From noncommutative optimal transport to limitations of quantum simulation

Peixue Wu

Institute for Quantum Computing, University of Waterloo

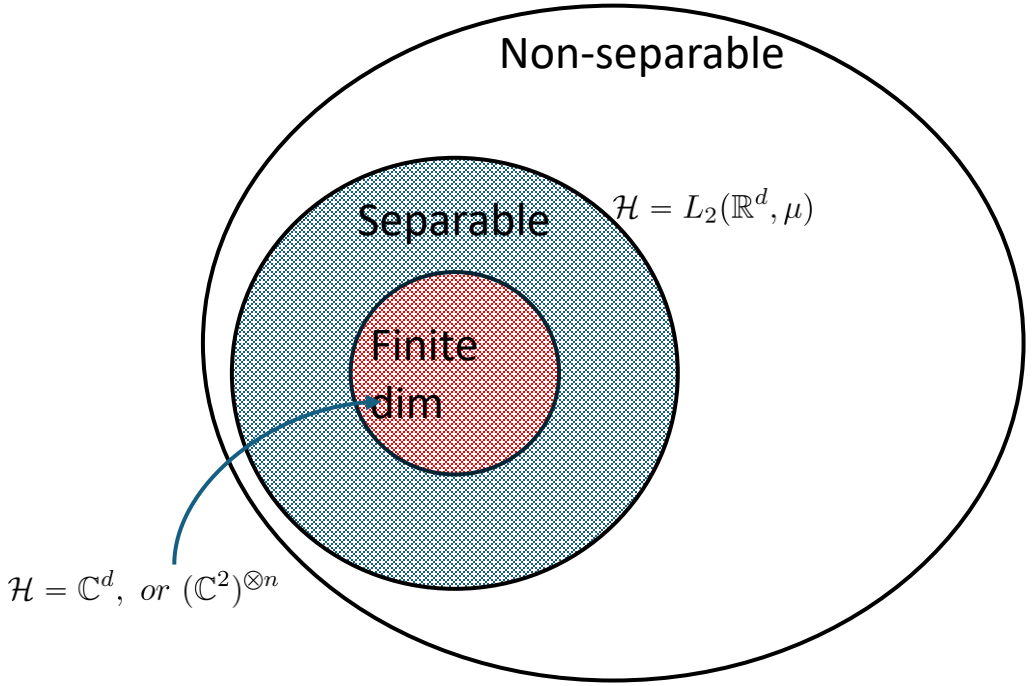
arXiv 2407.15357
arXiv 2303.11304

Discussion at IPAM

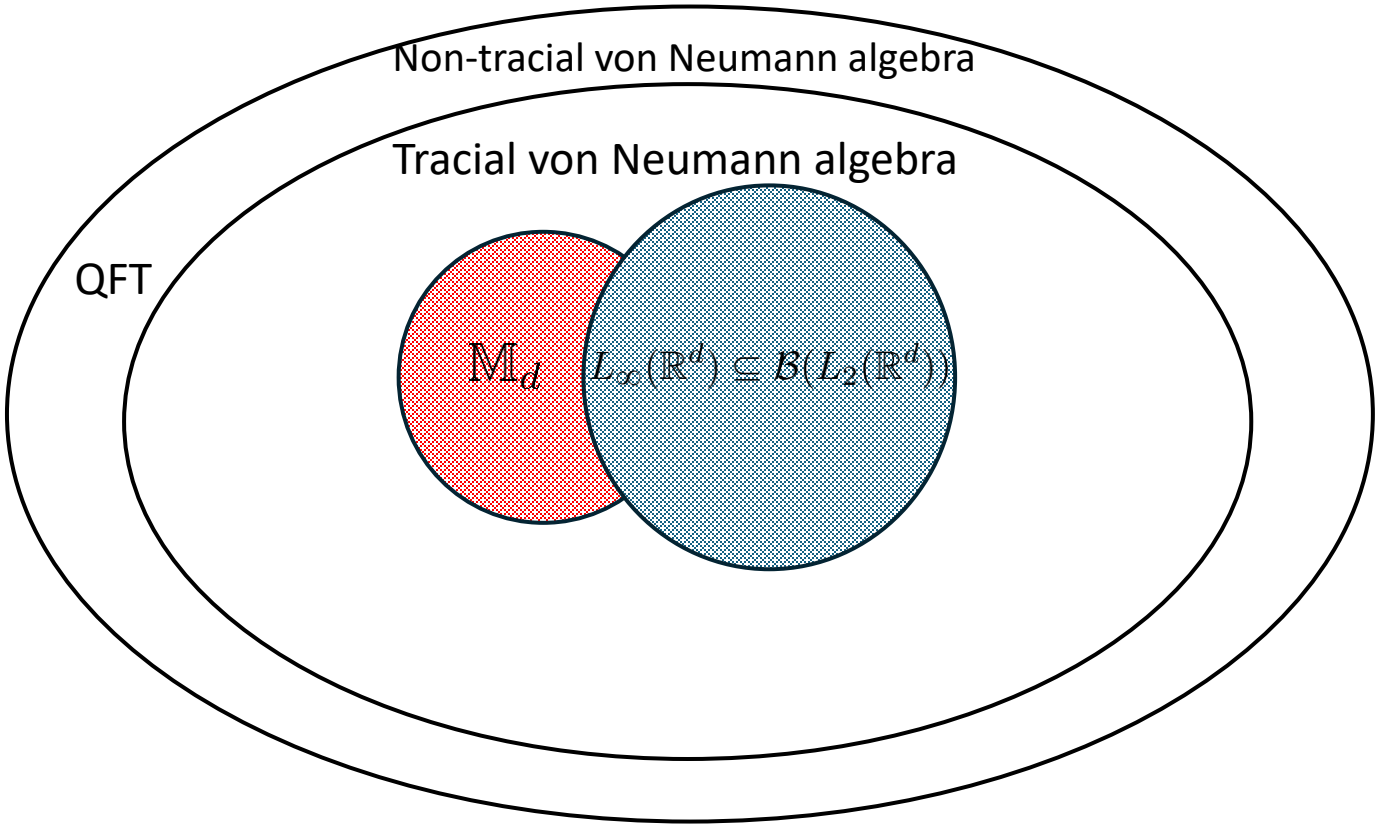
Discussion inside Junge team

Which Hilbert space do I live in?

We are living in a “Hilbert space” doing “algebra”



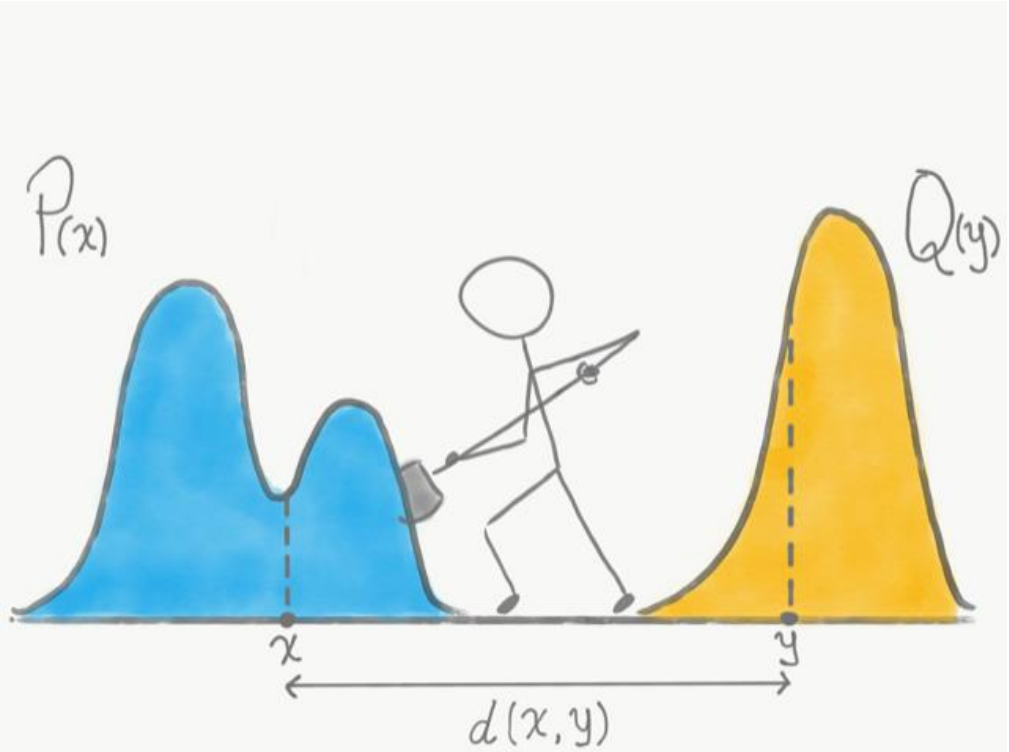
Hierarchy of Hilbert space



Hierarchy of algebras

Optimal transport theory

- What is the least “work” needed to reshape one probability distribution(state) into another?
- In the noncommutative setting, states are density operators(positive with trace 1) on a Hilbert space.
- Monge-Kantorovich transportation cost



$$\mathcal{T}(\rho,\sigma) = \inf_{\Pi \in \mathfrak{C}'(\rho,\sigma)} \mathrm{Tr}(C\Pi)$$

