APPROXIMATE SEPARATION OF QUANTUM GATES AND
SEPARATION EXPERIMENTS OF CNOT BASED ON PARTICLE
SWARM OPTIMIZATION ALGORITHM

KAN HE¹, SHUSEN LIU², JINCHUAN HOU¹

Abstract. Ying conceived of using two or more small-capacity quantum computers to produce a larger-capacity quantum computing system by quantum parallel programming ([M. S. Ying, Morgan-Kaufmann, 2016]). In doing so, the main obstacle is separating the quantum gates in the whole circuit to produce a tensor product of the local gates. It has been showed that there are few separable multipartite quantum gates, so the approximate separation problem involves finding local quantum gates that approximate a given inseparable gate. We propose and study a problem involving the approximate separation of multipartite gates based on quantum-gate fidelity. For given multipartite and local gates, we conclude that the smaller is the maximal distance between the products of an arbitrary pair of eigenvalues, the greater is their gate fidelity. This provides a criterion for approximate separation. Lastly, we discuss the optimal approximate separation of the CNOT gate.

1. Introduction

Programming for quantum computers has become an urgent task nowadays [1], [2], [3], [4]. As reported in [1], [5], [6], [7], extensive research has been conducted on quantum programming over the last decade, and several quantum programming platforms have been developed over the last two decades. The first quantum programming environment was the ‘QCL’ project proposed by Ömer in 1998 [8], [9]. Then, more quantum softwares are emerged, for instance, Q language as a C++ library [2], a scalable functional quantum programming language, called Quipper [10], [11], [12]. Wecker and Svore from QuArc (the Microsoft Research Quantum Architecture and Computation team) developed LIQUi as a modern tool-set embedded within F# [14]. At the end of 2017, QuARC announced a new programming language and simulator designed specifically for full-stack quantum computing, known as Q#, which represents a milestone in quantum programming. In the same year, Liu et al. released the quantum program Q\text{SI} that supports a more complicated loop structure [13]. To date, the structures of programming languages and tools have mainly been sequential.

Beyond the constraints of quantum hardware, there remain several barriers to the development of practical applications for quantum computers. One of the most serious barriers is

Key words and phrases. Separation of quantum gates; CNOT.
the number of physical qubits provided in physical machines. For example, IBMQ produces two five-qubits quantum computers \(^{18}\) and one 16-qubit quantum computer \(^{19}\), which are available to programmers through the cloud, but these are far fewer qubits than are required by practical quantum algorithms. Today, quantum hardware is in its infancy. As the number of available qubits is gradually increasing, many researchers are considering the possibility of combining various quantum hardware components to work as a single entity and thereby enable advances in the number of qubits \(^{7}\). To increase the number of accessible qubits in quantum hardware, one approach uses concurrent or parallel quantum programming. Although current quantum-specific environments are sequential in structure, some researchers are working to exploit the possibility of parallel or concurrent quantum programming on the general programming platform from different respects. Vizzotto and Costa applied mutually exclusive access to global variables to enable concurrent programming in Haskell \(^{21}\). Yu and Ying studied the termination of concurrent programs \(^{20}\). Researchers provide mathematics tools for process algebras to describe their interaction, communication and synchronization \(^{22}\). Recently, Ying and Li defined and established operational (denotational) semantics and a series of proof rules for ensuring the correctness of parallel quantum programs \(^{26}\). Not surprisingly, we showed that multipartite quantum gates that can be separated simply seldom exist \(^{28}\). Furthermore, in a practical quantum circuit, we must know how a given multipartite gate can be closed by local gates. In this paper, we show that for given multipartite and local gates, the smaller is the maximal distance between the products of an arbitrary pair of eigenvalues, the greater is their gate fidelity. This provides a criterion of approximate separation. We also discuss the optimal approximate separation of the CNOT gate.

It has been showed that only few kinds of multipartite gates can be separated directly. In this section, we turn to study the approximate separation problem of multipartite gates.

We introduce some notations. Let \(\mathcal{H}_k\) be a complex Hilbert space with \(\dim \mathcal{H} = m_k\), and \(\otimes_{k=1}^n \mathcal{H}_k\) the tensor product of \(\mathcal{H}_k\)s. Still denote by \(\mathcal{B}(\otimes_{k=1}^n \mathcal{H}_k), \mathcal{U}(\otimes_{k=1}^n \mathcal{H}_k)\) and \(\mathcal{B}_s(\otimes_{k=1}^n \mathcal{H}_k)\) the set of all bounded linear operators, all unitary operators, and all self-adjoint operators on the underline space \(\otimes_{k=1}^n \mathcal{H}_k\) respectively. The error of two gates \(U, V\) is

\[
E(U, V) = \max_{|x\rangle} \{d(U|x\rangle\langle x|U^\dagger, V|x\rangle\langle x|V^\dagger) : |||x\rangle|| = 1\},
\]

where \(d\) is an arbitrary distance between two matrices.
2. Results and experiments

The problem on \( \epsilon \)-approximate separation

Given a positive scalar \( \epsilon \) and a multipartite quantum gate \( U \in U(\bigotimes_{k=1}^{n} \mathcal{H}_k) \), determine whether there are local gates \( U_i \in U(\mathcal{H}_i) \) such that

\[
E(U, \bigotimes_{i=1}^{n} U_i) \leq \epsilon,
\]

where \( d(\cdot, \cdot) \) is an arbitrary distance between two operators. We refer to \( U \) as the \( \epsilon \)-approximate separable one if Eq. 1 holds true. Furthermore, how do we find these local gates \( U_i \)?

