Quantum Algorithm for Principal Component Analysis

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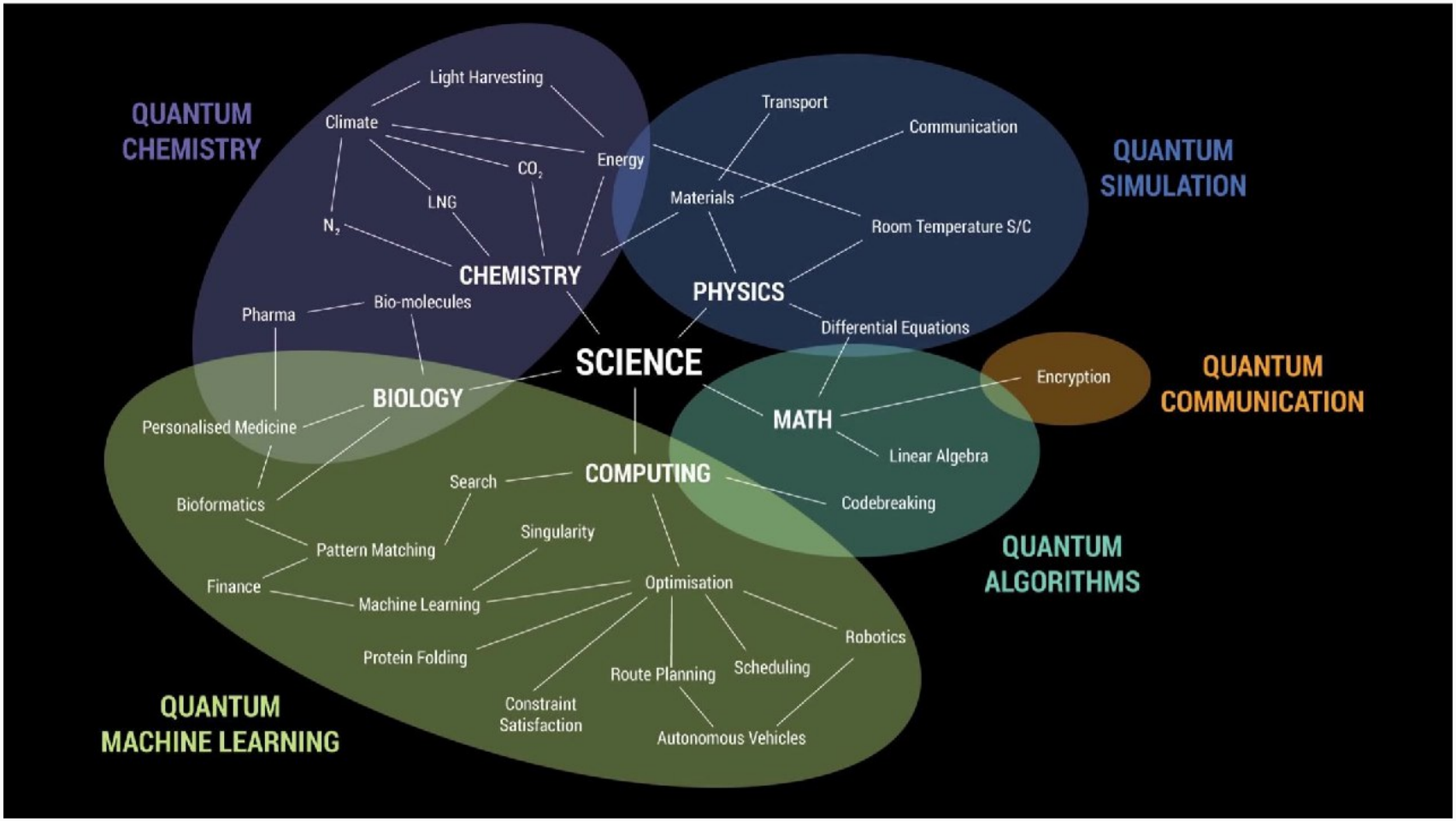
Introduction

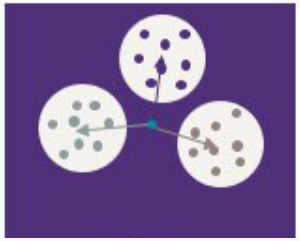
Applications of Quantum Computing



Quantum Machine Learning

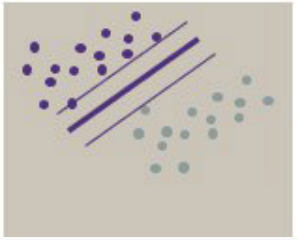
Quantum Clustering finding

When the data is represented in a very large dimension space, it is very difficult to perform the clusetring with a classical computer. The use of quantum computers is a very good solution.



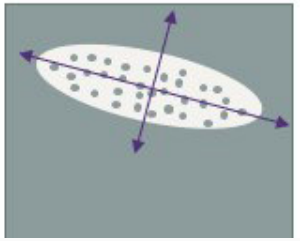
Quantum Support Vector Machine

Finding the hyperplane that separates many data points that are represented in a high dimensional space is so difficult on a classical computer. on a quantum computer, it can be solved extremely efficiently.



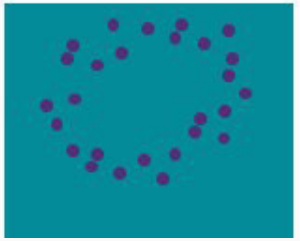
Quantum PCA

The goal of this algorithm is to find the proper axes along which to group this data. This is something that takes $O(N^3)$ on a classical computer.



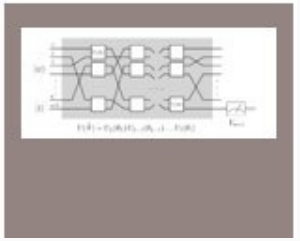
Feature topology

This is a method for finding the topological features of data. This problem can be mapped to a problem of finding the eigenvectors and eigenvalues of some huge, high-dimensional matrix.

