Quantum methods for Optimization and Machine Learning

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Quantum Algorithms for Optimisation / ML

The HHL algorithm [Harrow, Hassidim, Lloyd 2009]

Quantum computers provide a quantum solution to a system of linear equations in certain cases exponentially faster than classical algorithms, given quantum access to the data.

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"It opens the possibility of dramatic speedups for machine learning tasks, richer models for data sets and more natural settings for learning and inference"

Quantum Machine Learning Workshop during NIPS 2015

Remark: "Solving" systems of linear equations is BQP-complete

Three remarks on Quantum Machine Learning

QML needs a full-scale computer with quantum access to data for “exponential savings”

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Most overhyped and underestimated field at the same time

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Most overhyped and underestimated field at the same time

(One of) the most convincing reasons to build quantum computers

Quantum Machine Learning: the model

Data storage and quantum access

1. Data can be accessed quantumly directly
2. Quantum RAM : Efficient storage of classical data allowing quantum access to it
   - It takes polylogarithmic time to store/update/delete an element (i,j,a_{ij})
   - Query in polylogarithmic time $\sum c_{ij} |i,j,0\rangle \rightarrow \sum c_{ij} |i,j,a_{ij}\rangle$
3. Other access models…

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Computation on the data

- Given quantum access to data, learn some property of the data
- Running time of quantum algorithm can be more efficient that classical

Use-case: Recommendation Systems

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Matrix ~~Reconstruction~~ Sampling

Step 1

Products

Users

?	**1**	**…**	**?**
?	0	…	?
…	…	…	…
1	?	…	0

Use-case: Recommendation Systems

Matrix ~~Reconstruction~~ Sampling

Singular Value Estimation

Step 1

Products

Users

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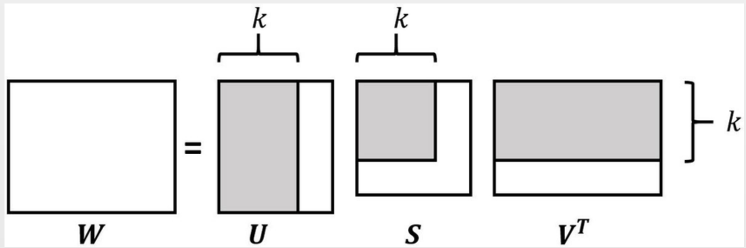
Step 2



Use-case: Recommendation Systems

NETFLIX

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Matrix ~~Reconstruction~~ Sampling

Products

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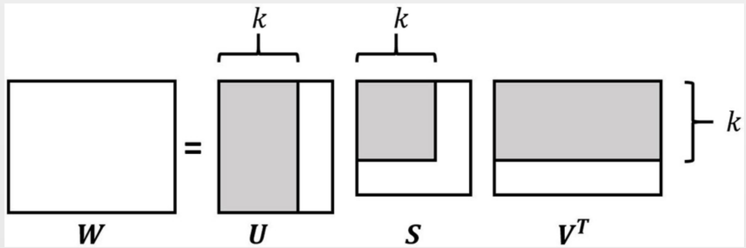

Step 3

Exponentially faster quantum algorithm for Singular Value Estimation

Use-case: Recommendation Systems

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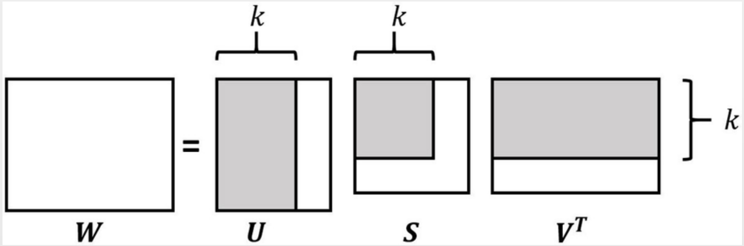

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Exponentially faster quantum algorithm for Singular Value Estimation

Quantum computers provide competitive recommendations exponentially faster than known classical algorithms
[Kerenidis, Prakash '17]

Use-case: Recommendation Systems

NETFLIX

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Matrix ~~Reconstruction~~ Sampling

