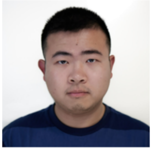
Quantum Signal Processing

Lin Lin

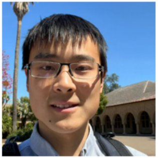
Department of Mathematics, UC Berkeley
Lawrence Berkeley National Laboratory
Challenge Institute for Quantum Computation

Modern Applied and Computational Analysis
ICERM, June 2023

Joint work with



Yulong Dong
(Berkeley)



Hongkang Ni
(Stanford)

Jiasu Wang
(Berkeley)

Also earlier work with Xiang Meng (MIT), Birgitta Whaley (Berkeley, Chem)

Outline

Introduction

Symmetric QSP and iterative algorithm

Infinite QSP

Outline

Introduction

Symmetric QSP and iterative algorithm

Infinite QSP

Solve nature with nature

Figure. A superposition of Feynmans

... if you want to make a simulation of nature (quantum many-body problem), you'd better make it quantum mechanical, and by golly it's a wonderful problem, because it doesn't look so easy.

– Richard P. Feynman (1981) 1st Conference on Physics and Computation, MIT

Representing polynomials using unitary matrices

Motivation:

- Quantum computers are fundamentally about manipulating unitary matrices.
- Polynomial function $f(A)$, e.g., A^{-1}, e^{-A} is generally non-unitary.
- Efficient quantum algorithms for $f(A)$:
  Quantum signal processing (QSP)[1], quantum singular value transformation (QSVT)[2], quantum eigenvalue transformation of unitary matrices (QETU)[3].

[1] (Low, Chuang, PRL 2017)

[2] (Gilyén, Su, Low, Wiebe, STOC, 2019) (Martyn et al, PRX Quantum 2021)

[3] (Dong-**Lin**-Tong, PRX Quantum 2022)

Grand Unification of Quantum Algorithms

John M. Martyn,[1,2,*] Zane M. Rossi,[2] Andrew K. Tan,[3] and Isaac L. Chuang[3,4]

[1] *Center for Theoretical Physics, Massachusetts Institute of Technology, Cambridge, Massachusetts 02139, USA*
[2] *Department of Physics, Massachusetts Institute of Technology, Cambridge, Massachusetts 02139, USA*
[3] *Department of Physics, Co-Design Center for Quantum Advantage, Massachusetts Institute of Technology, Cambridge, Massachusetts 02139, USA*
[4] *Center for Ultracold Atoms, and Research Laboratory of Electronics, Massachusetts Institute of Technology, Cambridge, Massachusetts 02139, USA*

(Received 7 May 2021; revised 20 August 2021; published 3 December 2021)

Quantum algorithms offer significant speed-ups over their classical counterparts for a variety of problems. The strongest arguments for this advantage are borne by algorithms for quantum search, quantum phase estimation, and Hamiltonian simulation, which appear as subroutines for large families of composite quantum algorithms. A number of these quantum algorithms have recently been tied together by a novel technique known as the quantum singular value transformation (QSVT), which enables one to perform a polynomial transformation of the singular values of a linear operator embedded in a unitary matrix. In the seminal GSLW'19 paper on the QSVT [Gilyén *et al.*, ACM STOC 2019], many algorithms are encompassed, including amplitude amplification, methods for the quantum linear systems problem, and quantum simulation. Here, we provide a pedagogical tutorial through these developments, first illustrating how quantum signal processing may be generalized to the quantum eigenvalue transform, from which the QSVT naturally emerges. Paralleling GSLW'19, we then employ the QSVT to construct intuitive quantum algorithms for search, phase estimation, and Hamiltonian simulation, and also showcase algorithms for the eigenvalue threshold problem and matrix inversion. This overview illustrates how the QSVT is a single framework comprising the three major quantum algorithms, suggesting a *grand unification* of quantum algorithms.