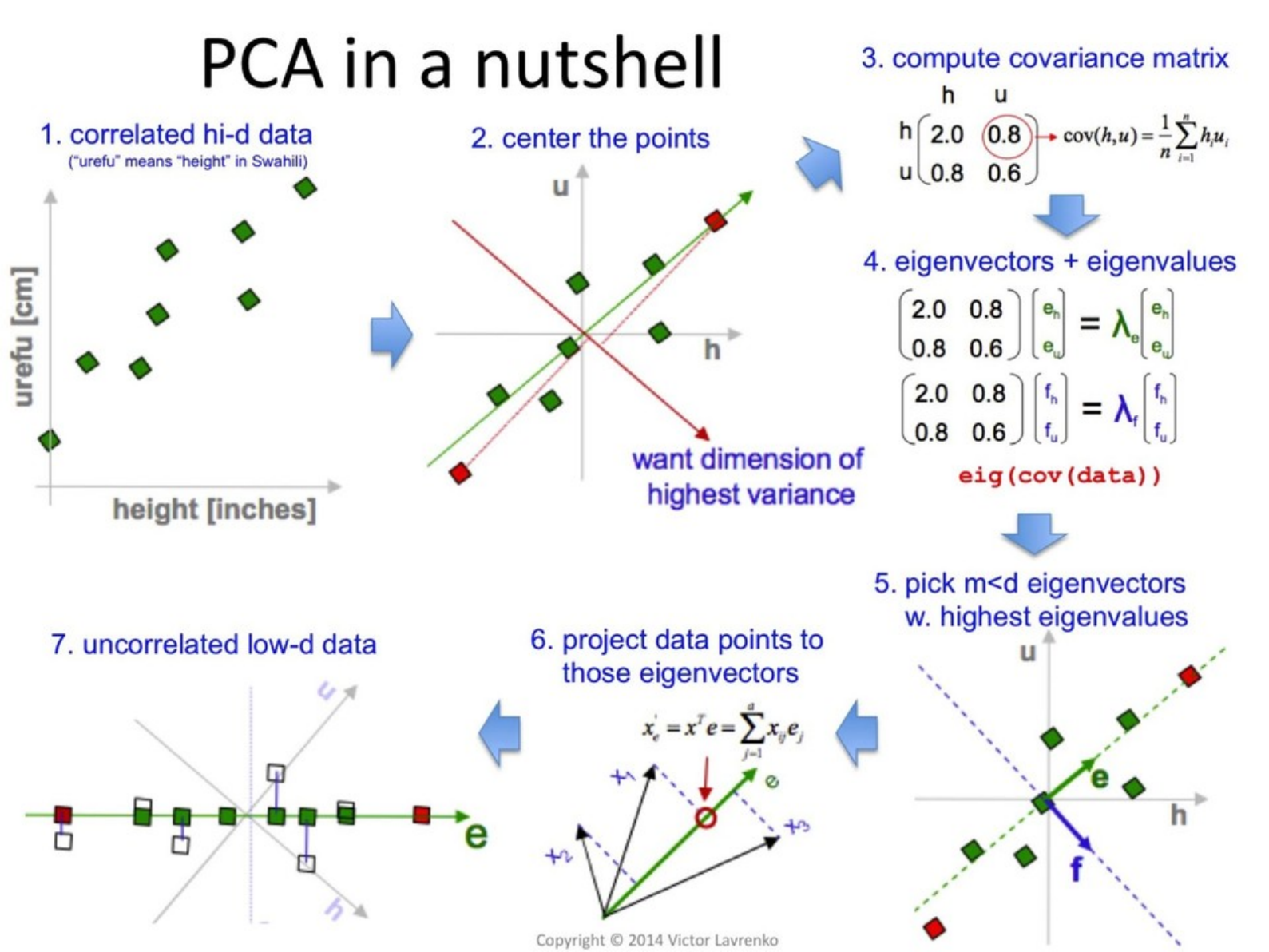


Quantum Deep Learning

Exciting breakthroughs may soon bring real quantum neural networks, specifically deep learning neural networks, to reality. Many research papers have shown remarkable results in quantum deep learning

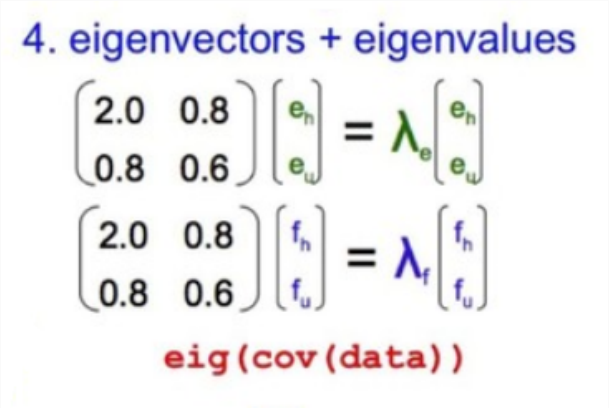


Principal Component Analysis



Complexity of Principal Component Analysis

- Must perform eigendecomposition, which is computationally intensive



- Given this bound, standard implementations of PCA usually run in $O(n^3)$, where n is the number of dimensions (features)
- This is the step we will focus on

The Quantum Algorithm

Quantum PCA

Given a covariance matrix X, normalized w.r.t. its trace, we aim at computing its top-k eigendecomposition by means of a quantum approach

The main technique we will exploit in order to do so is

- Quantum Phase Estimation
  - Phase Kickback
  - Inverse Quantum Fourier Transform

QPE - *Setup*

- X is a matrix having eigenvector v and corresponding eigenvalue λ
  i.e. $Xv = \lambda v$
- then v is also eigenvector of e^X, with corresponding eigenvalue e^λ
  i.e. $e^X v = e^\lambda v$

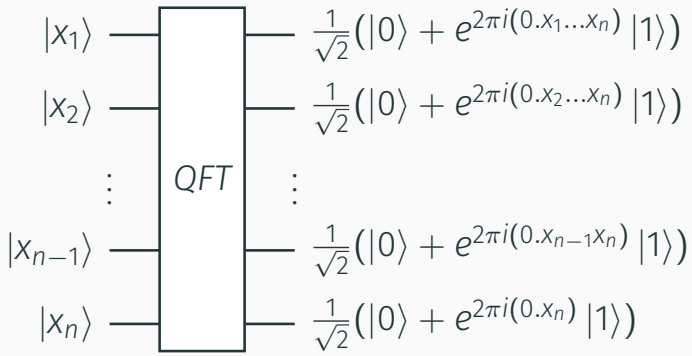
(Proven using Taylor series)

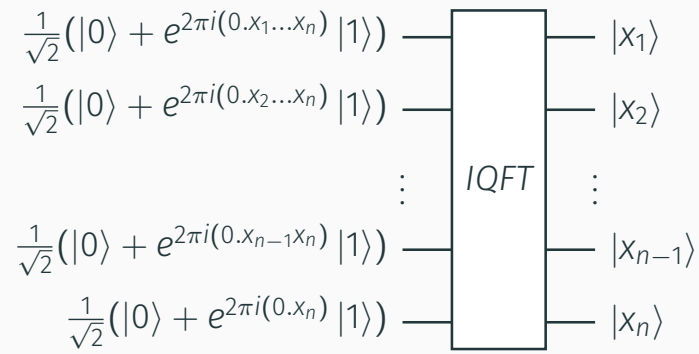
QPE - *Inverse Quantum Fourier Transform*

- Consider $U = e^{iX}$ and its eigenvalue $e^{i\lambda} = e^{i2\pi\varphi}$
- Given a quantum state of the form $\frac{1}{\sqrt{2^N}} \sum_{y=0}^{2^N-1} e^{2\pi i \varphi y} |y\rangle$ we can easily determine φ applying the inverse of the *Quantum Fourier Transform*

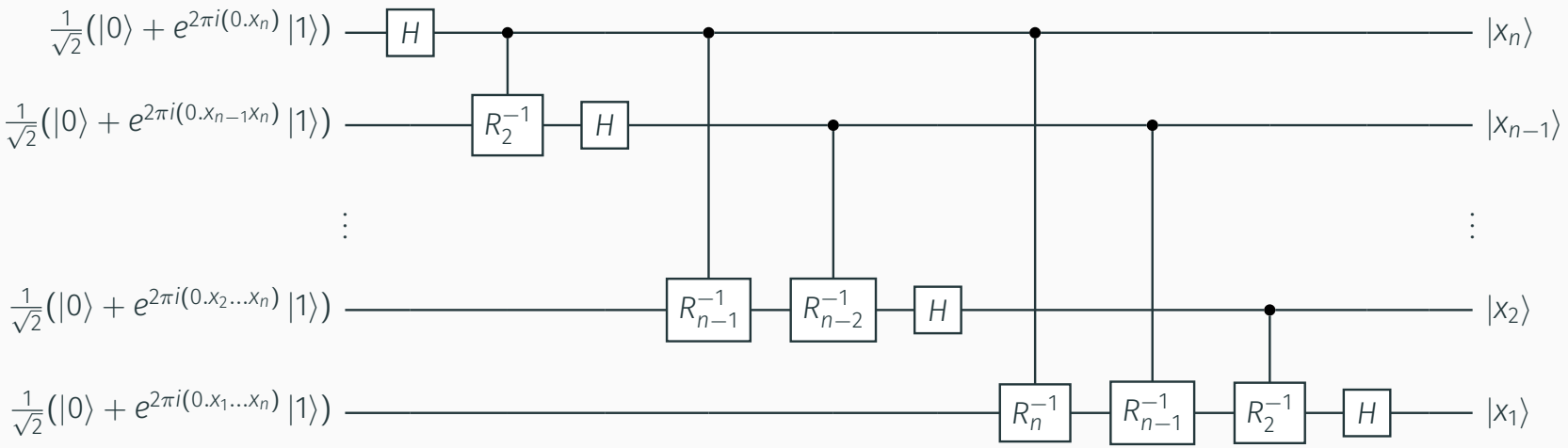
QPE - *Inverse Quantum Fourier Transform*

