Quantum classification of the MNIST dataset via Slow Feature Analysis

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Abstract

Quantum machine learning carries the promise to revolutionize information and communication technologies. While a number of quantum algorithms with potential exponential speedups have been proposed already, it is quite difficult to provide convincing evidence that quantum computers with quantum memories will be in fact useful to solve real-world problems. Our work makes considerable progress towards this goal.

We design quantum techniques for Dimensionality Reduction and for Classification, and combine them to provide an efficient and high accuracy quantum classifier that we test on the MNIST dataset. More precisely, we propose a quantum version of Slow Feature Analysis (QSFA), a dimensionality reduction technique that maps the dataset in a lower dimensional space where we can apply a novel quantum classification procedure, the Quantum Frobenius Distance (QFD). We simulate the quantum classifier (including errors) and show that it can provide classification of the MNIST handwritten digit dataset, a widely used dataset for benchmarking classification algorithms, with 98.5% accuracy, similar to the classical case. The running time of the quantum classifier is polylogarithmic in the dimension and number of data points. We also provide evidence that the other parameters on which the running time depends (condition number, Frobenius norm, error threshold, etc.) scale favourably in practice, thus ascertaining the efficiency of our algorithm.

1 Introduction

Quantum computing has the potential to revolutionize information and communication technologies and one of the most promising areas is quantum machine learning. The field of quantum machine learning stemmed from the well known HHL algorithm [HHL09], that takes as input a sparse and well conditioned system of equations A and an input vector \mathbf{b} , and in time polylogarithmic in the input dimensions produces a quantum state that encodes the classical solution $|x\rangle \approx |A^{-1}\mathbf{b}\rangle$. After that, other quantum algorithms with potential exponential speedups were proposed, using and extending techniques such as phase estimation, Hamiltonian simulation, and amplitude amplification, including for recommendation systems [KP16], topological data analysis [LGZ16], support vector machines [RML14], kernel PCA for anomaly detection [LR18], and data fitting [WBL12].

Nevertheless whether quantum processing machines can be used in practice along other processing units in order to solve efficiently and accurately real-world problems and lead to quantum innovation remains the billion-dollar question. Of course one would need powerful and robust quantum hardware but even in the case of full-scale quantum computers with quantum access to large datasets, it is essential, and rather not straightforward, to find practical applications of quantum computing that would have a real economic and societal impact.

Our work provides evidence that large-scale quantum computers with quantum access to data will be indeed useful for classification, one of the most important tasks in machine learning with applications in different industrial sectors, including automation, healthcare, Internet of Things etc. More precisely, we design efficient quantum algorithms for dimensionality reduction and

for classification and we also simulate their behaviour on the commonly-used MNIST dataset of handwritten digits and show that they would provide accurate and competitive classification.

Before providing more details on our results, we give a brief description of the notions of dimensionality reduction and classification. Dimensionality reduction (DR), a technique used in practice both in supervised and unsupervised learning, refers to the procedure by which the dimension of the input data is reduced as a first step before any further processing of the data. It is often necessary when trying to solve practical problems in machine learning and there are many classical techniques for performing it. For instance, it is used in order to decrease the variance of the learner, since it simplifies the model and reduces the noise in the data. It is also necessary when the running time of the algorithm has polynomial dependence on the number of features or dimensions which can be prohibited for large dimensional data sets. In the context of big data analysis, by removing features that carry low information (like features that are strictly proportional to other features, or features for which the data contains too little information), it is possible to optimize the storage space and allow for data visualization. Most importantly, supervised algorithms often suffer from the curse of dimensionality: by allowing large dimensionality of data, the informative power of the data points in the training set decreases, thus leading to a degradation in classification performances. One solution to improve the accuracy would be to increase the number of elements in the training set, but this is not always possible nor desirable, so the common route is to decrease the dimension of the data. Mathematically, the idea of the dimensionality reduction algorithms is to map vectors from a high dimensional space \mathcal{X} to a low dimensional space \mathcal{Y} , such that the most meaningful information (according to some criteria) is preserved. Of course, understanding which criterion to use is far from trivial.

The choice of the right DR algorithm depends on the nature of the data as well as on the type of algorithm that will be applied after the dimensionality reduction. A very well known DR algorithm is the Principal Component Analysis (PCA), that projects the data points onto the subspace spanned by the eigenvectors associated to the k largest eigenvalues of the covariance matrix of the data. In this way, the projection holds "most of the information" of the dataset. In fact it is possible to show that, for a subspace of dimension k, this choice of eigenvectors minimize the reconstruction error, i.e. the distance between the original and the projected vectors. However, PCA is not always the best choice of dimensionality reduction. PCA projects the data into the subspace along which the data has more variance. This does not take into consideration the information that different points might belong to different classes, and there are cases in which PCA can worsen the performance of the classifier. Other methods, like Fisher Linear Discriminant (FLD) also take into account the variance of each single class of points. Indeed, FLD projects the data in a subspace trying to maximize the distance between points belonging to different clusters and minimizing the distance between points belonging to the same cluster, thus preserving or increasing the accuracy. Slow Feature Analysis (SFA) is a different dimensionality reduction technique proposed in the context of computational neurosciences that projects the data points onto the subspace spanned by the eigenvectors associated to the k smallest eigenvalues of the derivative covariance matrix of the data. SFA has been shown to model a kind of neuron (called complex cell) situated in the cortical layer in the primary visual cortex (called V1) [BW05]. SFA can be used in machine learning as a DR algorithm, and it has been successfully applied to enhance the performance of classifiers [ZD12, Ber05]. It has been shown that solving the optimization problem upon which SFA is based is equivalent to other dimensionality reduction algorithms, like Laplacian Eigenmaps [Spr11] and Fisher Linear Discriminant [KM09], thus a quantum algorithm for SFA also provides algorithms for Laplacian Eigenmaps and Fisher Linear Discriminant.

The main goal of our work is to show that quantum computers will be able to provide efficient and accurate classification, a task of prominent importance in machine learning. The classification problem consists of finding the correct label for a new sample given a training set of N elements, each one associated with one of K possible labels. Classification algorithms can be used for solving problems like customer segmentation, medical diagnosis, image classification, spam detection, and others. Some classification algorithms could also be adapted for performing regression. Formally, we will show how to perform the following task: given a new sample x and quantum access to the training set T, find the correct class for x by building a function $h: \mathcal{X} \to [K]$. As we said, for most real-world datasets, the efficiency and accuracy of the classification can be considerably improved by performing dimensionality reduction before the actual classification.

In this work we first define quantum Slow Feature Analysis (QSFA), a quantum method for dimensionality reduction. The QSFA algorithm that we propose uses techniques based on the Singular Value Estimation and the projection procedure in [KP17, KP16], as well as recent improvements of these procedures in [CGJ18, GSLW18]. The idea is to approximately project the input vectors onto the space spanned by the eigenvectors corresponding to the smallest eigenvalues of the derivative covariance matrix. Our algorithm runs in time polylogarithmic in the dimension and number of points in the dataset, and - as is the case for algorithms based on HHL - depends on some characteristics of the input matrix (like the condition number), thus it can achieve an exponential speedup in certain cases. We use QSFA as the first step in an efficient and accurate procedure for solving the classification problem: given a set of labeled elements belonging to K different classes, the problem is to find the correct class for a new observation.

Second, we define the quantum Frobenius Distance (QFD) classification, a novel quantum method that classifies a new data point based on the average square ℓ_2 -distance between the new data point and each labeled cluster, i.e. the average of the square distances between the new data point and each point in the cluster. The running time is logarithmic in the number and dimension of the data points and proceeds by creating a weighted superposition of all points in a cluster and the new data point, and then estimating the distance of each point with the new data point in superposition, hence allowing to estimate the average square distance.

We started out wanting to provide concrete evidence that quantum computers will be able to solve real-world problems. To this end, we also provide the results of a simulation of the performance of the quantum classification algorithm on a standard dataset in machine learning: the MNIST dataset of handwritten digits. We simulated classically the procedures that the quantum algorithm performs including the errors in these procedures.

With respect to the accuracy, our classification using QSFA and QFD provides accuracy around 98.5%, which is comparable to classical machine learning algorithms, and better than many of the previous results registered in [LeC]. We note that the best classical classification algorithms, and our QFD classification as well, when applied directly on the raw data provide quite low accuracy, showing that the step of dimensionality reduction is indeed crucial.

With respect to the running time of our quantum procedure, it depends only polylogarithmically on the dimension and the number of data points, but it also depends on the characteristics of the input matrix, in particular its Frobenius norm (or maximum ℓ_1 norm depending on the quantum procedure used) and its condition number (or a condition threshold which can be used instead). We show that all these parameters increase very slowly with the number and dimension of the data points in the MNIST dataset. Moreover, we provide specific numbers for all other error parameters that appear in the running time.

We see our results as evidence that our quantum classifier can provide efficient and high accuracy classification. We note that the fact that the dependence on the dimension is only polylogarithmic can be seen from two points of view. First, as a much faster algorithm to provide classification with similar accuracy as the classical algorithms. Second, and maybe more importantly, by increasing the initial input dimension (number or dimension of data points), our quantum classifier may provide much higher accuracy classification in time similar to classical algorithms. Of course we will not be able to confirm the second statement before we can actually have quantum computers, but it is well known in the ML community that increasing the input dimension (up to some point) increases the accuracy of the classification, which is very important for much more interesting data sets than the MNIST one.

Let us remark also that our goal is to assess the power of quantum computers with access to a QRAM, i.e. a quantum computer that can access classical data in superposition, in a similar manner to classical high-performance computing machines which by default possess a RAM. Of course, we do not have such quantum computers right now and there is a possibility that they may never be realized. We think of our results as motivation for actually building such quantum processing machines. We will provide more details about the QRAM model in the following sections.

Note also that the quantum dimensionality reduction and classification proposed in this work can be used also on quantum data without the need of a QRAM, in other words, data produced by a quantum process that need to be further elaborated or classified. For instance, after Hamiltonian simulation used in quantum chemistry or for testing quantum devices, and so on. This way, one may not need to preload the classical data into the quantum memory, since there is an efficient procedure of creating the quantum states directly.

1.1 Previous Results

Despite the fact that quantum machine learning is a recent field, it already encompasses a rich set of techniques and approaches. In this section we describe the main trends, with special attention on classification algorithms.

