

Quantum Spectral Method for Gradient and Hessian Estimation

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joint work with Yuxin Zhang [arXiv:2407.03833](https://arxiv.org/abs/2407.03833)

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Two motivating quotes

Figure 1: Gian-Carlo Rota: Every mathematician has only a few tricks.



Figure 2: George Pólya: An idea which can be used once is a trick. If it can be used more than once it becomes a method.



Quantum computing

- ▶ **Quantum Fourier Transform (QFT)** plays an important in the design of quantum algorithms, for example,
Deutsch-Jozsa algorithm, Bernstein-Vazirani algorithm, Simon's algorithm, Shor's algorithm, Quantum phase estimation algorithm, the HHL algorithm for linear systems, ...



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- ▶ In this talk, we are considering the application of QFT at the estimation of **gradient vector** and **Hessian matrix** of multivariate functions.



Why estimate gradient and Hessian?

- ▶ Useful in many optimisation algorithms, such as gradient descent and Newton's algorithm. So corresponding results can be used to speed up optimisation problems. For example,
 - ▶ quantum speedup of convex optimisation
[van Apeldoorn, Gilyén, Gribling, de Wolf (QIP 2019)]
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 - ▶ quantum speedup of linear programming
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- ▶ Subroutine of many other quantum algorithms. For example,
 - ▶ quantum advantage of shallow circuits
[Bravyi, Gosset, Koenig (Science 2018)]
 - ▶ quantum tomography
[van Apeldoorn, Cornelissen, Gilyén, Nannicini (SODA 2023)]
 - ▶ quantum algorithm for estimating multiple expectation values
[Huggins, Wan, McClean, O'Brien, Wiebe, Babbush (PRL 129, 240501)]



Problem statement: quantum gradient estimation

Problem (Gradient estimation)

Let $\varepsilon \in (0, 1)$ be the accuracy. Given a differentiable function $f : \mathbb{R}^d \rightarrow \mathbb{R}$, and oracle to query f , compute an approximate gradient $\mathbf{g} \in \mathbb{R}^d$ such that $\|\mathbf{g} - \nabla f(\mathbf{0})\|_\infty \leq \varepsilon$.



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- **Query complexity:** the minimal number of calls to O_f to find \mathbf{g} .



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A **quantum query algorithm** of complexity T has the form: $U_T O_f \cdots U_1 O_f U_0$. Usually, U_0, U_1, \dots, U_T are simple gates, so the **gate complexity** \approx **query complexity**.



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In addition, for query complexity, we can **prove nontrivial lower bounds**. So it can be used to separate quantum and classical computing.



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We will obtain $|g_1, \dots, g_d\rangle$ by applying the inverse QFT to the above state.



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The query complexity of this algorithm is $O(1)$ when $f(x)$ is close to a linear function $g \cdot x$, which is **exponentially** faster than classical algorithms.



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The query complexity of this algorithm is $\tilde{O}(1)$ when $f(\mathbf{x})$ is close to a linear function $\mathbf{g} \cdot \mathbf{x}$, which is **exponentially** faster than classical algorithms.

Theorem (Jordan)

Let $\mathbf{g} \in \mathbb{R}^d$ and $a, \varepsilon \in \mathbb{R}_+$. Suppose we have \tilde{f} such that

$$|\tilde{f}(\mathbf{x}) - \mathbf{g} \cdot \mathbf{x}| \leq \frac{\varepsilon a}{8 \cdot 42\pi}, \quad (1)$$

and oracle $O : |\mathbf{x}\rangle \rightarrow e^{2\pi i 2^{n_\varepsilon} \tilde{f}(\mathbf{x})} |\mathbf{x}\rangle$, where $2^{n_\varepsilon} = 4/a\varepsilon$. Then $\tilde{O}(1)$ queries to O can give us $\tilde{\mathbf{g}} \in \mathbb{R}^d$ such that

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Consequently, for any function f , as long as we can **construct** \tilde{f} such that the condition (1) holds for $\mathbf{g} = \nabla f(\mathbf{0})$, then we can approximate $\nabla f(\mathbf{0})$.



Previous results: Gilyén-Arunachalam-Wiebe's algorithm (SODA 2019)

In 2019, Gilyén, Arunachalam, and Wiebe developed Jordan's algorithm and improved the efficiency using **higher-order finite difference methods**:

$$\nabla f(\mathbf{0}) \cdot \mathbf{x} \approx \sum_{\ell=1}^m \frac{(-1)^{\ell-1}}{\ell} \frac{\binom{m}{\ell}}{\binom{m+\ell}{\ell}} \left(f(\ell \mathbf{x}) - f(-\ell \mathbf{x}) \right).$$



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If $|\partial^\alpha f| \leq c^k k^{k/2}$ for all $k \in \mathbb{N}$ and $\alpha \in \mathbb{N}_0^d$ with $|\alpha| = k$, then error is bounded by

$$\sum_{k=2m+1}^{\infty} \left(8acm\sqrt{d} \right)^k$$

for most $\mathbf{x} \in aG_n^d$. Here G_n is the grid point that discretises $(-1/2, 1/2)$.