- More specifically, we obtain the best approximation for the binary fraction expansion of φ over n bits
- $\varphi \approx 0.x_1x_2...x_{n-1}x_n$





Circuit for the Inverse QFT



Where $R_k^{-1} = \begin{pmatrix} 1 & 0 \\ 0 & e^{\frac{2\pi i}{2^k}} \end{pmatrix}$

QPE

- We know how to obtain φ, and therefore also λ, provided we have the quantum state $\frac{1}{\sqrt{2^N}} \sum_{y=0}^{2^N-1} e^{2\pi i \varphi y} |y\rangle$
- But how can we build such a state?
- *Amplitude Encoding* and *Phase Kickback*

QPE - *Amplitude Encoding*

- The eigenvector corresponding to $e^{i\lambda}$, for U, is ψ_λ
- Using *Amplitude Encoding* then we could build the eigenstate (*i.e.* quantum state) $|\psi_\lambda\rangle$ over $log_2(|\psi_\lambda|)$ qubits

$$\psi_\lambda = \begin{pmatrix} \psi_{\lambda 0} \\ \psi_{\lambda 1} \\ \vdots \\ \psi_{\lambda n} \end{pmatrix} \Longrightarrow \psi_{\lambda 0} |0...00\rangle + \psi_{\lambda 1} |0...01\rangle + ... + \psi_{\lambda n} |1...11\rangle$$

- Then by definition $U |\psi_\lambda\rangle = e^{i\lambda} |\psi_\lambda\rangle$

QPE - *Phase Kickback*

- Recall that $\left|det(e^{iX})\right| = \left|e^{tr(iX)}\right| = \left|e^{i}\right| = 1$
  - X is normalized w.r.t. its trace!
- Since U is a unitary matrix we can implement the corresponding quantum gate, as well as its controlled version
- Let $c - U$ be the controlled version of gate U
- Then
  $|0\rangle |\psi_\lambda\rangle \xrightarrow{c-U} |0\rangle |\psi_\lambda\rangle$
  $|1\rangle |\psi_\lambda\rangle \xrightarrow{c-U} |1\rangle e^{i\lambda} |\psi_\lambda\rangle$

QPE - *Phase Kickback*

- It can be proven that, from a mathematical point of view, quantum states $|1\rangle e^{i\lambda} |\psi_\lambda\rangle$ and $e^{i\lambda} |1\rangle |\psi_\lambda\rangle$ are **the same state**
- The phase factor is *kicked back* from the controlled register to the control register

QPE - *Phase Kickback*

- The state $e^{i\lambda} |1\rangle |\psi_\lambda\rangle$ now encodes λ in its phase, but as a *global* phase shift, which is not measurable
- In order to introduce a *relative* phase shift that can then be measured, we must simply put the control register in a superposition prior to the application of the $c - U$
  - *e.g.* we apply the Hadamard gate!

$$\frac{1}{\sqrt{2}}(|0\rangle + |1\rangle) |\psi_\lambda\rangle \xrightarrow{c-U} \frac{1}{\sqrt{2}}(|0\rangle + e^{i\lambda} |1\rangle) |\psi_\lambda\rangle$$

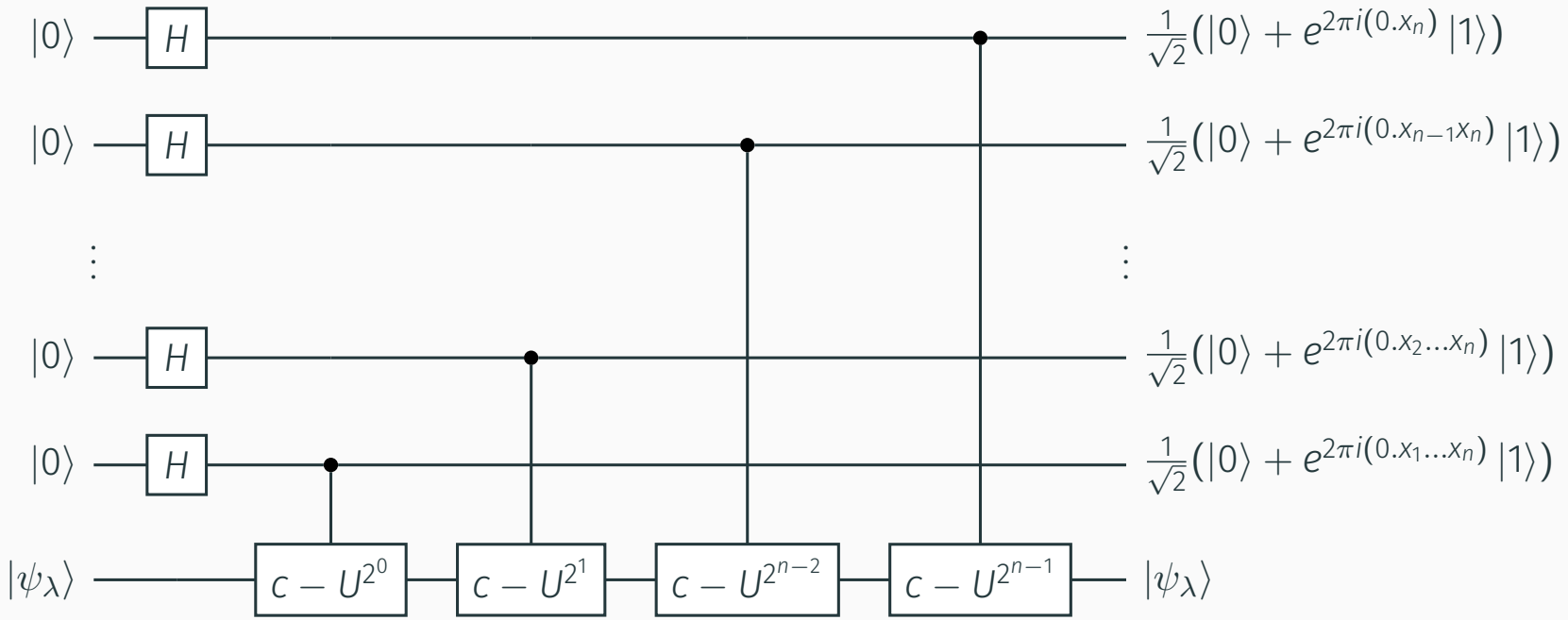
QPE - *Phase Kickback*

- As a last step, consider $c-U$ raised to power k
- Eigenvalue of $c-U^k$ corresponding to $|\psi_\lambda\rangle$ will be $e^{ik\lambda}$
- Applying $c-U^k$ using different control qubits, with k equals to **increasing powers of 2**, we obtain our goal configuration

$$\frac{1}{\sqrt{2}}\left(|0\rangle + e^{ik\lambda}|1\rangle\right)|\psi_\lambda\rangle = \frac{1}{\sqrt{2}}\left(|0\rangle + e^{2\pi i(0.x_{(\log_2 k+1)}\ldots x_n)}|1\rangle\right)|\psi_\lambda\rangle$$

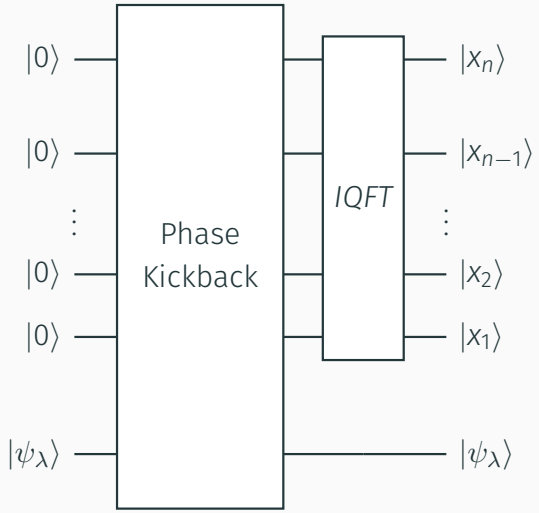
– Note that $|\psi_\lambda\rangle$ is left unchanged after every application, thus we can keep reusing it

Circuit for the Phase Kickback



QPE

Putting everything together



- This is how standard QPE works for computing an eigenvalue when the corresponding eigenvector is known
- In our case, however, **we don't know any of the eigenvectors of X a priori**, and therefore we cannot prepare the state $|\psi_\lambda\rangle$

Quantum PCA

- How can we exploit Quantum Phase Estimation to perform eigendecomposition in our scenario?