DOI: 10.1103/PRXQuantum.2.040203

Game rule

- Single qubit Pauli matrices

$$X = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \qquad Z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

- For $x = \cos\theta \in [-1, 1]$, rotation matrix
$$W(x) = e^{\mathrm{i}\theta X} = \begin{pmatrix} x & \mathrm{i}\sqrt{1-x^2} \\ \mathrm{i}\sqrt{1-x^2} & x \end{pmatrix}.$$

- Use products with phase factors $\Phi := (\phi_0, \cdots, \phi_d) \in \mathbb{R}^{d+1}$

$$U(x, \Phi) := e^{\mathrm{i}\phi_0 Z} W(x) e^{\mathrm{i}\phi_1 Z} W(x) \cdots e^{\mathrm{i}\phi_{d-1} Z} W(x) e^{\mathrm{i}\phi_d Z} \in \mathrm{SU}(2).$$

- Adjust Φ to fit a polynomial $f(x)$ using the real part of the upper left entry
$$\mathrm{Re}[U(x, \Phi)]_{1,1} = f(x), \quad x \in [-1, 1]$$

- A problem with rich mathematical structures.

MATLAB Demonstration

Try it: https://qsppack.gitbook.io/qsppack

Example 1: Chebyshev polynomial of the first kind

$$U(x,\Phi) := e^{\mathrm{i}\phi_0 Z} W(x) e^{\mathrm{i}\phi_1 Z} W(x) \cdots e^{\mathrm{i}\phi_{d-1} Z} W(x) e^{\mathrm{i}\phi_d Z}.$$

- $f(x) = T_d(x) = \cos(d \arccos(x)), x = \cos\theta$.
- Choose $\Phi = (\phi_0, \cdots, \phi_d) = (0, \ldots, 0)$.
- Then $U(x,\Phi) = W^d(x) = e^{\mathrm{i}d\theta X} \quad \Rightarrow$ $\mathrm{Re}[U(x,\Phi)]_{1,1} = \cos(d\theta) = \cos(d \arccos(x))$

Example 2: All zero vector

$$U(x, \Phi) := e^{\mathrm{i}\phi_0 Z} W(x) e^{\mathrm{i}\phi_1 Z} W(x) \cdots e^{\mathrm{i}\phi_{d-1} Z} W(x) e^{\mathrm{i}\phi_d Z}.$$

- $f(x) = 0$.
- $\Phi = (\pi/4, 0, \cdots, 0, \pi/4)$.
- $[U(x, \Phi)]_{1,1} = \mathrm{i}\cos(d\theta) \quad \Rightarrow \quad \mathrm{Re}[U(x, \Phi)]_{1,1} = 0$.

Example 3. 3rd order Chebyshev polynomial

- $f(x) = 0.2T_1(x) + 0.4T_3(x)$
- $\Phi = (0.5768, -0.1132, -0.1132, 0.5768)$.
- Some random Chebyshev polynomial. Symmetric phase factor.

Example 4. A smooth function

- $f(x) = \frac{1}{2} cos(100x)$.
- Cheyshev polynomial approximation.
- Symmetric phase factor. Decay behavior.

Phase factors used to be hard to compute..

Toward the first quantum simulation with quantum speedup

Andrew M. Childs[a,b,c,1], Dmitri Maslov[b,c,d], Yunseong Nam[b,c,e], Neil J. Ross[b,c,f], and Yuan Su[a,b,c]

[a]Department of Computer Science, University of Maryland, College Park, MD 20742; [b]Institute for Advanced Computer Studies, University of Maryland, College Park, MD 20742; [c]Joint Center for Quantum Information and Computer Science, University of Maryland, College Park, MD 20742; [d]Division of Computing and Communication Foundations, National Science Foundation, Alexandria, VA 22314; [e]IonQ, Inc., College Park, MD 20740; and [f]Department of Mathematics and Statistics, Dalhousie University, Halifax, NS B3H 4R2, Canada

Edited by John Preskill, California Institute of Technology, Pasadena, CA, and approved August 10, 2018 (received for review January 30, 2018)

Section H.3:

...However, this computation is difficult in practice, so we can only carry it out for very small instances. Specifically, we found the time required to calculate the angles to be prohibitive for values of M greater than about 32...It is a natural open problem to give a more practical method for computing the angles.

