Optimization Based Approach for Quantum Signal Processing and Its Energy Landscape

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Joint work with

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- Birgitta Whaley (Berkeley, Chem)

Outline

Introduction

Optimization based algorithm for finding phase factors

Energy landscape of the optimization

Matrix product state based optimization method

Open question

“Grand unification” of quantum algorithms

A Grand Unification of Quantum Algorithms

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Quantum algorithms offer significant speedups 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 were recently 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 QSVT [Gilyén, Su, Low, and Wiebe, 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 QSVT naturally emerges. Paralleling GSLW’19, we then employ 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 QSVT is a single framework comprising the three major quantum algorithms, suggesting a *grand unification* of quantum algorithms.

2105.02859;
QSVT: [GSLW18] 1806.01838

Quantum signal processing

$$U_\Phi(x) = e^{\mathrm{i}\phi_0 Z} \prod_{j=1}^{d} \left[W(x) e^{\mathrm{i}\phi_j Z} \right] = \begin{pmatrix} P(x) & \mathrm{i}Q(x)\sqrt{1-x^2} \\ \mathrm{i}Q^*(x)\sqrt{1-x^2} & P^*(x) \end{pmatrix}, \quad W(x) = \begin{pmatrix} x & \mathrm{i}\sqrt{1-x^2} \\ \mathrm{i}\sqrt{1-x^2} & x \end{pmatrix}.$$

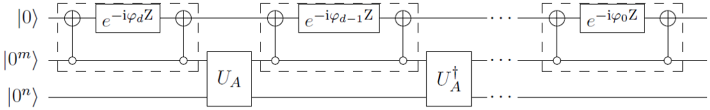
Quantum signal processing (QSP)

SU(2)

Quantum eigenvalue transformation (QET)

Quantum singular value transformation (QSVT)

Circuit



Low-Chuang, PRL 2017

Goal of QSP (real case)

- Given $f(x) \in \mathbb{R}[x]$. Polynomial of degree d. Even or odd. $|f(x)| < 1$ on $[-1, 1]$.

- Find phase factors $\Phi := (\phi_0, \cdots, \phi_d) \in \mathbb{R}^{d+1}$ so that

$$\mathrm{Re}[U(x, \Phi)]_{1,1} \equiv \mathrm{Re}[\langle 0|U(x, \Phi)|0\rangle] = f(x), \quad x \in [-1, 1]$$

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

- $W(x) = e^{\mathrm{i}\arccos(x) X} = \begin{pmatrix} x & \mathrm{i}\sqrt{1-x^2} \\ \mathrm{i}\sqrt{1-x^2} & x \end{pmatrix}.$

- Solution guaranteed to exist

Once upon a time, phase factors were hard to compute..

PNAS

Toward the first quantum simulation with quantum speedup

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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.

Algorithms for finding phase factors

- (Gilyen et al 1806.01838; Haah 1806.10236): compute the roots of a high-degree polynomial to high precision. Limit to $\sim$ hundreds of phase factors with double precision arithmetic.

- (Dong, Meng, Whaley, L., 2002.11649): Optimization based algorithm. No rigorous proof. Standard double precision arithmetic. $>$ 10000 phase factors.

- (Chao et al, 2003.02831): “capitalization”. No rigorous proof. Standard double precision arithmetic. $>$ 3000 phase factors.

- Should be able to compute much longer phase sequences. The problem is practically solved within 2 years!

- (Wang, Dong, L., in prep2): Matrix-product state based structure. Local convergence from fixed initial guess.

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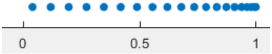
Optimization based formulation

- 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

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

- Global minimum $F(\Phi^*) = 0$.
- Dimension mismatch: $d > \widetilde{d}$, so solution cannot be unique.

Symmetric QSP

Recall

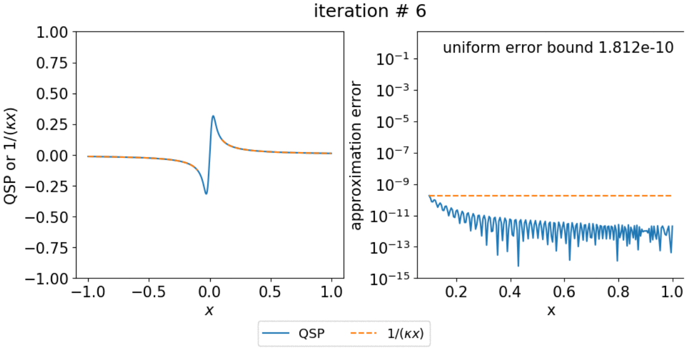
$$U(x,\Phi) = \begin{pmatrix} P(x) & \mathrm{i}Q(x)\sqrt{1-x^2} \\ \mathrm{i}Q^*(x)\sqrt{1-x^2} & P^*(x) \end{pmatrix}$$