The first category of algorithms use circuits of parametrized gates to perform machine learning tasks such as classification or regression [VBB17, SBSW18, CGAG17]. In the training phase, the parameters of the circuit are learned using classical optimization techniques, where the function to optimize is a loss function calculated on the output of the quantum circuit. A work in this direction [OMA+17] used the Quantum Approximative Optimization Algorithm (QAOA) to solve a clustering problem, exploiting a reduction from clustering to MaxCut, a combinatorial optimization problem which QAOA can solve. In the same work, a downscaled version of the algorithm was tested on real hardware. This model has similarities with classical neural networks, at the point that some of these works have been presented as quantum neural networks. For instance, in the work of [FN18] a quantum circuit of this kind has been trained on an extremely downsampled version of the MNIST dataset with only two digits and with a test error of 10%. A possible issue of this approach is outlined in [MBS⁺18], where the authors showed that for a large class of random quantum circuits, the gradient of the function under optimization can be exponentially small in the number of qubits, thus the probability to find a non-zero value of the gradient is vanishingly small. If the gradient is zero almost everywhere, gradient based methods for finding a correct set of parameters over large number of qubits are deemed to fail.

In [SFP17], the authors presented a kernelized binary distance-based classifier and tested it with two experiments on the IRIS dataset, first with numerical simulations and then on quantum hardware. Tested on a severly downsampled version of two linearly separable classes, the simulation lead to 100% accuracy, as expected.

Using quantum annealing it is possible to fit a generative model, as shown in [BRGBPO17]. This work used a dataset of handwritten digits as well, specifically the OptDigits dataset [Kay95] along with the BAS dataset of artificial images [Mac02]. The two datasets were studied for image reconstruction and classification. Preprocessing on the dataset helped to cope with the limitations of the hardware. The authors trained a quantum Boltzmann machine such that the samples from the annealer are as similar as possible to the distribution of the real data. One could potentially use this method to perform classification as well.

Another trend in quantum machine learning focuses on the use of amplitude amplification and estimation techniques, gaining a quadratic factor in the running time. Prominent examples of these approach is the quantum perceptron algorithm [KWS16], quantum k-nearest-neighbour [WKS14] and a genetic algorithm [LB16].

The approach that may achieve exponential speedups uses quantum computers to speed up the linear algebraic operations used in machine learning algorithms. The work of Robentrost et al. [RML14] consists of an algorithm for a Support Vector Machines classifier with an exponential speedup on the number of samples and the dimension of the feature space. There, the well known HHL algorithm is used to solve a linear system of equations associated to the optimization problem of SVM. Other results in this paradigm exploit novel Hamiltonian simulation techniques (called quantum self-testing) developed for the first time in [LMR13] and analyzed in [KLL+17]. Previous Hamiltonian simulation techniques were limited to sparse or local matrices, and this technique extends Hamiltonian simulation to dense but low-rank matrices. Based on quantum self-testing and assuming the existence of QRAM, the authors proposed a quantum version of PCA.

The work most related to ours is [CD16], where the authors described a dimensionality reduction and a classification algorithm for Linear and Nonlinear Fisher Discriminant Analysis using the model of Hamiltonian simulation. Their algorithm works for the case where the sparsity or rank of the matrix is polylogarithmic in the dimension and has complexity $O(r \ polylog(nd)\kappa_{\tau}^{3.5}/\epsilon^3)$ where r is the desired number of principal eigenvectors, and κ_{τ} is a pre-defined conditioning number which is chosen to be $O(1/\epsilon)$. At the end of the dimensionality reduction, the algorithm uses tomography to learn the corresponding eigenvectors and project clasically the data points onto this low-dimensional space. After this, the authors present an efficient QRAM-based classification algorithm using Quadratic Discriminant Analysis (QDA) with similar running time. The assumptions on the input matrix and the bad dependence of the running time on the error parameter make this algorithm hard to apply on real data.

1.2 Notation and Organisation

Let A be a matrix in $\mathbb{R}^{m \times n}$. It's singular value decomposition is $A := U\Sigma V^{\dagger}$, where U is a matrix whose columns are called the left singular vectors of A and are the eigenvectors of the AA^T matrix, Σ is a diagonal matrix whose diagonal elements are the singular values of A, and V is a matrix whose columns are called the right eigenvectors of A and are the eigenvectors of the A^TA matrix. We denote with [n] the set $\{1, 2, ..., n\}$. Unless otherwise stated, our vector are in \mathbb{R}^n . With $A_{\leq \sigma}$ we denote the projection of the matrix A onto the vector subspace spanned by the singular vectors associated to the singular values that are smaller than σ . The conditioning number of a matrix $\kappa(A)$ is defined as the ratio between the biggest and the smallest singular values.

Our training set is made of pairs $\mathcal{T} = \{(x(i), l(i))\}$ for $i \in [n]$: a vector and its associated label (also called class). With the notation $x(i), i \in [n]$ we denote the *i*-th sample of the training set, which we think of as a row of the matrix X. We consider K different labels $\mathcal{L} = \{l_1, l_2, ... l_K\}$, and for each label, we denote $T_k \subset [n]$ the set of training samples of this label, and X_k the corresponding matrix. With \tilde{O} we express the time complexity of an algorithm with polylogarithmic dependencies factored out.

The paper is organized as follows. In Section 2, SFA is introduced as an dimensionality reduction problem for classification. In Section 3, we show how to perform linear algebraic operations with a quantum computer. Here we give a new algorithm to perform singular value estimation of a product of two matrices. With these tools, we describe in Section 4 a quantum version of SFA that works with classical data. In Section 5, we describe a new distance based classification algorithm called quantum Frobenius Distance (QFD) classifier, and in Section 6 we show how the combination of QSFA and QFD has performance comparable to classical versions of the algorithm on the same dataset. We conclude our work in Section 7, by outlining applications, possible enhancements, and open problems.

2 Classical Slow Feature Analysis

SFA was originally proposed as an online, nonlinear, and unsupervised algorithm [WW99]. Its task was to learn slowly varying features from generic input signals that vary rapidly over time [Ber05, WW99]. SFA has been motivated by the temporal slowness principle, that postulates that while the primary sensory receptors (like the retinal receptors in an animal's eye) are sensitive to very small changes in the environment and thus vary on a very fast time scale, the internal representation of the environment in the brain varies on a much slower time scale. The slowness principle is a hypothesis for the functional organization of the visual cortex and possibly other sensory areas of the brain [WBF+11] and it has been introduced as a way to model the transformation invariance in natural image sequences [ZD12].

SFA is an algorithm that formalizes the slowness principle as a nonlinear optimization problem. In [BW04, SZW14], SFA has been used to do nonlinear blind source separation. Although SFA has been developed in the context of computational neurosciences, there have been many applications of the algorithm to solve ML related tasks. A prominent advantage of SFA compared to other algorithms is that it is almost hyperparameter-free. The only parameters to chose are in the preprocessing of the data, e.g. the initial PCA dimension and the nonlinear expansion that consists of a choice of a polynomial of (usually low) degree p. Another advantage is that it is guaranteed to find the optimal solution within the considered function space [EBW12]. For a detailed description of the algorithm, we suggest [SW08].

With appropriate preprocessing, SFA can be used in conjunction to a supervised algorithm to acquire classification capabilities. For instance it has been used for pattern recognition to classify images of digits in the famous MNIST database [Ber05]. SFA can be adapted to be used to solve complex tasks in supervised learning, like face and human action recognition [GLW13, ZD12, SJC⁺14].

The high level idea of using SFA for classification is the following: One can think of the training set as an input series $x(i) \in \mathbb{R}^d$, $i \in n$. Each x(i) belongs to one of K different classes. The goal is to learn K-1 functions $g_j(x(i))$, $j \in [K-1]$ such that the output $y(i) = [g_1(x(i)), \cdots, g_{K-1}(x(i))]$ is very similar for the training samples of the same class and largely different for samples of different classes. Once these functions are learned, they are used to map the training set in a low dimensional vector space. When a new data point arrive, it is mapped to the same vector space, where classification can be done with higher accuracy.

Now we introduce the minimization problem in its most general form as it is commonly stated for classification [Ber05]. Let $a = \sum_{k=1}^{K} {|T_k| \choose 2}$. For all $j \in [K-1]$, minimize:

$$\Delta(y_j) = \frac{1}{a} \sum_{k=1}^{K} \sum_{\substack{s,t \in T_k \\ s \neq t}} (g_j(x(s)) - g_j(x(t)))^2$$

with the following constraints:

1.
$$\frac{1}{n} \sum_{k=1}^{K} \sum_{i \in T_k} g_j(x(i)) = 0$$

2.
$$\frac{1}{n} \sum_{k=1}^{K} \sum_{i \in T_k} g_j(x(i))^2 = 1$$

3.
$$\frac{1}{n} \sum_{k=1}^{K} \sum_{i \in T_k} g_j(x(i)) g_v(x(i)) = 0 \quad \forall v < j$$

The minimization of the delta values $\Delta(y_j)$ encodes the requirement on the output signal to vary "as slow as possible", and thus the delta values are our measure of slowness. They are the average of the square of the first order derivative (over time) of the j-th component of the output signal y(t). The first requirement states that the average over time of each component of the signal should be zero, and it is stated just for convenience, such that the other two requirements take a simple form. The second requirement asks for the variance over time of each component of the signal to be 1. It is equivalent to saying that each signal should carry some information and avoid the trivial solution $g_j(\cdot) = 0$. The third requirement is to say that we want the signals to be decorrelated with each other. This also introduces an order, such that the first signal is the slowest, the second signal is the second slowest and so on. The first and the second constraint also avoid the trivial solution $y_i(t) = 0$. Intuitively, the decorrelation constraint forces different functions g_j to encode different "aspects" of the input, maximizing the information carried by the output signal.

In order for the minimization problem to be feasible in practice, the g_j 's are restricted to be linear functions w_j such that the output signal becomes $y(i) = [w_1^T x(i), \cdots w_{K-1}^T x(i)]^T$ or else Y = XW, where $X \in \mathbb{R}^{n \times d}$ is the matrix with rows the input samples and $W \in \mathbb{R}^{d \times (K-1)}$ the matrix that maps the input matrix X into a lower dimensional output $Y \in \mathbb{R}^{n \times (K-1)}$.

In case it is needed to capture nonlinear relations in the dataset, one performs a standard nonlinear polynomial expansion on the input data as preprocessing. Usually, a polynomial expansion of degree 2 or 3 is chosen. For example we can take

$$x = [x_1, x_2, x_3] \rightarrow \left[x_1^2, x_1 x_2, x_1 x_3, x_2^2, x_2 x_3, x_3^2, x_1, x_2, x_3\right].$$

The choice of the nonlinear expansion is important for using SFA in machine learning contexts. If it is a low dimensional expansion, it might not solve the task with high accuracy, while if the dimension is too high, it might overfit the training data, and therefore not generalize properly to test data. This technique also goes under the name of polynomial kernel.