$d = 32$ **was thought to be hard..**

Tremendous progress..

Direct methods (factorization of polynomials):

- (Gilyen et al 1806.01838; Haah 1806.10236): compute the roots of a high-degree polynomial to high precision. High precision arithmetic.
- (Chao et al, 2003.02831): "Capitalization".
- (Ying, 2202.02671): Prony's method.

Iterative methods: (symmetric phase factors)

- (Dong, Meng, Whaley, **Lin**, 2002.11649): Optimization based algorithm. Convergence proof (Wang, Dong, **Lin**, 2110.04993)
- (Dong, **Lin**, Ni, Wang, 2209.10162): fixed point iteration for solving nonlinear system. Improved convergence result.
- (Dong, **Lin**, Ni, Wang, in preparation): Newton's method. Most robust algorithm so far.

$d > 10000$. The problem is practically solved after 5 years!

Outline

Introduction

Symmetric QSP and iterative algorithm

Infinite QSP

Goal of QSP (real case)

$\mathrm{QSP}_d : \mathbb{R}^{d+1} \to \mathbb{R}_d[x]$. Map phase factor to polynomial.

$$U(x,\Phi) := e^{\mathrm{i}\phi_0 Z} W(x) e^{\mathrm{i}\phi_1 Z} W(x) \cdots e^{\mathrm{i}\phi_{d-1} Z} W(x) e^{\mathrm{i}\phi_d Z} = \begin{pmatrix} f(x) + i* & * \\ * & * \end{pmatrix}.$$

Question Range of the mapping, representability of f?

Theorem (Gilyen-Su-Low-Wiebe STOC 2019)

If $f \in \mathbb{R}_d[x]$ satisfies

1. *parity is $d \mod 2$,*
2. $\|f\|_\infty = \max_{x\in[-1,1]} |f(x)| \leq 1$,

then there exists phase factors $\Phi \in \mathbb{R}^{d+1}$.

Uniqueness?

- degree of freedom: $\mathrm{DOF}(\Phi) = d + 1$, $\mathrm{DOF}(f) = \lceil (d+1)/2 \rceil$
- one (natural) way towards uniqueness: symmetric QSP

Reduced phase factors

> Given any set of symmetric phase factors
>
> $$\Psi = (\psi_d, \psi_{d-1}, \psi_{d-2}, \cdot \boxed{\cdots, \psi_{d-2}, \psi_{d-1}, \psi_d)} \in \mathbb{R}^{d+1}$$
>
> Its set of *reduced phase factors* is defined as its **right half**
>
> $$\Phi = (\phi_0, \phi_1, \ldots, \phi_{\tilde{d}-1}) := \begin{cases} (\frac{1}{2}\psi_{\tilde{d}-1}, \psi_{\tilde{d}}, \cdots, \psi_d), & d \text{ is even,} \\ (\psi_{\tilde{d}}, \psi_{\tilde{d}-1}, \cdots, \psi_d), & d \text{ is odd.} \end{cases}$$

Symmetric QSP

$\mathrm{QSP}_d : \mathbb{R}^{d+1} \to \mathbb{R}_d[x]$. Map phase factor to polynomial.

$$U(x, \Phi) := e^{\mathrm{i}\phi_0 Z} W(x) e^{\mathrm{i}\phi_1 Z} W(x) \cdots e^{\mathrm{i}\phi_d Z} W(x) e^{\mathrm{i}\phi_0 Z} = \begin{pmatrix} f(x) + i* & * \\ * & * \end{pmatrix}.$$

Theorem (Wang-Dong-**Lin**, Quantum 2022)

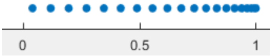
If $f \in \mathbb{R}_d[x]$ *satisfies*

1. *parity is* $d \mod 2$,
2. $\|f\|_\infty = \max_{x \in [-1,1]} |f(x)| \le 1$,

then there exists symmetric phase factors $\Phi \in \mathbb{R}^{d+1}$.

