A Practical Guide to Quantum Linear Algebra

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Quantum Computing in a Nutshell
– Keeping Quantum Computing Honest

- Exciting experiment
- New computational paradigm
- Is it competitive?
  $\rightarrow$ No
- Not – and never will be(?) – a silver bullet

Linear Algebra

$$Ax = b$$

$$Av = \lambda v$$
$$(H|\Psi\rangle = E|\Psi\rangle)$$

Linear Algebra

$$Ax = b \qquad \begin{gathered} Av = \lambda v \\ (H|\Psi\rangle = E|\Psi\rangle) \end{gathered}$$

- Underpins most of scientific computing
- Efficient algorithm development and implementation
  - BLAS
  - LAPACK
  - ATLAS
  - ...

  (Turing Award 2021 – Jack Dongarra)

Question: Can we do similar things with a quantum computer?

Quantum Linear Algebra: Desired Speedup

$$\mathrm{poly}(N) \qquad \textit{vs.} \qquad \mathrm{poly}\,\log(N)$$

Consider N-dimensional systems (say $N = 2^n$)

- Most classical simulations are $\mathrm{poly}(N)$
  $\rightarrow$ Storing a vector $\sim N$
  $\rightarrow$ Sparse MAT-VEC $\sim N$
- Quantum simulations we hope(!) for $\mathrm{poly}\,\log(N)$
  $\rightarrow$ An n-qubit state can be viewed as a 2^n-dim. unit vector
  $\rightarrow$ Matrix operations are implemented as quantum operations on these n qubits

!Careful!
!Caveats apply!

Rules of Quantum Simulation

In general, not all operations can be performed efficiently on a quantum device!

- Vectors (quantum states) are normalized
- Only a subset of operations can be efficiently implemented: unitary matrices
  $\rightarrow$ Other problems have to be rescaled (Block encoding)
  $\rightarrow$ Rescaling will introduce greater cost
- No cloning theorem
  $\rightarrow$ Iterative methods are not in general efficient

Quantum Algorithms for Scientific Computation

Lecture notes by Lin Lin:

- arXiv:2201.08309
- math.berkeley.edu/∼linlin/

Roadmap

Towards linear algebra on quantum devices

1. Basic quantum gates
2. (Real) Hadamard Test
3. Quantum Phase Estimation
4. Numerical performances on emulators and a real quantum device

Some Basic Gates & Conventions

Single qubit states:

$$|0\rangle := \begin{bmatrix} 1 \\ 0 \end{bmatrix} \quad \text{and} \quad |1\rangle := \begin{bmatrix} 0 \\ 1 \end{bmatrix}.$$

Single qubit gates, e.g.,

$$X := \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \quad \text{and} \quad H := \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}$$

Two-qubit gates, e.g.,

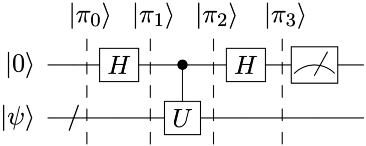
$$CNOT := \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix} \quad \text{and} \quad SWAP := \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}$$

The (real) Hadamard Test

- Simplest way to compute

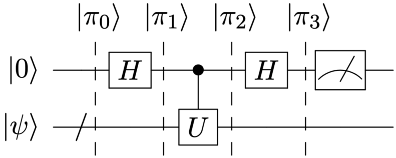
$$\langle U \rangle = \langle \psi | U | \psi \rangle$$

- Simple diagram



Why does it work?

The real Hadamard Test – Outcome



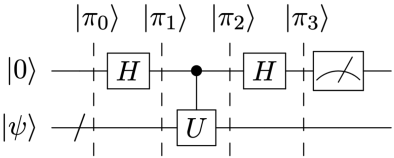
$$|\pi_0\rangle = |0\rangle \otimes |\psi\rangle = |0\rangle|\psi\rangle$$

$$|\pi_1\rangle = H|0\rangle I|\psi\rangle = \frac{1}{\sqrt{2}}\left(|0\rangle + |1\rangle\right)|\psi\rangle = |+\rangle|\psi\rangle$$

$$|\pi_2\rangle = (|0\rangle\langle 0| \otimes I + |1\rangle\langle 1| \otimes U)|\pi_1\rangle = \frac{1}{\sqrt{2}}|0\rangle I|\psi\rangle + \frac{1}{\sqrt{2}}|1\rangle U|\psi\rangle$$

$$|\pi_3\rangle = |0\rangle\frac{I+U}{2}|\psi\rangle + |1\rangle\frac{I-U}{2}|\psi\rangle$$

