Quantum algorithms for classification

Alessandro Luongo

Twitter: @scinawa https://luongo.pro/qml

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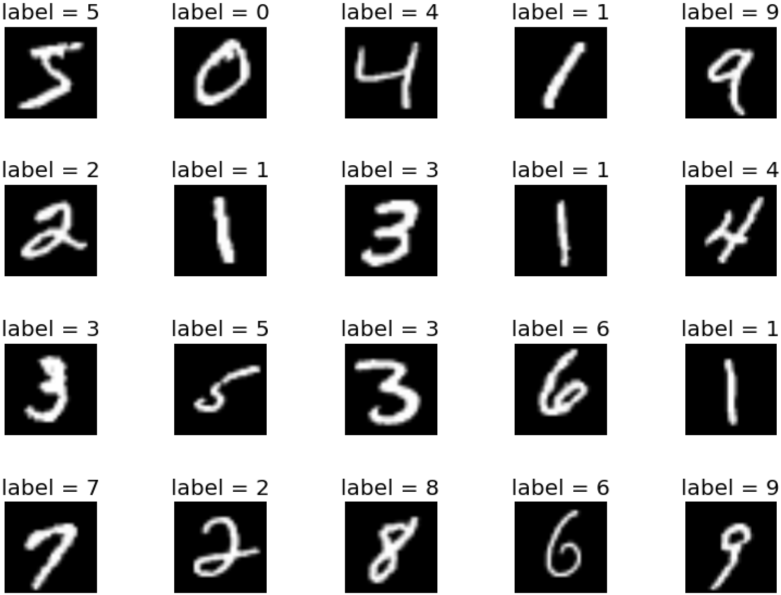
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1. Prologue

2. Toolbox

3. Quantum algorithms for classification..
   - Quantum Slow Feature Analysis
   - Quantum Frobenius Distance Classifier
   - q-means

4. ..on real data

Unsupervised methods

$$X \in \mathbb{R}^{n \times d}$$

- Anomaly detection
- Clustering
- Blind signal separation
- Text mining

Supervised methods

$$X \in \mathbb{R}^{n \times d}, Y \in \mathbb{R}^{n \times m}$$

- Regression
- Pattern recognition
- Time series forecasting
- Speech recognition

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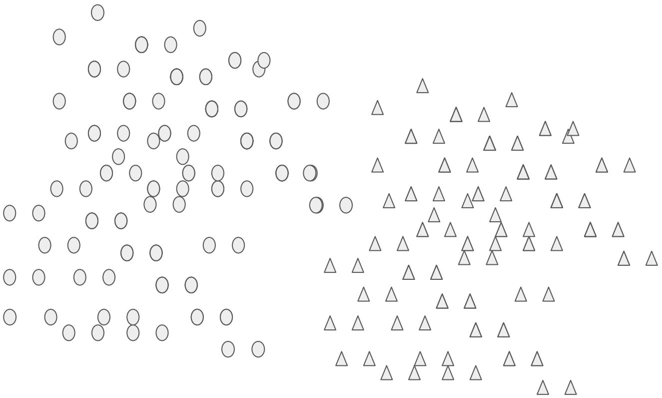
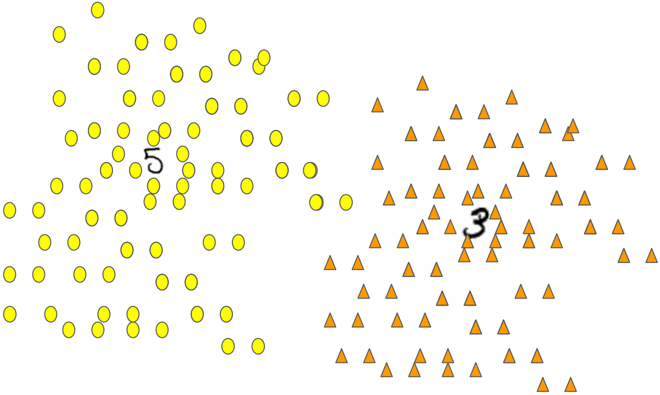
Unsupervised



