UNBIASED QUANTUM PHASE ESTIMATION

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Quantum phase estimation algorithm (PEA) is one of the most important algorithms in early studies of quantum computation. However, we find that the PEA is not an unbiased estimation, which prevents the estimation error from achieving an arbitrarily small level. In this paper, we propose an unbiased phase estimation algorithm (UPEA) based on the original PEA. We also show that a maximum likelihood estimation (MLE) post-processing step applied on UPEA has a smaller mean absolute error than MLE applied on PEA. In the end, we apply UPEA to quantum counting, and use an additional correction step to make the quantum counting algorithm unbiased.

Keywords: Quantum Algorithm, Phase Estimation, Quantum Counting

1 Introduction

Early quantum algorithms are mostly based on two algorithms, the Grover’s search algorithm [1] and the quantum Fourier transformation (QFT) [2, 3]. The quantum phase estimation algorithm (PEA) [2] is one of the most important applications of QFT, as well as a key for many other quantum algorithms, such as the quantum counting algorithm [4] and the Shor’s integer factorization algorithm [3]. The PEA based order finding sub-procedure is considered as the source of the exponential speedup of the Shor’s algorithm.

Though PEA was proposed over 20 years ago, it is still a research hotspot in recent years [5, 6, 7]. Phase estimation has also given rise to a more general topic, the amplitude estimation [8, 9, 10, 11, 12, 13], including maximum likelihood amplitude estimation [10], iterative amplitude estimation [12] and variational amplitude estimation [13]. Besides, the iterative phase estimation algorithm (IPEA) [14, 15, 16] is a more NISQ(noise-intermediate scale quantum)-friendly variant for PEA. With a certain strategy of selecting \( \phi \), IPEA is identical to PEA [14], so we do not discuss IPEA in this paper. The phase estimation and amplitude estimation have a wide range of applications like quantum chemistry [17, 18, 19] and machine learning [20, 21].

Given a quantum circuit that performs unitary transformation \( U \), and an eigenstate \( |\psi\rangle \)
of $U$ such that
\[ U |\psi\rangle = e^{2\pi i \phi} |\psi\rangle, \] (1)

the phase estimation algorithm (PEA) [2] provides an efficient way to estimate $\phi$. The QFT-based form of PEA [2, 3] uses the circuit shown in FIG. 1.

Let the integer-encoded measurement result be $s$, then
\[ \tilde{\phi} = \frac{s}{T} \] (2)
is an estimation of $\phi$, where $T = 2^t$, and $t$ is the number of qubits involved in QFT in FIG. 1. The result obeys the following distribution [22],
\[ P_{\text{PEA}}(\tilde{\phi}|\phi) = \left( \frac{\sin(T\pi(\tilde{\phi} - \phi))}{T \sin(\pi(\tilde{\phi} - \phi))} \right)^2, \quad \tilde{\phi} \in \left\{ 0, \frac{1}{T}, \frac{2}{T}, \ldots, \frac{T-1}{T} \right\} \] (3)

In Eq. 3, the estimation is accurate when $\phi$ is an integer multiplication of $T^{-1}$, and shows the biggest noise when $\phi$ is a half integer multiplication of $T^{-1}$. Using the theoretical distribution, it is not hard to find that PEA is biased periodically, as shown in FIG. 2. The bias can prevent the estimation error from reaching an arbitrarily small level by repetitions.

In this paper, we propose an unbiased phase estimation algorithm (UPEA) based on the original PEA. We also show that a maximum likelihood estimation (MLE) post-processing step applied on UPEA has a smaller mean absolute error than MLE applied on PEA. In the end, we apply UPEA to quantum counting, and use an additional correction step to make the quantum counting algorithm unbiased.

The meanings of UPEA are evident. The inaccuracy of PEA decreases of order $T^{-1}$. But on real quantum computers, $T$ is limited by the qubit numbers, decoherence time, gate fidelity and so on. And the accuracy of simple repetitions of PEA is limited by the bias. In comparison, repetitions of UPEA can bring down the error to arbitrary level due to the unbiasedness.