– **Quantum Algorithm Providing Exponential Speed Increase for Finding Eigenvalues and Eigenvectors** (Abrams & Lloyd, 1999) [1]

– **Quantum principal component analysis** (Lloyd, Mohseni & Rebentrost, 2014) [2]

  – **Towards Pricing Financial Derivatives with an IBM Quantum Computer** (Martin et al., 2019) [3]

Seth Lloyd

Quantum PCA

- As it happens, precise knowledge of $|\psi_\lambda\rangle$ is **not** required in order to estimate λ
- It suffices to have an estimate ψ_a, such that $|\langle\psi_a|\psi_\lambda\rangle|^2$ is not exponentially small (w.r.t. problem size), to measure the value of λ in a polynomial number of trials
- Even more interestingly, when the n qubits are measured to be in state λ, the register that initially stored $|\psi_a\rangle$ collapses to state $|\psi_\lambda\rangle$!
- How is this explained?

Quantum PCA

- The state we are using as input can be written as a **linear combination** of the true eigenvectors of X, labelled $|\Phi_k\rangle$

$$|\psi_a\rangle = \sum_k c_k |\Phi_k\rangle$$

- QPE on this state then yields measurements of each eigenvalue λ_k with probability $|c_k|^2$, while making the initial vector collapse to the corresponding true eigenvector $|\Phi_k\rangle$

Quantum PCA

- This is why using an estimate of a true eigenvector gives us the corresponding eigenvalue with sufficient reliability
- In this case, ”unexpected” measurements are not just meaningless noise, but are in fact occurrences of different eigenvalues
- Thus, for any random initial vector $|\psi\rangle$, the output configuration will in general reveal **all eigenvector-eigenvalue couples**

Quantum PCA

- In addition, if we are able to obtain an approximation for an eigenvector using a random initial state, we can sequentially improve the result by using such approximation as the new initial state
- This brings us to a crucial point for the algorithm: **extracting information from the output state**

Quantum PCA - *Reading the output*

- After applying QPE the eigenvectors are entangled with their eigenvalues and encoded in $log_2(|\psi_\lambda|)$ qubits
- Recall Amplitude Encoding:

$$|\psi_\lambda\rangle = \psi_{\lambda 0}\,|0...00\rangle + \psi_{\lambda 1}\,|0...01\rangle + ... + \psi_{\lambda n}\,|1...11\rangle$$

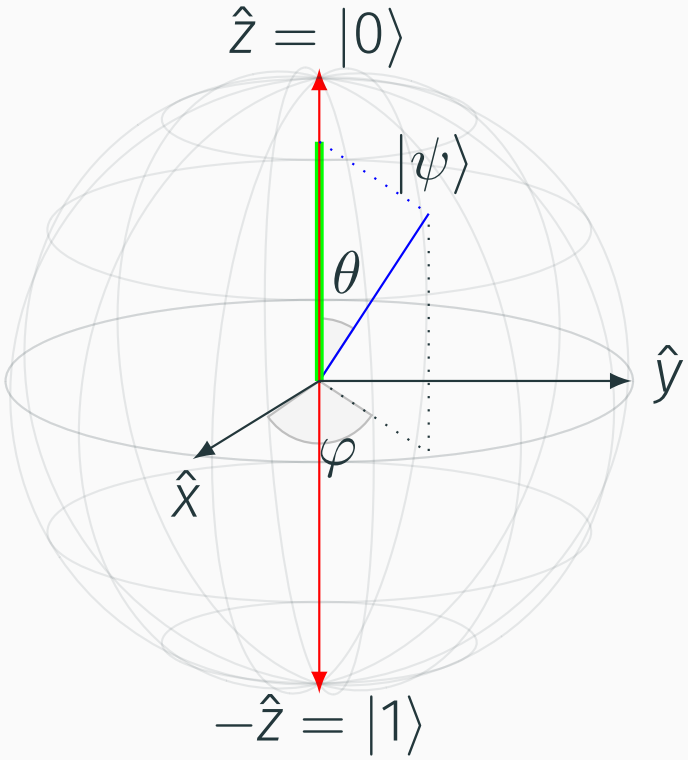
- Using data from N shots of the circuit, we can estimate these probabilities as relative frequencies $|\psi_{\lambda i}| = \sqrt{\frac{n_i}{N}}$
- How do we get the relative phases, *i.e.* detect signs?

Quantum Tomography

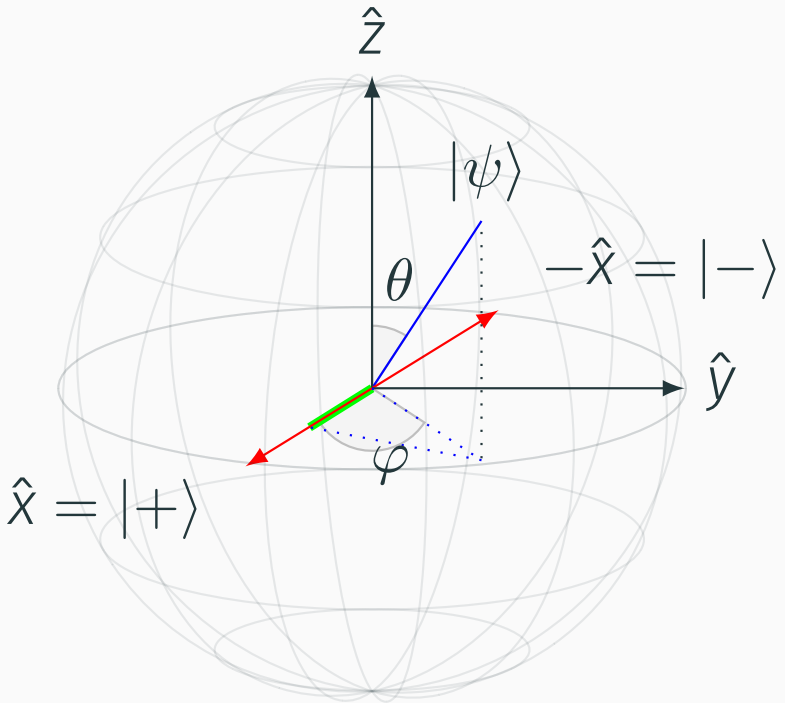
- The technique used to reconstruct information of a quantum state is called **Quantum State Tomography**
- Tomography is done by collecting and processing different types of measurements, or *observables*, of the system which correspond to various axes of the Bloch sphere

– Note that, still, the global phase of a state is not measurable, meaning that states $\alpha |0\rangle - \beta |1\rangle$ and $-\alpha |0\rangle + \beta |1\rangle$ are physically indistinguishable.
This is not relevant in our scenario as we are only interested in the direction of the vector and not in its sense

