Quantum state preparation without coherent arithmetic

arXiv:2210.14892

Sam McArdle (AWS), András Gilyén (Rényi Budapest), Mario Berta
Quantum state preparation problem

• Given the function $f : [a, b] \rightarrow \mathbb{R}$, prepare the $n$-qubit quantum state

$$|\Psi_f\rangle := \frac{1}{\mathcal{N}_f} \cdot \sum_{x=0}^{2^n-1} f(\bar{x}) |x\rangle$$

with uniform grid $\bar{x} := a + \frac{x(b-a)}{2^n}$, normalization $\mathcal{N}_f := \sqrt{\sum_{\bar{x}} |f(\bar{x})|^2}$

• Important sub-routine in a variety of quantum algorithms, for different functions of interest

• Minimize number of non-Clifford gates and ancilla qubits
Standard approach(es)

- Amplitude oracle $U_f : |x⟩|j⟩ \mapsto |x⟩|f(\bar{x}) \oplus j⟩$ that prepares $g$-bit approximation of the values $f(\bar{x})$

- Implemented via reversible computation, using piecewise polynomial approximation of the function $f(x)$

- Alternatively, reading values stored in a quantum memory

- Downsides:
  - Handcrafted for every function + discretization of values of function
  - Large ancilla cost – not suited for early fault-tolerant regime

- Other approaches with similar bottlenecks: Grover-Rudolph, adiabatic, repeat until success, matrix product states, etc.
Quantum eigenvalue transformation (QET)

• A framework to coherently apply functions to the eigenvalues of a Hermitian matrix

• An \((\alpha, m, \varepsilon)\)-block encoding of an \(n\)-qubit Hermitian \(A\) is an \((n + m)\)-qubit unitary \(U\) with

\[
||\alpha \langle 0|^{\otimes m} \otimes 1_n \rangle U \langle 0|^{\otimes m} \otimes 1_n \rangle - A|| \leq \varepsilon
\]

• Base functions are even degree \(d\) polynomials

\(\rightarrow\) QET circuit output is block encoding \(U_{A^d}\) of the matrix \(A^d\) (normalized)

• Implementation cost:
  • \(\frac{d}{2}\) applications of \(U\) and \(U^*\)
  • \(2d\) many \(m\)-controlled Toffoli gates (CNOT for \(m = 1\))
  • \(d\) single-qubit \(Z\)-rotations \(R_Z(\theta_k) := \exp(-i\theta_k Z)\) on additional ancilla qubit
QET continued

• Example circuit for even degree $d$ polynomial and $m = 1$:

• Efficient classical pre-computation of angle set $\{\theta_1, \theta_2, \ldots, \theta_d\}$

• Odd polynomials, general functions via polynomial approximation, complexity given by degree of polynomial – technical conditions omitted

(Extension: Quantum singular value transformation (QSVT) for general matrices $A$)
Main idea: State preparation via QET

• Create low-cost block encoding of \( A := \sum_{x=0}^{2^n-1} \sin \left( \frac{x}{2^n} \right) |x\rangle \langle x| \) via
  
  (exact (1,1,0) block encoding)

• Idea: Applying QET, convert this into block encoding of \( \sum_{x=0}^{2^n-1} f(\bar{x}) |x\rangle \langle x| \) using polynomial approximation of \( f \left( (b - a)\arcsin(\cdot) + a \right) \)

• Run relevant circuits on input \(|x_1 \cdots x_n\rangle \otimes |000\rangle_a = |+\rangle \otimes^n |000\rangle_a\) and use amplitude amplification to maximize probability of outputting \(|\Psi_f\rangle \otimes |000\rangle_a\)
Quantum circuits

1. $U_{\sin}$ block encoding circuit

2. $U_{\tilde{f}}$ block encoding circuit

3. Amplitude amplification (exact) circuit
Main result complexities

• Discretized $L_2$-norm filling-fraction ($N := 2^n$) as

\[ \mathcal{F}_f^{[N]} := \sqrt{\frac{(b-a)}{N} \sum_{x=0}^{N-1} |f(x)|^2 \over \sqrt{(b-a)|f|_{\text{max}}^2}} \approx \frac{\int_a^b |f(\bar{x})|^2 d\bar{x}}{\sqrt{(b-a)|f|_{\text{max}}^2}} =: \mathcal{F}_f^{[\infty]} \]

• **Theorem I**: Given a degree $d_\delta$ polynomial approximation $\tilde{f}$ of $f$, (*) we can prepare a quantum state $|\Psi_{\tilde{f}}\rangle$ that is $\varepsilon$-close in trace distance to $|\Psi_f\rangle$ using $O\left(\frac{nd_\delta}{\mathcal{F}_f^{[N]}(\tilde{f})}\right)$ gates + 4 ancilla qubits, for $\delta = \varepsilon \min\{\mathcal{F}_f^{[N]}, \mathcal{F}_{\tilde{f}}^{[N]}\}$.