- General QSP: $Q(x) \in \mathbb{C}[x]$.
- Symmetric QSP: $Q(x) \in \mathbb{R}[x] \quad \Rightarrow$
  $\Phi = (\phi_0, \phi_1, \ldots, \phi_1, \phi_0)$. Symmetric phase factors
- Degree of freedom: $\widetilde{d} = \lceil \frac{d+1}{2} \rceil \quad \Rightarrow$ matches that in $f(x)$!
- Modified optimization problem

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

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

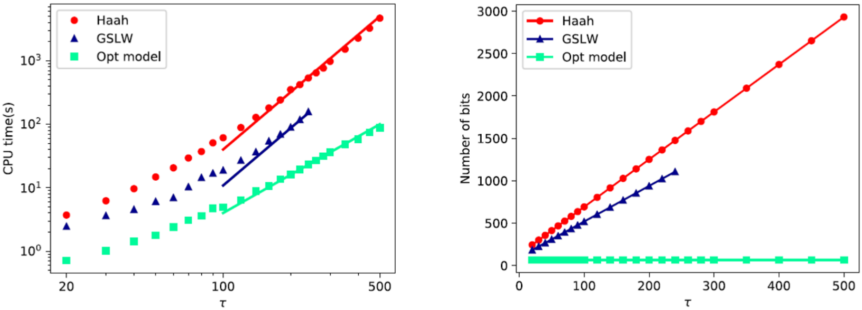
Example: solve linear systems



$$1/(\kappa x) \approx f(x),\ \kappa = 10,\ d = 303.$$

Applications

Hamiltonian simulation:



- Similar performance for other applications such as eigenstate filtering and solving linear systems

Streamlining the process of finding phase factors

Given a smooth function $f(x)$ (not necessarily a polynomial)

- Option 1: Numerically obtain near-best polynomial approximation (e.g. Remez method) + numerical optimization.
- Option 2: Direct optimization.

Option 1 is observed to be numerically more stable (objective function $= 0$ at global minima) when $f(x)$ is real.

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

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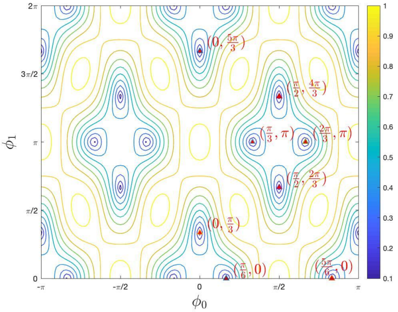
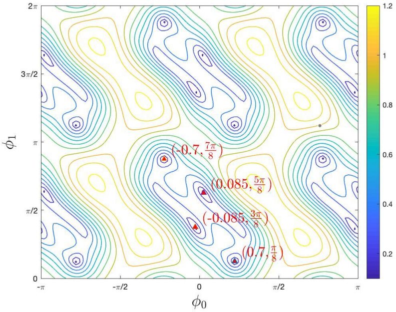
Optimization landscape

2 independent symmetric phase factors ϕ_0, ϕ_1.
Only global minima (so far).



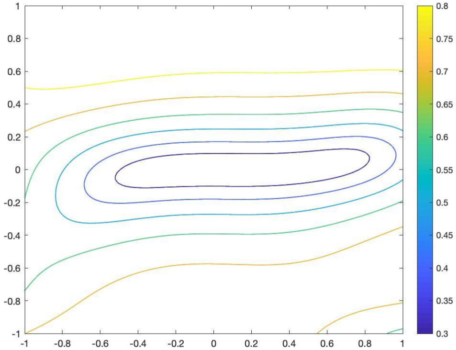
Even target function
$f(x) = x^2 - \frac{1}{2}$



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

Local minima exists (and there are many)

There are many local minima at large d.



$$F(\Phi^{\text{loc}} + xu_1 + yu_2)$$

Randomly generated odd target function ($d = 5$). $F(\Phi^{\text{loc}}) = 0.0084$

Two smallest eigenvalue of the Hessian: $0.015, 3.7897$ with eigenvectors u_1, u_2.

Uniqueness of symmetric phase factor

Theorem (Wang, Dong, L., in prep1)

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*

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

Global minimizer and (P, Q) pair

Corollary

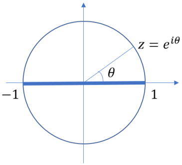
There is a bijection between global minimizers and all admissible $(P(x), Q(x))$ pairs with $\mathrm{Re}[P](x) = f(x)$.