Quantum Tomography



Measurement on Z basis



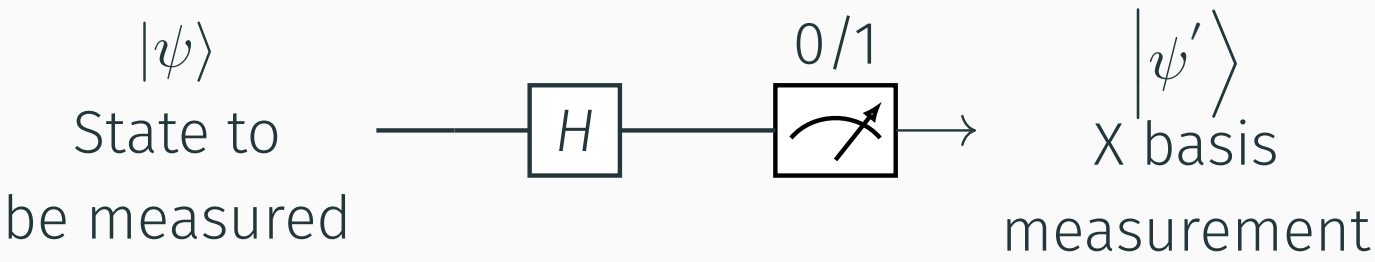
Measurement on X basis

Quantum Tomography

- Full Quantum State Tomography of a b-qubit system is in general computationally intensive
  - $O(4^b)$ different observables must be measured
  - Data processing involves common optimization algorithms
- However, we can exploit problem structure to do better
- In particular we assume to work with *real* amplitudes (not complex as in the general case)
  - Input state has real amplitudes
  - No rotations around the y axis performed by the algorithm in the ideal execution

Quantum Tomography

- We measure the register only in the Z basis (all qubits) and in the combinations of 1 qubit at a time in the X basis (*i.e.* $b + 1$ settings)
- We obtain measurements in the X basis from ones in the *standard computational basis* (Z basis) by applying an Hadamard gate before measurement



- This operation maps the state $|+\rangle$ to output 0 and the state $|-\rangle$ to output 1

Quantum Tomography

- Performing these measurements we can compare the probability of different outcomes in order to estimate the relative phases
- The total number of comparisons is $2^b - 1$, linear in the Hilbert space dimension
  - One for each amplitude!

Implementation and Analysis

Implementation

- We implement the algorithm in Python using Qiskit

```
def qpca(covmat, precision, initial, backend, req_shots)
```

- *covmat*: input covariance matrix
- *precision*: number of qubits to represent the eigenvalues
- *initial*: initial vector ($|\psi\rangle$)
- *backend*: to run the circuit (*qasm_simulator* by default)
- *req_shots*: shots of the circuit (8192 by default)

Demo

Here is a demo of the algorithm applied to the Iris dataset.

Analysis

In order to analyze the algorithm and its complexity there are different points to take into account

- Implementation of gate e^{iX}
- Quantum Phase Estimation
- Quantum State Tomography
- Executions of the circuit

Analysis - *Hamiltonian Simulation*

- Exponentiation of the covariance matrix is required to implement the (controlled) $U = e^{iX}$
- In Quantum Information, the process of finding a circuit that approximates such operator for a given Hamiltonian is called **Hamiltonian Simulation**
  - Note: also Hamiltonians are Hermitian matrices
- This was one of the original motivating problems of Quantum Computing proposed by Richard Feynman as a key part of simulating quantum mechanical systems.

Approaches to Simulation of non-sparse d-dimensional Hamiltonians

- Higher order Suzuki-Trotter expansion: $O(d \log d)$
- Lloyd-Mohseni-Rebentrost method: $O(\log d)$
  Assuming many copies of the Hamiltonian are available as quantum states (encoded in density matrix)
- Wang and Wossnig: $\tilde{O}(\sqrt{d})$
  Using a more practical qRAM data structure
  arXiv:1803.08273

Analysis - *QPE*

Gate-complexity of Quantum Phase Estimation is impacted by the precision of the eigenvalue estimation (m qubits)

- IQFT is $O(m^2)$
- m calls to powers of $c - U$
- If $c - U^k = k$ times $c - U$, gate-complexity is 2^m
- Then overall gate-complexity: $O(m^2 + 2^m)$
- Note: complexity scales linearly with accuracy $M = 2^m$

Analysis - *Tomography*

Already discussed.
Our implementation for d dimensional eigenvectors encoded in $b = \lceil \log_2 d \rceil$ qubits

- $b + 1$ different observables to be measured
- $O(2^b) = O(d)$ comparisons on the results of such measurements

Analysis - *Executions*

We know *what* we have to measure, but *how many* measurements should be taken?
Considering each eigenvalue/eigenvector couple

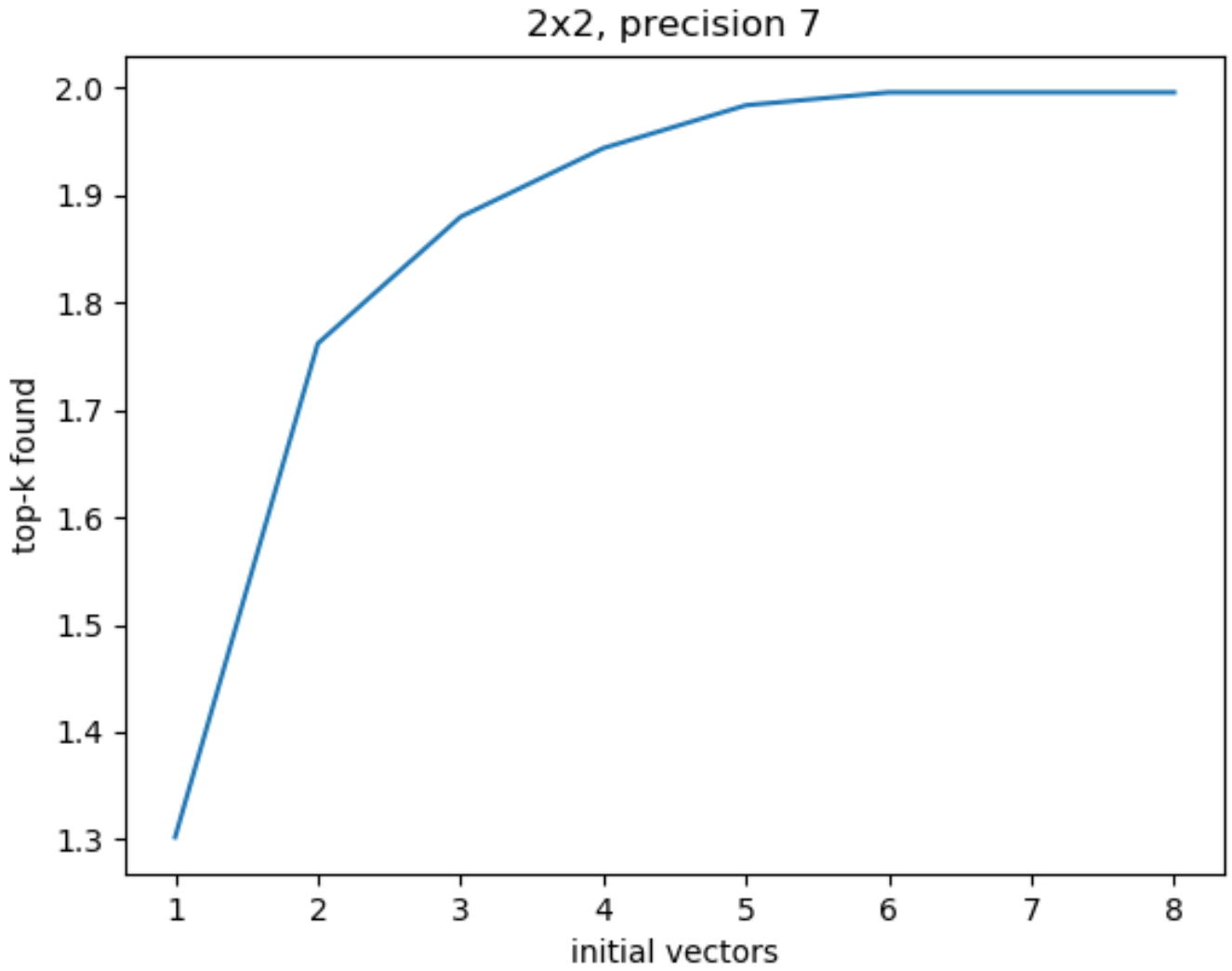
- Number of measurements in the *"all-Z basis"* scales only with precision of amplitude estimation
- Measurements in the *"one-X basis"* give clear results for strongly positive/negative amplitudes, ambiguous for values near 0