\((*)\) when $\tilde{f}(\cdot)$ applied to $\sin\left(\frac{x}{N}\right)$ approximates $\frac{f(\bar{x})}{|f|_{\text{max}}}$ to $L_\infty$-error on $[a, b]$
Main result complexities simplified

• **Theorem II**: For sufficiently smooth functions $f$, (*) we can prepare a quantum state $|\Psi_{\tilde{f}}\rangle$ that is $\varepsilon$-close in trace distance to $|\Psi_f\rangle$ using

$$\tilde{O}\left(\frac{n\log(\varepsilon^{-1})}{\mathcal{F}_f^{[N]}}\right)$$

 gates + 4 ancilla qubits.

(*) need $L_\infty$-approximation $\delta \propto \exp(-d_\delta)$ for degree $d_\delta$ polynomial

• Analytical minimax polynomial

• In practice use (works very well):
  • Remez approximation or just Local Taylor series
  • $L_2$-approximation on grid
# Complexity comparison literature

|                               | # Non-Clifford gates | # Ancilla qubits | Rigorous error bounds | Function                                      |
|-------------------------------|----------------------|------------------|------------------------|-----------------------------------------------|
| QET (this work)               | $\mathcal{O}\left(\frac{nd_\epsilon}{\mathcal{F}_f^{[N]}}\right)$ | 4                | ✓                      | Polynomial/Fourier approximation              |
| Black-box amplitude oracle    | $\mathcal{O}\left(\frac{g_\epsilon^2 \tilde{d}_\epsilon}{\mathcal{F}_f^{[N]}}\right)$ | $\mathcal{O}(g_\epsilon \tilde{d}_\epsilon)$ | ✓                      | General                                       |
| Grover-Rudolph amplitude oracle | $\mathcal{O}(ng_\epsilon^2 \tilde{d}_\epsilon)$ | $\mathcal{O}(g_\epsilon \tilde{d}_\epsilon)$ | ✓                      | Efficiently integrable probability distribution |
| Adiabatic amplitude oracle    | $\mathcal{O}\left(\frac{g_\epsilon^2 \tilde{d}_\epsilon}{(\mathcal{F}_f^{[N]})^4 \epsilon^2}\right)$ | $\mathcal{O}(g_\epsilon \tilde{d}_\epsilon)$ | ✓                      | General                                       |
| Matrix product state          | $\mathcal{O}(n)$   | 0                | ✓                      | Matrix product state $d = 2$ approximation     |

Note: $g_\epsilon$-bit amplitude oracles with degree $\tilde{d}_\epsilon$ piecewise polynomial approximation ($\tilde{d}_\epsilon \neq d_\epsilon$ in general)
Analytical performance: Gaussians

• Example function $f_{\beta}(x) := \exp\left(-\frac{\beta}{2}x^2\right)$

• **Theorem III**: For $\varepsilon \in \left(0, \frac{1}{2}\right)$ and $0 \leq \beta \leq 2^n$ we can prepare the $[-1,1]$ uniform grid Gaussian state on $n$ qubits up to $\varepsilon$-precision with gate complexity

$$O \left( n \cdot \log^5 \left( \frac{1}{\varepsilon} \right) \right) + 3 \text{ ancilla qubits}$$

• Note: All other approaches use hundreds of ancilla qubits

• Kaiser window state variant $|W_{\beta}^N (\bar{x})\rangle \propto \sum_{x=-N}^{N} \frac{1}{2N} I_0 \left( \frac{\beta \sqrt{1-x^2}}{I_0(\beta)} \right)$ on $[-1,1]$
Numerical benchmarking: \( \tanh(x) \)

- Example function \( \tanh(x) \) in the range \( x \in [0,1] \) on \( n = 32 \) gives

| Method                                      | # Ancilla qubits | # Toffoli gates |
|---------------------------------------------|------------------|-----------------|
| QET (this work)                             | 3                | \( 9.7 \times 10^4 \) |
| Black-box state amplitude oracle            | 216              | \( 6.9 \times 10^4 \) |
| Grover-Rudolph amplitude oracle             | \( > 959 \)      | \( > 2.0 \times 10^5 \) |

- Cost are lower bounds minimizing gate count, based on state-of-the-art amplitude oracles (which could potentially be improved)
- Other methods give even higher costs
Run Algorithm: Setup

• Treat special case: \( a = -1, b = 1 \), with function \( f(x) = f(-x) \)
• Goal: Prepare the \( n \)-qubit quantum state

\[
|\Psi_f\rangle = \frac{1}{\mathcal{N}_f} \cdot \sum_{x=-N/2}^{N/2-1} f(x) |x\rangle \quad \text{with} \quad \bar{x} = \frac{2x}{N}, \quad \text{and} \quad \mathcal{N}_f = \sqrt{\sum_{\bar{x}} f(\bar{x})}
\]