Unsupervised



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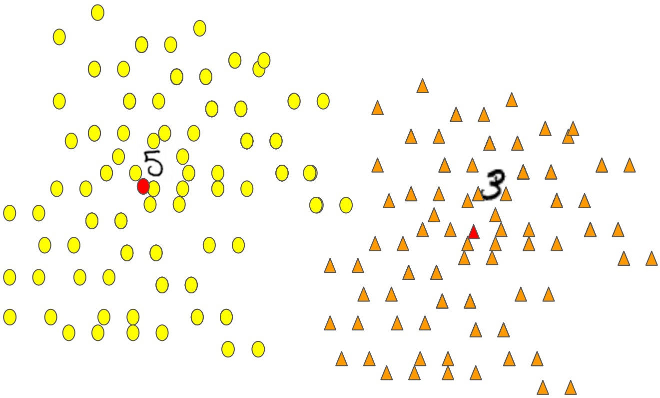
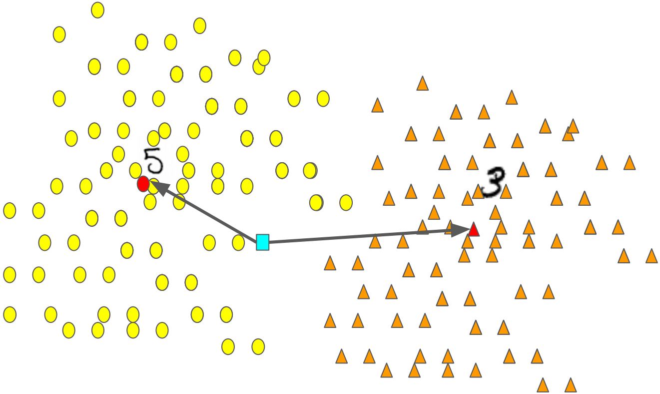


Supervised



ML's algos:
$runtime = O(poly(size)) = O(poly(n, d))$...

... but $size = O(2^{time})$... $\Rightarrow$ problem!

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$runtime = O(poly(size)) = O(poly(n, d))$...

... but $size = O(2^{time})$... $\Rightarrow$ problem!

We need Quantum Machine Learning!
$runtime = O(polylog(size))$

$[HHL09]$ ...

QML team @ IRIF

- Iordanis Kerenidis
- Jonas Landman
- Anupam Prakash

Takeaways

- There is an efficient quantum procedure for supervised dimensionality reduction: Quantum Slow Feature Analysis
- There is an efficient quantum procedure for supervised classification and distance calculation: Quantum Frobenius Distance Estimator .
- There is a new efficient quantum procedure for unsupervised classification: q-means
- We simulate quantum algorithm on real data: they work!
- QRAM based.

1 - QRAM

Let $X \in \mathbb{R}^{n \times d}$. There is a quantum algorithm that

$$|i\rangle|0\rangle \rightarrow |i\rangle|x_i\rangle \quad |x_i\rangle = \|x_i\|^{-1}|x_i\rangle$$

1 - QRAM

Let $X \in \mathbb{R}^{n \times d}$. There is a quantum algorithm that

$$|i\rangle\,|0\rangle \rightarrow |i\rangle\,|x_i\rangle \qquad |x_i\rangle = \|x_i\|^{-1}\,|x_i\rangle$$

$$\frac{1}{\sqrt{\sum_{i=0}^{n} \|x_i\|^2}} \sum_{i=0}^{n} \|x_i\|\,|i\rangle\,|x_i\rangle$$

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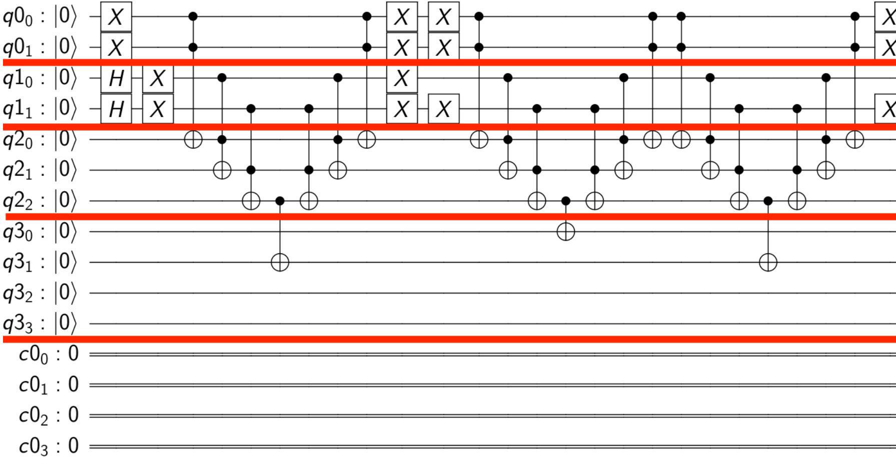
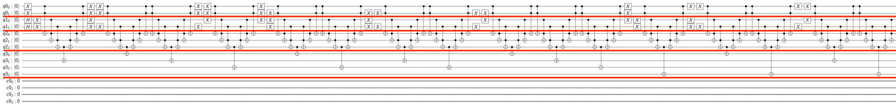
$$\frac{1}{\sqrt{\sum_{i=0}^{n} \|x_i\|^2}} \sum_{i=0}^{n} \|x_i\| \, |i\rangle \, |x_i\rangle$$