We also need to satisfy the constraint on the average of the signal being zero and have unit variance. This is not a strong assumption, since it takes linear preprocessing time with respect to the dimensions of the dataset to remove the mean and scale the components by their variance. Namely, we assume that the j-th component of the i-th vector in the dataset satisfies the condition:

$$x_j(i) := \frac{\tilde{x}_j(i) - E_i[\tilde{x}_j(i)]}{\sqrt{E_i[(\tilde{x}_j(i) - E_i[\tilde{x}_j(i)])^2]}},$$

where with $\tilde{x}(i)$ we define a raw signal with arbitrary mean and variance, $E_i[\tilde{x}_j(i)]$ the expected value of a single component of the vectors.

This allows us to rewrite the minimization problem including the constraints of zero mean and unit variance. We can restate the definition of the delta function as:

$$\Delta(y_j) = \frac{w_j^T A w_j}{w_i^T B w_j},\tag{1}$$

where the matrix B is called the covariance matrix and defined as:

$$B := \frac{1}{n} \sum_{i \in [n]} x(i)x(i)^T = X^T X$$
 (2)

and the matrix A is called the derivative covariance matrix and defined as:

$$A := \frac{1}{a} \sum_{k=1}^{K} \sum_{\substack{i,i' \in T_k \\ i \leq i'}} (x(i) - x(i'))(x(i) - x(i'))^T = \frac{1}{a} \sum_{k=1}^{K} \dot{X_k}^T \dot{X_k} := \dot{X}^T \dot{X}$$
(3)

Note also, that we can approximate the matrix A by subsampling from all possible pairs (x(i), x(i')) from each class and this is indeed what happens in practice.

It is not hard to see that the weight vectors w_j that correspond to the minima of equation (1) are the eigenvectors associated with the smallest eigenvalues of the generalized eigenvalue problem $AW = \Lambda BW$ [HTF09, SW82], where $\Lambda = Diag [\lambda_1, ... \lambda_n]$ is the diagonal matrix of eigenvalues, and W is the matrix of generalized eigenvectors. Picking the K-1 smallest eigenvectors will allow us to create the $d \times (K-1)$ matrix W that will project our data to the slow feature space. In other words, SFA reduces to a generalized eigenvalue problem.

2.1 The SFA algorithm

The SFA algorithm basically provides a solution to the generalized eigenvalue problem $AW = \Lambda BW$ and outputs the eigenvectors corresponding to the smallest eigenvalues. As we said we assume that the data has been normalized and polynomially expanded.

We are now ready for the main steps of the algorithm. The first step is to whiten the data that will reduce the problem into a normal eigenvalue problem; the second step is to perform PCA in order to find the eigenvalues and eigenvectors. We refer to [EBW12] for a more complete description.

2.1.1 Step 1: Whitening the data

Recall that $X \in \mathbb{R}^{n \times d}$, $A, B \in \mathbb{R}^{d \times d}$. We now show how to whiten the data by right multiplying with the matrix $B^{-1/2} = [(X^T X)]^{-1/2}$. Then, the input matrix becomes $Z = X B^{-1/2}$ and the covariance matrix of the whitened data $Z^T Z$ is thus the identity.

Claim 1. Let $Z := XB^{-1/2}$ be the matrix of whitened data. Then $Z^TZ = I$.

Proof. Let $X = U\Sigma V^T$. Remember that $B = X^TX = (U\Sigma V^T)^T(U\Sigma V^T) = V\Sigma^2 V^T$.

$$\begin{split} Z^T Z &= \left[X B^{-1/2} \right]^T X B^{-1/2} = (B^{-1/2})^T B B^{-1/2} \\ &= \left[((U \Sigma V^T)^T (U \Sigma V^T))^{-1/2} \right]^T (U \Sigma V^T)^T (U \Sigma V^T) \left[((U \Sigma V^T)^T (U \Sigma V^T))^{-1/2} \right] \\ &= \left[((V \Sigma U^T) (U \Sigma V^T))^{-1/2} \right]^T (V \Sigma U^T) (U \Sigma V^T) \left[((V \Sigma U^T) (U \Sigma V^T))^{-1/2} \right] \\ &= \left[(V \Sigma^2 V^T)^{-1/2} \right]^T (V \Sigma^2 V^T) \left[(V \Sigma^2 V^T)^{-1/2} \right] = \left[(V \Sigma^{-1} V^T) \right]^T (V \Sigma^2 V^T) (V \Sigma^{-1} V^T) \\ &= (V \Sigma^{-1} V^T) (V \Sigma^2 V^T) (V \Sigma^{-1} V^T) = (V I V^T) = I \end{split}$$

2.1.2 Step 2: Projection in slow feature space

The second step of SFA consists of outputing the K-1 "slowest" eigenvectors of the derivative covariance matrix of the whitened data $A := \dot{Z}^T \dot{Z}$, where \dot{Z} is defined similar to \dot{X} by using the whitened samples instead of the original ones. Note that taking the derivatives of the whitened data is equal to whitening the derivatives. In other words,

$$\begin{array}{c} X \xrightarrow{Der.} \dot{X} \\ \downarrow^{Whit.} & \downarrow^{Whit.} \\ Z \xrightarrow{Der.} \dot{Z} \end{array}$$

Claim 2. Let $A = \dot{Z}^T \dot{Z}$. Then $A = (B^{-1/2})^T \dot{X}^T \dot{X} B^{-1/2}$.

Proof.

$$A = \dot{Z}^T \dot{Z} = \frac{1}{a} \sum_{k=1}^K \sum_{\substack{i,i' \in T_k \\ i < i'}} (z(i) - z(i')) (z(i) - z(i'))^T$$

$$= (B^{-1/2})^T \frac{1}{a} \sum_{k=1}^K \sum_{\substack{i,i' \in T_k \\ i < i'}} (x(i) - x(i')) (x(i) - x(i'))^T B^{-1/2}$$

$$= (B^{-1/2})^T \dot{X}^T \dot{X} B^{-1/2}$$

This will in fact allow us to whiten the data with a quantum procedure. In practice, the matrix A is usually approximated with a small fraction of all the possible derivatives, roughly linear (and not quadratic) on the number of data points. In our case we take the number of rows of the derivative matrix to be just double the number of data points without compromising the accuracy.

SFA - Algorithm 1 (Classical) Slow Feature Analysis

Require:

Input $X \in \mathbb{R}^{n \times d}$ (normalized and polynomially expanded), and $K < d \in \mathbb{N}$

Ensure

Y=ZW, where $Z=XB^{-1/2}$ is the whitened input signal, and $W\in\mathbb{R}^{d\times(K-1)}$ are the K-1 eigenvectors of the matrix $A=\dot{Z}^T\dot{Z}$ corresponding to the smallest eigenvalues

- 1: Whiten the signal: $Z := XB^{-1/2}$, and create \dot{Z} from Z.
- 2: Perform PCA on the derivative covariance matrix $A = \dot{Z}^T \dot{Z}$ of the whitened data.
- 3: Return Y = ZW, the projection of whitened data onto W, the K-1 slowest eigenvectors of A

3 Quantum algorithms for machine learning

We start by stating some known results that we will use in the following sections.

Definition 1. The vector state $|x\rangle$ for $x \in \mathbb{R}^n$ is defined as $\frac{1}{||x||} \sum_{i \in [n]} x_i |i\rangle$.

Proposition 1. (Phase estimation [Kit96]) Let U be a unitary operator, with eigenvectors $|v_j\rangle$ and eigenvalues $e^{i\theta_j}$ for $\theta_j \in [-\pi, \pi]$, i.e. we have $U|v_j\rangle = e^{i\theta_j}|v_j\rangle$ for $j \in [n]$. For a precision parameter $\epsilon > 0$, there exists a quantum algorithm that runs in time $O(T(U)\log n/\varepsilon)$ and with probability 1 - 1/poly(n) maps a state $|\phi_i\rangle = \sum_{j \in [n]} \alpha_j |v_j\rangle$ to the state $\sum_{j \in [n]} \alpha_j |v_j\rangle |\bar{\theta_j}\rangle$ such that $\bar{\theta}_j \in \theta_j \pm \varepsilon$ for all $j \in [n]$.

Proposition 2. (Amplitude amplification and estimation [BHMT02]) If there is unitary operator U such that $U|0\rangle^l = |\phi\rangle = \sin(\theta)|x,0\rangle + \cos(\theta)|G,0^{\perp}\rangle$ then $\sin^2(\theta)$ can be estimated to multiplicative error η in time $O(\frac{T(U)}{\eta\sin(\theta)})$ and $|x\rangle$ can be generated in expected time $O(\frac{T(U)}{\sin(\theta)})$.

We will provide algorithms for a quantum computer that has quantum access to classical data through a structure called QRAM which allows for creating quantum states efficiently from classical data stored in a data structure. We say that a dataset is efficiently loaded in the QRAM, if the size of the data structure is linear in the dimension and number of data points and the time to enter/update/delete an element is polylogarithmic in the dimension and number of data points. In Appendix A we show how to construct such data structures. We also assume that the classical data is stored already polynomially expanded and scaled to zero mean and unit variance.

We first recall some known results about the power of quantum computers to perform linear algebraic procedures efficiently. In what follows we follow the convention that the matrices have been stored in QRAM normalized, i.e. $||M||_2 \le 1$ (see [KP17] for an efficient procedure for this normalization).

Theorem 1 (Singular Value Estimation [KP17]). Let $M \in \mathbb{R}^{n \times d}$ be a matrix with singular value decomposition $M = \sum_i \sigma_i u_i v_i^T$ stored in the data structure described in Appendix A. Let $\varepsilon > 0$

the precision parameter. There is an algorithm with running time $\tilde{O}(\mu(M))/\varepsilon$ that performs the mapping $\sum_i \alpha_i |v_i\rangle \to \sum_i \alpha_i |v_i\rangle |\tilde{\sigma}_i\rangle$, where $|\tilde{\sigma}_i - \sigma_i| \leq \varepsilon$ for all i with probability at least 1 - 1/poly(n).