Analysis - *Executions*

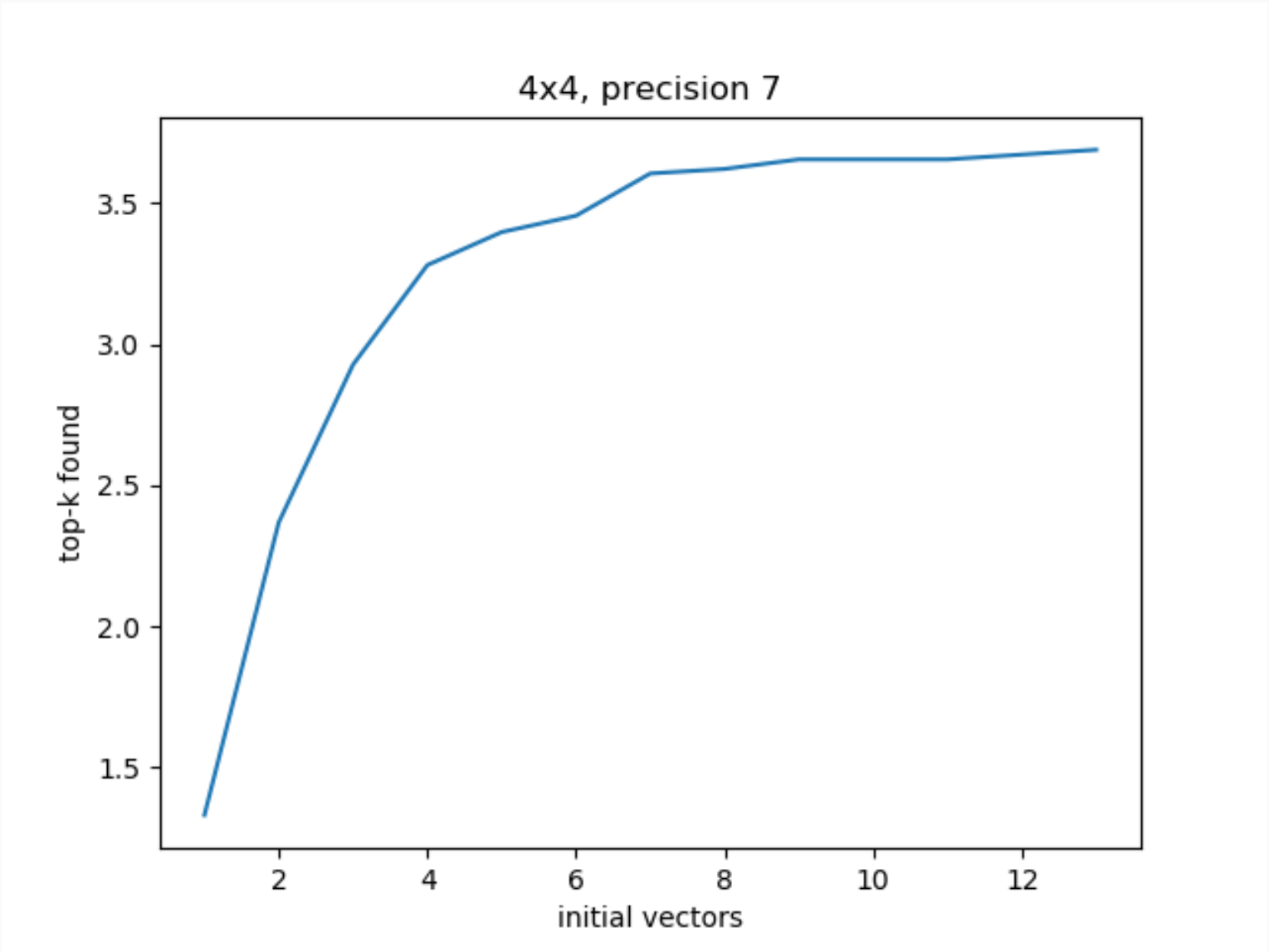
Recall: in principle, any random initialization reveals all eigenvalue/eigenvector couples.
In practice, some eigenvectors may have *exponentially small* contribution to an initial vector and appear rarely in output.
Different approaches

- Multiple initializations (random or by some criteria)
- Obtain rough estimate of eigenvector and iterate

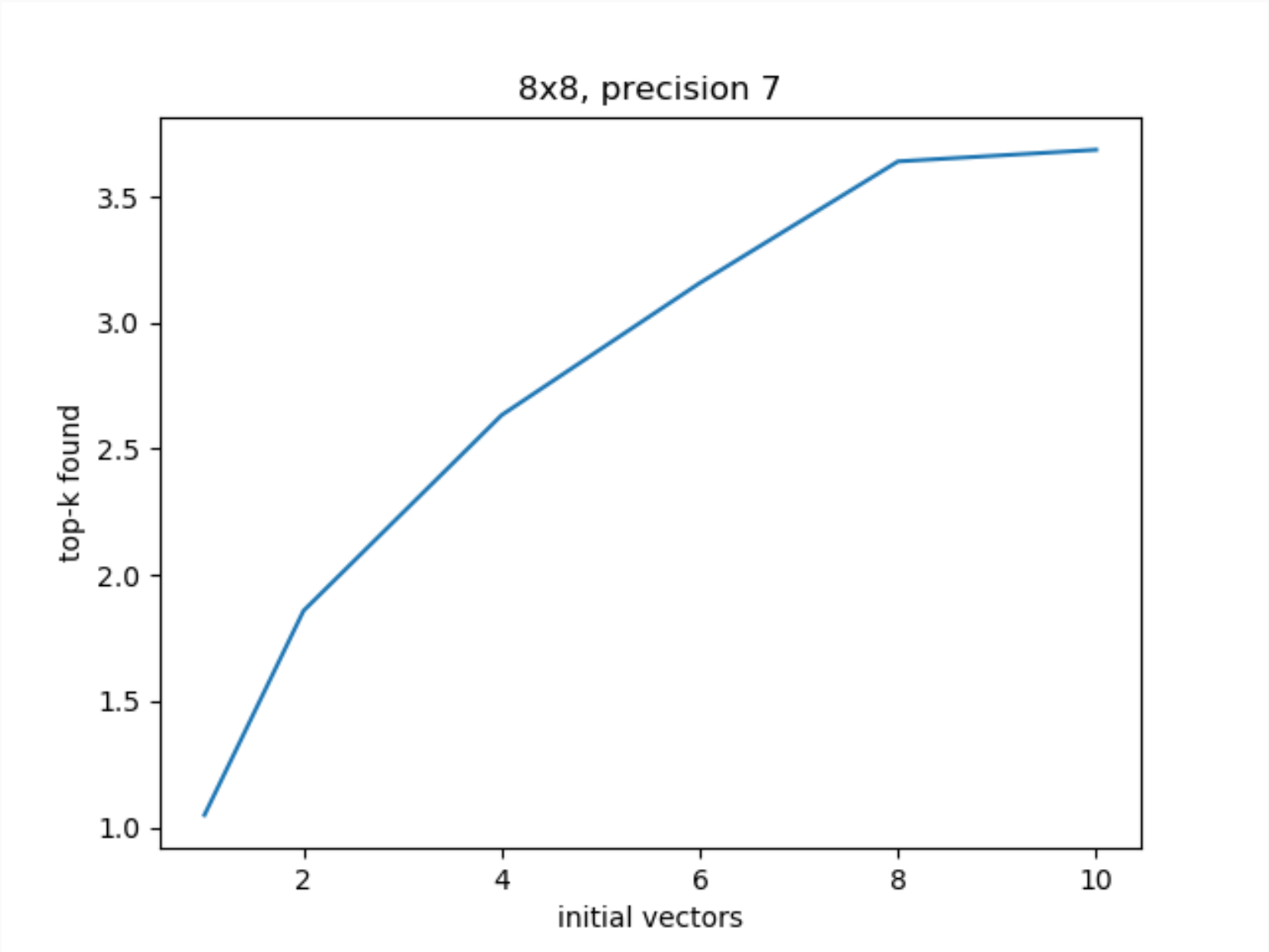
Some results for different numbers of random initializations