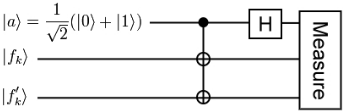
- Execution time: $O(\log nd)$
- Preparation time: $O(nd \log nd)$
- Size: $O(nd \log nd)$

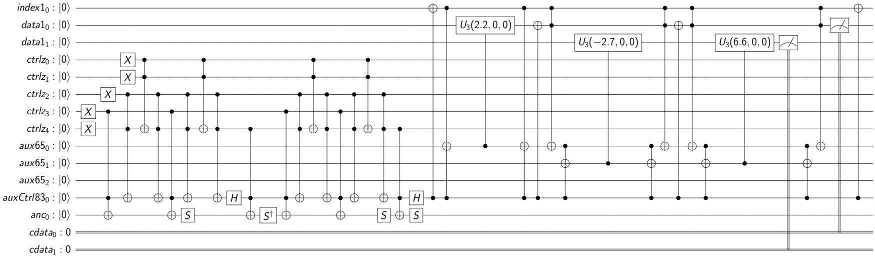

$q0_0 : |0\rangle$
$q0_1 : |0\rangle$
$q1_0 : |0\rangle$
$q1_1 : |0\rangle$
$q2_0 : |0\rangle$
$q2_1 : |0\rangle$
$q2_2 : |0\rangle$
$q3_0 : |0\rangle$
$q3_1 : |0\rangle$
$q3_2 : |0\rangle$
$q3_3 : |0\rangle$
$c0_0 : 0$
$c0_1 : 0$
$c0_2 : 0$
$c0_3 : 0$
X
H

QRAM [[2,3,4],[5,6,7],[8,9,10]]



QRAM + swaps... better





Thanks Alex Singh for the circuit

2 - Q-BLAS

- $M \in \mathbb{R}^{d \times d}$, s.t. $\|M\|_2 = 1$, in QRAM
- $x \in \mathbb{R}^d$ in QRAM.

There is a quantum algorithm that w.h.p. returns :

(i) $|z\rangle$ such that $\left\| |z\rangle - |M^{-1}x\rangle \right\| \leq \epsilon$
in time $\widetilde{O}(\kappa(M)\mu(M)\log(1/\epsilon))$

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(iii) a state $|M^{+}_{\leq\theta}M_{\leq\theta}x\rangle$
in time $\tilde{O}\left(\frac{\mu(M)\|x\|}{\delta\theta\left\|M^{+}_{\leq\theta}M_{\leq\theta}x\right\|}\right)$

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Get estimates of $\|z\| = f(M)x$ (with mult. error ϵ_2, time $O() \cdot \epsilon_2^{-1}$)

Gilyén, András, et al. "Quantum singular value transformation and beyond: exponential improvements for quantum matrix arithmetics." arXiv preprint arXiv:1806.01838 (2018).

2.5 - Q-BLAS

- $A, \quad B \in \mathbb{R}^{d\times d}$ in QRAM
$\|A\|_2 = \|B\|_2 = 1$, in QRAM
- $x \in \mathbb{R}^d$ in QRAM.

There is a quantum algorithm that w.h.p. returns :

- (i) $|z\rangle$ such that $\left\| |z\rangle - |(AB)^{-1}x\rangle \right\| \leq \epsilon$
- (ii) $|z\rangle$ such that $\| |z\rangle - |(AB)x\rangle \| \leq \epsilon$
- (iii) a state $|(AB)^{+}_{\leq\theta,\delta}(AB)_{\leq\theta,\delta}x\rangle$

Get estimates of $\|z\| = f(AB)x$ (with mult. error ϵ_2, time $O() \cdot \epsilon_2^{-1}$)

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- Before: Quantum Singular Value Estimation

$$\sum_i \alpha_i |v_i\rangle \mapsto \sum_i \alpha_i |v_i\rangle |\overline{\sigma}_i\rangle$$

- Now: Qubitization:

$$W = e^{i\phi_0 \sigma_z} e^{i\theta\sigma_x} e^{i\phi_1 \sigma_z} e^{i\theta\sigma_x} \cdots e^{i\phi_k \sigma_z} e^{i\theta\sigma_x}$$

Family of possible W is large enough...