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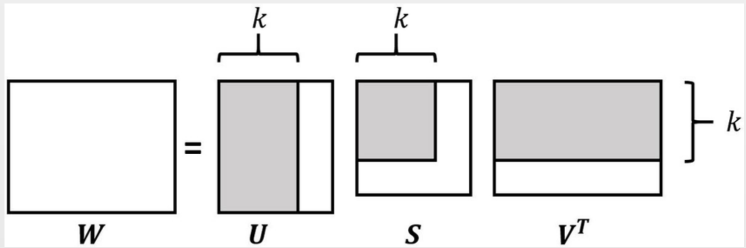

Step 3

Improved Linear Algebra for low-rank matrices

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NETFLIX

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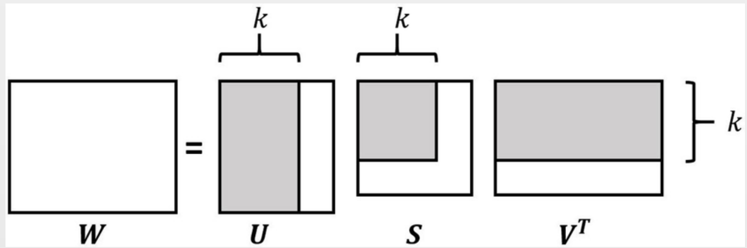

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Exponentially faster quantum algorithm for Singular Value Estimation

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Improved Linear Algebra for low-rank matrices

Running time: O(r*polylog(mn))

General quantum methods for Optimization

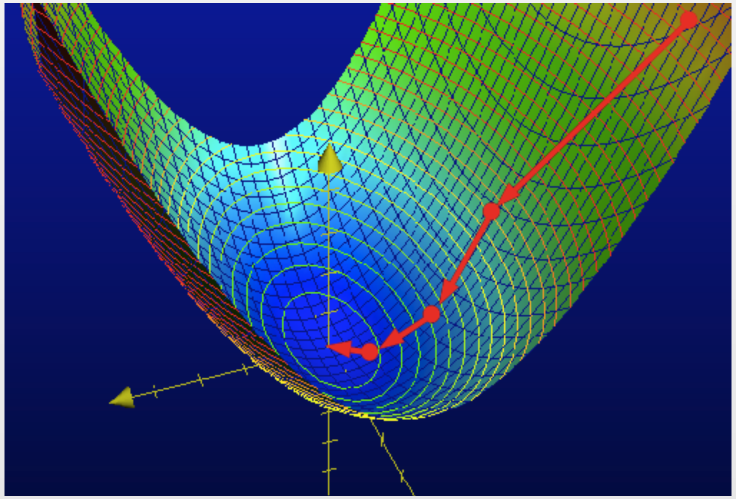
Iterative methods (ubiquitous in practice)

1. Start with an initial solution.
2. Update the solution according to an Update Rule
3. Repeat until the solution is satisfactory

Types of Iterative Methods

First order – Gradient Descent

Second order – Interior point methods



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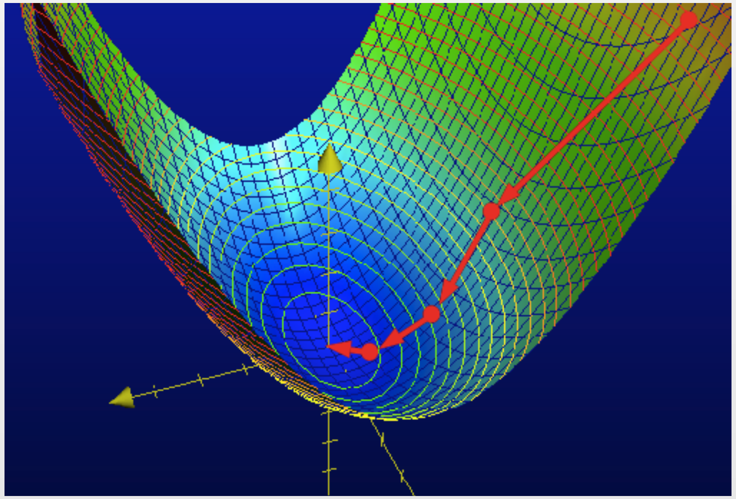