The structure of this paper is as follows. In section 2, we propose the unbiased phase estimation algorithm (UPEA). In section 3, we show that by repeating the UPEA procedure for several times and applying maximum likelihood estimation to obtain the final estimation, the unbiasedness of UPEA is maintained. Then in section 4, we apply UPEA to quantum counting and point out that the unbiasedness does not hold, but can be maintained by adding a correction step. Finally, in section 5, we make conclusions.
2 Unbiased Phase Estimation

The key idea of UPEA is intuitive. In each individual run of PEA, we uniformly randomly choose \( \theta \in [0, 1) \), or \( \theta \sim U(0, 1) \). The circuit of UPEA is shown in FIG. 3. The quantum state right before the QFT gate is,

\[
\sum_{j=0}^{T-1} e^{2\pi i j (\phi + \theta)} |j\rangle \langle \psi |.
\]

(4)

Let \( s \) be the measurement result, then \( s/T \) is an estimation of the quantity \( \phi + \theta \) in UPEA, in comparison with \( \phi \) in PEA. Note that \( \theta \) is a known classical parameter, our estimation of \( \phi \) is given by,

\[
\hat{\phi} = \frac{s}{T} - \theta.
\]

(5)

Different from PEA, the output \( \hat{\phi} \) in UPEA is a continuous random variable. Here we calculate the probability density function \( \rho_{UPEA}(\hat{\phi}) \). A necessary condition for obtaining an estimation \( \hat{\phi} \) is,

\[
\theta \in \frac{1}{T} \mathbb{Z} - \phi,
\]

(6)
(a) The bias calculated by simulating PEA for $2^{16}$ times.  
(b) The MAE calculated by simulating PEA for $2^{16}$ times.

Fig. 4. The bias and MAE of PEA and UPEA by sampling the theoretical distribution for $2^{16}$ times, with parameter $T = 16$. The $x$-axis stands for $\phi$, and the $y$-axis stands for bias or MAE.

which appears exactly $T$ times in the interval $[0, 1)$. Thus,

$$\rho_{UPEA}(\tilde{\phi}; \phi) = \sum_{\theta \in \frac{1}{T} \mathbb{Z} - \phi} P_{PEA}(\tilde{\phi} + \theta | \phi + \theta) = \frac{\sin^2(T \pi (\tilde{\phi} - \phi))}{T \sin^2(\pi (\tilde{\phi} - \phi))}. \quad (7)$$

We use bias and mean absolute error (MAE) to quantify the performance of PEA and UPEA. Using the theoretical distribution in Eq. 3, the bias and MAE of PEA is given by,

$$B_{PEA}(\phi) = \sum_{\hat{\phi}} d(\hat{\phi}, \phi) P_{PEA}(\hat{\phi} | \phi), \quad (8)$$

$$M_{PEA}(\phi) = \sum_{\hat{\phi}} |d(\hat{\phi}, \phi)| P_{PEA}(\hat{\phi} | \phi), \quad (9)$$

where the signed circular distance $d(\hat{\phi}, \phi)$ is defined as the unique element in the set $(\hat{\phi} - \phi + \mathbb{Z}) \cap [-0.5, 0.5)$. The boundary choice of $\pm 0.5$ does not really matter, as $P_{PEA}(\phi \pm 0.5 | \phi)$ is always zero.

For UPEA, the bias and MAE is the expectation value of $d(\hat{\phi}, \phi)$ and $|d(\hat{\phi}, \phi)|$ over $\theta$ and $\tilde{\phi}$. If $\theta$ is fixed, the bias and MAE is given by $B_{PEA}(\phi + \theta)$ and $M_{PEA}(\phi + \theta)$, where $B_{PEA}$ and $M_{PEA}$ are periodically extended from $[0, 1]$ to $\mathbb{R}$. Thus,

$$B_{UPEA}(\phi) = \int_0^1 B_{PEA}(\phi + \theta) \, d\theta = \int_{-1/2}^{1/2} B_{PEA}(\theta) \, d\theta, \quad (10)$$

$$M_{UPEA}(\phi) = \int_0^1 M_{PEA}(\phi + \theta) \, d\theta = \int_{-1/2}^{1/2} M_{PEA}(\theta) \, d\theta. \quad (11)$$

Observing that $P(\tilde{\phi} | \phi) = P(-\tilde{\phi} | -\phi)$ and $d(\tilde{\phi}, \phi) = -d(-\tilde{\phi}, -\phi)$, $B_{PEA}(\theta)$ is an odd function about $\theta$, thus $B_{UPEA}(\phi) = 0$. This proves the unbiasedness of our UPEA algorithm. Also, $M_{UPEA}(\phi)$ is constant over $\phi$. By the way, from the deduction we see that since the function $B_{PEA}$ has period $1/T$, it is sufficient to choose $\theta \sim U(0, 1/T)$.