3 - Compute distances

$V \in \mathbb{R}^{n\times d}, C \in \mathbb{R}^{k\times d}$ in the QRAM, and $\epsilon > 0$
There is a quantum algorithm that w.h.p. and in time $\widetilde{O}\left(\frac{\eta}{\epsilon}\right)$

$$|i\rangle\,|j\rangle\,|0\rangle \mapsto \; |i\rangle\,|j\rangle\,|\overline{d(v_i, c_j)}\rangle$$

where $|\overline{d(v_i, c_j)} - d(v_i, c_j)| \leqslant \epsilon$, where $\eta = \frac{max||v_i||}{min||v_i||}$.

Based on: Wiebe, N., Kapoor, A., & Svore, K. (2014). Quantum algorithms for nearest-neighbor methods for supervised and unsupervised learning. arXiv preprint arXiv:1401.2142.

3 - sketch proof

- Use Quantum Frobenius Dinstance to build:

$$\frac{\|v_i\|}{\sqrt{Z_{ij}}} |i\rangle |j\rangle |0\rangle |v_i\rangle + \frac{\|c_j\|}{\sqrt{Z_{ij}}} |i\rangle |j\rangle |1\rangle |c_j\rangle$$

- Hadamard on 3rd qubit.

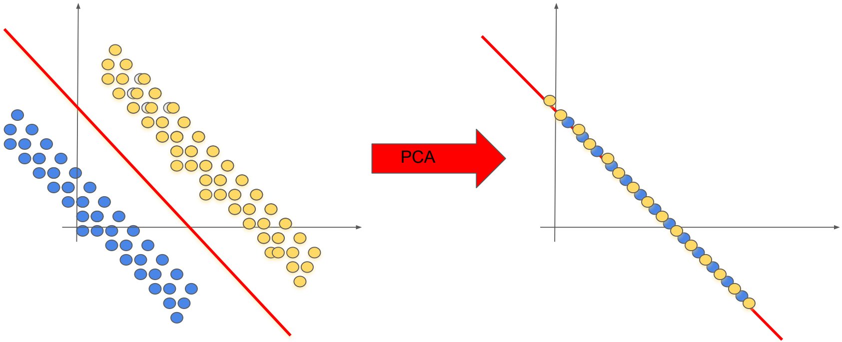
$$p(1)_{ij} = \frac{1}{2Z_{ij}}(\|v_i\|^2 + \|c_j\|^2 - 2\|v_i\| \|c_j\| \langle v_i, c_j\rangle) = \frac{d(v_i, c_j)^2}{2Z_{ij}}$$

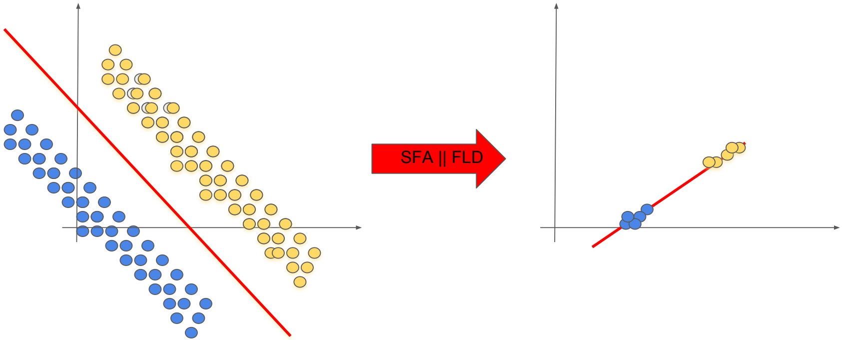
- Perform amplitude estimation on L copies.
- Use Median Lemma (Wiebe et. al.)
- Invert circuit (garbage collection), multiply by $2Z_{ij}$.

4 - Tomography

For a pure quantum state $|x\rangle$, there is a tomography algorithm with sample and time complexity $O(d \log d/\epsilon^2)$ that produces an estimate $\widetilde{x} \in \mathbb{R}^d$ with $\|\widetilde{x}\|_2 = 1$ such that $\|\widetilde{x} - x\|_2 \leq \epsilon$ with probability at least $(1 - 1/d^{0.83})$.

Kerenidis, Iordanis, and Anupam Prakash. ”A quantum interior point method for LPs and SDPs.” arXiv preprint arXiv:1808.09266 (2018).


PCA


SFA || FLD

Slow Feature Analysis (Supervised)

Input signal: $x(i) \in \mathbb{R}^d$. Task: Learn K functions:

$$y(i) = [g_1(x(i)), \cdots, g_K(x(i))]$$

Such that $\forall j \in [K]$. Minimize:

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

Constraints on output signal: average of components is 0, variance of components is 1, signals are decorrelated.

Def Cov. matrix $B := X^T X$, Derivative cov. matrix $A := \dot{X}^T \dot{X}$

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$$AW = BW\Lambda$$

Step 1: Whitening

Data is whitened (sphered) if $B = X^T X = I$.

