Energy Landscape of Optimizing Symmetric Phase Factors in Quantum Signal Processing

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Construct quantum algorithms for many numerical problems with a proper set of phase factors.

- Quantum linear system problem, x^{-1},
- Hamiltonian simulation, $e^{-\mathrm{i}tx}$,
- Thermal state preparation problem, $e^{-\beta x}$
- ......

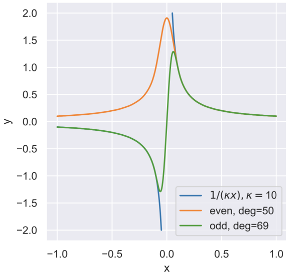


Fig: Polynomial approximation of $\frac{1}{x}$.

Quantum Signal Processing(QSP)

Given a sequence of phase factors $\Phi := (\phi_0, \cdots, \phi_d) \in [-\pi, \pi)^{d+1}$, define

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

where $x \in [-1, 1]$, $X := \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, Z := \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$ are Pauli matrices.

- The real component of the upper-left matrix element [1]

$$g(x, \Phi) := \mathrm{Re}[U(x, \Phi)_{11}] \quad (2)$$

can be any real polynomial with parity (d mod 2) and of degree $\leq d$ up to scaling.

[1] A. Gilyén, Y. Su, G. H. Low, and N. Wiebe, Quantum singular value transformation and beyond: exponential improvements for quantum matrix arithmetics, 2018.

How to find phase factors

Recent progress:

- Gilyén-Su-Low-Wiebe [STOC'19],
- Haah [Quantum'19],
- Dong-Meng-Whaley-Lin [Phys.Rev.A'21],
- Chao-Ding-Gilyén-Huang-Szedegy [arXiv:2003.02831].

- The first two methods are constructive, but need to find the roots of high degree polynomials to high precision.
- The third method is an optimization based method and imposes the symmetry constraint on the phase factors.

Optimization problem

Given a polynomial $f \in \mathbb{R}[x]$ of degree d, with parity ($d \mod 2$) and $\max_{x\in[-1,1]} |f(x)| \leq 1$, the optimization problem is

$$\Phi^* = \underset{\substack{\Phi\in[-\pi,\pi)^{d+1}, \\ \text{symmetric}}}{\operatorname{argmin}} F(\Phi), \ F(\Phi) := \frac{1}{\widetilde{d}} \sum_{k=1}^{\widetilde{d}} \left| g(x_k, \Phi) - f(x_k) \right|^2, \qquad (3)$$

where $\widetilde{d} := \lceil \frac{d+1}{2} \rceil$ and $x_k = \cos\left(\frac{2k-1}{4\widetilde{d}}\pi\right)$, $k = 1, ..., \widetilde{d}$ are positive Chebyshev nodes of $T_{2\widetilde{d}}(x)$.

- The selection of $T_{2\widetilde{d}}(x)$ is enough, because it matches the degree of freedom. For convenience, we choose the first half of phase factors $(\phi_0, \cdots, \phi_{\widetilde{d}-1})$ as free variables.
- Usually scale the L^∞ norm of f to be less than 1 in order to enhance numerical stability.

Symmetric phase factors

Theorem 1 (Existence and uniqueness)

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

$$U(x, \Phi) = \begin{pmatrix} P(x) & iQ(x)\sqrt{1-x^2} \\ iQ(x)\sqrt{1-x^2} & P^*(x) \end{pmatrix}, \tag{4}$$

if and only if $P \in \mathbb{C}[x]$ *and* $Q \in \mathbb{R}[x]$ *satisfy*

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 nonzero leading coefficient of* Q *is positive.*

Here, $R_d := \begin{cases} [0, \pi)^k \times [-\pi, \pi) \times [0, \pi)^k & \text{if } d = 2k, k \in \mathbb{N}^*, \\ [0, \pi)^{d+1} & \text{otherwise.} \end{cases}$

- There is a bijection between the global minimizer and the pair of (P, Q) satisfying the conditions 1-4 in Theorem 1.
- The global minimizer is not unique.

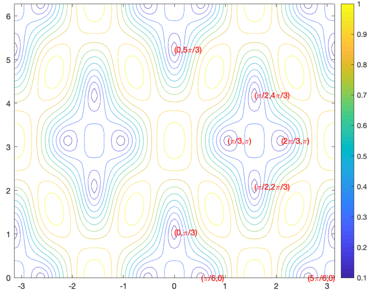


Fig: The contour of the objective function.

