CSC 591 Project B4 report3 Quantum Enhanced Simulation Optimization

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1 Introduction

As we mentioned before, we need to focus three things: Quantum Amplitude Estimation (QAE), Operator \mathcal{P}_X , and F. At this report, we will focus on QAE and show simple example.

2 Quantum Amplitude Estimation

QAE is a fundamental quantum algorithm with the potential to achieve a quadratic speedup for many applications that are classically solved through Monte Carlo (MC) simulation. While the estimation error of classical MC simulation scales as $\mathcal{O}(M^{-1/2})$, where M denotes the number of (classical) samples, QAE achieves a scaling of $\mathcal{O}(M^{-1})$ for M (quantum) samples, which implies the aforementioned quadratic speedup.

The canonical version of QAE (figure 1) is a combination of Quantum Phase Estimation(QPE) and Grover's Algorithm. However, since QPE consists of many controlled amplification operations followed by a quantum Fourier transform, the whole procedure is hard to implement with current and near-term quantum computers. Hence, there is new version of QAE which is called Iterative QAE (IQAE).

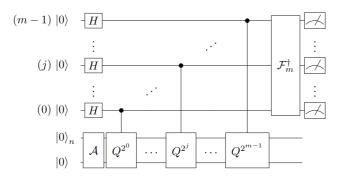


Figure 1: The quantum circuit of cannonical QAE

2.1 Canonical Quantum Amplitude Estimation

Suppose the problem of interest is given by an operator A acting on n+1 qubits such that

$$\mathcal{A} \left| 0 \right\rangle_n \left| 0 \right\rangle = \sqrt{1 - a} \left| \psi_0 \right\rangle_n \left| 0 \right\rangle + \sqrt{a} \left| \psi_1 \right\rangle_n \left| 1 \right\rangle$$

,where $a \in [0,1]$ is the unknown, and $|\psi_0\rangle_n$ and $|\psi_1\rangle_n$ are two normalized states, not necessarily orthogonal. QAE allows to estimate a with high probability. To this extent, an operator $\mathcal{Q} = -\mathcal{S}_{\psi_0} \mathcal{A}^{\dagger} \mathcal{S}_0 \mathcal{A}$ is defined where $\mathcal{S}_{\psi_0} = \mathbf{I} - 2 |\psi_0\rangle_n \langle \psi_0|_n \otimes |0\rangle \langle 0|$ and $\mathcal{S}_0 = \mathbf{I} - 2 |0\rangle_{n+1} \langle 0|_{n+1}$.

The canonical QAE follows the form of QPE: it uses m ancilla qubits – initialized in equal superposition to represent the final result, it defines the number of quantum samples as M=2m and applies geometrically increasing powers of $\mathcal Q$ controlled by the ancillas. Eventually, it performs a QFT on the ancilla qubits before they are measured, as illustrated in figure 1. Subsequently, the measured integer $y \in \{0,\ldots,M-1\}$ is mapped to an angle $\hat{\theta}_a = y\pi/M$. Thereafter, the resulting estimate of a is defined as $\hat{a} = \sin^2(\hat{\theta}_a)$.

2.2 Iterative Quantum Amplitude Estimation

As mentioned before, we use the quantum computer to approximate $P(|1\rangle) = \sin^2((2k+1)\theta a)$ for the last qubit in $\mathcal{Q}^k \mathcal{A} |0\rangle_n |0\rangle$ for different powers k. The main idea is as follows. Suppose a confidence interval $[\theta_l, \theta_u] \in [0, \pi/2]$ for θ_a and a power k of \mathcal{Q} as well as an estimate for $\sin^2((2k+1)\theta_a)$. Through exploiting the trigonometric identity $\sin^2(x) = (1-\cos(2x))/2$, we can translate our estimates for $\sin^2((2k+1)\theta_a)$ into estimates for $\cos((4k+2)\theta_a)$. We cannot estimate the sine (only its square), and the cosine alone is only invertible without ambiguity if we know the argument is restricted to either $[0,\pi]$ or $[\pi,2\pi]$, i.e., the upper or lower half-plane. Thus, we want to find the largest k such that the scaled interval $[(4k+2)\theta_l, (4k+2)\theta_u]_{mod2\pi}$ is fully contained either in $[0,\pi]$ or $[\pi,2\pi]$. If this is given, we can convert $\cos((4k+2)\theta_a)$ and improve our estimate for θ_a with high confidence. This implies an upper bound of k, and the heart of the algorithm is the procedure used to find the next k given $[\theta_l, \theta_u]$. Table 1 shows the sketch of the algorithm. Figure 2 shows the step 2 and 3 in the algorithm.