Optimization based formulation

- Parity: only $\widetilde{d} := \lceil \frac{d+1}{2} \rceil$ degrees of freedom to determine $f(x)$.
- Sampling on Chebyshev nodes $x_k = \cos\left(\frac{2k-1}{4\widetilde{d}}\pi\right)$, $k = 1, ..., \widetilde{d}$.



- Minimization problem

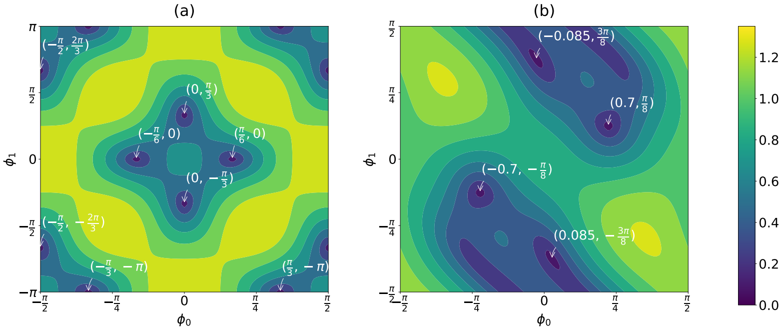
$$\Phi^* = \underset{\substack{\Phi\in[-\pi,\pi)^{d+1}, \\ \text{symmetric.}}}{\operatorname{argmin}} F(\Phi), \; F(\Phi) := \frac{1}{\widetilde{d}} \sum_{i=1}^{\widetilde{d}} \left|\mathrm{Re}[U(x_i, \Phi)]_{1,1} - f(x_i)\right|^2,$$

- Global minimum $F(\Phi^*) = 0$.

(Dong, Meng, Whaley, **Lin**, 2002.11649 PRA 2021),https://github.com/qsppack/qsppack

Optimization landscape

2 independent symmetric phase factors ϕ_0, ϕ_1.



Even target function

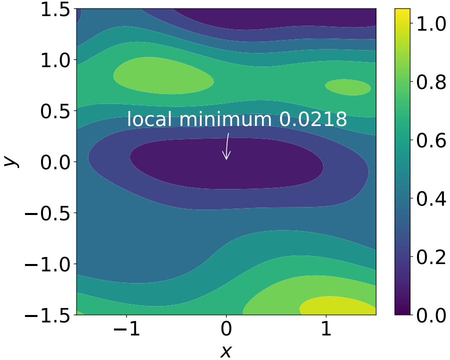
$$f(x) = x^2 - \frac{1}{2}$$

Only global minima (so far).

Odd target function

$$f(x) = \frac{1}{\sqrt{3}}x^3 - \frac{2}{\sqrt{3}}x$$

Local minima exists (and there are many)



Random $F(\Phi^{\text{loc}} + xu_1 + yu_2)$. $F(\Phi^{\text{loc}}) = 0.0218$

There are **combinatorially many** global minima at large d.
Can we characterize them?

Uniqueness of symmetric phase factor

Theorem (Wang-Dong-**Lin**, Quantum 2022)

For any $P \in \mathbb{C}[x]$ and $Q \in \mathbb{R}[x]$ satisfying

1. *$deg(P) = d$ and $deg(Q) = d - 1$.*
2. *P has parity $(d \mod 2)$ and Q has parity $(d - 1 \mod 2)$.*
3. *(Normalization condition) $\forall x \in [-1, 1] : |P(x)|^2 + (1 - x^2)|Q(x)|^2 = 1$.*
4. *If d is odd, then the leading coefficient of Q is positive.*

there exists a unique set of symmetric phase factors $\Phi := (\phi_0, \phi_1, \cdots, \phi_1, \phi_0) \in D_d$ such that

$$U(x, \Phi) = \begin{pmatrix} P(x) & iQ(x)\sqrt{1 - x^2} \\ iQ(x)\sqrt{1 - x^2} & P^*(x) \end{pmatrix}$$

Without specifying $\operatorname{Im} P$ and Q, the phase factors are still not unique.