The function $\mu(M)$ is defined as $\min_{p \in [0,1]} \left(\|M\|_F, \sqrt{s_{2p}(M)s_{2(1-p)}(M^T)} \right)$, while s_p is defined as $\max_{i \in [m]} \|m(i)\|_p^p$. The optimal value for p depend on the matrix under consideration, but we have that $\mu(M)$ is smaller than the maximum l_1 norm of the row vectors, which is always smaller than the sparsity. For a matrix M and a vector x, we define as $M_{\leq \theta, \delta}^+ M_{\leq \theta, \delta} x$ the projection of x onto the space spanned by the singular vectors of M whose corresponding singular values are smaller than θ , and some subset we do not control of singular vectors whose corresponding singular values are in the interval $[\theta, (1+\delta)\theta]$.

The relevance of Theorem 1 in machine learning is the following: if we are able to estimate the singular values of a matrix, then we can perform a conditional rotation controlled by these singular values and hence perform a variety of linear algebraic operations, including matrix inversion, matrix multiplication or projection onto a subspace. We present these procedures from [KP16, KP17] in Algorithm 2.

Theorem 2 (Matrix algebra [KP16, KP17]). Let $M := \sum_i \sigma_i u_i v_i^T \in \mathbb{R}^{d \times d}$ such that $||M||_2 = 1$, and a vector $x \in \mathbb{R}^d$ stored in QRAM as described in Appendix A. There exist quantum algorithms that with probability at least 1 - 1/poly(d) return

- (i) a state $|z\rangle$ such that $|z\rangle |Mx\rangle| \le \epsilon$ in time $\tilde{O}(\kappa^2(M)\mu(M)/\epsilon)$
- (ii) a state $|z\rangle$ such that $|z\rangle |M^{-1}x\rangle| \le \epsilon$ in time $\tilde{O}(\kappa^2(M)\mu(M)/\epsilon)$
- $(iii) \ \ a \ \ state \ \ |M^+_{\leq \theta, \delta} M_{\leq \theta, \delta} x \rangle \ \ in \ \ time \ \ \tilde{O}\big(\frac{\mu(M) \|x\|}{\delta \theta \left\|M^+_{\leq \theta, \delta} M_{\leq \theta, \delta} x\right\|}\big)$

One can also get estimates of the norms with multiplicative error η by increasing the running time by a factor $1/\eta$.

In recent work [CGJ18, GSLW18], QRAM based procedures for matrix multiplication and inversion have been discovered where the dependence on the error parameter was greatly improved to $\operatorname{polylog}(1/\epsilon)$ and that on κ to linear. There, the notion of block encodings is used which is shown to be equivalent to our notion of having an efficient data structure as the one described in Appendix A. In order to get the polylogarithmic dependence on the precision parameter ϵ , the authors show how to perform the linear algebra procedures directly through the technique of qubitization and without explicitly estimating the singular values.

Hence, we can restate the above theorem with the improved times as

Theorem 3 (Matrix algebra [CGJ18, GSLW18]). Let $M := \sum_i \sigma_i u_i v_i^T \in \mathbb{R}^{d \times d}$ such that $||M||_2 = 1$, and a vector $x \in \mathbb{R}^d$ stored in QRAM as described in Appendix A. There exist quantum algorithms that with probability at least 1 - 1/poly(d) return

- (i) a state $|z\rangle$ such that $|z\rangle |Mx\rangle| \le \epsilon$ in time $\tilde{O}(\kappa(M)\mu(M)\log(1/\epsilon))$
- (ii) a state $|z\rangle$ such that $|z\rangle |M^{-1}x\rangle| \le \epsilon$ in time $\tilde{O}(\kappa(M)\mu(M)\log(1/\epsilon))$

One can also get estimates of the norms with multiplicative error η by increasing the running time by a factor $1/\eta$.

Another important advantage of the new methods is that it provides easy ways to manipulate sums or products of matrices.

Theorem 4 (Matrix algebra on products of matrices [CGJ18, GSLW18]). Let $M_1, M_2 \in \mathbb{R}^{d \times d}$ such that $||M_1||_2 = ||M_2||_2 = 1$, $M = M_1M_2$, and a vector $x \in \mathbb{R}^d$ stored in QRAM as described in Appendix A. There exist quantum algorithms that with probability at least 1 - 1/poly(d) return

- (i) a state $|z\rangle$ such that $|z\rangle |Mx\rangle| \le \epsilon$ in time $\tilde{O}(\kappa(M)(\mu(M_1) + \mu(M_2))\log(1/\epsilon))$
- (ii) a state $|z\rangle$ such that $|z\rangle |M^{-1}x\rangle| \le \epsilon$ in time $\tilde{O}(\kappa(M)(\mu(M_1) + \mu(M_2))\log(1/\epsilon))$
- (iii) a state $|M_{\leq \theta, \delta}^+ M_{\leq \theta, \delta} x\rangle$ in time $\tilde{O}(\frac{(\mu(M_1) + \mu(M_2))||x||}{\delta \theta ||M_{\leq \theta, \delta}^+ M_{\leq \theta, \delta} x||})$

One can also get estimates of the norms with multiplicative error η by increasing the running time by a factor $1/\eta$.

Matrix Operations - Algorithm 2 Matrix multiplication, inversion, and subspace projection

 $M = \sum_i \sigma_i u_i v_i^T \in \mathbb{R}^{n \times d}$ and $x \in \mathbb{R}^d$ stored in QRAM. Threshold θ and precision parameter $\delta > 0$ for matrix projection, error $\varepsilon > 0$ for matrix multiplication and inversion. Estimator

Ensure:

Quantum states $|Mx\rangle$, $|M^{-1}x\rangle$, or $|M^+_{<\theta,\delta}M_{\leq\theta,\delta}x\rangle$ respectively.

- 1: Create the state: $|x\rangle = \sum_{i} \alpha_{i} |v_{i}\rangle$ using the QRAM.
- 2: Perform SVE on M with precision $\epsilon/\kappa(M)$ for matrix multiplication and inversion and with precision $\delta\theta$ for matrix projection. This step creates the state: $\sum_{i} \alpha_{i} |v_{i}\rangle |\overline{\sigma}_{i}\rangle$
- 3: Perform a conditional operation on an ancilla qubit to get
 - (i) for matrix multiplication: $\sum_{i=1}^{d} \alpha_i |v_i\rangle |\overline{\sigma}_i\rangle \left(\overline{\sigma}_i |0\rangle + \sqrt{1-\overline{\sigma}_i^2} |1\rangle\right)$
 - (ii) for matrix inversion: $\sum_{i=1}^{d} \alpha_i |v_i\rangle |\overline{\sigma_i}\rangle \left(\frac{\overline{\sigma}_{min}}{\overline{\sigma}_i} |0\rangle + \sqrt{1 \left(\frac{\overline{\sigma}_{min}}{\overline{\sigma}_i} \right)^2} |1\rangle \right)$
 - (iii) for projecting in the subspace spanned by singular values smaller than θ , map $|\overline{\sigma}_i\rangle|0\rangle \rightarrow$ $|\overline{\sigma}_i\rangle|0\rangle$ if $\overline{\sigma}_i<(1+\delta)\theta$ and to $|\overline{\sigma}_i\rangle|1\rangle$ otherwise.
- 4: Uncompute the SVE to get the following states:
 - (i) for matrix multiplication: $\sum_{i=1}^{d} \alpha_i \overline{\sigma}_i |v_i\rangle |0\rangle + |G\rangle |1\rangle$
 - (ii) for matrix inversion: $\overline{\sigma}_{min} \sum_{i=1}^{d} \frac{\alpha_i}{\overline{\sigma}_i} |v_i\rangle |0\rangle + |G\rangle |1\rangle$
 - (iii) for projection in a subspace: $\sum_{j \in S} \alpha_j |v_j\rangle |0\rangle + \sum_{j \in \overline{S}} \alpha_j |v_j\rangle |1\rangle$ where S is the set of j's such that $\sigma_j \leq \theta$ and some j's such that $\sigma_j \leq [\theta, (1+\delta)\theta)$, and \bar{S} is the complement of S.
- 5: Perform amplitude amplification on the register $|0\rangle$ with the unitary U implementing steps 1 to 4, to obtain
 - (i) for matrix multiplication: $|z\rangle$ such that $|z\rangle |Mx\rangle | \le \epsilon$, using $O(\kappa(M))$ iterations
 - (ii) for matrix inversion: $|z\rangle$ such that $|z\rangle |M^{-1}x\rangle| \leq \epsilon$, using $O(\kappa(M))$ iterations
 - (iii) for projection in a subspace: $|M_{\theta,\delta}^+ M_{\theta,\delta} x\rangle$, using $O(\frac{\|x\|}{\|M_{<\theta,\delta}^+ M_{\leq\theta,\delta} x\|})$ iterations
- 6: Perform amplitude estimation on the register $|0\rangle$ with the unitary U implementing steps 1 to 4, to obtain
 - (i) for matrix multiplication: ||Mx|| such that $||Mx|| ||Mx|| \le \eta ||Mx||$, using $O(\kappa(M)/\eta)$
 - (ii) for matrix inversion: $\overline{\|M^{-1}x\|}$ such that $|\overline{\|M^{-1}x\|} \|M^{-1}x\|| \le \eta \|M^{-1}x\|$, using $O(\kappa(M)/\eta)$ iterations

Quantum Slow Feature Analysis 4

Our goal is to quantumly map the input matrix X to the output matrix Y. For this, we assume that the matrices X and \dot{X} are stored in QRAM and we provide efficient data structures for that in Appendix A. Let us define the state $|X\rangle:=\frac{1}{\|X\|_F}\sum_{i=1}^n\|x(i)\|\,|i\rangle\,|x(i)\rangle$. We will describe how to build a circuit that approximately performs the unitary $U_{QSFA}:|X\rangle \to |Y\rangle$ where $|Y\rangle:=\frac{1}{\|Y\|_F}\sum_{i=0}^n||y(i)||\,|i\rangle\,|y(i)\rangle$. As the classical algorithm, QSFA is divided in two parts. In the first step we whiten the data, i.e. we map the state $|X\rangle$ to the state $|Z\rangle=|XB^{-1/2}\rangle$, and in the second step we approximately project $|Z\rangle$ onto the subspace spanned by the smallest eigenvectors of the whitened derivative covariance matrix $A=\dot{Z}^T\dot{Z}$.