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Main results

We propose a new quantum algorithm for gradient estimation for another class of functions, achieving **exponential speedups** over classical algorithms.



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Theorem (Our result, informal)

Let $f : \mathbb{R}^d \rightarrow \mathbb{R}$ be analytic and well defined at a neighborhood of $\mathbf{0}$ in the complex field. Then there exists a quantum algorithm that computes an approximate $\mathbf{g} \in \mathbb{R}^d$ such that $\|\mathbf{g} - \nabla f(\mathbf{0})\|_\infty \leq \varepsilon$, using $\tilde{O}(1/\varepsilon)$ queries to phase oracles.



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Oracle settings:

Phase oracles O_{f_1}, O_{f_2} for real and imaginary parts of $f(\mathbf{x}) = f_1(\mathbf{x}) + if_2(\mathbf{x})$:

$$O_{f_1} : |\mathbf{x}\rangle \rightarrow e^{if_1(\mathbf{x})}|\mathbf{x}\rangle, \quad O_{f_2} : |\mathbf{x}\rangle \rightarrow e^{if_2(\mathbf{x})}|\mathbf{x}\rangle.$$



Key ideas

Different from previous algorithms, our algorithm employs the **spectral method** to approximate gradient $\nabla f(\mathbf{0})$.

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Consider a univariate function $f(x)$ that is sufficiently smooth such that it can be represented by the Taylor series in $\bar{B}(x_0, r) \subset \mathbb{C}$, i.e.

$$f(x) = \sum_{n=0}^{\infty} a_n (x - x_0)^n, \quad a_n = \frac{f^{(n)}(x_0)}{n!}, \quad |a_n| \leq \max_{x \in \bar{B}(x_0, r)} |f(x)| r^{-n}.$$



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Then for $\delta \in (0, r)$, $N \in \mathbb{N}$, and $\omega = e^{-2\pi i/N}$, we have

$$f(x_0 + \delta \omega^k) = \sum_{n=0}^{\infty} a_n (\delta \omega^k)^n = \sum_{n=0}^{N-1} \omega^{kn} c_n,$$

where $c_n = \sum_{m=0}^{\infty} a_{n+mN} \delta^{n+mN}$.



Key ideas

To understand how to obtain derivative information from c_n , let us consider c_1 and c_2 as examples.

$$c_1 = a_1\delta + a_{1+N}\delta^{1+N} + a_{1+2N}\delta^{1+2N} + \dots$$

and there is a constant $\kappa > 0$ such that $|a_n| \leq \kappa r^{-n}$ for all $n \in \mathbb{N}$, which implies that series $\{a_n\}$ decreases faster than r^{-n} .



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The same holds for c_2 as

$$c_2 = a_2\delta^2 + a_{2+N}\delta^{2+N} + a_{2+2N}\delta^{2+2N} + \dots$$

Similarly, c_2/δ^2 is close to $a_2 = f''(x_0)/2$.



Key ideas

Now we have $f_k := f(x_0 + \delta\omega^k) = \sum_{n=0}^{N-1} \omega^{kn} c_n$. The inverse discrete Fourier transform gives us

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The error is bounded by

$$\left| a_n - \frac{c_n}{\delta^n} \right| \leq \kappa r^{-n} \sum_{m=1}^{\infty} (\delta/r)^{mN} = \kappa r^{-n} \frac{(\delta/r)^N}{1 - (\delta/r)^N}$$

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for some constant κ . Particularly, when $n = 1$,

$$\left| f'(0) - \frac{c_1}{\delta} \right| \leq \kappa r^{-1} \frac{(\delta/r)^N}{1 - (\delta/r)^N}.$$



Key ideas

For multivariable function $f(\mathbf{x})$, we consider $h(\tau) = f(\tau\mathbf{x})$. Then $h'(0) = \nabla f(0) \cdot \mathbf{x}$. Using the above analysis, we derive a real-valued function $F(\mathbf{x})$

$$F(\mathbf{x}) = \frac{1}{N\delta} \sum_{k=0}^{N-1} \omega^{-k} f(\delta\omega^k \mathbf{x})$$

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When $N = O(\log(\kappa/\varepsilon))$, we can get an **additive error ε** , which is **significantly smaller** than the one obtained by finite difference formulas. This is a crucial point in our work.