Characterization of all global minimizers

Corollary (Wang-Dong-Lin, Quantum 2022)

There is a bijection between global minimizers and all admissible $(P(x), Q(x))$ pairs with $\mathrm{Re}[P](x) = f(x)$.

- $P(x) = f(x) + iP_{\mathrm{Im}}(x)$. Complementary polynomials $P_{\mathrm{Im}}(x), Q(x) \in \mathbb{R}[x]$.
- Normalization condition

$$1 - f(x)^2 = P_{\mathrm{Im}}(x)^2 + (1 - x^2)Q(x)^2.$$

- Pin down all roots of RHS via Laurent polynomial $\mathbb{C}[z, z^{-1}] \Rightarrow$ finite # of global minimizers.
- Generalize results in [Gilyen et al 2019; Haah 2019] to find all global minimizers.

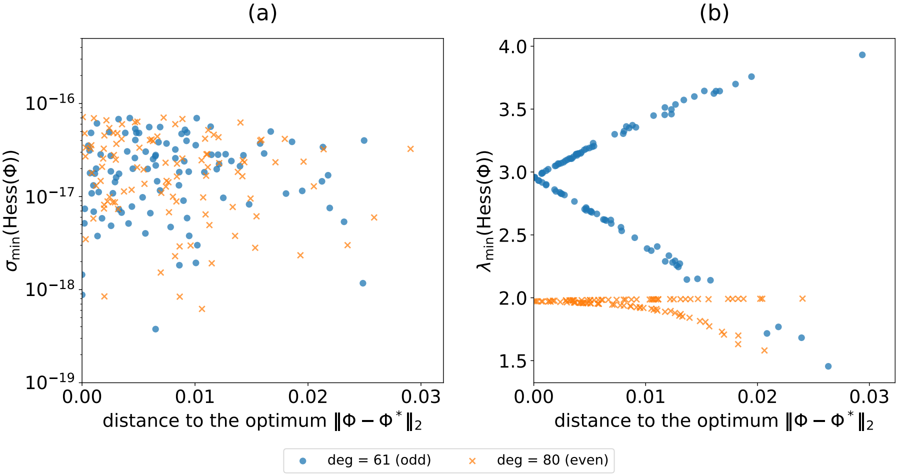
Magical initial guess

Fixed initial guess $\Phi_0 = (\pi/4, 0, \ldots, 0, \pi/4)$.

- Used in qsppack for all examples.
- Robust for all target functions seen so far.
- Corresponds to $P(x) = \mathrm{i}T_d(x), Q(x) = U_{d-1}(x)$.
- One special solution for $f(x) = 0$.
- Why does it work?

(Dong, Meng, Whaley, **Lin**, 2002.11649 PRA 2021)

Symmetric phase factors are important to the landscape



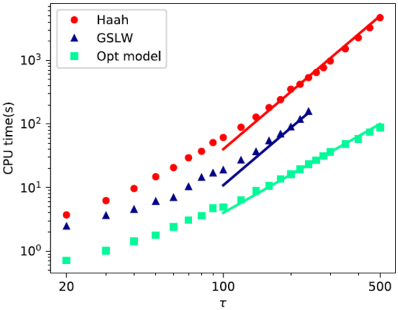
The Hessian at the minima is singular if the symmetric condition is not imposed.

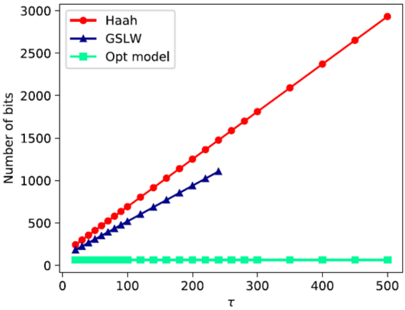
Example: Hamiltonian simulation

- Simulate a Hamiltonian means (mathematically)..

$$H \mapsto e^{-\mathrm{i}\tau H} \Rightarrow x \mapsto \cos(\tau x) - \mathrm{i}\sin(\tau x)$$

- Optimal polynomial approximates simulation $d \approx \frac{e}{2}\tau$





Why does optimization algorithm work?