We also do numerical experiments for PEA and UPEA. Instead of using quantum simulators, our experiments sample the theoretical distribution function Eq. 3 and Eq. 7 directly.
3 Maximum Likelihood Phase Estimation

As is introduced, UPEA shows more of its power when we allow repeating it for several times. Suppose we have repeated PEA or UPEA for $R$ times, and get a set of estimation \( \{ \tilde{\phi}_1, \tilde{\phi}_2, \cdots, \tilde{\phi}_R \} \). The estimation $\tilde{\phi}$ is obtained by maximizing the likelihood function,

$$L(\tilde{\phi}; \{ \tilde{\phi}_j \}) = \prod_{j=1}^{R} \left( \frac{\sin(T(\pi(\tilde{\phi}_j - \tilde{\phi}))}{T \sin(\pi(\tilde{\phi}_j - \tilde{\phi}))} \right)^2.$$

(12)
Here we prove that the unbiasedness of UPEA still holds. The bias is,

\[ B_{UPEA}(\varphi; R) = \int_0^1 \rho_{UPEA}(\hat{\varphi}_1; \varphi) d\hat{\varphi}_1 \cdots \int_0^1 \rho_{UPEA}(\hat{\varphi}_R; \varphi) d\hat{\varphi}_R \cdot d \left( \arg\max_{\varphi'} L(\varphi'; \{\hat{\varphi}_j\}), \varphi \right) \]  

(13)

Observing that,

\[ \arg\max_{\varphi'} L(\varphi'; \{\hat{\varphi}_j - \varphi\}) = \arg\max_{\varphi'} L(\varphi'; \{\hat{\varphi}_j\}) - \varphi, \]  

(14)

we can deduce that,

\[ B_{UPEA}(\varphi; R) = \int_0^1 \rho_{UPEA}(\hat{\varphi}_1 - \varphi; 0) d\hat{\varphi}_1 \cdots \int_0^1 \rho_{UPEA}(\hat{\varphi}_R - \varphi; 0) d\hat{\varphi}_R \cdot d \left( \arg\max_{\varphi'} L(\varphi'; \{\hat{\varphi}_j\}), 0 \right) \]  

(15)

\[ = \int_{-\varphi}^{1-\varphi} \rho_{UPEA}(\hat{\varphi}_1; 0) d\hat{\varphi}_1 \cdots \int_{-\varphi}^{1-\varphi} \rho_{UPEA}(\hat{\varphi}_R; 0) d\hat{\varphi}_R \cdot d \left( \arg\max_{\varphi'} L(\varphi'; \{\hat{\varphi}_j\}), 0 \right) \]  

(16)

Finally, using the period-1 and oddity of \( \rho_{UPEA}(\hat{\varphi}_j) \) and \( \arg\max_{\varphi'} L(\varphi'; \{\hat{\varphi}_j\}) \), we conclude that \( B_{UPEA}(\varphi; R) = 0 \).

We do simulation experiments on PEA and UPEA with \( R = T = 16 \), and the results are shown in FIG. 5 (a) (b). We also fix \( T = 16 \) and study the bias and MAE behavior with respect to \( R \), as shown in FIG. 6. In summary,

- The maximum likelihood estimation algorithm maintains the unbiasedness of UPEA;
- For \( R \geq 3 \), there is a sudden decrement of error for both PEA and UPEA;
- For \( R \geq 3 \), UPEA has a smaller MAE than PEA.

We conclude that UPEA behaves even better than PEA when combined with the maximum likelihood estimation.

4 Application in Quantum Counting

The quantum counting algorithm (QCA) is an important application of PEA. Given a Boolean function \( f : \{0, 1, \cdots, N - 1\} \to \{0, 1\} \), where \( N = 2^n (n \in \mathbb{Z}_+) \), the quantum counting algorithm can estimate the quantity,

\[ M = \sum_{j=0}^{N-1} f(j). \]  

(17)

The key idea of quantum counting is that the uniform superposition state,

\[ |u\rangle = \frac{1}{\sqrt{N}} \sum_{j=0}^{N-1} |j\rangle, \]  

(18)
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Fig. 7. The bias and MAE of quantum counting, with parameter $T = 16$. The $x$-axis stands for $m$, and the $y$-axis stands for bias or MAE.

is on a plane spanned by two eigenvectors $|\psi_\pm\rangle$ of the Grover’s iteration $[1, 22] G_f$ for Boolean function $f$, with eigenvalues $e^{\pm 2\pi i \varphi}$, where

$$M = N \sin^2(\pi \varphi).$$  \hspace{1cm} (19)

