A Quantum Algorithm for Spectral Measurement based on Block-Encodings

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Based on arXiv:2103.09717

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Outline

1. Block-encodings: non-unitary matrices on quantum computer

$$U = \begin{bmatrix} A & \cdot \\ \cdot & \cdot \end{bmatrix}$$

Low, Chuang arXiv:1610.06546 Gilyén et al arXiv:1806.01838

Applications: Hamiltonian simulation, Thermal state preparation, Fast-Forwarding, Observable estimation...

2. Spectral measurement: measuring in an eigenbasis of H

$$\sum_j \alpha_j |0^n\rangle |\psi_j\rangle \quad \rightarrow \quad \sum_j \alpha_j |\lambda_j\rangle |\psi_j\rangle$$

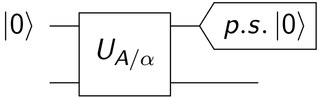
Rall arXiv:2103.09717

What is a block-encoding?

- A is *any* matrix, $|A| \leq \alpha$:

$$U_{A/\alpha} = \begin{bmatrix} A/\alpha & \cdot \\ \cdot & \cdot \end{bmatrix}$$

- Quantum circuit implementation: $|\psi\rangle \to (A/\alpha)\,|\psi\rangle$



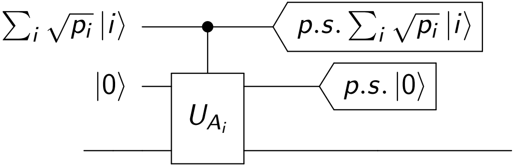
Linear Combinations of Block-Encodings

- Given block-encodings of A, B, can construct:

$$A \cdot B \qquad A \otimes B \qquad pA + (1-p)B$$

- Linear combinations of block-encodings

$$U_{\sum_i p_i A_i} =$$



- Linear combinations of Pauli matrices
  $\rightarrow$ most practical Hamiltonians have a block-encoding

Singular Value Transformation

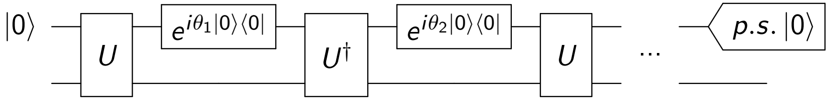
- Given block-encoding of

$$A = \sum_i \lambda_i \left|\psi_i\right\rangle \left\langle\psi_i\right|$$

and some polynomial $p(x)$, construct a block-encoding of:

$$p(A) = \sum_i p(\lambda_i) \left|\psi_i\right\rangle \left\langle\psi_i\right|$$

- Cost: degree of $p(x)$. Several restrictions on $p(x)$ required.
- Circuit: for some angles $\theta_1, ..., \theta_d$



Applications

- Hamiltonian simulation
  Low, Chuang arXiv:1610.06546 Gilyén et al arXiv:1806.01838

$$p(x) \approx \cos(tx), \qquad q(x) \approx \sin(tx), \qquad e^{itx} \approx p(x) + iq(x)$$

- Thermal state preparation Chowdhury, Somma arXiv:1603.02940

$$p(x) \approx e^{-\beta x/2}, \qquad \sqrt{\rho_{\text{therm}}} \approx p(H)$$

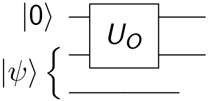
$$\frac{I}{D} \to \sqrt{\rho_{\text{therm}}}\frac{I}{D}\sqrt{\rho_{\text{therm}}} \propto \rho_{\text{therm}}$$

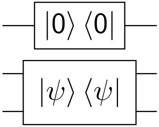
- Fast-forwarding Apers, Sarlette arXiv:1804.02321

$$U^n \approx p(U) \text{ of degree } \sqrt{n \cdot 2 \ln \frac{2}{\varepsilon}}$$

Estimating observables: $\mathrm{Tr}(\rho O)$ Rall arXiv:2004.06832

- Given a block-encoding of O, and $|\psi\rangle$, a purification of ρ
- Perform amplitude estimation with:

$|\Phi\rangle :=$ 

$\Pi :=$ 

- Estimates:

$$|\Pi |\Phi\rangle | = | \langle 0| \langle \psi| (U_O \otimes I) |0\rangle |\psi\rangle | = | \langle \psi| (O \otimes I) |\psi\rangle |$$

$$= |\mathrm{Tr} [|\psi\rangle \langle \psi| (O \otimes I)] | = |\mathrm{Tr} (\rho O) |$$

Spectral Measurement

Rall arXiv:2103.09717

- Input:

$$U = \sum_j e^{2\pi i \lambda_j} |\psi_j\rangle \langle\psi_j| \quad \text{or} \quad H = \sum_j \lambda_j |\psi_j\rangle \langle\psi_j|$$

- Output:

$$\sum_j \alpha_j |0^n\rangle |\psi_j\rangle \quad \rightarrow \quad \sum_j \alpha_j |\lambda_j\rangle |\psi_j\rangle$$

$$|\lambda_j\rangle := n\text{-bit estimate of } \lambda_j$$

- Applications:
  - Quantum Metropolis Sampling: Temme et al arXiv:0911.3635 Yung, Guzik arXiv:1011.1468 Lemieux et al arXiv:1910.01659
  - Non-destructive amplitude estimation, required for: Harrow, Wei arXiv:1908.10856 Arunachalam et al arXiv:2009.11270

Prior Art

- 'Textbook method' - Phase Estimation [Nielsen, Chuang]
  - Construct $\sum_t \frac{1}{\sqrt{2^n}} |t\rangle \otimes U^t$, then Quantum Fourier Transform
  - High ancilla cost from median amplification, requires quantum sorting network
- Iterative Phase Estimation [Kitaev quant-ph/9511026]
  - Assumes we are given an eigenstate $|\psi_j\rangle$
  - Obtains λ_j one bit at a time
- Novel Methods for Amplitude Estimation
  - Destructive: requires many copies of the input state
    [Aaronson, Rall arXiv:1908.10846] [Grinko et al arXiv:1912.05559]
  - State repair methods require lots of adaptivity
    [Poulin et al arXiv:1711.11025] [Harrow, Wei arXiv:1908.10856]

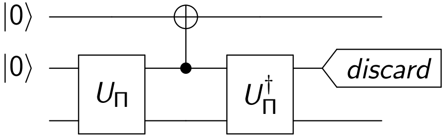
Block-measurement lemma

Let Π be a projector and let V be the isometry:

$$V = \Pi \otimes |1\rangle + (I - \Pi) \otimes |0\rangle$$

Given a δ-approximate block-encoding of Π, there exists a quantum channel Λ that is 2δ close in $\diamond$-norm to V.

- Say U_Π is the approximate block-encoding of Π:



- Analysis trick:

$$\text{total error} \leq \text{error when postselecting } |0\rangle$$
$$+ \text{ probability postselection fails}$$

Method Outline

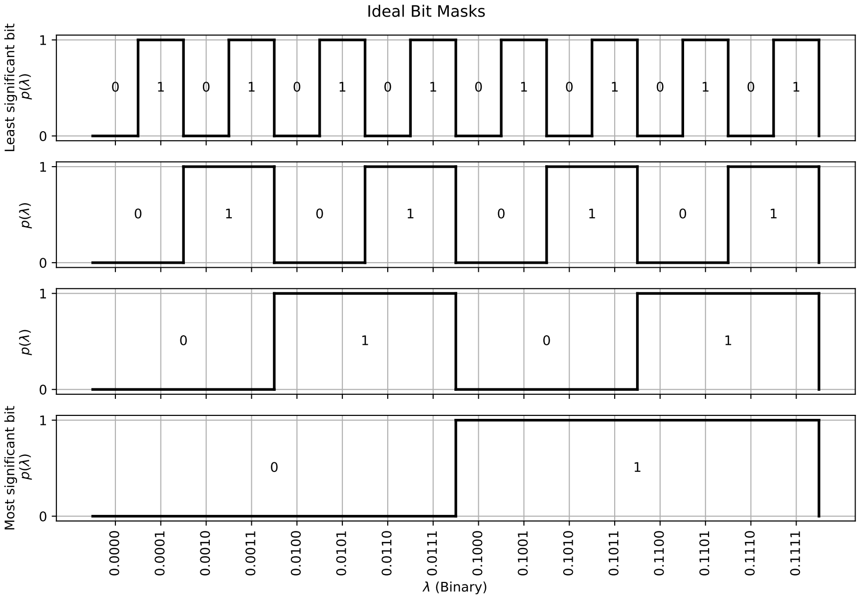
- Goal: n-bit approximation of λ_j
- For each bit $k \in \{0, ...n-1\}$ fix a projector:

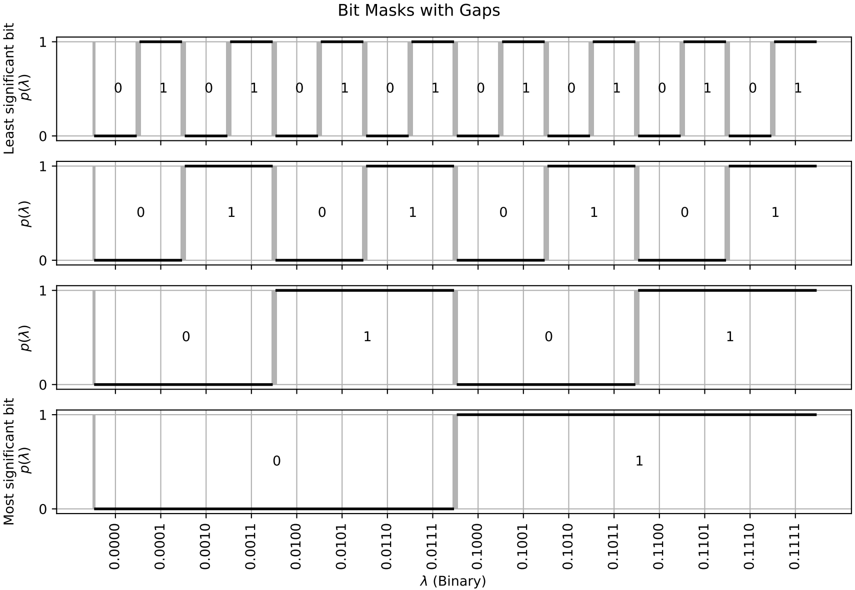
$$\Pi_k = \sum_j k\text{'th bit of } \lambda_j \cdot |\psi_j\rangle \langle\psi_j|$$

- Make projectors via singular value transformation: $\Pi_k \approx p_k(H)$

$$k\text{'th bit of } \lambda \approx p_k(\lambda)$$

- Use block-measurement lemma to compute $|\lambda_j\rangle$


Ideal Bit Masks
Least significant bit
$p(\lambda)$
Most significant bit
0
1
0.0000
0.0001
0.0010
0.0011
0.0100
0.0101
0.0110
0.0111
0.1000
0.1001
0.1010
0.1011
0.1100
0.1101
0.1110
0.1111
λ (Binary)


Bit Masks with Gaps
Least significant bit
$p(\lambda)$
Most significant bit
0
1
0000 0001 0010 0011 0100 0101 0110 0111 1000 1001 1010 1011 1100 1101 1110 1111
0.0000
0.0001
0.0010
0.0011
0.0100
0.0101
0.0110
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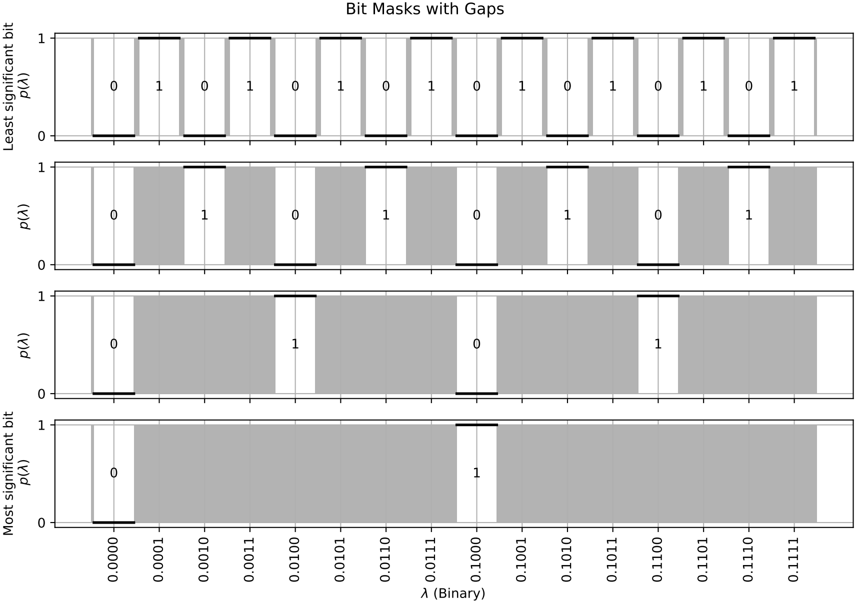
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λ (Binary)