4.1 Step 1: Whitening the data

Recall that $X = \sum_i \sigma_i u_i v_i^T \in \mathbb{R}^{n \times d}$, and $A, B \in \mathbb{R}^{d \times d}$. We now show how to whiten the data having quantum access to the matrix X. We know that the data is whitened by multiplying X with the matrix $B^{-1/2} = (X^T X)^{-1/2}$. Note that $B^{-1/2}$ is a symmetric matrix with eigenvectors the column singular vectors of X and eigenvalues equal to $1/|\sigma_i|$. In fact the results in [CGJ18] easily imply that the time to multiply with $B^{-1/2}$ is the same as the time to multiply with X and hence we have

Theorem 5 (Whitening algorithm). Let $X = \sum_i \sigma_i u_i v_i^T \in \mathbb{R}^{n \times d}$ stored in QRAM as described in Appendix A. Let $Z = XB^{-1/2} = X(X^TX)^{-1/2}$ the matrix of whitened data. There exists a quantum algorithm that produces as output a state $|\bar{Z}\rangle$ such that $||\bar{Z}\rangle - |Z\rangle| \leq \varepsilon$ in expected time $\tilde{O}(\kappa(X)\mu(X)\log 1/\varepsilon)$).

4.2 Step 2: Projection in slow feature space

Remember that the previous step produced the state $|Z\rangle$ of the whitened data up to some error ϵ . Now we want to project this state onto the subspace spanned by the eigenvectors associated to the K-1 "slowest" eigenvectors of the whitened derivative covariance matrix $A:=\dot{Z}^T\dot{Z}$, where \dot{Z} is the whitened derivative matrix $\dot{Z}=\dot{X}B^{-1/2}=\dot{X}(X^TX)^{-1/2}$. Let θ a threshold value and δ a precision parameter. With $A_{\leq\theta,\delta}$ we denote a projection of the matrix A onto the vector subspace spanned by the union of the singular vectors associated to singular values that are smaller than θ and some subset of singular vectors whose corresponding singular values are in the interval $[\theta,(1+\delta)\theta]$. As in the previous section, we note that the eigenvalues of A are the squares of the singular values of \dot{Z} , and the two matrices share the same column space: $\dot{Z}=U\Sigma V^T$, and $A_{\dot{Z}}=V\Sigma^2 V^T$. Note also that whitening the derivatives is equal to taking the derivatives of the whitened data.

Using the projection ideas in [KP16] and the recent more efficient procedures in [CGJ18, GSLW18] for easily manipulating products of matrices we can project the input onto the "slow" subspace of A and also estimate the norm. To perform the projection, we will need a threshold for the eigenvalues that will give us the subspace of the K-1 slowest eigenvectors. A priori, we don't know the appropriate threshold value, and thus it must be found experimentally through binary search since it depends on the distribution of singular values of the matrix representing the dataset.

We provide the full analysis in the next section that describes the entire QSFA algorithm.

4.3 Analysis of QSFA

We can now describe and analyse the entire QSFA algorithm. Our goal is to use QRAM access to the input data X and \dot{X} and output a quantum state $|Y\rangle$ that corresponds to the projection of the whitened data onto the slow eigenvectors of the derivative covariance matrix, i.e. output $A_{<\theta,\delta}^+A_{\leq\theta,\delta}Z$.

QSFA Quantum Slow Feature Analysis

Require:

Matrices $X \in \mathbb{R}^{n \times d}$ and $\dot{X} \in \mathbb{R}^{n \times d}$ in QRAM, parameters $\epsilon, \theta, \delta, \eta > 0$.

Ensure:

A state $|\overline{Y}\rangle$ such that $||Y\rangle - |\overline{Y}\rangle| \le \epsilon$, with $Y = A^+_{\le \theta, \delta} A_{\le \theta, \delta} Z$

- 1: Create the state $|X\rangle := \frac{1}{\|X\|_F} \sum_{i=1}^n \|x(i)\| |i\rangle |x(i)\rangle$
- 2: (Whitening algorithm) Map $|X\rangle$ to $|\overline{Z}\rangle$ with $|\overline{Z}\rangle |Z\rangle| \le \epsilon$ and $Z = XB^{-1/2}$.
- 3: (Projection in slow feature space) Project $|\overline{Z}\rangle$ onto the slow eigenspace of A using threshold θ and precision δ (i.e. $A^+_{<\theta,\delta}A_{\leq\theta,\delta}\overline{Z}$)
- 4: Perform amplitude amplification and estimation on the register $|0\rangle$ with the unitary U implementing steps 1 to 3, to obtain $|\overline{Y}\rangle$ with $|\overline{Y}\rangle |Y\rangle| \le \epsilon$ and an estimator $|\overline{Y}|$ with multiplicative error η .

We conclude this section by stating the main dimensionality reduction theorem of this paper.

Theorem 6 (QSFA algorithm). Let $X = \sum_{i} \sigma_{i} u_{i} v_{i}^{T} \in \mathbb{R}^{n \times d}$ and its derivative matrix $\dot{X} \in \mathbb{R}^{n \log n \times d}$ stored in QRAM as described in Appendix A. Let $\epsilon, \theta, \delta, \eta > 0$. There exists a quantum algorithm that produces as output a state $|\overline{Y}\rangle$ with $||\overline{Y}\rangle - |A_{\leq \theta, \delta}^{+} A_{\leq \theta, \delta} Z\rangle| \leq \epsilon$ in time $\tilde{O}\left(\left(\kappa(X)\mu(X)\log(1/\varepsilon) + \frac{(\mu(X) + \mu(\dot{X}))}{\delta\theta}\right) \frac{||Z||}{||A_{\leq \theta, \delta}^{+} A_{\leq \theta, \delta} Z||}\right)$ and an estimator $\overline{||Y||}$ with $||\overline{||Y||} - ||Y|| |\leq \eta \, ||Y||$ with an additional $1/\eta$ factor.

Proof. QSFA consists of two steps. The first step is the whitening, which can be performed in time $\tilde{O}(\kappa(X)\mu(X)\log(1/\epsilon))$ and provide the state $|\overline{Z}\rangle$ (see Theorem 5).

The second step is the projection in the slow feature space. Using Theorems 2,3, and 4, we know that the projection (without the amplitude amplification) takes time equal to the ratio μ over the threshold parameter, and since the matrix is the product of matrices, the parameter μ is the sum of the μ 's, namely we have that the second step takes time $\tilde{O}(\frac{(\mu(X) + \mu(\dot{X})}{\delta \theta})$.

Finally, the amplitude amplification and estimation depends on the size of the projection of $|\overline{Z}\rangle$ onto the slow eigenspace of A, more precisely it corresponds to the factor $\tilde{O}(\frac{||\overline{Z}||}{||A^+_{\epsilon\theta,\kappa}A_{\leq\theta,\kappa}\overline{Z}||})$.

First, this term is roughly the same if we look at Z instead of \overline{Z} . Note also that Z is the whitened data, which means that each whitened vector should look roughly the same on each direction. This implies that the ratio should be proportional to the ratio of the dimension of the whitened data over the dimension of the output signal. We will see in the following sections that in the case of the MNIST dataset this ratio is small enough.

5 Quantum Frobenius Distance classifier

In this section we provide a novel quantum classification algorithm, called Quantum Frobenius Distance Classifier (QFD), whose running time is logarithmic in the dimension and number of data points, assuming that the training dataset as quantum states is efficiently preparable, namely it is either stored in QRAM as described in Appendix A or comes directly from some quantum process. The classification algorithm assigns a test point x(0) to the cluster k whose points have minimum normalized average squared ℓ_2 distance to x(0).

Let X_k be defined as the matrix whose rows are the vectors corresponding to the k-th cluster, and $|T_k|$ is the number of elements in the cluster. For the test point x(0), define the matrix $X(0) \in \mathbb{R}^{|T_k| \times d}$ which just repeats the row $x(0) |T_k|$ times. Then, we define

$$F_k(x(0)) = \frac{\|X_k - X(0)\|_F^2}{2(\|X_k\|_F^2 + \|X(0)\|_F^2)},$$

which corresponds to the average normalized squared distance between x(0) and the cluster k. Let $h: \mathcal{X} \to [K]$ our classification function. We assign to x(0) a label according to the following rule:

$$h(x(0)) := \underset{k \in [K]}{\arg \min} F_k(x(0))$$
 (4)

We will estimate $F_k(x(0))$ efficiently using the algorithm below. From our QRAM construction we know we can create a superposition of all vectors in the cluster as quantum states, have access to their norms and to the total number of points and norm of the cluster (see also Appendix A). We define $N_k = \|X_k\|_F^2 + \|X(0)\|_F^2 = \|X_k\|_F^2 + |T_k| \|x(0)\|^2$.

QFE 4 Frobenius Distance Estimator

Require:

QRAM access to the matrix X_k of cluster k and to a test vector x(0). Error parameter $\eta > 0$.

An estimate $\overline{F_k(x(0))}$ such that $|F_k(x(0)) - \overline{F_k(x(0))}| < \eta$.

- 1: s:=0
- 2: **for** $r = O(1/\eta^2)$ **do**
- 3: Create the state

$$\frac{1}{\sqrt{N_k}} \left(\sqrt{|T_k|} \left\| x(0) \right\| \left| 0 \right\rangle + \left\| X_k \right\|_F \left| 1 \right\rangle \right) \left| 0 \right\rangle \left| 0 \right\rangle$$

4: Apply the unitary that maps:

$$\left|0\right\rangle \left|0\right\rangle \mapsto \left|0\right\rangle \frac{1}{\sqrt{\left|T_{k}\right|}} \sum_{i \in T_{k}} \left|i\right\rangle \ \ \text{and} \ \ \left|1\right\rangle \left|0\right\rangle \mapsto \left|1\right\rangle \frac{1}{\left\|X_{k}\right\|_{F}} \sum_{i \in T_{k}} \left\|x(i)\right\| \left|i\right\rangle$$

to the first two registers to get

$$\frac{1}{\sqrt{N_k}} \left(\left. |0\rangle \sum_{i \in T_k} \left\| x(0) \right\| \left| i \right\rangle + \left| 1 \right\rangle \sum_{i \in T_k} \left\| x(i) \right\| \left| i \right\rangle \right) \left| 0 \right\rangle$$

5: Apply the unitary that maps

$$|0\rangle |i\rangle |0\rangle \mapsto |0\rangle |i\rangle |x(0)\rangle$$
 and $|1\rangle |i\rangle |0\rangle \mapsto |1\rangle |i\rangle |x(i)\rangle$

to get the state

$$\frac{1}{\sqrt{N_k}}\Big(\left.\left|0\right\rangle \sum_{i\in T_k}\left\|x(0)\right\|\left.\left|i\right\rangle\left|x(0)\right\rangle + \left.\left|1\right\rangle \sum_{i\in T_k}\left\|x(i)\right\|\left.\left|i\right\rangle\left|x(i)\right\rangle \right.\Big)$$

6: Apply a Hadamard to the first register to get

$$\frac{1}{\sqrt{2N_k}}\left|0\right\rangle \sum_{i\in T_k} \left(\left\|x(0)\right\| \left|i\right\rangle \left|x(0)\right\rangle + \left\|x(i)\right\| \left|i\right\rangle \left|x(i)\right\rangle\right) + \frac{1}{\sqrt{2N_k}}\left|1\right\rangle \sum_{i\in T_k} \left(\left\|x(0)\right\| \left|i\right\rangle \left|x(0)\right\rangle - \left\|x(i)\right\| \left|i\right\rangle \left|x(i)\right\rangle\right)$$

- 7: Measure the first register and if the outcome is $|1\rangle$ then s:=s+1
- 8: end for
- 9: Output $\frac{s}{r}$.