1. Start with block encoding of \( A = \sum_{x=-N/2}^{N/2-1} \sin\left(\frac{2x}{N}\right) |x\rangle \langle x| \)
2. QET to convert into block encoding of \( \sum_{x=-N/2}^{N/2-1} f(\bar{x}) |x\rangle \langle x| \)
3. \( O\left(\frac{1}{\mathcal{F}_f^{[N]}}\right) \) rounds of exact amplitude amplification (extra ancilla)
• Need to start with (extensive) classical pre-processing
Run algorithm: Quantum circuits

1. $U_{\sin}$ block encoding circuit

2. $U_{\tilde{f}}$ block encoding circuit

3. Amplitude amplification (exact) circuit
Run algorithm: Classical pre-computation

• Compute polynomial $h(y)$ such that

$$|h(y)|_{\max}^{y \in [-1,1]} \leq 1 \text{ and } \left| h(\sin(y)) - \frac{f(y)}{|f(y)|_{\max}^{y \in [-1,1]}} \right|_{\max}^{y \in [-1,1]} \leq \delta$$

leading to approximation $\tilde{f}(x) := h(\sin(\bar{x}))$

(Remez algorithm / local Taylor series / $L_2$-approximation on grid / ...)

• Compute discretized $L_2$-norm filling-fraction $\mathcal{F}_{\tilde{f}}^{[N]} \approx \mathcal{F}_{\tilde{f}}^{[\infty]}$ of $\tilde{f}(x)$

(choose depending on how large $N = 2^n$ is)

• Compute QET angle set $\{\theta_1, \theta_2, \ldots, \theta_d\}$ of polynomial $\tilde{f}(x)$

(different analytically and/or numerically good methods available)
Extensions
Extensions: Non-smooth functions

• First approach: Use coherent inequality test with flag qubit for piecewise QET polynomial implementation

\[ \text{for } k \text{ discontinuities this requires } (k + n) \text{ ancilla qubits and } 2kn \text{ Toffoli gates for the inequality comparison} \]

• Second approach: Example triangle function for \( \tilde{x} \in [0,1] \)

\[
\begin{align*}
    f(\tilde{x}) &= \begin{cases} 
        \tilde{x} & 0 \leq \tilde{x} \leq 1/3 \\
        \frac{1}{2}(1 - \tilde{x}) & 1/3 < \tilde{x} \leq 1
    \end{cases} \\
    \text{instead use} \quad \tilde{f}(\tilde{x}) &= \begin{cases} 
        \tilde{x} & 0 \leq \tilde{x} \leq \frac{1}{3} \\
        \text{Unspecified} & \frac{1}{3} < \tilde{x} < 2 \\
        \frac{1}{2}\left(\frac{7}{3} - \tilde{x}\right) & 2 \leq \tilde{x} \leq \frac{7}{3}
    \end{cases}
\end{align*}
\]

\[ \text{use coherent inequality test to flip for } \tilde{x} > \frac{1}{3} \text{ and in the end reverse this inequality check} \]
Extensions: Fourier based QET

- Block-encoding of $A$ is replaced by controlled time evolution
  \[ V(A) := |0\rangle\langle 0| \otimes 1 + |1\rangle\langle 1| \otimes \exp(iAt) \]
- Fourier-based QET uses calls to $V(A)$, together with single-qubit-rotations, to apply a function $f(\cdot)$ in Fourier series form to $A$
- We can implement $V(A)$ for diagonal $A = \sum_x \bar{x}\ket{x}\bra{x}$ using $n$ controlled $Z$-rotations
- Example with compact Fourier series: Cycloid function
  \[ n = 32 \text{ for } \bar{x} \in [0,2\pi], \text{ gives } 7.35 \times 10^5 \text{ Toffoli gates} \]
  + 3 ancillas qubits

From Wikipedia
Outlook

• Introduced versatile method for preparing a quantum state whose amplitudes are given by some known function
• Based on the QET, orders of magnitude savings in ancilla qubits
• Needed: More detailed practical resource estimates, more functions, combination with other methods, etc.
• Open questions:
  • Example square root function $\sqrt{\bar{x}}$ for $\bar{x} \in [0,1]$, non-differentiable at $\bar{x} = 0$
    $\rightarrow$ use $\sqrt{\bar{x} + a}$ instead?
  • Multivariate functions via multivariate QET?

Thank you
Some references (highly incomplete)

Black box prep: Grover (2000), Bhaskar et al. (2016), Haener et al. (2018), Sanders et al. (2019), Wang et al. (2021/22), Bausch (2022), Krishnakumar (2022), ...

Grover/Rudolph prep: Grover & Rudolph (2002)

Adiabatic prep: Rattew & Koczor (2022)

Matrix product prep: Holmes & Matsuura (2020), Garcia-Ripoll (2021)

QET: Low & Chuang (2017/19), Gilyen et al. (2019)

QET angles: Gilyen et al. (2019), Haah (2019), Dong et al. (2021)

Fourier based QET: Dong et al. (2022), Perez-Salinas et al. (2021), Silva et al. (2022)

Multivariate QET: Rossi & Chuang (2022)