Efficient Quantum Gradient Descent algorithm for Linear Systems and Stochastic Least Squares.
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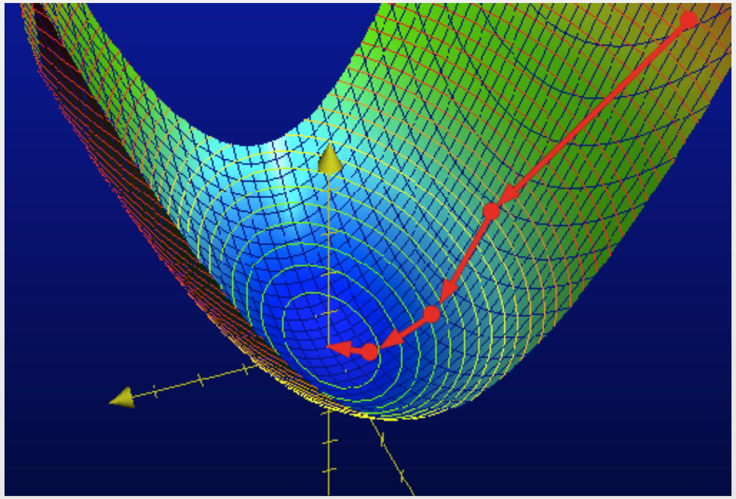

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Efficient Quantum Gradient Descent algorithm for Linear Systems and Stochastic Least Squares.
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Remark 1: Improved Linear Algebra

Remark 2: Great savings in QRAM

Quantum Linear Algebra

Problem:

Given matrix A and vector x, output Ax, $A^{-1}x$, …

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Step 1
Map A to some unitary U s.t.
1. The spectra of A and U are related
2. U is efficient to implement

$A/\mu(A) = P \circ Q$, $U = (2PP^t - I)(2QQ^t - I)$

Efϕiciency via QRAM data structures

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Efficiency via QRAM data structures

Step 2
~~Phase Estimation on U~~
LCU, Qubitization on U

Apply a circuit with $O(\log 1/\varepsilon)$ U's

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Step 3
Amplitude Amplification (VT)

$O(\kappa(A))$ iterations

Quantum Linear Algebra

Problem:
Given matrix A and vector x, output Ax, $A^{-1}x$, …

Running time: $O(\kappa(A)\mu(A)\log 1/\varepsilon)$

Quantum Linear Algebra

Problem:
Given matrix A and vector x, output Ax, $A^{-1}x$, …

Open Question:
What is the optimal $\mu(A)$?

Running time: $O(\kappa(A)\mu(A)\log 1/\varepsilon)$

Could QML work on real data?

Classification

[KL 18]

Could QML work on real data?

Frobenius Distance Classification

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 $\eta > 0$.

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

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

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1. Create the state

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

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Remark 1:
Classification as easy as creating the states

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Remark 2:
Comparable accuracy to classical classifiers

Could QML work on real data?

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Classification

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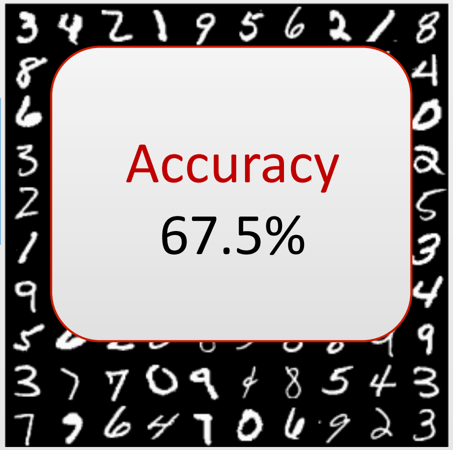

Accuracy

67.5%

Remark 2:
Comparable accuracy to classical classifiers

Could QML work on real data?

Dimensionality Reduction: Slow Feature Analysis

Classification

[KL 18]

Could QML work on real data?

Dimensionality Reduction: Slow Feature Analysis

Classification

[KL 18]

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

Could QML work on real data?