Whitening its just matrix (Moore-Penrose) inversion
$Z := X^+ X$ .. now $Z^T Z = I$
Freebie Theorem!
There exists an efficient quantum algorithm for whitening that builds $|Z\rangle$

Step 2: Projection

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

- Whiten data $|X\rangle \mapsto |Z\rangle$
- Project data in slow feature space $|Z\rangle \mapsto |Y\rangle$

New algo! QSFA

- Let $X = \sum_i \sigma_i u_i v_i^T \in \mathbb{R}^{n \times d}$, $\dot{X} \in \mathbb{R}^{n \log n \times d}$ QRAM.
- Let $\epsilon, \theta, \delta, \eta > 0$.

There exists a quantum algorithm that produces:

- $|\overline{Y}\rangle$ with $|\,|\overline{Y}\rangle - |A^{+}_{\leq\theta,\delta} A_{\leq\theta,\delta} Z\rangle\,| \leq \epsilon$ in time

  $$\tilde{O}\left(\left(\kappa(X)\mu(X)\log(1/\varepsilon) + \frac{(\mu(X) + \mu(\dot{X}))}{\delta\theta}\right) \times \frac{||Z||}{||A^{+}_{\leq\theta,\delta} A_{\leq\theta,\delta} Z||}\right)$$

- $\overline{\|Y\|}$ s.t. $|\overline{\|Y\|} - \|Y\|\,| \leq \eta \|Y\|$ with an additional $1/\eta$ factor.

New algo! QFDC (Supervised)

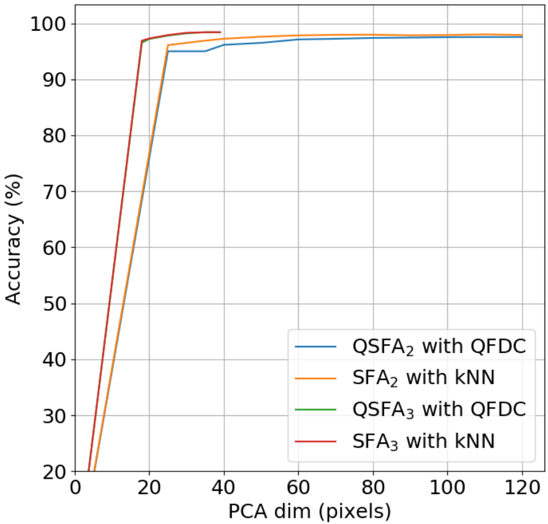
$X_k \in \mathbb{R}^{|T_k| \times d}$ matrix of elements labeled k
$X_0 \in \mathbb{R}^{|T_k| \times d}$ repeats the row x_0 for $|T_k|$ times.

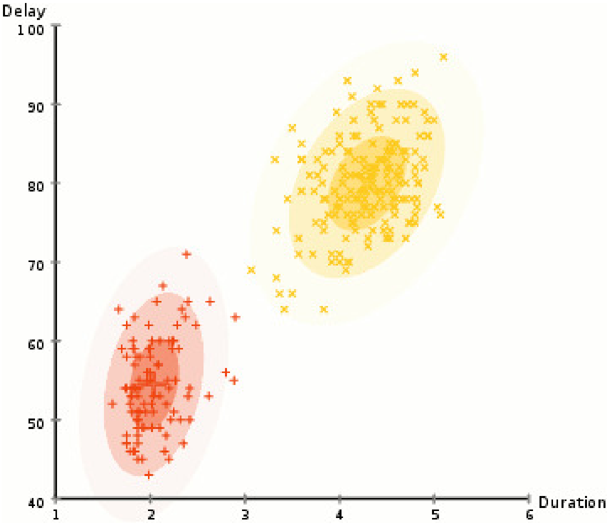
$$F_k(x_0) = \frac{\|X_k - X_0\|_F^2}{2(\|X_k\|_F^2 + \|X_0\|_F^2)},$$

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

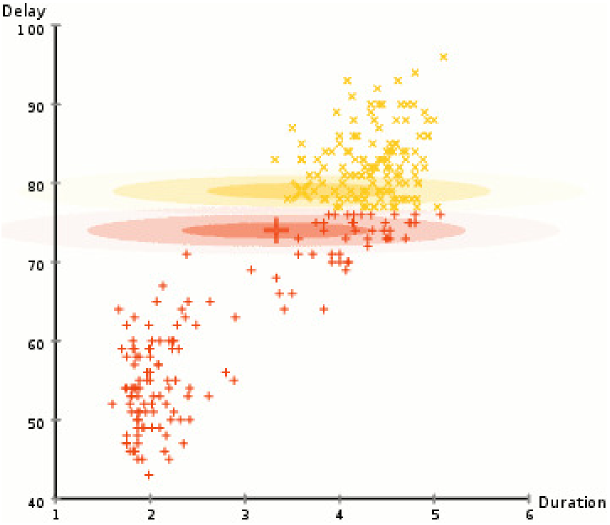
$$h(x_0) = min_k\{F_k(y_0) = p(|1\rangle)\}$$

