risk. If $|Y| < \infty$, there exists a minimiser $\hat{f} \in \mathcal{H}$ such that

$$\inf_{f \in \mathcal{H}} \hat{\mathcal{E}}(f) = \hat{\mathcal{E}}(\hat{f}).$$

If the size of the training set is sufficiently large it is possible to prove, under suitable assumptions on the hypothesis space, that minimising the empirical risk leads to an hypothesis that minimises the true risk. Bounds on the difference between risk and empirical risk are called generalisation bounds.

A fundamental result in statistical learning theory [VV98; Blu+89; SB14], often referred in the literature as the fundamental theorem of statistical learning, is that for every $\epsilon, \delta \in (0, 1)$, and every distribution $\rho$ over $X \times Y$ there exists a $m_\mathcal{H}(\epsilon, \delta)$ such that, with probability at least $1 - \delta$, for all $n \geq m_\mathcal{H}(\epsilon, \delta)$

$$\left| \mathcal{E}(\hat{f}) - \inf_{f \in \mathcal{H}} \mathcal{E}(f) \right| \leq \left| \hat{\mathcal{E}}(f) - \mathcal{E}(f) \right| \leq \epsilon. \quad (1)$$

It is also possible to prove that $m_\mathcal{H}(\epsilon, \delta)$, known as the sample complexity of $\mathcal{H}$, scales as

$$m_\mathcal{H}(\epsilon, \delta) = \Theta\left(\frac{c + \log(1/\delta)}{\epsilon^2}\right) \quad (2)$$
where $c$ is a measure of the complexity of $H$. From Eq. 2 we have that the optimal error for a dataset of size $n$ scales as

$$
\epsilon = \Theta \left( \frac{\sqrt{c + \log(1/\delta)}}{n} \right).
$$

Eq. 3 can be interpreted by saying that the optimal error scales as $1/\sqrt{n}$. Intuitively, the dependency on $c$ models the phenomenon known as overfitting in which a large hypothesis space describes well the training set but performs poorly on the true risk. This problem can be addressed with so-called regularisation techniques, which essentially limit the expressive power of the learned estimator in order to avoid overfitting the training dataset.

Different regularisation strategies have been proposed in the literature (see [VV98; Bis06; BPR07] for an introduction to the main ideas), and one of the well-established approaches which directly imposes constraints on the hypotheses class of candidate predictors is the Tikhonov regularisation. Regularisation ideas have led to popular machine learning approaches which are widely used in practice, such as Regularised Least Squares [CS02], Gaussian Process (GP) Regression and Classification [RW06], Logistic Regression [Bis06], and Support Vector Machines (SVM) [VV98]. All these algorithms can be studied within the framework of kernel methods [S+04].

From a computational perspective, these approaches compute a solution for the learning problem by optimising over the constraint objective, which typically consists of a sequence of standard linear algebra operations such as matrix multiplication and inversion. For most classical algorithms, such as GP or SVM, the computational time is therefore $O(N^3)$, which is similar to the time it requires to invert a square matrix that has size equal to the number $N$ of examples in the training set. Notably this can be improved depending on the sparsity and the conditioning of the specific optimisation problem.

To reduce the computational cost, instead of considering the optimisation problem as a separate process from the statistical one, more recent methods hinge on the intuition that reducing the computational burden of the learning algorithm can be interpreted as a form of regularisation on its own. For instance, early stopping approaches are now widely used in practice, and perform only a limited number of steps of an iterative optimisation algorithm, to avoid overfitting the training set. They thereby entail less operations, while provably maintaining the same generalisation performance of approaches such as Tikhonov regularisation [BPR07].

A different approach, also known as divide and conquer, is based on the idea of distributing portions of the training data onto separate machines, each solving a smaller learning problem, and then combining individual predictors into a joint one. This computation hence benefits from both the parallelisation and the reduced dimension of distributed datasets while similarly maintaining statistical guarantees [ZDW13].