Theorem (Local strong convexity)

If $\|f\|_\infty \leq Cd^{-1}$, $\left\|\widetilde{\Phi} - \widetilde{\Phi}^0\right\|_2 \leq C' d^{-1}$, *($C, C'$ are universal), then:*

$$\frac{1}{4} \leq \lambda_{\min}\left(\mathrm{Hess}(\widetilde{\Phi})\right) \leq \lambda_{\max}\left(\mathrm{Hess}(\widetilde{\Phi})\right) \leq \frac{25}{4}. \quad (1)$$

Corollary (Convergence from Φ^0)

If $\|f\|_\infty \leq Cd^{-1}$*, starting from* Φ^0*, at the* ℓ*-th iteration of the (projected) gradient method*

$$\left\|\widetilde{\Phi}^\ell - \widetilde{\Phi}^*\right\|_2 \leq e^{-\gamma\ell}\left\|\widetilde{\Phi}^0 - \widetilde{\Phi}^*\right\|_2. \quad (2)$$

Here γ, C *are universal constants.*

Dependence $\mathcal{O}(d^{-1})$ is undesirable.

(Wang-Dong-**Lin**, Quantum 2022)

Outline

Introduction

Symmetric QSP and iterative algorithm

Infinite QSP

QSP representation for smooth functions

👉 polynomial sequence approximates continuous function

$$f(x) = \begin{cases} \sum_{j=0}^{\infty} c_j T_{2j}(x), & f \text{ is even,} \\ \sum_{j=0}^{\infty} c_j T_{2j+1}(x), & f \text{ is odd,} \end{cases}$$

truncated polynomial sequence

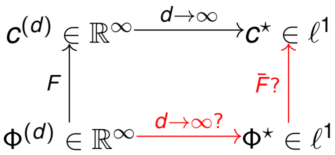
$$f^{(d)} = \sum_{j=0}^{\tilde{d}-1} c_j T_{2j \text{ or } 2j+1}(x) \to f \quad \text{in } \|\cdot\|_\infty.$$

Questions about consequences of this convergence

❓ (1) if each $f^{(d)}$ has a symmetric $\Phi^{(d)} \in \mathbb{R}^{\tilde{d}}$

(2) then can we find a phase-factor sequence converges to some limit $\Phi^{(d)} \overset{d\to\infty}{\longrightarrow} \Phi^\star$?

Question of infinite QSP



? (1) extension to $\bar{F} : \ell^1 \to \ell^1$ (iQSP is well defined)?
(2) inevitability of $\bar{F}$ (iQSP is solvable)?

Theorem (Dong, **Lin**, Ni, Wang, 2209.10162)

Universal constant $r_c \approx 0.902$, $\overline{F}$ *has an inverse map* $\overline{F}^{-1} : B(0, r_c) \subset \ell^1 \to \ell^1$, *where* $B(a, r) := \{v \in \ell^1 : \|v - a\|_1 < r\}$.

Fixed-point iteration for solving iQSP

Solve nonlinear equation

$$F(\Phi) = c$$

via a very simple algorithm, i.e., fixed point iteration:

$$\Phi^{\ell+1} = \Phi^{\ell} - \frac{1}{2}\left(F\left(\Phi^{\ell}\right) - c\right)$$

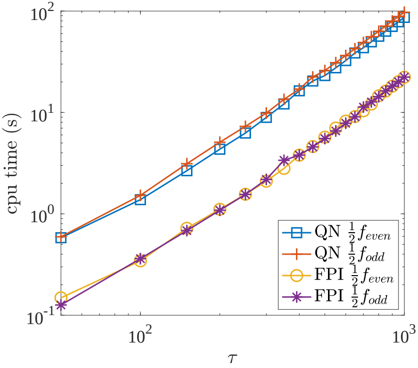
Theorem (Dong, Lin, Ni, Wang, 2209.10162)

$\exists$ universal constants C_1, C_2, γ, so that when $\|c\|_1 \leq C_1$, fixed point iteration converges to $\Phi^\star = \overline{F}^{-1}(c)$.

$$\left\|\Phi^{(\ell)} - \Phi^\star\right\|_1 \leq C_2 \gamma^{\ell}. \qquad (3)$$

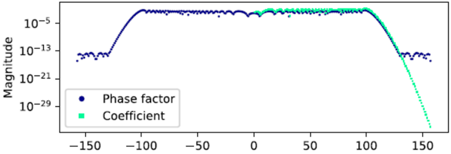
No explicitly dependence on d!