For the analysis, just note that the probability of measuring $|1\rangle$ is:

$$\frac{1}{2N_k} \left(\left| T_k \right| \left\| x(0) \right\|^2 + \sum_{i \in T_k} \left\| x(i) \right\|^2 - 2 \sum_{i \in T_k} \left\langle x(0), x(i) \right\rangle \right) = F_k(x(0)).$$

By Hoeffding bounds, to estimate $F_k(x(0))$ with error η we would need $O(\frac{1}{\eta^2})$ samples. For the running time, we assume all unitaries are efficient either because the quantum states can be prepared directly by some quantum procedure or given that the classical vectors are stored in the QRAM as described in Appendix A, hence the algorithm runs in time $\tilde{O}(\frac{1}{\eta^2})$. We can of course use amplitude estimation and save a factor of η . Depending on the application one may prefer

to keep the quantum part of the classifier as simple as possible or optimize the running time by performing amplitude estimation.

Given this estimator we can now define the QFD classifier.

QFD 5 Quantum Frobenius Distance classifier

Require

QRAM access to K matrices X_k of elements of different classes. A test vector x(0). Error parameter $\eta > 0$.

Ensure:

A label for x(0).

- 1: for $k \in [K]$ do
- 2: Use the QFE algorithm to compute $F_k(x(0))$ on X_k and x(0) with precision η .
- 3: end for
- 4: Output $h(x(0)) = \arg\min_{k \in [K]} F_k(x(0))$.

The running time of the classifier can be made $\tilde{O}(\frac{K}{\eta})$ when using amplitude amplification. We will see that in fact η does not have to be very small in order to classify correctly the MNIST dataset after the dimensionality reduction (we can take $\eta=1/10$), since the clusters are pretty well separated.

6 Classification of MNIST dataset of handwritten digits

6.1 Description of the quantum classifier

The MNIST dataset [LeC] is composed of n = 60000 images in the training set and 10000 images in the test set, where each image is a black and white image of a handwritten digit of 28×28 pixels. The MNIST dataset is a commonly used benchmark for the accuracy of proposed classifiers, where accuracy is defined as the percentage of correctly classified elements in the test set. See for example [LeC] or [LBBH98] for a long list of MNIST classification results. Classical classification techniques can achieve around 98-99% accuracy, with neural network solutions exceeding 99% (the MNIST dataset is quite simple and this is why it is used as a first benchmark). Classical SFA has also been applied previously on the same dataset with accuracy 98.5%, with initial PCA of dimension 35 and polynomial expansion of degree 3 [Ber05], and we will closely follow that classification procedure.

Our goal in this section is to propose a hybrid classical-quantum classifier with two properties: very good accuracy and efficiency. We describe our quantum classifier by going through the three parts in any classical classifier: preprocessing, training, and testing.

Data preprocessing In the preprocessing stage, we need to basically decide on the dimension of the input vectors that we will provide as input to the training algorithm. In fact, the bottleneck for the training part is the fact that when the dimension of the input vectors becomes too large, procedures like full PCA or SFA become infeasible since their complexity is $\tilde{O}(min(n^2d, d^2n))$ [RLLY08]. This is why, as we will also see below, the dimension of the input is kept under control, even though bigger dimension would probably mean better accuracy in the classification.

Let us see in more details what this dimension should be. The methodology is as follows: first, the dimension of the dataset, which is initially $28 \times 28 = 784$, is reduced with a PCA to something like 35 (or around 90, depending on the polynomial expansion degree we use in the following step). Fortunately, efficient incremental algorithms for PCA exist, where it is not required to fully diagonalize a covariance matrix, and the running time depends on the number of dimensions required as output. Second, a polynomial expansion of degree 2 or 3 is applied, hence making the dimension up to 10^4 . The reason for this preprocessing is that we need to capture the nonlinear relationships of the input, hence it is necessary to do the polynomial expansion. However, it would already challenge current HPC architectures if we performed polynomial expansion on the initial dimension of 784, thus we perform PCA first. The main intuition is that most of the information about the input vectors can be captured in the subspace spanned by the top 40 eigenvectors and the nonlinear correlations can be captured by a polynomial expansion of at most degree 3 on that

subspace. Third, the data is normalized so as to satisfy the SFA requirements of zero mean and unit variance

Overall, the preprocessing stage creates around $n = 10^5$ vectors $x(i), i \in [n]$ of size roughly $d = 10^4$ and the running time of the preprocessing is of the order of $\tilde{O}(nd)$, with $nd \approx 10^9$.

In the quantum classifier, apart from the above steps, we will add a first quantum step, which is to load the preprocessed data in the QRAM as described in Appendix A. The loading takes time polylogarithmic for each data coordinate, makes only one pass over the data and creates a data structure linear on the size of the data. Hence, we can add this step to the preprocessing, keeping the overall preprocessing time to $\tilde{O}(nd)$.

Training We are now ready to proceed to the training stage, which will be performed through Slow Feature Analysis. The classical SFA procedure outputs a small number (K-1) of "slow" eigenvectors of the derivative covariance matrix, where K is the number of different classes in the classification and here K=10. This is in fact the bottleneck for classical algorithms and this is why the dimension was kept to $d=10^4$, which still requires intensive HPC calculations. In high level, the running time is cubic and hence of the order 10^{13} . Once these eigenvectors are found, each data point is projected onto this subspace to provide n vectors of (K-1) dimensions which are stored in memory. Note that the training set is labelled, so we have the clustering of these points and we can use it to find for example the centroid of each cluster. As we said, this dimensionality reduction is the computationally hardest part of the classifier and its complexity is cubic on the dimension chosen in the preprocessing stage. This is why the dimension is kept small, thus deteriorating the classification.

In the quantum case, we have shown how to perform a version of QSFA in time which is only polylogarithmic in the dimension and number of data points. One can use this property either to have a much faster algorithm, or to increase the dimension of the data in the previous step, hence increasing the accuracy of the classifier. Note that at the end, the quantum procedure does not output a classical description of the eigenvectors, neither does it compute all vectors y(i) as the classical counterpart could do. Nevertheless, given a quantum state $|x(i)\rangle$ it can produce the quantum state $|y(i)\rangle$ with high probability and accuracy.

Testing For the testing stage, the trained classifier is used to classify the 10000 images in the test set.

Classically, the testing works as following: using the output of the SFA procedure, one projects the test data point x(0) onto the subspace spanned by the (K-1) slow eigenvectors found in the training stage, to get a (K-1)-dimensional vector y(0). Then, a classification algorithm is performed, for example kNN (i.e. one finds the k closest neighbours of y(0) and assigns the label that appears the majority of times). The complexity of this step is O(Kd) for the projection of the test vector, plus the time of the classification in the K-1-dimensional space. The kNN algorithm is for example linear in the number of data points times the dimension of the points $(\tilde{O}(nd))$. If in the training stage we have found the centroids of the clusters then classification can be done in time $\tilde{O}(Kd)$, as in Nearest Centroid classification.

In our quantum classifier, we use the QFD procedure which runs in time logarithmic in the number and dimension of the data points. In fact, our final algorithm is performing the training and testing together, i.e. using QSFA and QFD together. In high level, for each cluster k, we perform the QFD classifier, where now instead of using directly the states x(i) via the QRAM, we use the QSFA procedure before in order to create the states y(i). More precisely, we use the QSFA procedure that maps $|0\rangle$ to a state $|\overline{Y}\rangle$, which is ε -close to the state $|Y\rangle = \frac{1}{\|Y\|_F} \sum_{i=1}^n \|y(i)\| \, |i\rangle \, |y(i)\rangle$. We can also use the same procedure to construct a single vector $|y(0)\rangle$ or to construct a state ε -close to $|Y_k\rangle$ and estimate the norm $\|Y_k\|_F$, where we only use the data from the k-th cluster. We let $N_k = \|Y_k\|_F^2 + |T_k| \, \|y(0)\|^2$.

Quantum Classifier for MNIST 6 Quantum Classifier for MNIST

Require:

QRAM access to matrices X and \dot{X} , a new test vector x(0), and $\varepsilon, \eta > 0$ the error parameters. **Ensure:**

A label for x(0)

- 1: for $k = 1 \rightarrow K$ do
- 2: $s_k := 0$
- 3: Use QSFA to estimate the norm $||Y_k||_F$ and the norm ||y(0)|| (to error η).
- 4: **for** $r = O(1/\eta^2)$ **do**
- 5: Create the state (to error $O(\eta)$)

$$\frac{1}{\sqrt{N_k}} \left(\sqrt{|T_k|} \|y(0)\| |0\rangle + \|Y_k\| |1\rangle \right) |0\rangle |0\rangle$$

6: Use QSFA to apply the following mapping (to error ε):

$$|0\rangle |0\rangle |0\rangle \mapsto |0\rangle \frac{1}{\sqrt{|T_k|}} \sum_{i \in T_k} |i\rangle |y(0)\rangle \quad \text{and} \quad |1\rangle |0\rangle |0\rangle \mapsto |1\rangle \frac{1}{\|Y_k\|} \sum_{i \in T_k} \|y(i)\| |i\rangle |y(i)\rangle$$

to the first two registers to get a state (to error $O(\varepsilon + \eta)$)

$$\frac{1}{\sqrt{N_k}} \left(\left. \left| 0 \right\rangle \sum_{i \in T_k} \left\| y(0) \right\| \left| i \right\rangle \left| y(0) \right\rangle + \left| 1 \right\rangle \sum_{i \in T_k} \left\| y(i) \right\| \left| i \right\rangle \left| y(i) \right\rangle \right)$$

7: Apply a Hadamard to the first register to get the state (to error $O(\varepsilon + \eta)$)

$$\frac{1}{\sqrt{2N_k}}\left|0\right\rangle \sum_{i\in T_k} \left(\left\|y(0)\right\|\left|i\right\rangle\left|y(0)\right\rangle + \left\|y(i)\right\|\left|i\right\rangle\left|y(i)\right\rangle\right) + \frac{1}{\sqrt{2N_k}}\left|1\right\rangle \sum_{i\in T_k} \left(\left\|y(0)\right\|\left|i\right\rangle\left|y(0)\right\rangle - \left\|y(i)\right\|\left|i\right\rangle\left|y(i)\right\rangle\right)$$

- 8: Measure the first register and if the outcome is $|1\rangle$ then $s_k := s_k + 1$
- 9: end for
- 10: Estimate the Frobenius distance as $F_k(y(0)) := \frac{s_k}{r}$ (to error $O(\varepsilon + \eta)$).
- 11: end for
- 12: Assign the new vector to the cluster with the minimum Frobenius distance estimator:

$$h(x(0)) = min_k \{ F_k(y(0)) \}$$

6.2 Analysis of accuracy and efficiency

We provide an analysis of the accuracy and the running time of the quantum classifier for different sets of parameters. In Table 1 we report the results of our quantum classification of the MNIST data set.