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Combining this with previous results, we obtain a quantum algorithm that estimates gradient $\nabla f(\mathbf{0})$ with query complexity $\tilde{O}(1/\varepsilon)$.



Differences

Difference 1. The functions used to approximate $\nabla f(\mathbf{0}) \cdot \mathbf{x}$.

- ▶ GAW deal with analytic real-valued functions $f : \mathbb{R}^d \rightarrow \mathbb{R}$ with specific smoothness conditions. They use the degree- $2m$ **central difference approximation**.
- ▶ We deal with analytic complex-valued functions $f : \mathbb{C}^d \rightarrow \mathbb{C}$ such that $f(\mathbb{R}^d) \subset \mathbb{R}$. We derive the approximating formula using the **spectral method**.



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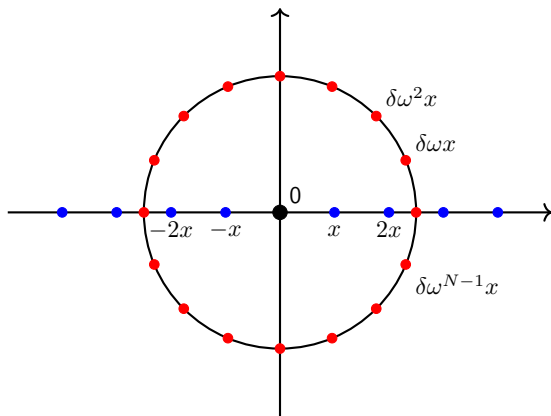
Remark

The spectral method also outperforms finite difference method for solving ODEs on a quantum computer. [Childs, Liu, CMP 2019], [Berry J. Phys. A 2010]



Differences

Our method offers better error performance in approximating derivatives. In our opinion, one of the key reasons is the way **sampling points** are selected. As illustrated for 1-dimensional functions.



Spectral method (our):

$$\frac{1}{N\delta} \sum_{k=0}^{N-1} \omega^{-k} f(\delta\omega^k x) \approx f'(0)x$$

Finite difference method [GAW]:

$$\sum_{\substack{\ell=-m \\ \ell \neq 0}}^m \frac{(-1)^{\ell-1}}{\ell} \frac{\binom{m}{|\ell|}}{\binom{m+|\ell|}{|\ell|}} f(\ell x) \approx f'(0)x$$



Differences

Difference 2. The oracle settings.

- ▶ GAW assumes access to **phase oracle** $O_f: |\mathbf{x}\rangle \rightarrow e^{if(\mathbf{x})}|\mathbf{x}\rangle$ for $f: \mathbb{R}^d \rightarrow \mathbb{R}$.
- ▶ We assume **phase oracles for the real and imaginary parts** of $f(\mathbf{x}) = f_1(\mathbf{x}) + if_2(\mathbf{x})$, denoted as O_{f_1}, O_{f_2} , respectively.

While our oracle assumptions differ from GAW, they are still standard and natural, resembling how data is stored in classical computing.



Quantum Hessian estimation

As a generalization, we present four quantum algorithms for estimating the Hessian: using either finite difference method or spectral for estimating dense or sparse Hessians.



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Theorem (Hessian estimation based on spectral method)

Let $f : \mathbb{C}^d \rightarrow \mathbb{C}$ be analytic and maps \mathbb{R}^d to \mathbb{R} . Then there is a quantum algorithm that computes $\tilde{\mathbf{H}}$ such that $\|\tilde{\mathbf{H}} - \mathbf{H}_f(\mathbf{0})\|_{\max} \leq \varepsilon$, using $\tilde{O}(d/\varepsilon)$ queries to O_{f_1}, O_{f_2} , where $\mathbf{H}_f(\mathbf{0})$ is the Hessian of f at $\mathbf{0}$.



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- ▶ We obtain a lower bound of $\tilde{\Omega}(d)$.
- ▶ If $\mathbf{H}_f(\mathbf{0})$ is promised to be s -sparse, then the complexity can be reduced to $\tilde{O}(s/\varepsilon)$.



Quantum Hessian estimation

To illustrate how to derive a quantum algorithm for Hessian estimation from a gradient estimation algorithm, we will provide a brief explanation using the simple case of $f(\mathbf{x}) = \langle \mathbf{x} | H | \mathbf{x} \rangle$.

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For fixed $\mathbf{y} \in \mathbb{R}^d$, we can get the following linear function h using 2 queries to f

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When H is sparse, then randomly generate $k = O(s \log d)$ vectors $\mathbf{y}_1, \dots, \mathbf{y}_k$ are enough to recover H from $\mathbf{y}_1, \dots, \mathbf{y}_k$ and $H\mathbf{y}_1, \dots, H\mathbf{y}_k$.



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Thanks very much for your time!