A third approach that has recently received significant attention from the machine learning community, along with the quantum computing community, is based on random sub-sampling, a form of dimensionality reduction. Depending on how such sampling is performed, different methods have been proposed, the most well-known being random features [R+07] and Nyström approaches [SS00; WS01]. Here the computational advantage is clearly given by the smaller dimensionality of the hypotheses space, and it has also recently been shown that it is possible to obtain equivalent generalisation performance to classical methods in these settings [RCR15].

For all these methods, training times can be typically reduced from the $O(N^3)$ of standard approaches to $\tilde{O}(N^2)$ or $\tilde{O}(Nz)$, where $z$ is the number of non-zero entries, while keeping the statistical performance of the learned estimator essentially unaltered.
3 Quantum learning algorithms

Linear algebra subroutines are a central computational element of learning algorithms. A large class of quantum machine learning algorithms claim exponential speed-ups compared to classical algorithms by making use of fast quantum linear algebra subroutines \cite{WBL12,SSP16,RML14,Wan17,PKP17,CGJ18,ZZW18}. One widely used algorithm is the quantum linear system solver \cite{HHL09} (also known as HHL after the three authors Harrow, Hassidim, and Lloyd). The algorithm takes as input a quantum encoding of the vector $b \in \mathbb{R}^n$ and an $s$-sparse matrix $A \in \mathbb{R}^{n \times n}$, with $\| A \| \leq 1$, and outputs an approximation $|\tilde{w}\rangle$ of the solution $|w = A^{-1}b\rangle$ of the linear system such that

$$\| |\tilde{w}\rangle - |w\rangle \| \leq \gamma$$

for an error parameter $\gamma > 0$. The current best implementation of the algorithm runs in time \cite{CGJ18}

$$O(\| A \|_F \kappa \text{polylog}(\kappa, n, 1/\gamma)),$$

where $\| A \|_F$ is the Frobenius norm of $A$ and $\kappa$ its condition number. Note that the HHL algorithm requires to access the data matrix $A \in \mathbb{R}^{n \times d}$ in $O(\text{polylog}(nd))$ time. All the quantum learning algorithms we discuss in this paper inherit this assumption. Recently, it was proven that such strong oracular assumptions (when the data matrix is low-rank) also lead to exponentially faster classical algorithms \cite{Tan18,CLW18,GLT18,Chi+19b}. We recommend \cite{Cil+18,Aar15} for more detailed discussions of the limits of quantum learning algorithms based on fast linear algebra subroutines.

Before proceeding to the statistical analysis of quantum learning algorithms we review some quantum algorithms for the least squares problem. These will serve as the main examples in our analysis.

3.1 Quantum least squares

Least squares is an algorithm for minimising the empirical risk, with respect to the squared loss, for the hypothesis class of linear functions. More specifically let $X = \mathbb{R}^d$ and $Y = \mathbb{R}$, and let $\mathcal{H} := \{ f : X \to Y \mid \exists w \in \mathbb{R}^d : f(x) = w^T x \}$ be the hypothesis class of linear functions. The empirical risk is

$$\hat{\mathcal{E}}(f) := \frac{1}{n} \sum_{i=1}^{n} \left( w^T x_i - y_i \right)^2.$$ 

We can minimise the empirical risk by setting its gradient to zero. Using $X := \sum_i x_i x_i^T$ and $b := \sum_i y_i x_i$ one can write a close form solution to the least squares problem as $w = X^{-1}b$.

Several quantum algorithms for least squares (or, more generally, linear regression problems) have been proposed \cite{WBL12,PKP17,CGJ18,Wan17,ZZW18}. A common feature is that they use a fast quantum linear system algorithm to find a quantum encoding $|w\rangle$ of the solution vector $w = X^{-1}b$. The fastest known algorithm in the class \cite{CGJ18}, which improves the dependency on the error from polynomial to logarithmic, solves the (regularized) least squares or linear regression problem in time

$$O(\| X \|_F \kappa \text{polylog}(n, \kappa, 1/\gamma)),$$

where $\kappa^2$ is the condition number of $X$ and $\gamma > 0$ is an approximation parameter. As for every other quantum algorithm discussed in this paper the quantum least squares solver requires a quantum-accessible data structure. The dependency on the Frobenius norm implies that it is possible to obtain a speedup only when $X$ is low-rank (but non-sparse). Due to approximation errors, the output of the algorithm is not $|w\rangle$ but a quantum state $|\tilde{w}\rangle$, such that $\| |\tilde{w}\rangle - |w\rangle \| \leq \gamma$. 