In our solution, the gate fidelity is selected as the replacement of the distance between matrices in the above question. The gate fidelity between two unitary gates \( U, V \) is defined as

\[
F_{\min}(U, V) = \min_{|x\rangle} \{ F(U|x\rangle\langle x|U^\dagger, V|x\rangle\langle x|V^\dagger) : ||x|| = 1 \},
\]

where \( F(A, B) = \text{tr}(\sqrt{\sqrt{A}B\sqrt{A}}) \) is the Uhlmann fidelity. Considering the specialty of the gate fidelity, we re-describe the question on \( \epsilon \)-approximate separation as follows:

The question on \( \epsilon \)-approximate separation based on the gate fidelity

Given a positive scalar \( \epsilon \) and a multipartite quantum gate \( U \in U(\bigotimes_{k=1}^{n} \mathcal{H}_k) \), whether or not there are local gates \( U_i \in U(\mathcal{H}_i) \) such that

\[
F_{\min}(U, \bigotimes_{i=1}^{n} U_i) \geq 1 - \epsilon.
\]

And how do we find these local gates \( U_i \)?

Next we answer the question on \( \epsilon \)-approximate separation based on the gate fidelity by connecting the gate fidelity to numerical ranges. Recall the numerical range of a bounded linear operator \( A \) is

\[
W(A) = \{ \lambda = \langle x|A|x\rangle, ||x|| = 1 \}.
\]

The numerical radius of \( A \) is

\[
w(A) = \max\{ ||\lambda|| : \lambda \in W(A) \}.
\]

Let us introduce the distance from 0 to \( W(A) \) is defined as

\[
w_{\min}(A) = \min\{ ||\lambda|| : \lambda \in W(A) \}.
\]

The maximal distance of the eigenvalues of a matrix \( A \) with its spectral set \( \sigma(A) \):

\[
d_{\max}(A) = \max_{\lambda_i \in \sigma(A)} \{ |\lambda_i - \lambda_j| \}.
\]
**Theorem 2.1** For arbitrary $m \times m$ unitary matrices $U, V$, 

\[ F_{\min}(U, V) = \sqrt{1 - \left( \frac{d_{\max}(V^\dagger U)}{2} \right)^2}. \]

**Remark.** From Theorem 2.1, we conclude that the $\epsilon$-approximate separation question that is based on the gate fidelity can be solved in the following manner: for a given multipartite quantum gate $U \in \mathcal{U}(\otimes_{k=1}^n \mathcal{H}_k)$, we design a search program to find the unitary matrix $U_i \in \mathcal{U}(\mathcal{H}_i)$ for each $i$ such that $d_{\max}(\otimes_{i=1}^n U_i^\dagger U)$ converges to its infimum. Simultaneously, the gate fidelity $F_{\min}(U, \otimes_{i=1}^n U_i)$ can touch its supremum. Therefore, $\otimes_{i=1}^n U_i$ can become an $\epsilon$-approximate separation to $U$ based on the gate fidelity if and only if $d_{\max}(\otimes_{i=1}^n U_i^\dagger U) \leq 2\sqrt{2\epsilon - \epsilon^2}$ (assume without loss of generality $\epsilon < 1$).

**Proof of Theorem 2.1.** First, it is easy to check that 

\[ F_{\min}(U, V) = \min_{\|x\| = 1} |\langle x | V^\dagger U | x \rangle| = w_{\min}(V^\dagger U). \]

Note that the numerical range of each an $m \times m$ unitary matrix is a convex polygon with its $m$ vertex lying on the circumference of the disc with the unit radius. It follows that the value $w_{\min}(V^\dagger U)$ equals to the distance from the original point to the longest edge of the convex polygon. We therefore have that 

\[ w_{\min}(V^\dagger U) = \sqrt{1 - \left( \frac{d_{\max}(V^\dagger U)}{2} \right)^2}. \]

Thus, we complete the proof. \hfill \Box

We can understand this through Figure 1, where we describes the $m = 4$ case. Note that where all eigenvalues of $V^\dagger U$ lie on the circumference of the circle with the unit radius.