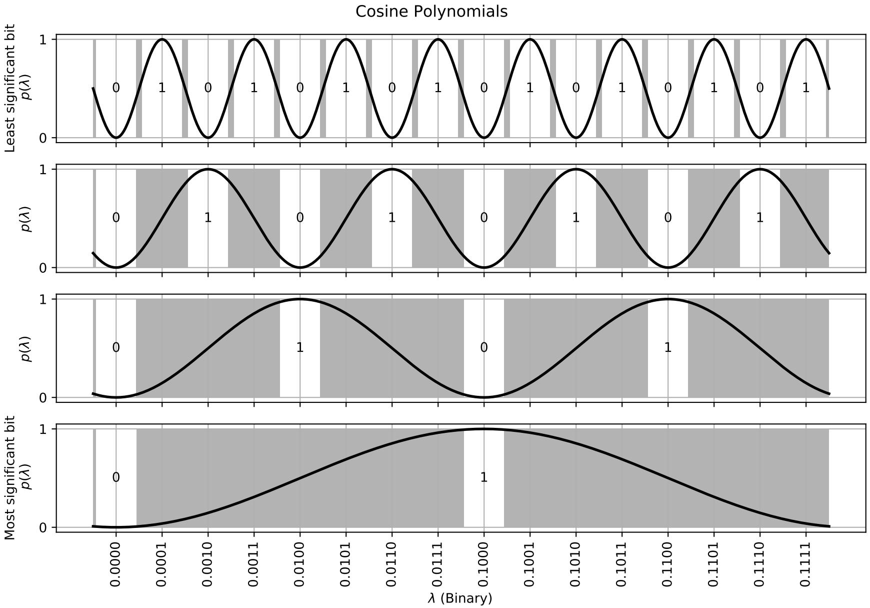
Making a Cosine

- First, make $\frac{1+\cos(2^{n-k}\pi\lambda)}{2} = \cos^2\left(\frac{2^{n-k}\pi\lambda}{2}\right)$
- For unitaries with phases $e^{2\pi i\lambda}$, just use a linear combination

$$\frac{e^{2^{n-k}\pi i\lambda}+1}{2} \propto \cos\left(\frac{2^{n-k}\pi\lambda}{2}\right)$$

- For Hamiltonians with eigenvalues λ, use the Jacobi-Anger expansion

$$p_{\cos}(\lambda) = J_0(t) - 2\sum_k^R (-1)^k J_{2k}(t)\, T_{2k}(x) \approx \cos(tx)$$


Cosine Polynomials
Least significant bit
p(λ)
Most significant bit
λ (Binary)
0.0000
0.0001
0.0010
0.0011
0.0100
0.0101
0.0110
0.0111
0.1000
0.1001
0.1010
0.1011
0.1100
0.1101
0.1110
0.1111