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It is possible to get rid of the dependency on the Frobenius norm using the sample based Hamiltonian simulation method [LMR14; Kim+17]. Leveraging this technique, [SSP16] proposed a least squares algorithm whose scaling does not depend on the Frobenius norm but requires a higher number copies (with respect to [CGJ18]) of the input density matrix. Note that, because the algorithm in [SSP16] is posed in the query model, i.e. the computational complexity is given in number of calls to the oracle which returns the data already encoded in form of a quantum state, it is not possible to make a direct comparison between the two algorithms. The computational complexity of the algorithm given in [SSP16] is 

\[ O(n^2\gamma^{-3}\text{polylog}(n)), \]

and the dependency on the error is polynomial.

4 Quantum speed-ups and statistical bounds

In this section we analyse the speed-up claims of quantum machine learning algorithms using the framework of statistical learning theory. Our main point is that if one considers the \( \Theta(n^{-1/2}) \) scaling of the generalisation error—see Eq. 3—quantum learning algorithms cannot achieve polylogarithmic runtime in \( n \).

The starting point of our discussion is the following standard error decomposition. Consider an hypothesis \( f \). We want to bound how far the generalisation error of \( f \) is from the best possible generalisation error; this is known as the Bayes risk and is indicated by \( \mathcal{E}^*: := \inf_{f \in \mathcal{F}} \mathcal{E}(f) \), where \( \mathcal{F} \) denotes the set of all measurable functions \( f : X \to Y \). We want to decompose this general error into different components and for this reason we introduce \( \mathcal{E}_H := \inf_{f \in H} \mathcal{E}(f) \), that is the best risk attainable by function in the hypothesis space \( H \). In order to simplify our discussion let us assume that \( \mathcal{E}_H \) always admits a minimizer \( f_H \in H \) (it is possible to levy this assumption using the theory of regularisation). Recalling that \( \hat{\mathcal{E}}(\hat{f}) := \inf_{f \in H} \hat{\mathcal{E}}(f) \), we can decompose the total error as:

\[ \mathcal{E}(f) - \mathcal{E}^* = \underbrace{\mathcal{E}(f) - \mathcal{E}(\hat{f})}_{\text{Optimisation error}} + \underbrace{\mathcal{E}(\hat{f}) - \mathcal{E}_H}_{\text{Estimation error}} + \underbrace{\mathcal{E}_H - \mathcal{E}^*}_{\text{Irreducible error}} \] (4)

The first term in Eq. 4 is the optimisation error and measures how good is the optimisation that generated \( f \) with respect to the ideal minimisation of the empirical risk. This error is related to the approximation error of the algorithm. We discuss this error contribution more in detail in Section 4.1. The second term is the estimation error and models the error that we make by estimating the true risk using samples from the distribution \( \rho \). This is the generalisation bound we discussed in Eq. 1. The third term is the irreducible error and measures how well the hypothesis space models the problem. It is an irreducible source of error that we indicate with the letter \( \mu \). If the irreducible error is zero than we say that \( H \) is universal. For simplicity, we assume throughout the paper that \( \mu = 0 \).

From the error decomposition in Eq. 4 we see that in order to have the best possible generalisation error we must make sure that the optimisation error matches the scaling of the estimation error. For classical algorithms the optimisation error typically scales with \( O(\log(1/\epsilon)) \) and matching the bounds is usually not a relevant problem (unless one wants to reduce the overall time complexity, in this case one could use an algorithm that is less accurate but converges faster to the solution with the best statistical error—this is the approach taken by methods such as early stopping discussed in Section 2). For many quantum algorithms, such as some of the quantum linear regression and least squares algorithms we discussed in the previous section.
| Algorithm              | Train time | Test time |
|-----------------------|------------|-----------|
| Classical             |            |           |
| SVM / KRR             | $n^3$      | $n$       |
| KRR [Y+17; MB17; GOS16; ACW17; FM12] | $n^2$      | $n$       |
| Divide and conquer [ZDW13] | $n^2$      | $n$       |
| Nyström [WS01; RCR15] | $n^2$      | $\sqrt{n}$ |
| FALKON [RCR17]        | $n\sqrt{n}$| $\sqrt{n}$ |
| Quantum               |            |           |
| QKLS / QKLR [CGJ18]   | $\sqrt{n}$ | $n\sqrt{n}$ |
| QSVM [RML14]          | $n\sqrt{n}$| $n^2\sqrt{n}$ |