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Table 1. Sketch of the algorithm STEP 1. Set [\theta_l, \theta_u] = [0, \pi/2], k_i = 0, i = 0 STEP 2. Set K_i = 4k_i + 2 Measure the last qubit until get certain level of confidence interval ((K_i\theta_u - K_i\theta_l)/2 < L) STEP 3 Find the largest k such that the scaled interval [K_i\theta_l, K_i\theta_u]_{mod2\pi} is fully contained either in [0, \pi] or [\pi, 2\pi] STEP 4 If \theta_u - \theta_l > 2\epsilon, i = i + 1 and go to STEP2 Otherwise, return [a_l, a_u] = [\sin^2\theta_l, \sin^2\theta_u]
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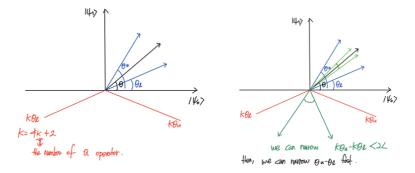


Figure 2: STEP2 and STEP3 description in the algorithm

Then, why Grover algorithm gives quantum advantage in terms of MC simulation? Since $\sin^2(\theta_a)$ follows Bernoulli distribution, we can get the confidence interval with certain number (n) of measurement.

$$p - \frac{1.96\sqrt{p(1-p)}}{n} \le \sin^2(\theta_a) \le p + \frac{1.96\sqrt{p(1-p)}}{n}$$

Since θ_a is included in interval $[0, \pi/2]$, θ_a can be as follows.

$$\arcsin\left(\sqrt{p-\frac{1.96\sqrt{p(1-p)}}{n}}\right) \le \theta_a \le \arcsin\left(\sqrt{p+\frac{1.96\sqrt{p(1-p)}}{n}}\right)$$

Hence, if we have larger n, we can get more precise θ_a . This is classical MC simulation. In contrast, if we apply one Q operator, the above equation becomes as follows.

$$\arcsin\left(\sqrt{p - \frac{1.96\sqrt{p(1-p)}}{n}}\right) \le 3\theta_a \le \arcsin\left(\sqrt{p + \frac{1.96\sqrt{p(1-p)}}{n}}\right)$$

As a result, we can get much narrower confidence interval with the same number of measurement.

3 Example

In this section, we introduce simple example with 2-qubits and $f(x) = x^2$, where $x \in \{0, 1, 2, 3\}$. Figure 3 and following equation shows what we prepared in previous report.

$$\mathcal{A}\left|0\right\rangle_{2}\left|0\right\rangle = \sum_{i=0}^{3}\sqrt{1-cf(i)}\sqrt{p_{i}}\left|i\right\rangle_{2}\left|0\right\rangle + \sum_{i=0}^{3}\sqrt{cf(i)}\sqrt{p_{i}}\left|i\right\rangle_{2}\left|1\right\rangle$$

,where c = 0.001.



Figure 3: The entire circuit for A

$$P(1) = \sum_{i=0}^{3} cf(i)p_i = E(cf(x)) = cE(f(x)) = \sin^2(\theta_a)$$

3.1 \mathcal{Q} operator

Before, apply IQAE, we want to show what happen when we apply \mathcal{Q} operator once. Figure 5 shows the entire circuit with $\mathcal{Q} = -\mathcal{S}_{\psi_0} \mathcal{A}^{\dagger} \mathcal{S}_0 \mathcal{A}$.

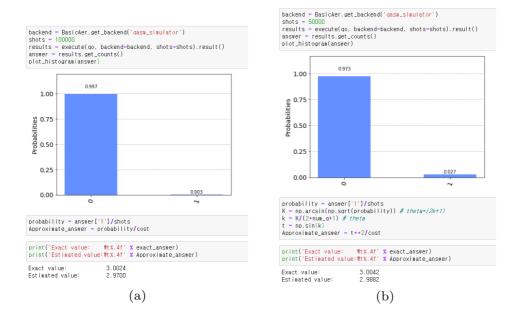


Figure 4: (a): The results with \mathcal{A} (b): The results with one \mathcal{Q} and \mathcal{A}

Figure 4(a) shows the result with \mathcal{A} and measurement and (b) shows the result with \mathcal{A} , \mathcal{Q} once, and measurement. Figure 4(a) shows that we can approximate the expected value (2.97) with 100,000 measurements. In contrast, figure 4(b) shows that we can approximate the expected value (2.9882) with 50,000 measurements. The reason is what we explained in page 3.

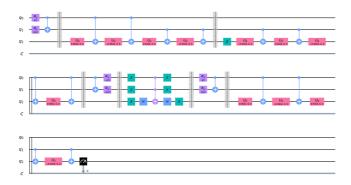


Figure 5: The entire circuit with one \mathcal{Q} operator and \mathcal{A}

3.2 Iterative Quantum Amplitude Estimation

Now, we want to apply IQAE. Since IQAE circuit is very complicated, we cannot show the figure. Instead, we will show the results simply and entire code is uploaded at Github (https://github.ncsu.edu/yha3/CSC591).

```
print('theta_lower: #t%.4f' % theta_l)
print('theta_upper: #t%.4f' % theta_u)
print('lower CI for E(x^2): #t%.4f' % A_l)
print('upper CI for E(x^2): #t%.4f' % A_u)
print('Number of measurement: #t%.4f' % N_measure)

theta_lower: 0.0538
theta_upper: 0.0554
lower CI for E(x^2): 2.8921
upper CI for E(x^2): 3.0625
Number of measurement: 10000.0000
```

Figure 6: IQAE results

As it can be seen in figure 6, we can get the 99% confidence interval [2.8921, 3.0625] with only 10,000 measurements and as mentioned in report2, the exact expected value is 3.

Reference

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URL: https://github.ncsu.edu/yha3/CSC591