To be specific,

$$|u\rangle = \frac{1}{\sqrt{2}} \left( e^{i\pi \varphi} |\psi_+\rangle + e^{-i\pi \varphi} |\psi_-\rangle \right).$$  \hspace{1cm} (20)

Applying PEA to $G_f$ and $|\psi\rangle$, the output $\tilde{\varphi} = s/T$ obeys the distribution $\frac{1}{2}[P(\tilde{\varphi} | \varphi) + P(\tilde{\varphi} | -\varphi)]$. Finally, the result of QCA is,

$$\tilde{M} = N \sin^2(\pi \tilde{\varphi}).$$  \hspace{1cm} (21)

If we replace the PEA step in quantum counting with UPEA, then $s/T$ is an estimation of $\varphi + \theta$ or $-\varphi + \theta$ with equal probability. Similarly, the estimation is given by

$$\tilde{M} = N \sin^2 \left[ \pi \left( \frac{s}{T} - \theta \right) \right].$$  \hspace{1cm} (22)

For convenience, we define $m = M/N$ and $\tilde{m} = \tilde{M}/N$. Though our estimation about $\varphi$ or $-\varphi$ is unbiased, the nonlinear mapping from $\varphi$ to $m$ will break the unbiasedness, as confirmed by our simulation experiments in FIG. 7. Here the bias and MAE is defined as,

$$B_{QCA}(m) = \sum_M (\tilde{m} - m) P_{QCA}(\tilde{m} | m),$$  \hspace{1cm} (23)

$$M_{QCA}(m) = \sum_M |\tilde{m} - m| P_{QCA}(\tilde{m} | m),$$  \hspace{1cm} (24)

where $P_{QCA}(\tilde{m} | m) = P_{PEA}(\tilde{\varphi} | \varphi)$. In FIG. 7, the quantity $B_{UQCA}(m)$ shows a linear relationship with $m$. 
Theoretically, the bias of UQCA is,

\[ B_{UQCA}(m) = \int_0^1 (\tilde{m} - m) \rho_{UQCA}(\tilde{m}|m) \, d\tilde{m} \]
\[ = \int_0^1 [\sin^2(\pi \tilde{\varphi}) - \sin^2(\pi \varphi)] \rho_{UPEA}(\tilde{\varphi}|\varphi) \, d\tilde{\varphi}, \]

(25)

where \( \rho_{UQCA}(\tilde{m}|m) \) is the probability density function of obtaining an estimation \( \tilde{m} \) using UQCA when the ground truth is \( m \), and \( \rho_{UPEA}(\tilde{\varphi}|\varphi) \) is the probability density function of obtaining an estimation \( \tilde{\varphi} \) using UPEA when the ground truth is \( \varphi \). Then,

\[ B_{UQCA}(m) = \int_0^1 [\sin^2(\pi \tilde{\varphi}) - \sin^2(\pi \varphi)] \frac{\sin^2(T \pi (\tilde{\varphi} - \varphi))}{T \sin^2(\pi (\tilde{\varphi} - \varphi))} \, d\tilde{\varphi} \]
\[ = \frac{1}{T} \int_{-1/2}^{1/2} \left[ \sin^2(\pi (\varphi + \phi)) - \sin^2(\pi \varphi) \right] \frac{\sin^2(T \pi \phi)}{T \sin^2(\pi \phi)} \, d\phi \]
\[ = \frac{1}{T} \cos(2\pi \varphi) \int_0^1 \sin^2(T \pi \phi) \, d\phi \]
\[ = \frac{1}{2T} \cos(2\pi \varphi) \]
\[ = 1 - 2m \frac{1}{2T}. \]

(26)

Therefore, QCA cannot be made unbiased by simply replacing PEA with UPEA. Indeed, we can add an extra correction step,

\[ m' = \left( 1 - \frac{1}{T} \right)^{-1} \left( \tilde{m} - \frac{1}{2T} \right), \]

(27)

and output \( m' \) instead of \( \tilde{m} \) to make it unbiased. But such correction step can bring a little cost in MAE, as shown in FIG. 7, since the error is amplified \( (1 - 1/2T)^{-1} \) times along with \( m' \).