6.2.1 Accuracy estimation

We provide evidence that our quantum algorithm will provide classification with good accuracy. Note that this is not by definition, since - due to errors - the QSFA procedure we perform is not exactly the same as the classical SFA one, and the classification algorithm we use is not among the ones used classically. We also have to make sure that the errors in the procedures will not deteriorate the accuracy.

Since currently available quantum hardware cannot run our algorithm or any significant part of it, we will simulate the quantum algorithms on an Atos QLM with 6 TB of RAM. We tested our algorithm increasing the dimension of an initial PCA on the training set. One can surely hope that the accuracy will get even better when we increase the dimension of the preprocessed input.

First, for the derivative matrix \dot{X} we subsample from all the possible derivatives for a given class. In this experiment we used a constant sample size (with replacement) of 10000 derivatives. Adding more derivatives would not increase the accuracy and will only deteriorate other parameters.

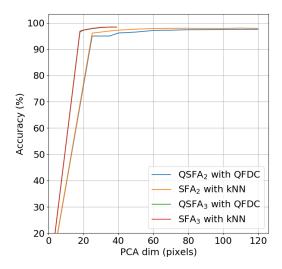


Figure 1: We plot the accuracy of our quantum classifier (QSFA + QFD) versus the classical classifier (SFA + kNN) for polynomial expansion 2 and 3 and different initial PCA dimensions. For polynomial expansion 2, our quantum classifier reaches the accuracy of the classical one for large enough dimensions. For polynomial expansion 3, the two are almost indistinguishable. In this experiment we took for the quantum classifier the error to be $\epsilon = 10^{-5}$ and κ_t to be 200.

Since doing a simulation of the quantum circuit implementing QSFA and classification is not within the reach of the possible classical quantum simulator platforms, our simulation implemented the linear algebraic operations executed by the quantum computer in the Hilbert space. Our software relied on the state-of-the-art python package for numerical computation and machine learning: scikit-learn [PVG⁺11] and the scipy ecosystem [JOP⁺18].

We look at the error that our quantum algorithm commits in the two parts. First, let ϵ the error parameter for the whitening procedure. To simulate the error in the whitening we added noise from a truncated Gaussian distribution centered in each singular value σ_i with unit variance. The new value of σ_i is distributed in $\sigma_i \pm \sigma_i \epsilon$. The running time depends only logarithmically on this error, so we can take this error to be very small. For the error in the projection part, this comes only from potentially projecting on a different space than the one wanted. We recall that the projection procedure performs an SVE with error $\delta\theta$, and then using a threshold gate keeps the singular values which are smaller than $(1 + \delta)\theta$. By taking a correct θ (around 0.3 or 0.05 depending on the polynomial expansion) and a small enough δ (around 1/20), we guarantee in practice that the projection is indeed on the smallest K-1 eigenvectors.

In Figure 1 we plot the accuracy of the (QSFA + QFD) quantum classifier using polynomial expansion of degree 2 and 3, showing that we achieve very good accuracy. In the x axis we change the initial resolution of the image using PCA, and on the y axis we plot the accuracy, namely the percentage of well classified digits from the test set. The highest performance accuracy was 98.5% with polynomial expansion of degree 3 and PCA dimension of 36. The best execution for polynomial expansion of degree 2 is with an initial PCA dimension of 90, and was of 97.4%. For comparison, we also plot the accuracy of a classical (SFA + kNN) classifier and see that our quantum classifier practically achieving the accuracy as the classical one. Our simulations also lead to results comparable to the literature [Ber05], where a Gaussian classifier is used after SFA with PCA dimension 35 and polynomial expansion of degree 3 to achieve 98.5% accuracy.

We remark that the dimensionality reduction step is necessary for good accuracy. Indeed, the classification algorithm proposed in Section 5 reaches 67.13% accuracy with the original vectors, which is comparable to classical classification on the raw data. Moreover, the degree of polynomial expansion is important in capturing the non-linearity in the input and we see that the accuracy increases almost 1% by going from polynomial expansion of degree 2 to 3. We expect that with a polynomial expansion of degree 4 and a sufficient PCA dimension it will be possible to reach even higher accuracy. Such parameters would be impossible for classical classifiers but our quantum classifier can handle them, since the dependence on the dimension is favourable.

Table 1: Accuracy of relevant experiments for various combination of classifiers and polynomial expansion. Here we have chosen $\epsilon/\kappa(X) = 10^{-7}, \delta = 0.054, \eta = 1/10$ and 10.000 derivatives per class.

$QSFA_2$										
PCA	d	X	$ \dot{X} $	$ x(i) _1$	$\ \dot{x}(i)\ _1$	$\kappa(X)$	$\kappa_t(X)$	θ	$\%_t$	%
40	860	22	102	0.9	1.4	41	32	0.38	96.4	96.4
80	3220	41	197	2.7	3.8	119	65	0.32	97.3	97.4
90	4185	46	215	3.1	4.4	143	72	0.31	97.4	97.4
$QSFA_3$										
PCA	d	X	$ \dot{X} $	$ x(i) _1$	$\ \dot{x}(i)\ _1$	$\kappa(X)$	$\kappa_t(X)$	θ	$\%_t$	%
30	5455	73	81	5.9	4.3	276	149	0.06	98.2	98.3
35	8435	96	102	7.8	5.7	369	146	0.05	97.5	98.4
36	9138	101	108	8.0	5.3	388	149	0.04	97.7	98.5

We also recorded in Table 1 the accuracy of our classifier when instead of the condition number κ we use a conditioning threshold κ_t which improves the running time by a factor of 2. The threshold of the conditioning number of X is chosen to retain 99.5% of the singular values. In this case, the accuracy for polynomial expansion 2 remains practically unchanged, while for polynomial expansion 3 there is a small decline, with the maximum becoming 98.2%. We can increase this accuracy in the following way: instead of running the classifier once, we run it a few times (around 10) and do a majority vote before labelling the new data point. This increases the accuracy of polynomial expansion 3 a bit, for example for PCA 36, the accuracy goes from 97.7% to 97.9%.

Note that while we tried to optimize the parameters in order to achieve the best possible accuracy, it is very probable there are even better parameters that in practice can be found by a hyper-parameter tuning algorithm. This could further increase the accuracy of the quantum classifier.

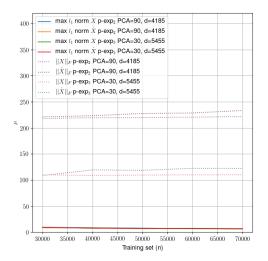
6.2.2 Running time estimation

It is easy to see that the asymptotic running time of the quantum classifier is given by the running time of the QSFA times a factor K/η^2 (or K/η with amplitude amplification) that comes from the QFD. We will now provide estimates for all the parameters that appear in the running time of our quantum classifier for the MNIST dataset. Let us stress that our goal now is not to prove asymptotic bounds on the running time, but estimate these parameters on the MNIST dataset, hence providing a good idea of what the running time will be in practice. Our algorithm runs for each of the K=10 classes.

Number and dimension of data points. For the MNIST data set we have that nd is of the order of 10^9 (including data points and derivative points). The main advantage of our quantum classifier is the logarithmic dependence on the number and dimension of the data points. This way, one can either opt for a more efficient quantum algorithm, or even more interestingly, achieve higher accuracy by increasing the number and the dimension of the data points.

The parameter μ for the matrices X and X. We analyze the parameter μ of the matrices X and X as the number of data points in the training set and the dimension of the input vectors (PCA dimension + polynomial expansion) increases. In the original algorithms for linear systems the parameter μ was in fact the sparsity of the matrix which for the MNIST dataset is linear to the dimension, (i.e. around 10^4). Using the QRAM construction presented in the Appendix, we know that μ is bounded by the Frobenius norm of the matrix. We also look at the case where μ depends on the maximum l_1 norm of the rows of the matrices, as presented in [KP17]. In Figure 2 we analyze these values (where the matrices are normalized to have spectral norm 1 as needed) and see that they are practically constant as we increase the number of points in the dataset. All the l_1 norms in the experiment were less than 10. We also plot the Frobenius norm and the maximum l_1 norm as the dimension of the vectors in the dataset increases. While the Frobenius norm somewhat increases with the dimension, the maximum l_1 norm remains stable and less than 10.

This could be expected since in the preprocessing a PCA is done, making the input matrices in fact quite low rank. Indeed, after the polynomial expansion the Frobenius norm does not increase



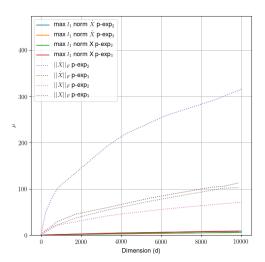


Figure 2: Sensitivity analysis of the parameter μ for the matrices X and \dot{X} while increasing n and d. The graphs show the value of the Frobenius norm and the max ℓ_1 -norm as two options for μ . For the MNIST dataset, we see that both the Frobenius norm and the maximum l_1 norm are practically constant when we increase the number of data points in the training set, with values of the order of 10^2 and 10 respectively. When we increase the dimension of the data points, the Frobenius norm increases slowly to values around 10^2 , while the maximum ℓ_1 norm remains practically constant and below 10.

much since we only add higher order terms and note that all entries of the matrices are smaller than 1, since $||X||_{max} \leq ||X||_2 \leq 1$. On the other hand, the scaling and normalization of X helps keeping the l_1 norm even lower.