**Example 2.2** Applying the above theoretical analysis, we consider the approximate separation question of CNOT gates. The CNOT gate is of the following form: 

\[
\begin{pmatrix}
1 & 0 & 0 & 0 \\
0 & 1 & 0 & 0 \\
0 & 0 & 0 & 1 \\
0 & 0 & 1 & 0
\end{pmatrix}
\]

Assume that $U = \begin{pmatrix} u_{11} & u_{12} \\
u_{21} & u_{22} \end{pmatrix}$ and $V = \begin{pmatrix} v_{11} & v_{12} \\
v_{21} & v_{22} \end{pmatrix}$ are two $2 \times 2$ unitary matrices. Since a $2 \times 2$ unitary matrix with its four real parameters can be represented in the form 

\[
\begin{pmatrix}
e^{\alpha} & e^{-i\beta} \\
e^{i\beta} & e^{-\alpha} \end{pmatrix}
\begin{pmatrix}
\cos \frac{\gamma}{2} & -\sin \frac{\gamma}{2} \\
\sin \frac{\gamma}{2} & \cos \frac{\gamma}{2} \end{pmatrix}
\begin{pmatrix}
e^{-i\delta} & 0 \\
0 & e^{i\delta} \end{pmatrix}
\]

we denote $U, V$ by $U[\alpha_U, \beta_U, \gamma_U, \delta_U]$ and $V[\alpha_V, \beta_V, \gamma_V, \delta_V]$ respectively.

We find the $\epsilon$-approximate separation solution of CNOT by the following optimization problem:
A, B, C, D are eigenvalues of $V^\dagger U$. The quadrangle ABCD is the numerical range $W(V^\dagger U)$. The line segment AD is $d_{\text{max}}(V^\dagger U)$. Furthermore, the line segment OG equals to $w_{\min}(V^\dagger U)$, which is $F_{\min}(U, V)$. It is clear from the graph that the theorem holds true.

Maximize: $d_{\text{Max}}(U^\dagger \otimes V^\dagger \text{CNOT})$

subject to: $U, V$ are 2x2 unitary matrices

Since $U = U[\alpha_U, \beta_U, \gamma_U, \delta_U]$ and $V = V[\alpha_V, \beta_V, \gamma_V, \delta_V]$, $d_{\text{Max}}(U^\dagger \otimes V^\dagger \text{CNOT})$ is a non-negative function with eight parameters $f_m[\alpha_U, \beta_U, \gamma_U, \delta_U, \alpha_V, \beta_V, \gamma_V, \delta_V]$. Thus, the above optimization problem is equivalent to:

Maximize: $f_m[\alpha_U, \beta_U, \gamma_U, \delta_U, \alpha_V, \beta_V, \gamma_V, \delta_V]$

subject to: $\alpha_U, \beta_U, \gamma_U, \delta_U, \alpha_V, \beta_V, \gamma_V, \delta_V \in \mathbb{R}$

Applying the particle swarm optimization algorithm, we obtain the optimal output as $d_{\text{Max}}(U^\dagger \otimes V^\dagger \text{CNOT}) \approx 1.4159$, $U \approx U[218.0000, 157.0000, 159.0000, 471.0000]$, $V \approx V[633.0000, 84.0000, 628.0000, 387.0000]$. From Theorem 2.1, it follows that the corresponding value of the gate fidelity is approximately 0.7063. At the moment, the two unitary matrices that approximately separate the CNOT gate with $\epsilon \approx 1 - 0.7063 = 0.2937$ are in form

$$U = \begin{pmatrix} 0.4057 - 0.5795i & 0.5800 + 0.4040i \\ 0.5793 + 0.4049i & 0.4039 - 0.5808i \end{pmatrix}$$

and

$$V = \begin{pmatrix} 0.6724 + 0.7402i & -0.0016i \\ 0.0002 - 0.0016i & 0.7386 - 0.6741i \end{pmatrix}.$$
Next we make a numerical experiment on the above approximate separation shown above. Each one among 1000 random pure two-qubit states $|\psi\rangle$ is acted upon by CNOT and the tensor product $U \otimes V$ respectively. In Figure 2, for an arbitrary random two-qubit input $|\psi\rangle$, the values of the y-axis represent the Unh MLM fidelity of $\text{CNOT}(|\psi\rangle)$ and $U \otimes V(|\psi\rangle)$. It can be seen that the values of the y-axis is bounded from below by 0.7063, and part of them values are close to 1.

![Graph](image)

**Figure 2.** The numerical experiment on the approximate separation of CNOT.

**Conclusion and discussion**

In this paper, we proposed and discussed the approximate separation question, which has more practical import. Here we identified an interesting connection between gate fidelity and the numerical range of operators, and solved the approximate separation question of multipartite quantum gates based on the gate fidelity. Furthermore, we provided an example of the approximate separation of the CNOT gate.

**Acknowledgements** Thanks for comments. This work is partly supported by National Natural Science Foundation of China No. 11771011, 12071336. Correspondence should be addressed to K. He(hekanquantum@163.com).

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1. College of Mathematics, Taiyuan University of Technology, Taiyuan 030024, P. R. China;
2. Institute for Quantum Computing, Baidu Research, Beijing 100193, P. R. China

Email address, K. He: hekanquantum@163.com