Figure 1: Summary of time complexities for training and testing of different classical and quantum algorithms when statistical guarantees are taken into account. We omit $\text{polylog}(n,d)$ dependencies for the quantum algorithms. As per the argument presented in Section 4, we assume $\epsilon = \Theta(1/\sqrt{n})$ and count the effects of measurement errors. The acronyms in the table refer to: support vector machines (SVM), kernel ridge regression (KRR), quantum kernel least squares (QKLS), quantum kernel linear regression (QKLR), and quantum support vector machines (QSVM). Note that for quantum algorithms the state obtained after training cannot be maintained or copied and the algorithm must be retrained after each test round. This brings a factor proportional to the train time in the test time of quantum algorithms. Because the condition number may also depend on $n$ and for quantum algorithms this dependency may be worse, the overall scaling of the quantum algorithms may be slower than the classical.

For quantum algorithms with polylogarithmic error dependency, such as [CGJ18] this argument is no longer valid. In this case, we show that quantum algorithms argument cannot achieve polylogarithmic runtime in the dimension of the training set based on an argument that analyses the error dependency introduced via the finite sampling process that is required to extract a classical output from the algorithm. This will be discussed in Section 4.2.

We begin by discussing the dependency on the error and then proceed to discuss the dependency on the measurement errors. We summarise the results of our analysis in Table 1.

### 4.1 Error dependency of the quantum algorithms

In this section we show that in order to have a total error (see Eq. 4) that scales as $1/\sqrt{n}$ we must introduce a polynomial $n$-dependency in the quantum algorithm. For simplicity, we present our argument by discussing the case of quantum least squares algorithms with inverse polynomial dependency on the error [WBL12; SSP16; Wan17]. Our results generalize easily generalise for all kernel methods.

For a $\gamma$ error guarantee on the final output state, the quantum algorithms we consider have a time complexity that scales as $O(\kappa^c\gamma^{-\beta}\text{polylog}(n))$ for some $\beta, c > 0$. For example, $\beta = 3$ in [SSP16] and $\beta = 4$ in [LCW19].

Since for the quantum algorithm the data matrix needs either to be Hermitian or encoded in a larger Hermitian matrix such that the dimensionality of the matrix is $n + d$ for $n$ data points in $\mathbb{R}^d$, we assume here for simplicity that the data is given by a $n \times n$ Hermitian matrix,
i.e., \( n \) points in \( \mathbb{R}^n \).

In order give a precise bound to the optimisation error term in Eq. 4 in terms of the approximation error of the quantum algorithm we consider the following decomposition between the ideal minimizer of the empirical risk \( \hat{f} \) and the approximate minimizer output of the learning algorithm

\[
\mathcal{E}(\hat{f}) - \mathcal{E}(\hat{\hat{f}}) = \mathcal{E}(\hat{f}) - \mathcal{E}(\hat{\hat{f}}) + \mathcal{E}(\hat{\hat{f}}) - \mathcal{E}(\hat{\hat{f}})
\]

\[
= \Theta(n^{-1/2}) + O(\gamma),
\]

where the first and third contributions result from the generalization performance bounds while the second comes from the approximation error of the quantum algorithm.