Accuracy QSFA+QFDC





From Wikipedia



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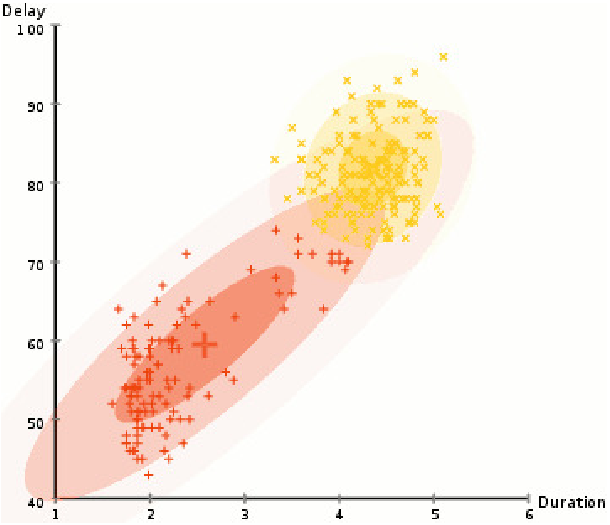

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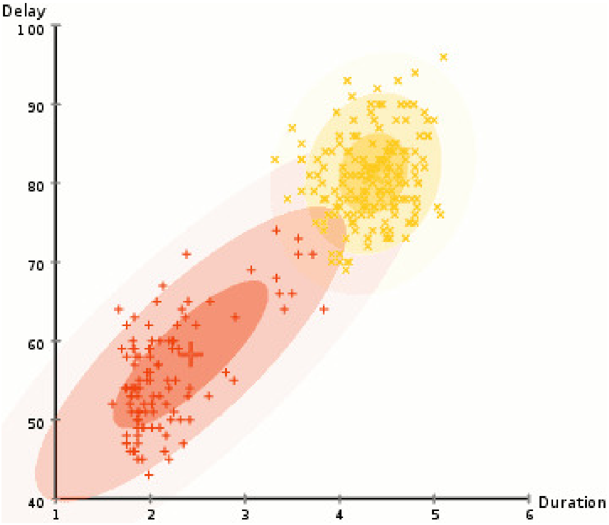

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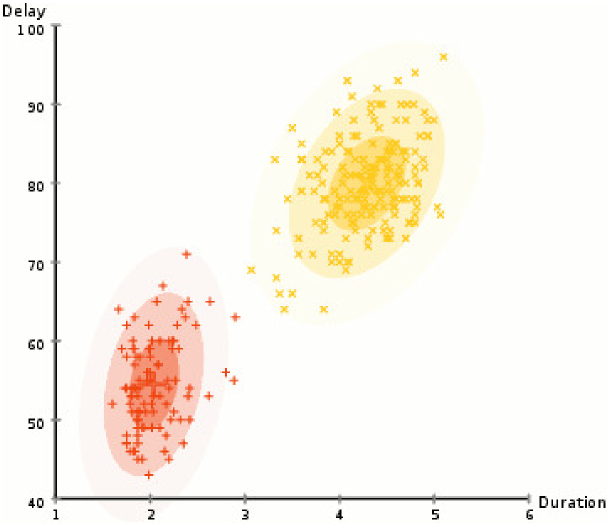

From Wikipedia

k-means (Unsupervised)

Find initial centroids c_j

Repeat until centroids are steady: $|c_j^t - c_j^{t+1}| \leq \tau$

- Calculate distances between all points and all clusters

$$\forall i \in [n], c \in [k] \quad d(v_i, c_i)$$

- Assign points to closer cluster

$$l(v_i) = \arg\min_{c \in [k]} d(v_i, c_i)$$

- Calculate new centroids

$$c_j = \frac{1}{|C_j|} \sum_{i \in C_j} v_i$$

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... is $O(tndk)$:(

δ-k-means (Unsupervised)

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$$\forall i \in [n], c \in [k] \quad d(v_i, c_i)$$

- Assign points to closer cluster

$$L_\delta(v_i) = \{ c_p \ |d^2(c_i^*, v_i) - d^2(c_p, v_i)| \leq \delta \ \}$$

$$l(v_i) = rand(L_\delta(v_i))$$

- Calculate new centroids

$$c_j = \frac{1}{|C_j|} \sum_{i \in C_j} v_i$$

q-means (Unsupervised)