Dimensionality Reduction: Slow Feature Analysis

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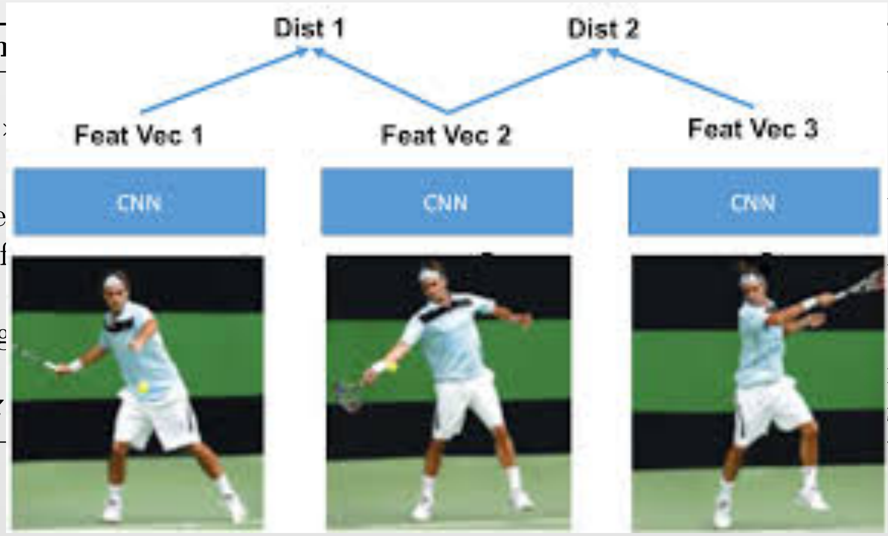

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Quantum Slow Feature Analysis

Efficient Quantum Linear Algebra
(Matrix Multiplication, Inversion, Projection)

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Classification

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Quantum Slow Feature Analysis

Efficient Quantum Linear Algebra
(Matrix Multiplication, Inversion, Projection)

Remark:
Classification only needs quantum states

Could QML work on real data?

Quantum Classifier

Input: X, a new vector x(0)

1. Do QSFA to quantumly project X and x(0) to Y and y(0)
2. Use Frobenius Distance Classification on Y, y(0)

Classification

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Accuracy

We simulate the quantum procedures including errors in an HPC machine and test it on the 10000 test digits of MNIST for different parameters

Classification

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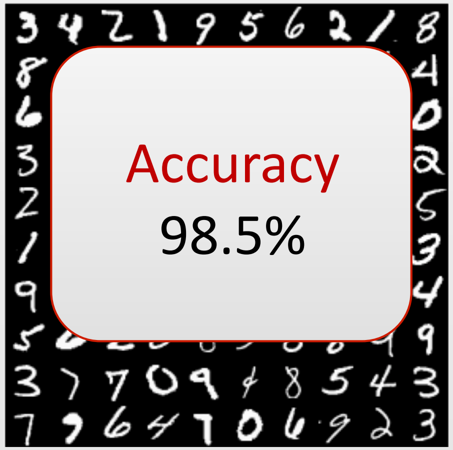

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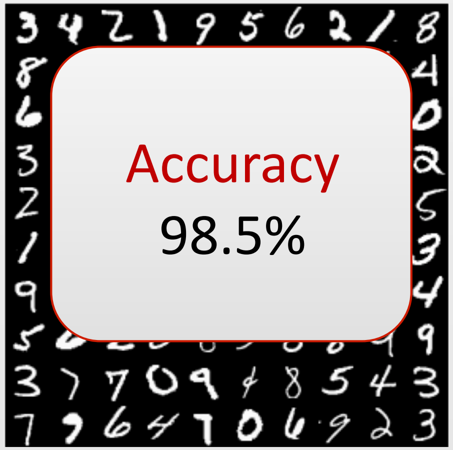
Running time

Classical: $O(n\ d^2)$ ~= 10^{13} (1 hour on 6Tb RAM HPC)

Classification

[KL 18]



Could QML work on real data?

Quantum Classifier

Input: X, a new vector x(0)

1. Do QSFA to quantumly project X and x(0) to Y and y(0)
2. Use Frobenius Distance Classification on Y, y(0)

Accuracy

We simulate the quantum procedures including errors in an HPC machine and test it on the 10000 test digits of MNIST for different parameters

Running time

Classical: $O(n\, d^2) \sim= 10^{13}$ (1 hour on 6Tb RAM HPC)
Quantum: $O(\kappa, \mu, 1/\theta, 1/\delta, 1/\eta, K, \mathrm{polylog}(n, d, 1/\varepsilon), \ldots)$

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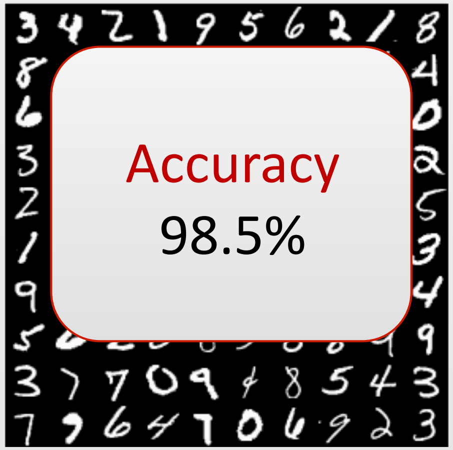