Let us analyse the algorithmic error term for the problem of linear regression and least squares problem. Assuming that the output of the quantum algorithm is a state \( |\tilde{w}\rangle \) while the exact minimizer of the empirical risk is \( |w\rangle \), with \( ||\tilde{w} - w|| \leq \gamma \), we find that (assuming \( |X| \) and \( |Y| \) are bounded)

\[
|\hat{\mathcal{E}}(\hat{f}) - \mathcal{E}(\hat{f})| \leq \frac{1}{n} \sum_{i=1}^{n} \left| (\tilde{w}^T x_i - y_i)^2 - (w^T x_i - y_i)^2 \right|
\]

\[
\leq \frac{1}{n} \sum_{i=1}^{n} L |(\tilde{w} - w)^T x_i|
\]

\[
\leq \frac{1}{n} \sum_{i=1}^{n} L ||\tilde{w} - w|| ||x_i|| \leq O(\gamma),
\]

where we used Cauchy-Schwarz and the fact that because \( |X| \) and \( |Y| \) are bounded we have that for the square loss \( \ell_{sq} \) it holds \( |\ell_{sq}(f(x_1), y_1) - \ell_{sq}(f(x_2, y_2)| \leq L |(f(x_1) - y_1) - (f(x_2) - y_2)| \) for some \( L > 0 \).

In order to have the best possible accuracy, we need to match the different error bounds. We set \( \gamma = n^{-1/2} \) and get that the overall scaling of the algorithm is of the order

\[
O \left( \kappa^c n^{\beta/2} \log(n) \right),
\]

for some constant \( c \). For an extensive comparison of the runtime of classical and quantum algorithms see Table 1.

### 4.2 Measurement errors in quantum algorithms

So far we have ignored the error introduced by the measurement process used to compute a classical estimate of the output of the quantum algorithm. It is well known that this error scales as \( O(1/\sqrt{m}) \), where \( m \) is the number of measurements.

Let us consider again the case of quantum least squares. The (quantum) output of the algorithm is the state \( |\tilde{w}\rangle \) an is approximation of the ideal output \( |w\rangle \). We can produce a classical estimate \( \hat{\tilde{w}} \) of the vector \( \tilde{w} \) with accuracy

\[
||\tilde{w} - \hat{\tilde{w}}|| \leq \tau = O(1/\sqrt{m}),
\]

where \( m \) is the number of measurements performed on the state.
Let \( y \) be the ideal prediction. We have two sources of error, the algorithmic error and the error coming from the estimation process

\[
|y - \hat{y}| = |w^T x - \hat{w}^T x| \\
\leq \|w - \hat{w}\| \|x\| \\
\leq (\gamma + \tau) \|x\|
\]

where we used Cauchy-Schwarz and \( \|w - \hat{w}\| \leq \gamma \).

If we look again at Eq. 5, we have that, in order to match the bound on the generalisation error we must repeat the algorithm \( \Theta(1/\sqrt{n}) \) times. We note that it might be possible to quadratically improve this dependency using metrology [GLM06].

5 Conclusions

Quantum machine algorithms promise to be exponentially faster than classical methods. In this paper, we use standard results from statistical learning theory to rule out quantum machine algorithms with polylogarithmic time complexity in the input dimensions. Considering that virtually all practical machine learning algorithms have polynomial runtimes, our results effectively rule out the possibility of superpolynomial advantages for quantum machine learning.

Our argument leverages the fact that the statistical error of the algorithm has a provable polynomial dependence on the number of samples in the training set. Since the statistical error and the approximation error of the algorithm are additive, in order to achieve the best possible error rate, the scale of the statistical error must match that of the approximation error. This matching forces the approximation error of quantum algorithms to scale polynomially with the number of samples. This effectively kills quantum speedups for algorithms that have polynomial dependence on the error.

For algorithms where the dependency on the error is logarithmic, this argument does not apply. In this case, we show that the sampling error coming from the measurement process also adds up additively to the total error and—matching this error to the generalization one—introduces a polynomial dependency in the number of samples that kills the superpolynomial speedup.

Notably, our results hold even assuming that quantum algorithms can access a quantum data structure at no cost. In this respect, we prove a stronger ‘no-go’ result for quantum learning than the one proved by Tang in [Tan18]. Indeed this result relies on a classical data structure that mimics a quantum data structure but is unrealistic in practice.

As future directions, it is worth mentioning that it may be possible strengthen our results by analysing the \( n \) dependency of the condition number. Previous results in this direction can be found in [CS02; Hoc11].

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