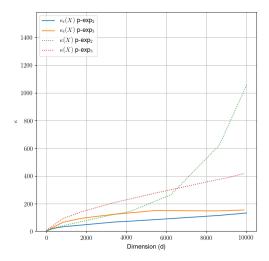
What is important to state here is that one can gain a factor 10^3 by taking the correct quantum algorithm for performing linear algebra and not just an off-the-shelf one. Such decisions will be crucial in reaching the real potential of quantum computing for machine learning applications.

Condition number for the matrix X. For the condition number of the input matrix, first we plot it while increasing the number of data points and see that indeed the condition number is stable, in fact decreasing. Note also that we do not need to have the real condition number in the running time but a threshold under which we ignore the smaller eigenvalues. In fact, by consider a conditioning threshold which retains 99.5% of the singular values and which does not considerably penalise the accuracy, and we achieve a behaviour of growing much more slowly as we increase the dimension and with a value around 10^2 .

Error parameters. There are four error parameters, ε for the matrix multiplication procedure, δ and θ for the projection procedure, and η for the estimate in the classification. For ε , it appears only within a logarithm in the running time, so we can take it to be rather small. In our experiments we took it to be as small as 10^{-5} . For the projection, we took $\delta \approx 1/20$ and from the simulations we have that $\theta \approx 0.3$ for polynomial expansion 2 and $\theta \approx 0.05$ for polynomial expansion 3. Last, it is enough to take $\eta = 1/10$. Note also, that these parameters are pretty stable when increasing the dimension, they only depend on whether we perform a polynomial expansion of 2 or 3.

Projection ratio. Our running time also depends on one last thing, the ratio between the norm of the vector in the whitened space over the projected vector in the slow feature space. To estimate this, we computed the average and the variance of this ratio among the vectors in the test set. For an initial PCA dimension of 40 and polynomial expansion of degree 2, this ratio is 0.1 with variance 0.0022, while for a polynomial expansion of degree 3 and a PCA dimension of 30 is 0.05 with 0.0007 variance.

Overall, putting the orders of all parameters together, we get that the rough estimate of the



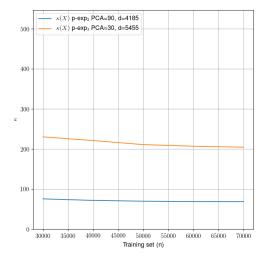


Figure 3: Sensitivity analysis of the condition number of X while increasing n and d. We plot the condition number while increasing the number of data points in the training set and see that it slowly decreases to reach values around 10^2 . We also plot the condition number and the condition threshold (that keeps 99.5% of the eigenvalues) while increasing the dimension of the data points. While the real condition number increases, the condition threshold is stable around 10^2 .

running time of the quantum classifier's training and testing part is of the order of 10⁷. Again, we are not arguing that this is the precise number of steps of the quantum algorithm, but these estimates, and more importantly the behaviour of the parameters as the dimension increases, give further evidence that the quantum classifier can be more efficient that a classical classifier, whose running time is of the order of 10¹³ for the same input dimension. Moreover, the fact that all parameters that appear in the running time of the quantum classifier seem to increase very slowly (or not at all) as we increase the number and dimension of the data points leads us to believe that one could still have an efficient quantum classifier with much higher number and dimension of points, thus eventually providing much higher classification accuracy.

7 Conclusions

We provided evidence that quantum computers with quantum memories can be useful for solving real-world problems by designing an efficient classifier. Benchmarked on the MNIST dataset, we proved high accuracy classification, comparable to the best classical classifiers. The running time of the quantum procedure is only logarithmic with respect to the dimension and number of data points, thus allowing the quantum classifier to run on higher dimensional input.

It would be interesting to see if the same performance is achievable also on different dataset. We believe our quantum algorithm for Dimensionality Reduction can find applications in many other contexts. For instance, it can be used directly on processes that produce quantum data that might be high dimensional. In this case, constructing the QRAM would not be a necessary condition anymore. Moreover, we envision its utility in conjunction with other quantum machine learning algorithms. For instance, Projective Simulation [MMDB17] is a Reinforcement Learning algorithm based on a random walk over a graph. The graph represents the memory of an agent that acts on a certain environment. The random walk start from a node (or superposition of nodes) decided by an input-coupling function. QSFA could be used to treat and pre-process high-dimensional input signals in agents that use Projective Simulation as input-coupling function of external stimuli in the memory model of the agent. This would resemble even further what we believe to be the current architecture of the brain, where SFA is used to model complex cells in the primary visual cortex (V1: the first cortical area dedicated to visual processing), and Projective Simulation is used to model high level cognitive functions which emerges from a model of an episodic and compositional memory for the agent (so to model creativity, curiosity, and so on..).

Note also, that the same quantum algorithm for SFA also can acquire the classification capabilities of Fisher Linear Discriminant [KM09] and Laplacian Eigenmaps [Spr11].

Last, our classification procedure provides a simple but powerful way for classifying both quantum data or QRAM-loaded classical data. Note that the procedure, apart from the loading of the data, is extremely simple, including a few extra quantum operations, like a Hadamard and a computational basis measurement. Despite its simplicity, the accuracy of the classifier is comparable to classification algorithms. Even though the loading of the data might be costly, we remark that this cost is amortized, since we prepare the QRAM once, but we can use it for all new test point that arrives in the system. Again, what is important in the classical machine learning world is not the time of the preprocessing, but the efficiency of the training procedure and the accuracy of the classifier on new data. This is exactly where the quantum classifier provides remarkable savings.

Note also that it might be more important not to see our quantum classifier as a faster algorithm but as a way to increase the accuracy. As we said, the training stage is limited by the dimension of the input and the fact that our quantum classifier depends only polylogarithmically on the dimension and all other parameters remain stable when the dimension increases, will enable us to use much higher dimension in the training stage, thus hopefully improving the accuracy of the classifier.

Acknowledgement

We thank Anupam Prakash and Andras Gilyen for helpful discussions.

Appendices

A Construction of the QRAM

In this section we show how to construct the QRAM oracles needed in QSFA. QRAM has been used in quantum algorithmics literature as a generic way of retrieving classical data and build a corresponding quantum state. The name QRAM is meant to evoke the way classical RAM address the data in memory using a tree structure. Classically, given an address to retrieve in memory, each bit of the address is used to take a binary decision on which path to take on a tree-like circuit, until a leaf - which contains the data - is found. Proposals for QRAM have followed this model [GLM08].

We will show here that if we have the ability to ask quantum queries in superposition, then all quantum states we need for the procedures in the quantum classifier can be efficiently created.

A quantum query is defined very simply as

$$|i\rangle |0\rangle \rightarrow |i\rangle |b_i\rangle$$
 for $b_i \in \mathbb{R}$ and $i \in [N]$

One, of course can write down the real b_i with some precision δ using $\log 1/\delta$ bits.

We show what our QRAM data structure looks like for the input matrix X (and similarly for the matrix \dot{X}) if the choice of μ is the Frobenius norm of the matrix. A similar construction for the case where μ is the maximum of the l_1 norms of the rows can be found in [KP17].

Stemmed from ideas in [GR02], which gave the idea of constructing quantum states using precomputed amplitudes, building a QRAM oracle for a matrix of real values has already been described in previous literature [KP17, KP16]: Each row of the matrix is encoded as a tree, where the leves correspond to the matrix elements, while the intermediate nodes store the square amplitudes that corresponds to their subtree.

We extend this data structure to allow us to efficiently create superpositions corresponding to the rows of the matrices, states with amplitudes equal to the norms of the rows of the matrices, and also state corresponding to the inputs that belong to a specific class k.

We assume that the preprocessing (the optional PCA step, polynomial expansion, and removing the mean from the vectors and scaling the components to have unit variance) is performed classically, taking $\tilde{O}(nd)$ time. The creation of the QRAM also takes $\tilde{O}(nd)$ time.

Using the notation of the paper, we have $X \in \mathbb{R}^{n \times d}$, $X = \bigcup_{i=1}^K X_i$ and $X_k \in \mathbb{R}^{|T_k| \times d}$. As we see in the figure, all rows of the matrix X are saved as a tree with leaves the entries and root the

corresponding norm ||x(i)||. We arrange the rows per class and we join all trees corresponding to rows of a class k into a tree built on top of the individual trees, with leaves the norms of each row in the class (i.e. the roots of the previous trees) and root the norm of the class $||X_k||$. On top of these K trees, we built one last tree with leaves the norms of each class (i.e. the roots of the previous trees) and root the norm of the entire matrix ||X||. We also store the number of elements per class $T_k \in [K]$. It is easy to see that the states we need in the quantum classifier can be created efficiently using this data structure.

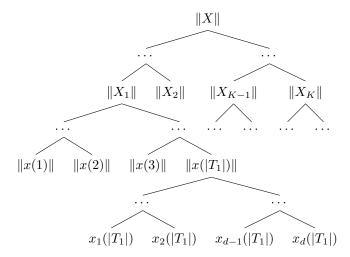


Figure 4: QRAM tree for matrices X_k and for the Frobenius norms of the sub matrices of each class

Theorem 7 (QRAM for X_k [KP16]). Let $X \in \mathbb{R}^{n \times d}$ and $X_k \in \mathbb{R}^{|T_k| \times d}$ for $k \in [K]$. There exists a data structure to store the rows of X such that:

- 1. The size of the data structure is $O(nd \log^2(nd))$
- 2. The time to store a row x(i) is $O(d \log^2(nd))$, and the time to store the whole matrix X is thus $O(nd \log^2(nd))$
- 3. A quantum algorithm that can ask superposition queries to the data structure can perform in time polylog(nd) the following unitaries:
 - $U: |i\rangle |0\rangle \rightarrow |i\rangle |x(i)\rangle$ for $i \in [n]$
 - $V: |0\rangle \to \sum_{i \in [n]} ||x(i)|| |i\rangle$
 - $U_k: |i\rangle |0\rangle \rightarrow |i\rangle |x(i)\rangle$ for $i \in T_k$, for all $k \in [K]$
 - $V_k: |0\rangle \to \sum_{i \in T_k} ||x(i)|| |i\rangle$, for all $k \in [K]$

The procedure to create and store the matrix \dot{X} is exactly the same as the procedure needed for the X. Note that the classical matrix \dot{X}_k is created in the following way: for each sample class T_k in the training set, we are going to create $m = T_k log(T_k)$ new derivative vectors $\dot{x}(i) := x(i) - x(j)$ with $i, j \in T_k$ by sampling from the uniform distribution m pairs of vectors with the same label.

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