The real Hadamard Test – Outcome



We then perform a (single qubit) measurement and find

$$\mathbb{P}_{\mathrm{Re}|0\rangle} = |\langle 0|\pi_3\rangle|^2 = \frac{2 + \langle\psi|(U + U^\dagger)|\psi\rangle}{4} = \frac{1}{2}(1 + \mathrm{Re}\langle\psi|U|\psi\rangle)$$

and

$$\mathbb{P}_{\mathrm{Re}|1\rangle} = |\langle 1|\pi_3\rangle|^2 = \frac{1}{2}(1 - \mathrm{Re}\langle\psi|U|\psi\rangle)$$

The real Hadamard Test – Experiment

Consider

$$U = \begin{bmatrix} 1 & 0 \\ 0 & e^{i\theta} \end{bmatrix} \quad \text{where} \quad \theta = \frac{1}{2} + \frac{1}{2^4} = 0.5625$$

Then

$$\lambda_1 = 1, v_1 = |0\rangle \quad \text{and} \quad \lambda_2 = e^{i\theta} = \cos(\theta) + i\sin(\theta), v_2 = |1\rangle$$

and

$$\langle 1|U|1\rangle = \cos(\theta) + i\sin(\theta)$$

The real Hadamard Test – Experiment

Initializing with

$$|\Psi\rangle = |1\rangle$$

yields

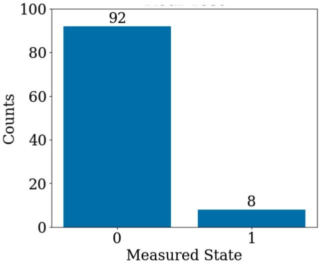
$$\mathrm{Re}\langle 1|U|1\rangle = \cos(\theta)$$

We find

$$\mathbb{P}_{\mathrm{Re}|0\rangle} = \frac{1}{2}(1+\cos(\theta)) \approx 0.9230$$
$$\mathbb{P}_{\mathrm{Re}|1\rangle} = \frac{1}{2}(1-\cos(\theta)) \approx 0.0770$$

Quantum simulation:

- AerSimulator
- Real Hadamard test
- 100 samples



The real Hadamard Test – Convergence

- Every sample is a random variable with two outcomes:

$$|0\rangle \quad \text{or} \quad |1\rangle$$

$\Rightarrow$ Bernoulli distribution

$$X_i \sim \mathcal{B}(p) \quad \text{with} \quad p = \mathbb{P}_{\mathrm{Re}|0\rangle}$$

- Given N_s i.i.d. samples, we estimate

$$\hat{p}_{N_s} = \frac{1}{N_s} \sum_{i=1}^{N_s} \mathbb{1}_{\{|0\rangle\}}(X_i)$$

[empirical distribution function]

- By the weak law of large numbers

$$\hat{p}_{N_s} \xrightarrow{\mathbb{P}} \mathbb{E}(X) \quad \Leftrightarrow \quad \lim_{N_s \to \infty} \mathbb{P}(|\hat{p}_{N_s} - p| > \varepsilon) = 0 \ \forall \varepsilon > 0$$

The real Hadamard Test – Convergence rate

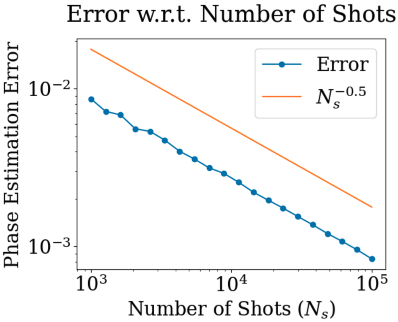
- For the empirical distribution function the STD is

$$\sigma^2 = \mathbb{V}(\hat{p}_{N_s}) = \frac{p(1-p)}{N_s}$$

- Then

$$\epsilon \geq \sigma = \sqrt{\frac{p(1-p)}{N_s}} \quad \Rightarrow \quad N_s \geq \frac{p(1-p)}{\epsilon^2} \in \Omega\left(\frac{1}{\epsilon^2}\right)$$

The real Hadamard test – Convergence rate

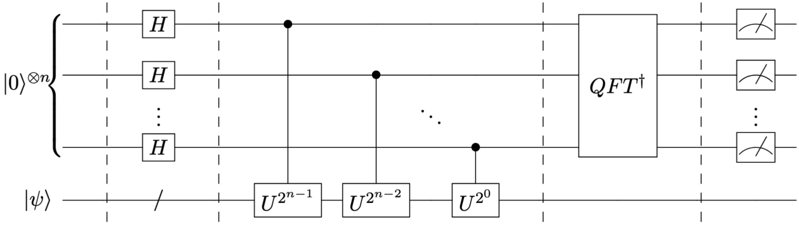


Shot Count	Estim. Angle θ	Error
100	0.4027	0.1598
500	0.4864	0.0761
1000	0.5394	0.0231
5000	0.5830	0.0205
10000	0.5698	0.0073
50000	0.5569	0.0056
100000	0.5620	0.0005