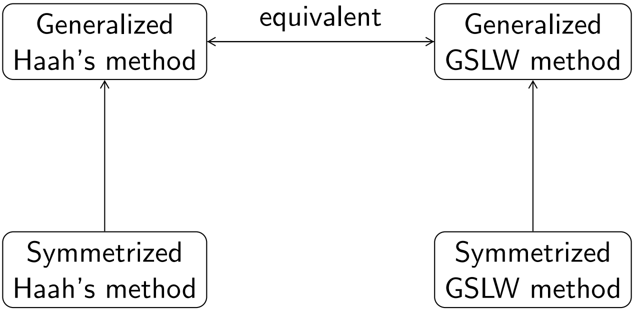
$$f(x) = x^2 - \frac{1}{2}$$

$$\begin{cases} P_{\mathrm{Im}} = \pm\frac{\sqrt{3}}{2}(2x^2 - 1) \\ Q = \pm 2x \end{cases}$$

$$\begin{cases} P_{\mathrm{Im}} = \pm\frac{\sqrt{3}}{2} \\ Q = \pm x \end{cases}$$

Find all global minimizers

- We notice that Haah's method and GSLW method can be modified for symmetrical phase factors, but provide only the global minimizer around $(\frac{\pi}{4}, 0, \cdots, 0)$.
- We propose the generalized versions of both methods which are able to find all global minimizers to the optimization problem.



Characterize all global minimizers

Theorem 2

Given $f(x) \in \mathbb{R}[x]$ *with* $\max_{x\in[-1,1]} |f(x)| < 1$, $P \in \mathbb{C}[x]$ *and* $Q \in \mathbb{R}[x]$ *satisfy*

1. $P_{\mathrm{Re}}(x) = f(x)$,
2. *the conditions 1-4 in Theorem 1,*

if only if there exists a multiset $\tilde{\mathcal{D}}$ *such that*

1. $\tilde{\mathcal{D}} \uplus \tilde{\mathcal{D}}^{-1} = \mathcal{S}$, *where* $\mathcal{S}$ *contains all roots of* $1 - f(\frac{z+z^{-1}}{2})^2$ *with multiplicity and* $\tilde{\mathcal{D}}^{-1} := \{z^{-1} : z \in \tilde{\mathcal{D}}\}$,
2. $\tilde{\mathcal{D}}$ *is closed under complex conjugation and additive inverse,*
3. $P_{\mathrm{Im}}(\frac{z+z^{-1}}{2}) = c_1 \frac{e(z)+e(z^{-1})}{2}$ *and* $Q(\frac{z+z^{-1}}{2}) = c_2 \frac{e(z)-e(z^{-1})}{2(z-z^{-1})}$, *where* $e(z) := z^{-d} \prod_{r\in\tilde{\mathcal{D}}}(z - r)$ *and* $c_1^2 = c_2^2 = \frac{1-f(\frac{z+z^{-1}}{2})^2}{e(z)e(z^{-1})} \in \mathbb{R}_+$.
4. *If* d *is odd, then* $c_2 > 0$.

Existence of local minimizer

The local minimizer exists for $d \geq 3$. Here is an example.

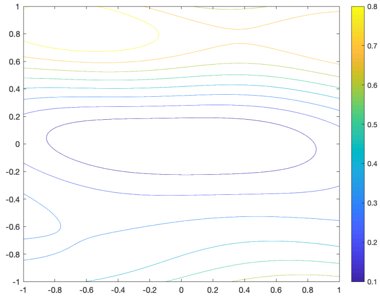


Fig: The contour of the objective function on the hyperplane spanned by the eigenvectors corresponding to the two largest eigenvalues.

$d = 4$

Objective value: $1.33e - 2$

Eigenvalues of Hessian matrix:

$(0.1075, 4.4849, 7.7454)$

Others

- The global energy landscape is bad.
- However, the optimization problem is locally strong convex around $(\frac{\pi}{4}, 0, \cdots, 0)$ thanks to the symmetry constraint.
- This accounts for the good performance of optimization algorithms around that point.

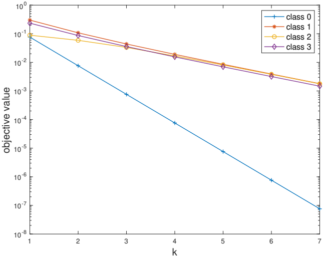


Fig: The convergence rate of different global minimizers corresponding to $0.1^k f(x)$ with $f(x) = \frac{1}{4}x^6 + \frac{5}{4}x^4 + \frac{1}{8}x^2 - \frac{1}{8}$.

Different convergence limit

class 0:$(\frac{\pi}{4}, 0, 0, 0)$

class 1:$(\frac{\pi}{4}, 0, \frac{\pi}{4}, -\frac{\pi}{2})$

class 2:$(\frac{\pi}{4}, 0, -\frac{\pi}{4}, \frac{\pi}{2})$

class 3:$(\frac{\pi}{4}, \frac{\pi}{4}, 0, -\frac{\pi}{2})$

Thank you!