- Amplify the signal:

$$p \leq \frac{1}{2} - \eta \quad \rightarrow \quad A(p) \leq \delta$$

$$p \geq \frac{1}{2} + \eta \quad \rightarrow \quad A(p) \geq 1 - \delta$$

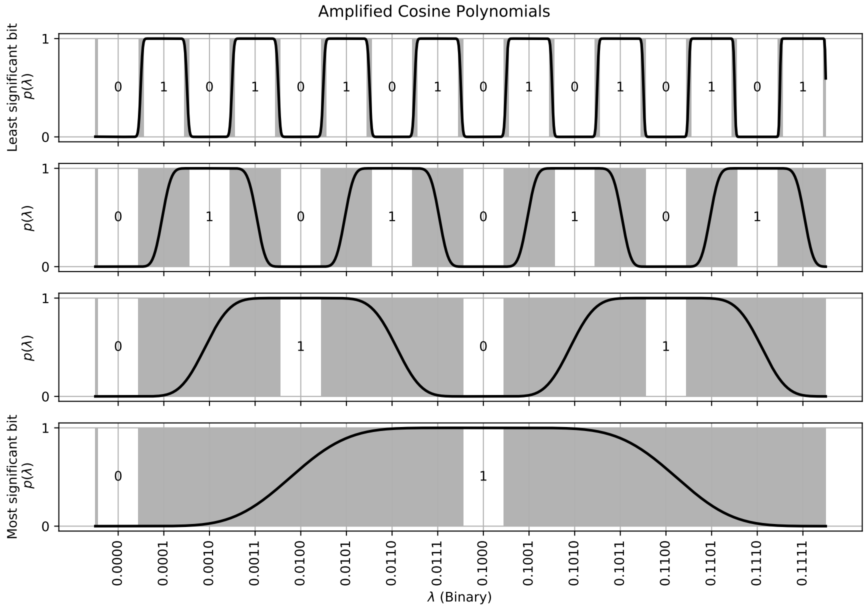
- Classical approach, achieves $m \in O(\eta^{-2} \log(\delta^{-1}))$

$$A_m(p) = \Pr[\text{more than half of } m \text{ coin tosses come up heads}]$$

- Quantum approach, achieves $m \in O(\eta^{-1} \log(\delta^{-1}))$

$$A_m(p) \approx \frac{2k}{\sqrt{\pi}} \int_0^p e^{-(kp)^2} \approx \text{erf}(kp) \approx \text{sign}(p)$$

See Appendix A of Low, Chuang arXiv:1707.05391


Amplified Cosine Polynomials
Least significant bit
Most significant bit
p(λ)
0
1
0000
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λ (Binary)

Performance

- Parameters: precision n, accuracy δ, and gap parameter α.

$$\alpha = 2^n \cdot \text{mininum gap size} = \text{total fraction ignored } \lambda$$

- Asymptotic performance: both PE and new method already optimal

$$O\left(2^n \alpha^{-1} \log(\delta^{-1})\right)$$

- Ancilla cost
  - Phase estimation needs $O((n + \log(\alpha^{-1})) \log(\delta^{-1}))$
  - New method needs only $O(n)$.
- Query complexity
  - Stabilizes at around $n \gtrsim 10, \alpha \lesssim 2^{-10}$ and $\delta \leq 10^{-30}$
  - For unitaries: $\sim 14x$. For Hamiltonians: $\sim 20x$.

Application: Amplitude Estimation

- Given one copy of $|\Psi\rangle$ and the reflections

$$R_\Pi = 2\Pi - I, \qquad R_{|\Psi\rangle} = 2\,|\Psi\rangle\,\langle\Psi| - I$$

estimate $a = |\Pi\,|\Psi\rangle\,|$.

- Use linear combinations to make the block-encodings:

$$\Pi = \frac{R_\Pi + I}{2}, \qquad |\Psi\rangle\,\langle\Psi| = \frac{R_{|\Psi\rangle} + I}{2}$$

$$A := |\Psi\rangle\,\langle\Psi| \cdot \Pi \cdot |\Psi\rangle\,\langle\Psi| = a^2\,|\Psi\rangle\,\langle\Psi|$$

- Then apply energy estimation to perform the map:

$$|0^n\rangle\,|\Psi\rangle \to |a^2\rangle\,|\Psi\rangle$$

Thank you for your attention!

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