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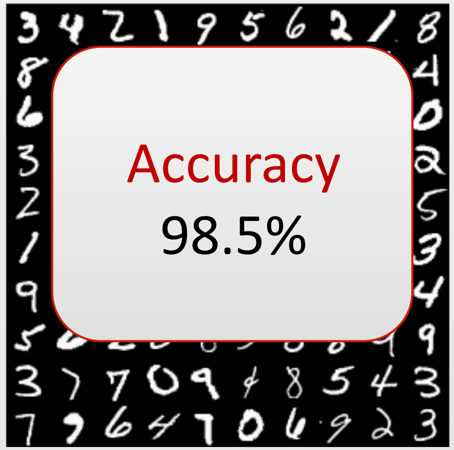
Classification

[KL 18]



Could QML work on real data?

Main question:

Better accuracy by increasing the dimension, keeping efficient time?

Quantum time: O(κ, μ, 1/θ, 1/δ, 1/η, K, polylog(n, d, 1/ε),...)

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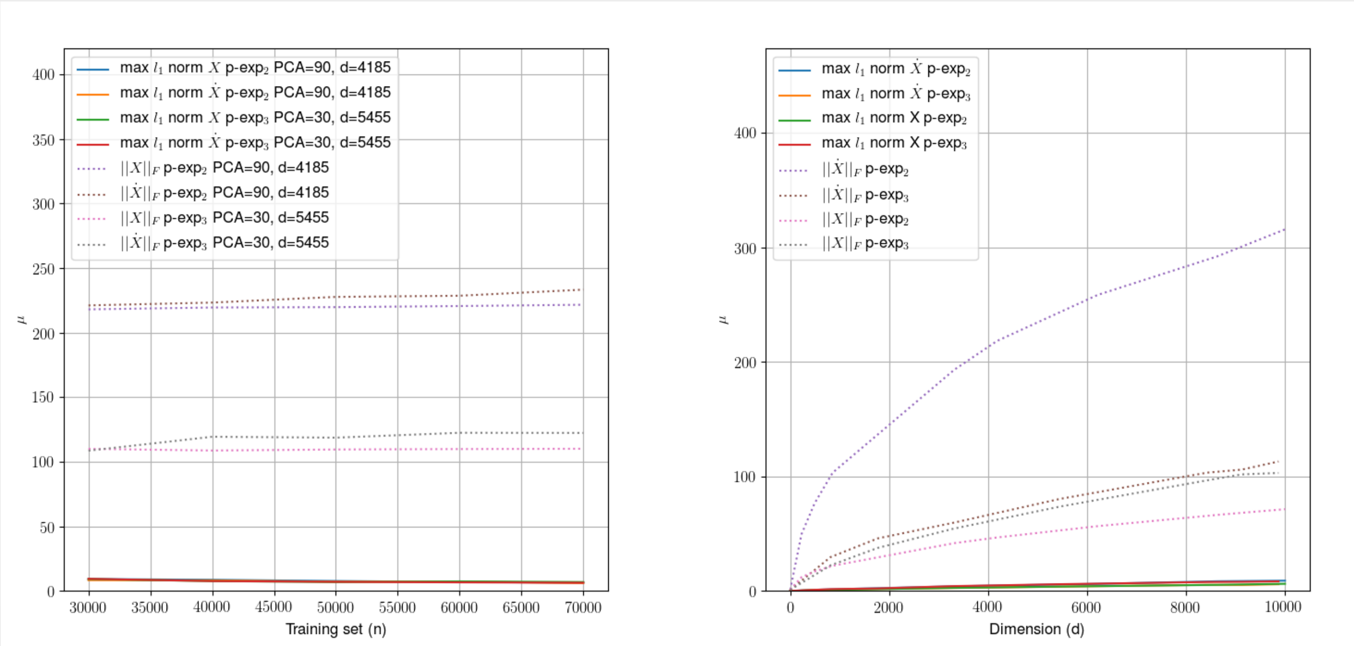