Find initial centroids c_j

Repeat until centroids are steady: $|c_j^t - c_j^{t+1}| \leq \tau$

- Calculate distances between all points and all clusters

$$\bigotimes_{j=0}^{K} \sum_{i=0}^{n} |i\rangle |j\rangle |d(v_i, c_i)\rangle$$

- Assign points to closer cluster

$$\sum_{i=0}^{n} |i\rangle |l(i)\rangle$$

- Calculate centroids again

$$\sum_{j=1}^{k} \sqrt{\frac{|C_j|}{N}} |c_j^{t+1}\rangle |j\rangle$$

Well-clusterable data

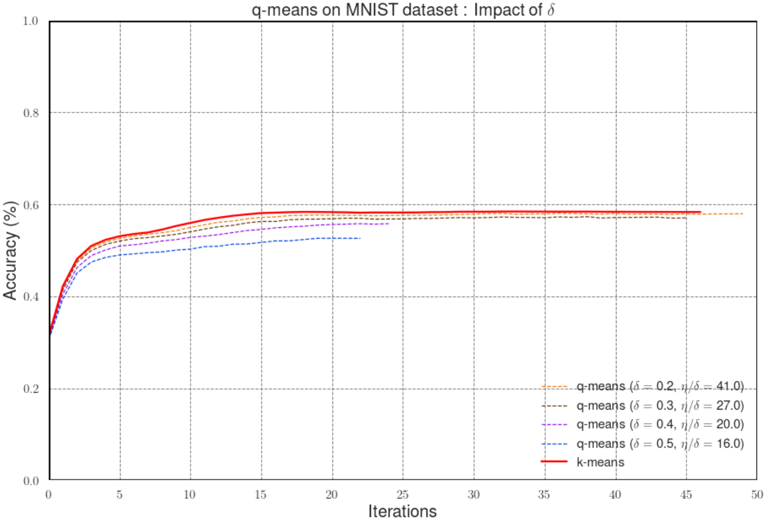
The data is $(\xi, \beta, \lambda, \eta)$-well clustered if there are $\xi > 0, \;\; \beta > 0, \;\; 0 \ll \lambda < 1, \;\; \eta > 1:$

1. clusters' separation: $d(c_i, c_j) \geq \xi \quad \forall i, j \in [k]$
2. proximity to centroid: A fraction λn of points v_i in the dataset verify: $d(v_i, c_{l(v_i)}) \leq \beta$.
3. dataset's width: All the norms are between 1 and $\eta = \max_i (\|v_i\|)$

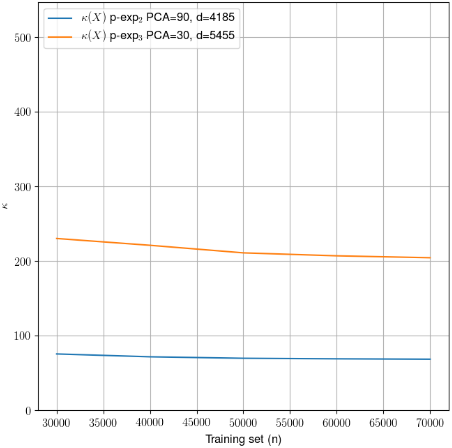
New algo! q-means

For a $(\xi, \beta, \lambda, \eta)$-well clusterable dataset $V \in \mathbb{R}^{n \times d}$ in QRAM, there is a quantum algorithm that returns in t steps the k centroids that cluster the dataset consistently with the classical δ-k-means algorithm in time $\widetilde{O}\left(t \cdot \frac{k^3 d \eta^3}{\delta^3}\right)$.

Accuracy q-means

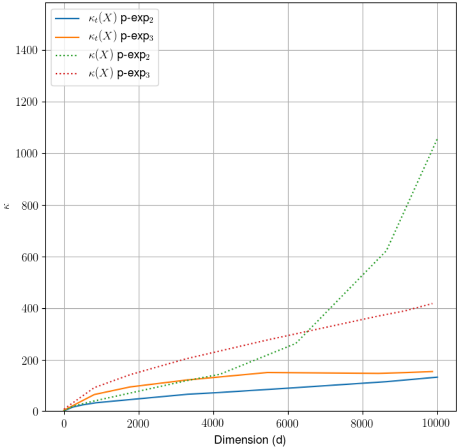


$\lambda_{max}/\lambda_{min}$: more data



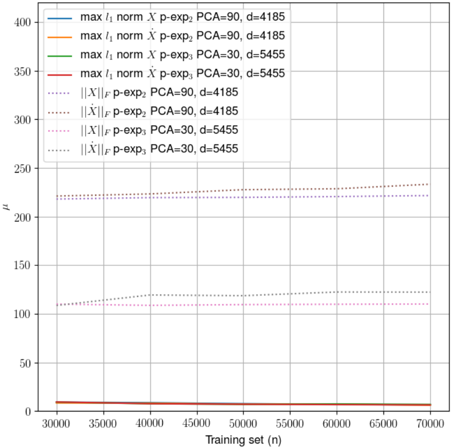
Condition number by increasing the number of elements in training set