$\Rightarrow$ Converges slowly... very slowly!
(like molasses in January)

Quantum Phase Estimation (QPE)

- The Hadamard test performs a single qubit measurement
- Can we achieve higher accuracy measuring multiple qubits?
  $\Rightarrow$ Yes, this is the idea of QPE



- The rate of convergence:

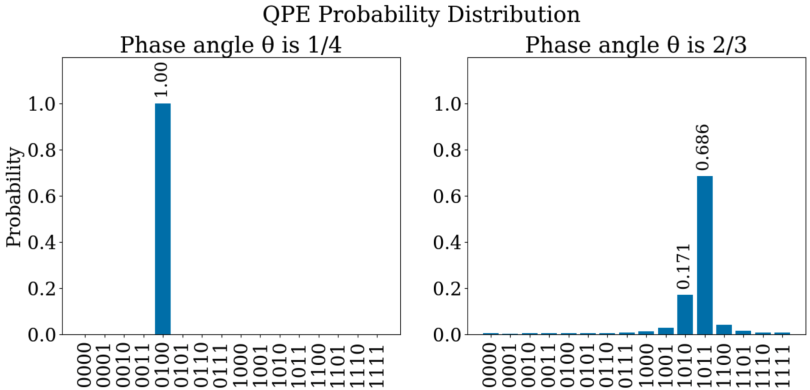
$$n \in \Omega\left(\frac{1}{\epsilon}\right)$$

QPE – Convergence

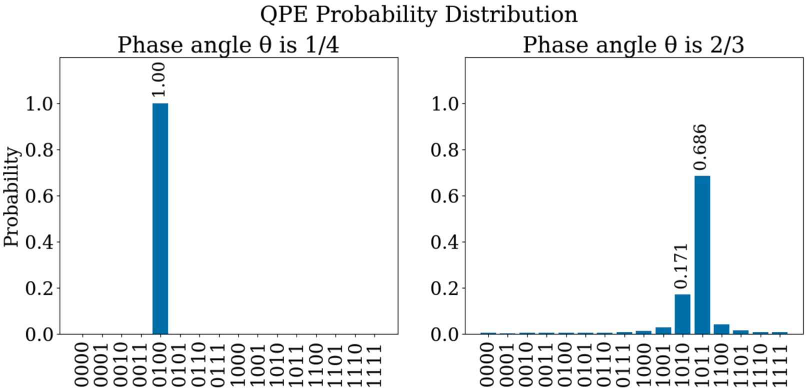
- Consider

$$U = \begin{bmatrix} 1 & 0 \\ 0 & e^{i2\pi\theta} \end{bmatrix}$$

- 4 ancilla qubits
- phase angles $\theta = 1/4$ and $\theta = 2/3$

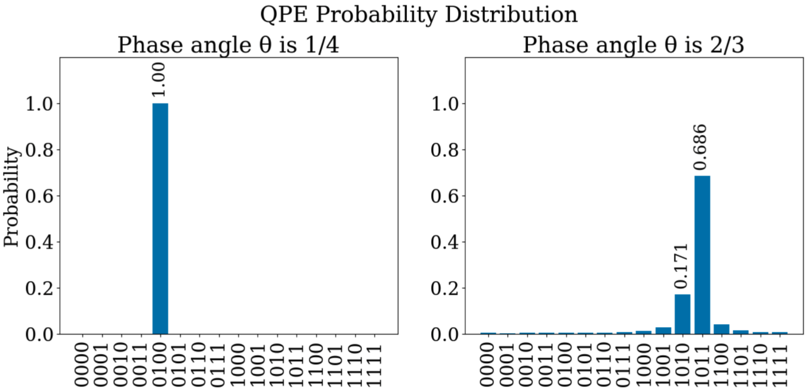


QPE – Computing the Phase



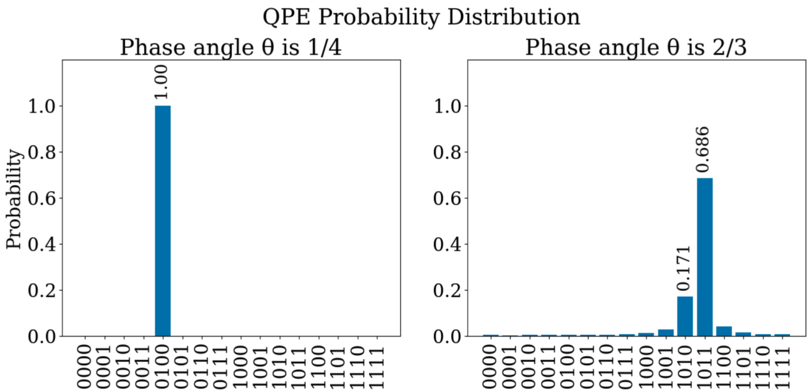
- Find the maximal state:
  0100 and 1011, respectively