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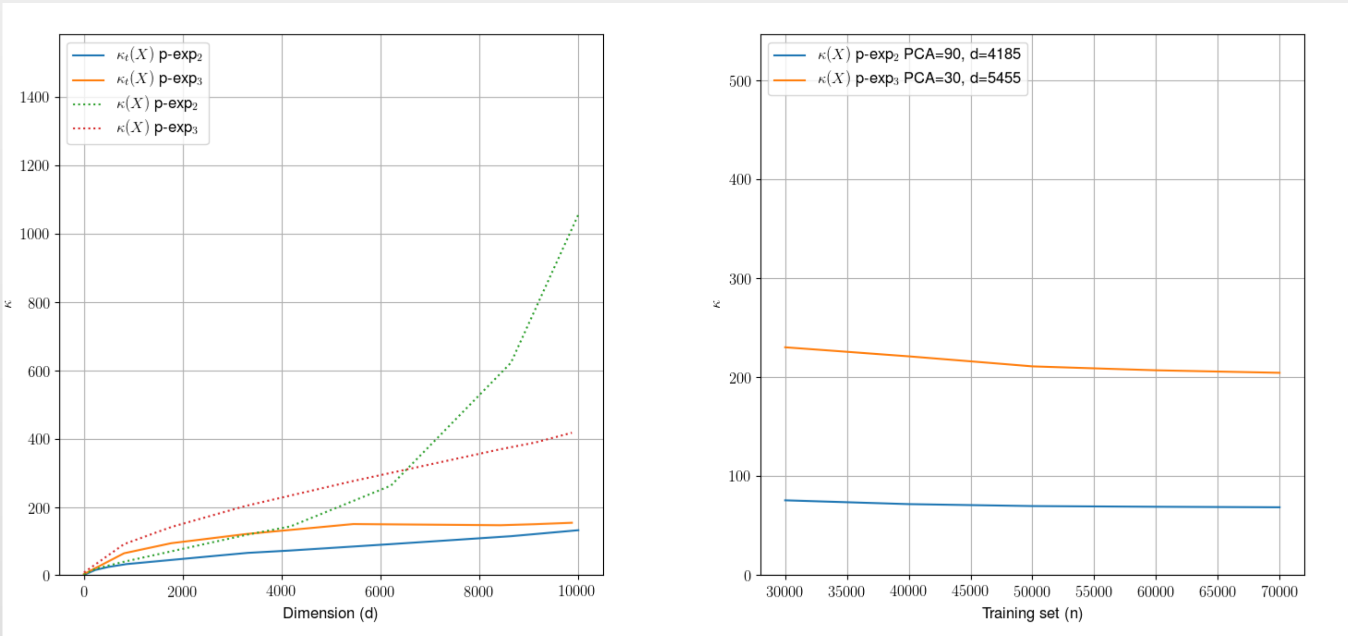

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Main question:
Better accuracy by increasing the dimension, keeping efficient time?
Quantum time: O(κ, μ, 1/θ, 1/δ, 1/η, K, polylog(n, d, 1/ε),...)

Hope (and some evidence):
Quantum classification algorithms can handle bigger dimensions (hence be more accurate), since their running time scales much more favourably with the dimension.

Classification

[KL 18]

Unsupervised Classification: Q-means [KLLP 18]

K-means

Input: M N-dimensional points, K clusters

1. Start with some random points as centroids

Repeat until convergence

2. For each point compute distances to the centroids and assign to closest cluster O(KMN)
3. Recompute the centroids O(MN)

Unsupervised Classification: Q-means [KLLP 18]

K-means

Input: M N-dimensional points, K clusters

1. Start with some random points as centroids

Repeat until convergence

2. For each point compute distances to the centroids and assign to closest cluster $O(KMN)$
3. Recompute the centroids $O(MN)$

Q-means

Input: M N-dimensional points with quantum access, K clusters

1. Start with some random points as centroids

Repeat until convergence

2. For all points in superposition compute distances to centroids and assign to closest cluster $O(K \log(MN))$
2. Use Matrix Multiplication and tomography to recompute the centroids $O(KN \log(MN))$

Summary and open questions

Summary

QML is (one of) the best reason to build quantum computers

- Use case: Quantum recommendation systems
- General Methods: Quantum gradient descent for linear gradients
- Benchmarking: Classification of MNIST dataset
- ML data has some hidden structure (e.g. low rank approximations)
- ML is very robust to errors

Open Questions

Build quantum computers and QRAMs

Find new quantum methods (Interior point methods, fully quantum methods,…)

Find more real-world applications

Benchmark hardware via applications