Analysis - *Results*

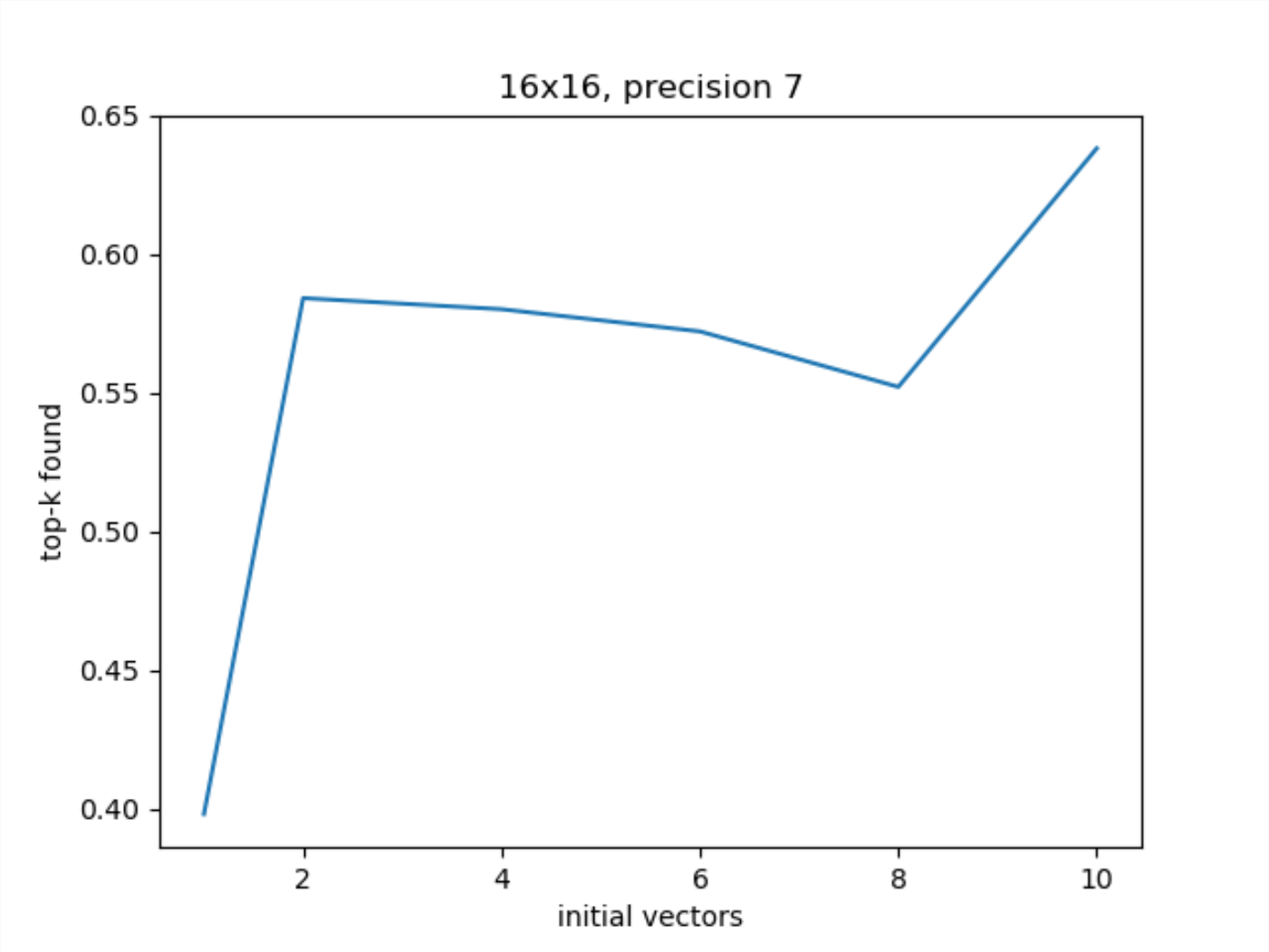


Analysis - *Results*



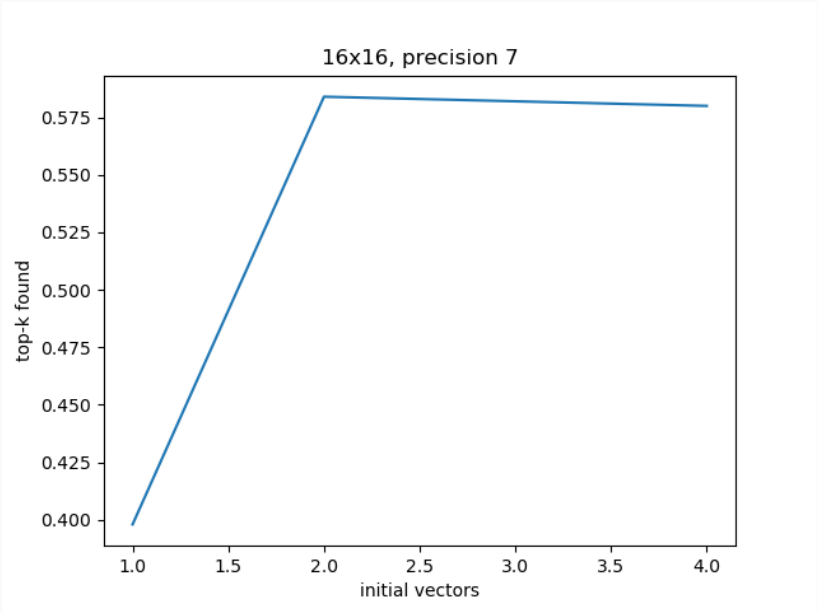
Analysis - *Results*

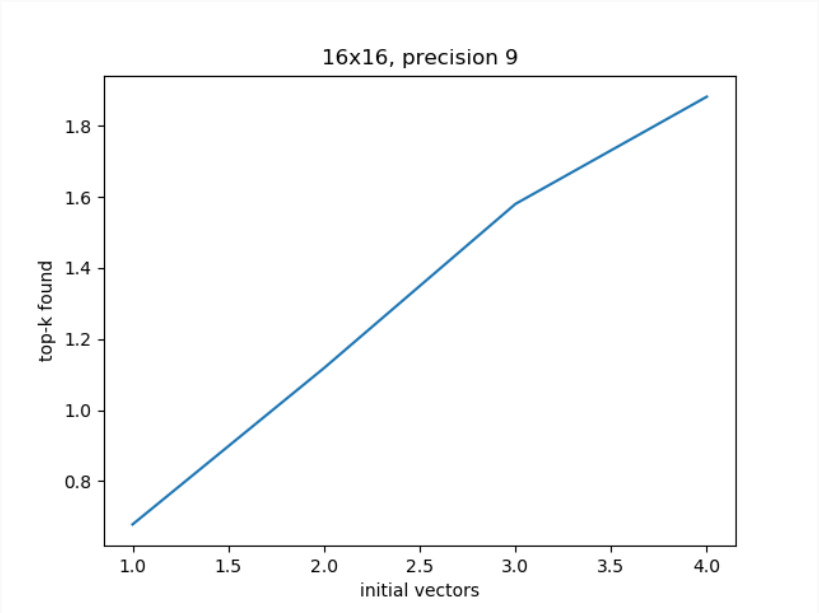
With 7 qubits precision, results on 16x16 covariance matrices start degrading.