Similarly, if we repeat UPEA for \( R \) times and obtain \{\( \tilde{\varphi}_1, \tilde{\varphi}_2, \ldots, \tilde{\varphi}_R \}\}, we can use maximum likelihood estimation to make the result more robust. The bias is,

\[ B_{UQCA}(m; R) \]
\[ = \int_0^1 \rho_{UPEA}(\tilde{\varphi}_1; \varphi) \, d\tilde{\varphi}_1 \cdots \int_0^1 \rho_{UPEA}(\tilde{\varphi}_R; \varphi) \, d\tilde{\varphi}_R \cdot \left[ \sin^2 \left( \pi \argmax_{\varphi'} L(\varphi'; \{\tilde{\varphi}_j\}) \right) - \sin^2(\pi \varphi) \right] \]
\[ = \int_0^1 \rho_{UPEA}(\tilde{\varphi}_1; 0) \, d\tilde{\varphi}_1 \cdots \int_0^1 \rho_{UPEA}(\tilde{\varphi}_R; 0) \, d\tilde{\varphi}_R \cdot \left[ \sin^2 \left( \pi \varphi + \pi \argmax_{\varphi'} L(\varphi'; \{\tilde{\varphi}_j\}) \right) - \sin^2(\pi \varphi) \right] \]
\[ = \int_{-1/2}^{1/2} \rho_{UPEA}(\tilde{\varphi}_1; 0) \, d\tilde{\varphi}_1 \cdots \int_{-1/2}^{1/2} \rho_{UPEA}(\tilde{\varphi}_R; 0) \, d\tilde{\varphi}_R \cdot \left[ \sin^2 \left( \pi \argmax_{\varphi'} L(\varphi'; \{\tilde{\varphi}_j\}) \right) \cos(2\pi \varphi) + \frac{1}{2} \sin \left( 2\pi \argmax_{\varphi'} L(\varphi'; \{\tilde{\varphi}_j\}) \right) \sin(2\pi \varphi) \right] \]
\[ = B_{UQCA}(0; R) \cos(2\pi \varphi) \]
\[ = B_{UQCA}(0; R)(1 - 2m), \]

(28)
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Fig. 8. The bias and MAE of quantum counting, with parameter $T = 16$ and $R = 3$.

where the second term in Eq. (28) vanishes because of its oddity.

Thus, the bias of UQCA with $R$ repetitions is also linear about $m$. The only thing left for the correction formula is $B_{UQCA}(0; R)$, which can be pre-calculated by simulation. To be specific, for $N_{\text{test}}$ times, draw $R$ random numbers with probability density function,

$$\rho(x) = \frac{\sin^2(T\pi x)}{T\sin^2(\pi x)},$$

(29)

says $\{\{x_{j,k}\}_{k=1}^{R}\}_{j=1}^{N_{\text{test}}}$, then the estimated of $B_{UQCA}(0; R)$ is,

$$b = \frac{N_{\text{test}}}{2} \arg\max_{x} L(x; \{x_{j,k}\}_{k=1}^{R}).$$

(30)

Before performing correction for UQCA with parameters $T$ and $R$, one should first run simulations to calculate the corresponding $b$, then the correction formula is,

$$m' = \frac{\tilde{m} - b}{1 - 2b},$$

(31)

where $\tilde{m}$ is the result of maximum likelihood estimation, and $m'$ is the correction output. For example, by simulating UQCA with $m = 0, T = 16, R = 3$ for $2^{16}$ times we get $b \approx 0.004775$. Then we do experiments to compare UQCA with or without correction, as shown in FIG. 8.

We also do experiments for UQCA with or without correction for $T = 16$ and different $R$. The results in FIG. 9 shows that the extra error brought by the correction decays significantly as $R$ grows.

5 Conclusion

The original form of phase estimation algorithm suffers a periodical bias, which prevents its accuracy from reaching an arbitrary level. We propose an unbiased phase estimation algorithm, by introducing a uniformly distributed variable $\theta$ to the original phase estimation algorithm. We also show that a maximum likelihood estimation post-processing step can
Fig. 9. The MAE of UQCA with or without correction for $T = 16$ and different $R$.

make UPEA more robust when $R \geq 3$, as it keeps the unbiasedness and reduce the MAE quickly.

Finally, we apply UPEA to quantum counting. We point out that a direct substitution of UPEA for PEA cannot make quantum counting unbiased, and there is a linear relationship between the bias and $m$, the ground truth of quantum counting. By applying a correction step, the bias can vanish, with an extra cost of MAE in the meantime. Moreover, by repeating for $R$ times and using maximum likelihood estimation, we prove that the linear relationship still holds, and the extra cost decays quickly while the unbiasedness is maintained.

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