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

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

- Seems like an infinite number of choices ([Gilyen et al 2019; Haah 2019] constructs a class of solutions)

Key: Laurent polynomials



- For any $x \in [-1, 1]$, $x = \frac{z+z^{-1}}{2}$ with $z = e^{i\theta}$.
- $f(x) \to f(\frac{z+z^{-1}}{2})$: Laurent polynomial $\mathbb{C}[z, z^{-1}]$.
- Factorization:

$$1 - f\left(\frac{z+z^{-1}}{2}\right)^2 = \left(p_{\mathrm{Im}}(z) + \frac{z-z^{-1}}{2} q(z)\right)\left(p_{\mathrm{Im}}(z) - \frac{z-z^{-1}}{2} q(z)\right),$$

$$p_{\mathrm{Im}}(z) := P_{\mathrm{Im}}\left(\frac{z+z^{-1}}{2}\right), \quad q(z) := Q\left(\frac{z+z^{-1}}{2}\right),$$

$$1 - f\left(\frac{z+z^{-1}}{2}\right)^2 = \beta z^{-2d} \prod_{r \in \mathcal{S}} (z - r), \text{ for some } \beta \in \mathbb{R}.$$

- Pin down the roots of RHS $\Rightarrow$ finite # of global minimizers.
- Generalize results in [Gilyen et al 2019; Haah 2019] to find all global minimizers.

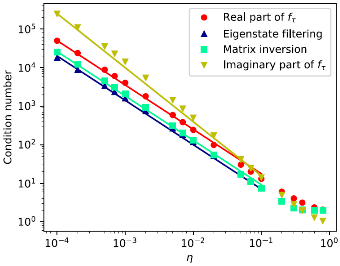
One special initial guess

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

- Used in qsppack for all examples.
- Robust for virtually all real target functions.
- Corresponds to $P(x) = \mathrm{i}\, T_d(x), Q(x) = U_{d-1}(x)$.
- One special solution for $f(x) = 0$, i.e. $c = 0$.

Condition number and the magnitude

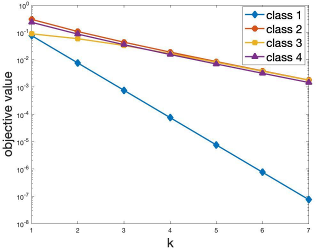
$$\|f\|_\infty = \max_{x\in[-1,1]} |f(x)| = 1-\eta.$$



Condition number of the Hessian at Φ^*.

- Ill-conditioned optimization problem as $\eta \to 0$.
- Given $\|f\|_\infty < 1$, consider $cf(x)$ with $|c| < 1$.

Not all global minima are equivalent



$$\left\|\Phi^*(k) - \Phi_0^{\text{class}}\right\|_2$$

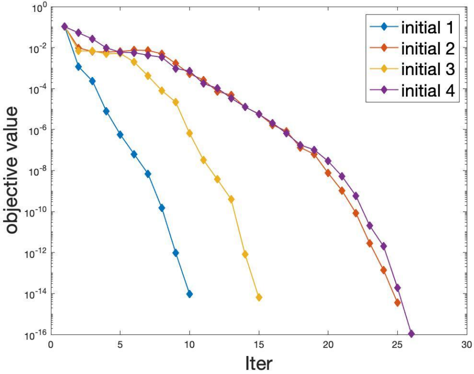
$$f(x) = 10^{-k}\left(\frac{1}{4}T_6 + \frac{5}{4}T_4 + \frac{1}{8}T_2 - \frac{1}{8}T_0\right).$$

- class 1 $\rightarrow \left(\frac{\pi}{4}, 0, 0, 0, 0, 0, \frac{\pi}{4}\right)$
- class 2 $\rightarrow \left(\frac{\pi}{4}, 0, \frac{\pi}{4}, -\frac{\pi}{2}, \frac{\pi}{4}, 0, \frac{\pi}{4}\right)$
- class 3 $\rightarrow \left(\frac{\pi}{4}, 0, -\frac{\pi}{4}, \frac{\pi}{2}, -\frac{\pi}{4}, 0, \frac{\pi}{4}\right)$
- class 4 $\rightarrow \left(\frac{\pi}{4}, \frac{\pi}{4}, 0, -\frac{\pi}{2}, 0, \frac{\pi}{4}, \frac{\pi}{4}\right)$

- The branch converging to $\Phi_0 = (\pi/4, 0, \ldots, 0, \pi/4)$ is called maximal solution (also generated by GSLW/Haah method)
- Φ_0 has the largest “convergence basin”.

Actual faster convergence near Φ_0

Initial 1: Φ_0



Distance of maximal solution to Φ_0

Recall $\Phi_0 = (\pi/4, 0, \ldots, 0, \pi/4)$.

Theorem (Wang, Dong, L., in prep1)

Let Φ^* be the symmetric phase factors corresponding to the maximal solution for the target function $f(x)$ with $\|f\|_\infty < \frac{1}{\sqrt{2}}$. Then

$$||\Phi^* - \Phi_0||_2 \leq \sqrt{12}\,\|f\|_\infty .$$

- Bound independent of d!
- Capitalization (perturbation with high order polynomials) is not effective for symmetric phase factors.