Analysis - *Results*

Raising precision to 9 qubits makes results immediately improve





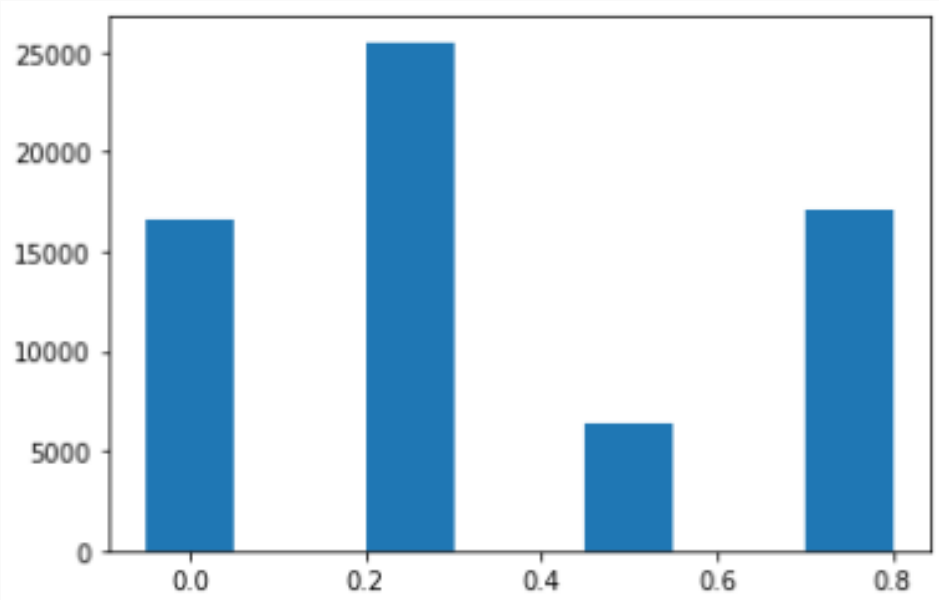
We test the algorithm on IBM's 5-qubit quantum device Vigo

- 2*x*2 covariance matrix
- 2 qubits precision for the eigenvalues

Real eigendecomposition

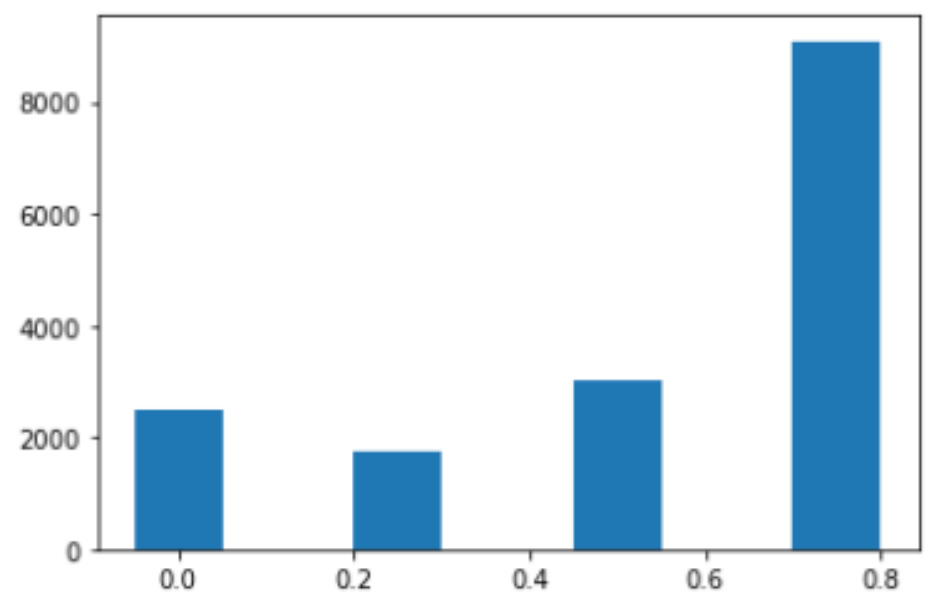
$$\lambda_1 = 0.84212698,\ v_1 = \begin{bmatrix} 0.91854462 & -0.39531732 \end{bmatrix}$$
$$\lambda_2 = 0.15787302,\ v_2 = \begin{bmatrix} 0.39531732 & 0.91854462 \end{bmatrix}$$

Histogram of eigenvalues found using 4 random initial vectors



Vector corresponding to 0.75, $v_a = \begin{bmatrix} 0.85450074 & -0.51945017 \end{bmatrix}$

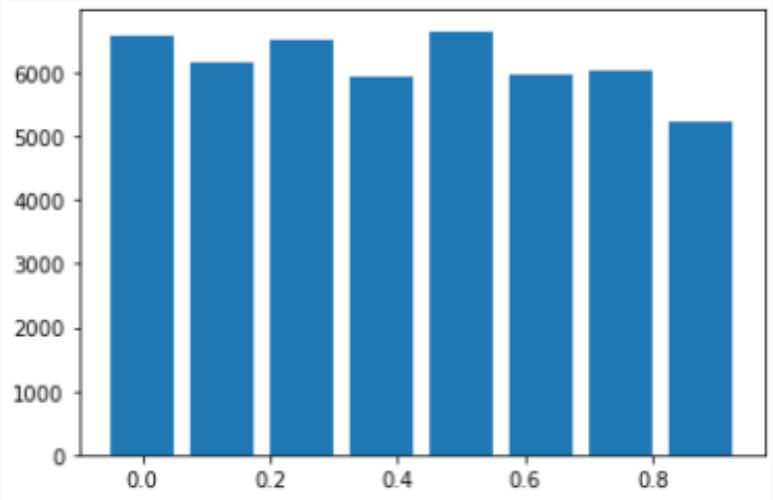
Running the algorithm using v_a as initial vector now measures



and improved vector $v = \begin{bmatrix} 0.91533142 & -0.40270137 \end{bmatrix} \approx v_1$

Analysis - *Results on Real Device*

- Iterative Approach proves effective with today's noisy quantum computers
- For 2*x*2 matrix we obtained decent results
- Attempts on 4*x*4 with 3 qubit precision are already too noisy



References

- Daniel S. Abrams, Seth Lloyd *A quantum algorithm providing exponential speed increase for finding eigenvalues and eigenvectors.* *https://arxiv.org/pdf/quant-ph/9807070v1.pdf*
- Seth Lloyd , Masoud Mohseni and Patrick Rebentrost *Quantum principal component analysis.* *https://arxiv.org/pdf/1307.0401.pdf*
- Ana Martin, Bruno Candelas, Ángel Rodríguez-Rozas et al. *Towards Pricing Financial Derivatives with an IBM Quantum Computer.* *https://arxiv.org/pdf/1904.05803.pdf*