QPE – Computing the Phase



- Find the maximal state:
  0100 and 1011, respectively
- Convert to decimal basis:
  4 and 11, respectively

QPE – Computing the Phase



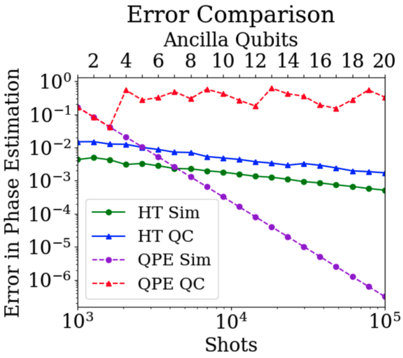
- Find the maximal state:
  0100 and 1011, respectively
- Convert to decimal basis:
  4 and 11, respectively
- Normalize w.r.t. number ancilla qubits (2^n):
  $4/16 = 1/4$ and $11/16 = 0.6875 \approx 2/3$, respectively

Comparison and quantum computation

- Consider

$$U = \begin{bmatrix} 1 & 0 \\ 0 & e^{i2\pi\frac{1}{3}} \end{bmatrix}$$

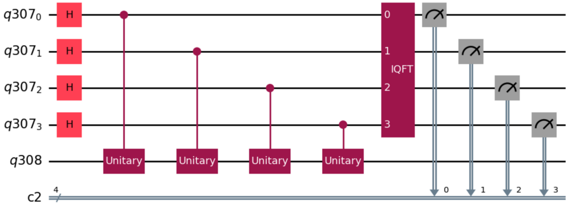
- 1 to 20 ancilla qubits for QPE (each at 10^3 shots)
- 10^3 to 10^5 shots for HT



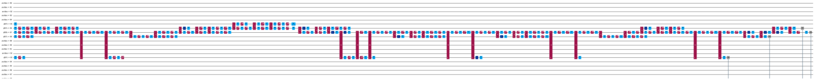
Why is QPE on the quantum device so bad?

Quantum Simulation – Transpilation

Original circuit:

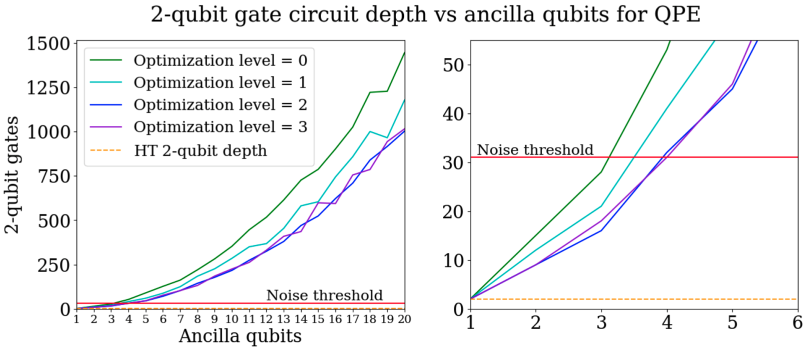


Transpiled circuit:
(Qiskit 1.1.1, optimization_level=3)

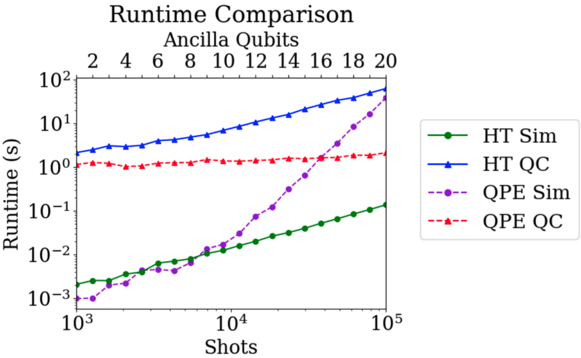


2-qubit gate depth

- The dominant noise contribution comes from two-qubit gates e.g. controlled or swap gates



Quantum Simulation – Runtime



$\Rightarrow$ Quantum simulation of QPE has constant runtime

High-accuracy electronic structure methods

What:
Introduction to high-accuracy electronic structure methods

Where:
Institute for Mathematical and Statistical Innovation (IMSI)
Chicago, Illinois, USA

When:
June 30 – July 10, 2025

Funding is available!
Application deadline: Dec. 15

Team

Alexander Weiss

Paul Bruzzi

Thank you for your attention!