Well-conditioned Hessian at maximal solution

Corollary

If $\|f\|_\infty \leq \frac{1}{48\tilde{d}}$, *then*

$$||\Phi^* - \Phi_0||_2 \leq \frac{\sqrt{3}}{24\tilde{d}}$$

Furthermore,

$$\lambda_{\min}\left(\mathrm{Hess}(\Phi^*)\right) \geq 1.$$

- $\mathrm{Hess}(\Phi^*)$ is positive definite.
- Optimization algorithm expects to converge locally.

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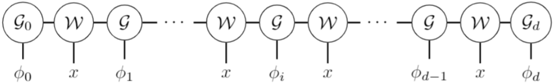
Matrix product state structure of QSP

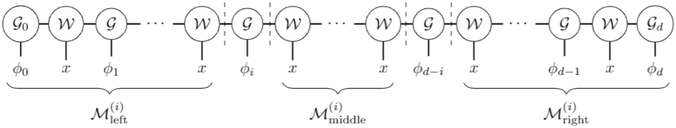
- MPS structure for $\langle 0|U(x,\Phi)|0\rangle$.



- $\mathcal{G}_0(\phi_0) = (e^{\mathrm{i}\phi_0}, 0), \mathcal{G}_d(\phi_d) = (e^{\mathrm{i}\phi_d}, 0)^\top$
- $\mathcal{W}(x) = e^{\mathrm{i}\arccos(x)X}, \mathcal{G}(\phi_j) = e^{\mathrm{i}\phi_j Z}$

Gradient calculation

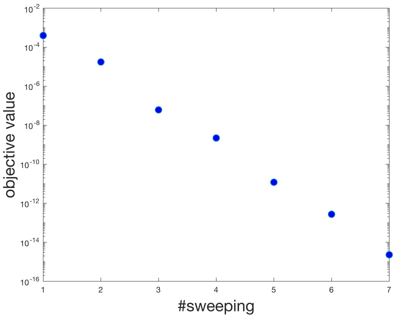
- Computing the gradient $\langle 0|\partial_{\phi_i} U(x,\Phi)|0\rangle$ (note the symmetric structure)



- Sweeping based algorithm: $\mathcal{O}(d^2)$ per sweep.

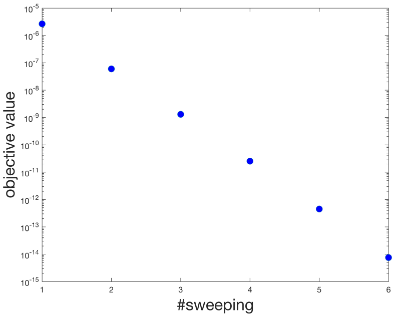
- Sweeping directions: Edge to center; Edge to center to edge; Center to edge; Center to edge to center; etc

Fast convergence (very few sweeps)



Even target function

$f(x) = \cos(500x)$, $\widetilde{d} = 367$



Odd target function

$f(x) = \frac{1}{\kappa x}$ with $\kappa = 50$, $\widetilde{d} = 760$.

Convergence from Φ_0

Recall $\Phi_0 = (\pi/4, 0, \ldots, 0, \pi/4)$.

Theorem (Wang, Dong, L., in prep2)

There exists a constant C (independent of d and target function) s.t. for any $f(x)$ with $\|f\|_\infty \leq \frac{1}{C\tilde{d}}$,

$$F(\Phi^k) \leq \left[1 - \frac{1}{12(1+\tilde{d})}\right]^k F(\Phi^0) \tag{1}$$

where k is the number of sweeping.

Number of sweeps seems to be independent of d. Cost close to $\mathcal{O}(d^2)$.

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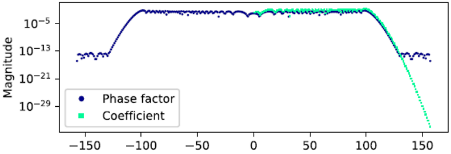
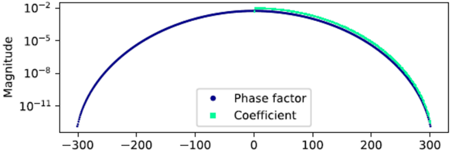
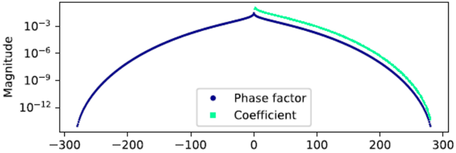
Open question: decay behavior of the phase sequence



Hamiltonian simulation



Eigenstate filtering



Solving linear systems

Acknowledgment

Thank you for your attention!

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

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