Fixed-point iteration for solving iQSP

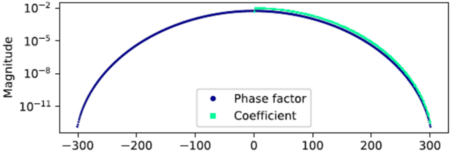


- $f(x) = \sin(\tau x)$ or $f(x) = \cos(\tau x)$.
- Fixed ϵ, degree of approximating polynomial $d = \mathcal{O}(\tau)$.
- Complexity is $\mathcal{O}(d^2 \log(1/\epsilon))$ theoretically and numerically.

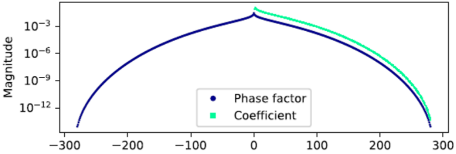
Decay behavior of the phase sequence



Hamiltonian simulation



Eigenstate filtering



Solving linear systems

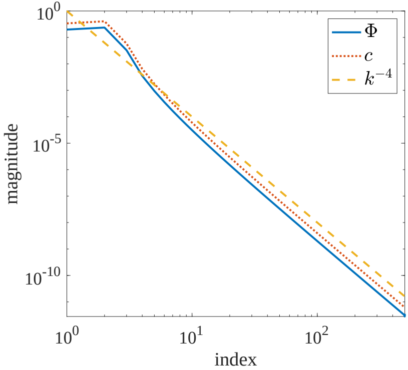
Decay properties of reduced phase factors

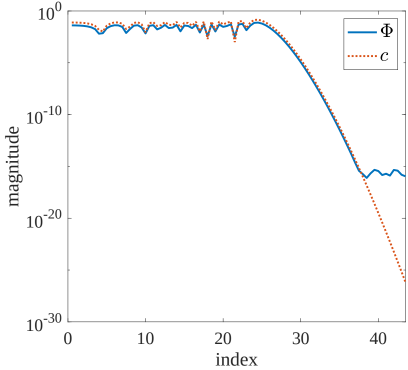
Theorem (Dong, Lin, Ni, Wang, 2209.10162)

$\exists$ universal constants C, C_1, C_2. Given target function f with $\|c\|_1 < C$, then for any n,

$$C_1 \sum_{k>n} |c_k| \leq \sum_{k>n} |\phi_k| \leq C_2 \sum_{k>n} |c_k| . \qquad (4)$$

Sharper tests of decay properties





- $f(x) = 0.8\,|x|^3$.
- $|c_k| \sim k^{-4}$, $|\phi_k| \sim k^{-4}$.

- $f(x) = 0.5\sin(1000x)$.
- Superalgebraic decay.

Conclusion

- QSP: Polynomial representation using parts of a unitary matrix.
- Iterative methods can survive in the presence of complex energy landscape from a problem-independent initial guess
- Surprising relation between (a branch of) phase factors, Chebyshev coefficients, and regularity of target functions.
- Open question: Why iterative method works for $f(x) = c\cos(\tau x)$ when (1) τ is large (2) $c \approx 1$? (violates both ℓ_∞ and ℓ_1 bound).
- Not discussed: fully-coherent limit $\|f\|_\infty = 1$ and Newton's method.

Acknowledgment

Thank you for your attention!

Lin Lin
https://math.berkeley.edu/~linlin/

U.S. DEPARTMENT OF ENERGY | Office of Science
NSF
AFOSR AIR FORCE OFFICE OF SCIENTIFIC RESEARCH
Google AI Quantum
SIMONS FOUNDATION