$\lambda_{max}/\lambda_{min}$: more features



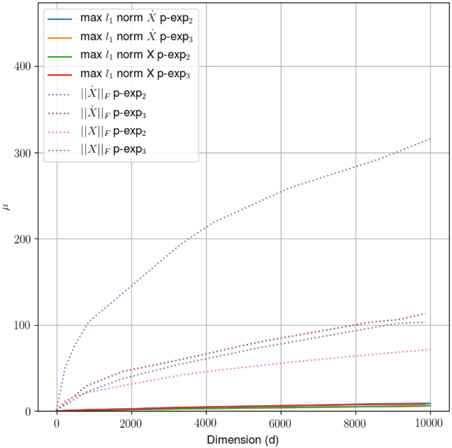
Condition number by increasing the features (pixels)

$\mu(X)$: more data



$\mu(X)$ and $\mu(\dot{X})$ by increasing the number of elements in training set.

$\mu(X)$: more features



$\mu(X)$ and $\mu(\dot{X})$ by increasing the number of features.

Conclusions

Quantum Slow Feature Analysis and Quantum Frobenius Distance Classifier on MNIST

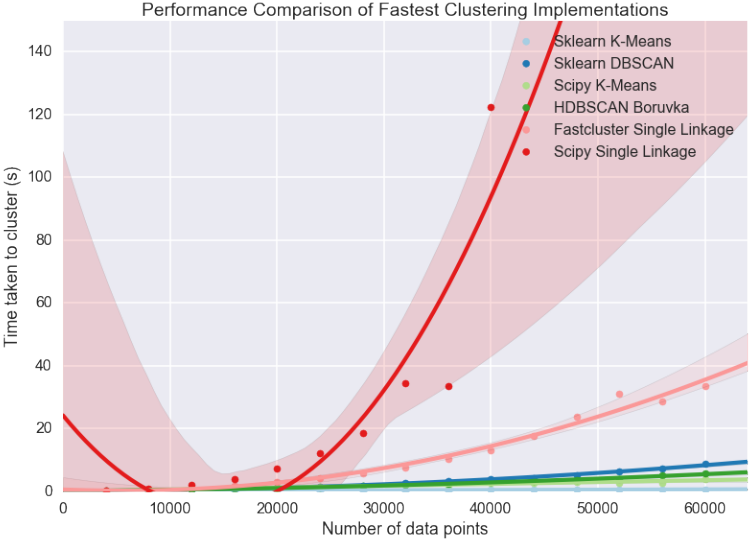
- $\propto 150 \,||\, 200$ (Logical) qubits
- Classifying the test set (10^4 vectors) with quantum algos is $\simeq 100$ times faster
- Possibility to extract the model classically! $|i\rangle |i\rangle \mapsto |i\rangle |g_i\rangle$.
- Not only fast but might be more accurate!

Conclusions

q-means

- Exponentially faster in the number of data points: $O(n) \to O(\log n)$.
- Finding new datasets to apply q-means.
- We recover the centroids classically

... Yet an uneven comparison?



From: `https://hdbscan.readthedocs.io/en/latest/performance_and_scalability.html`

#TODOs

- Generalizations…
- Experiments…
- Code…
- New algos…
- Compositions…
- Adversarial QML…
- Privacy preserving QML…

Thanks for your time

there is never enough.
(cit. Dan Geer)

@scinawa

- Quantum Machine Learning ⇒ https://luongo.pro/qml
- QSFA + QFDC ⇒ https://arxiv.org/abs/1805.08837
- q-means ⇒ stay tuned...

- Projective Simulation
- Quantum Recommendation Systems
- Quantum SVM
- Quantum Anomaly detection
- Quantum Gradient Descent
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- Quantum PCA
- ...

1. Ewin Tang. **A quantum-inspired classical algorithm for recommendation systems**. arXiv:1807.04271, 2018. (undergraduate thesis, advised by Scott Aaronson)
2. Ewin Tang. **Quantum-inspired classical algorithms for principal component analysis and supervised clustering.** arXiv:1811.00414, 2018.
3. Ewin Tang et al. **Quantum-inspired low-rank stochastic regression with logarithmic dependence on the dimension** arXiv: 1811.04909, 2018