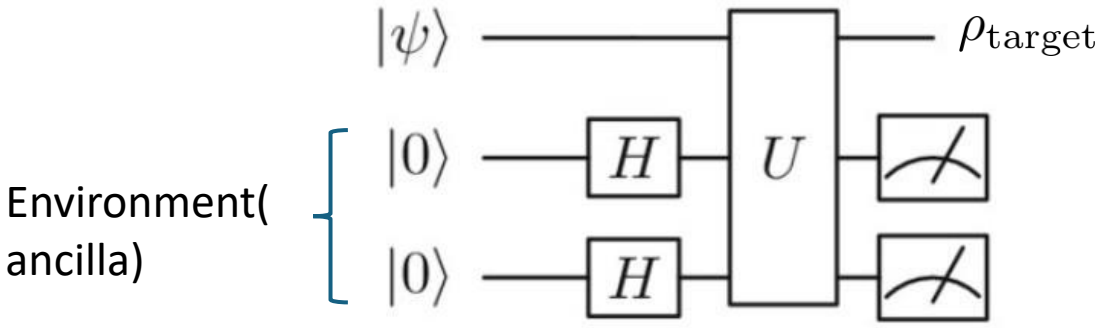
$\mathfrak{C}'(\rho,\sigma)$: a subset of couplings of ρ,σ.

C: a cost operator.

$$\mathcal{T}(\rho,\sigma) = \sup_{(A,B)\in\mathcal{B}_c} |\mathrm{Tr}(\rho A) - \mathrm{Tr}(\sigma B)|$$

$\mathcal{B}_c \subseteq \mathcal{B}(\mathcal{H}) \times \mathcal{B}(\mathcal{H})$: a suitably chosen dual pairs

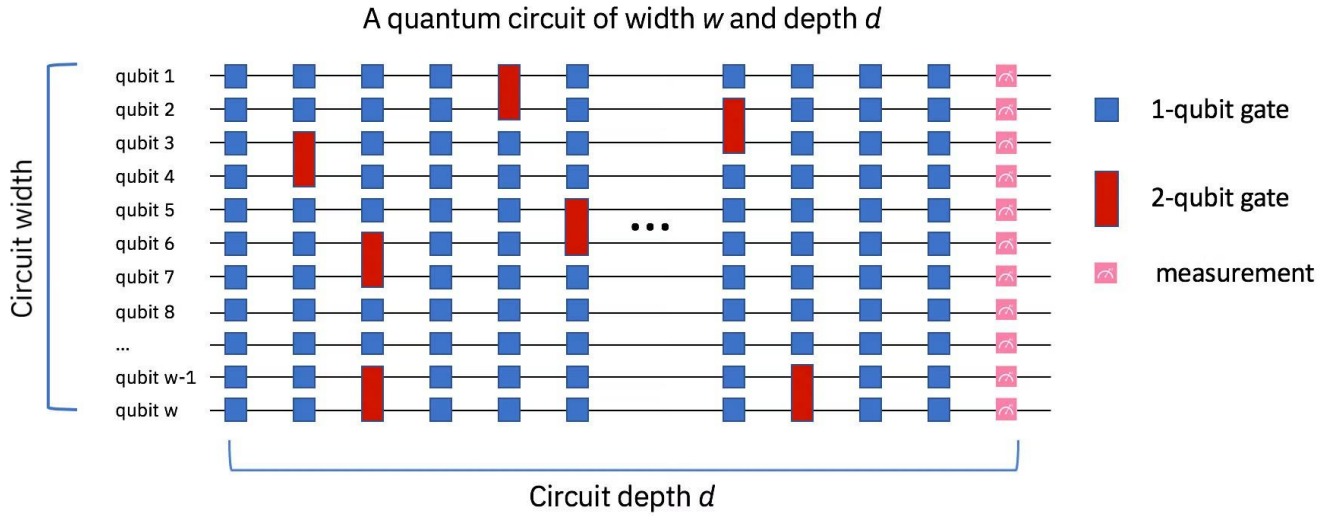
Quantum simulation



$$\text{Count}(U) = \min\{l \geqslant 1 : U = u_1 u_2 \cdots u_l, u_i \in S\}.$$

- Given an initial “easy” state and a target state, what is the minimal number of unitary operators to transform one to another?
- S is a set of “cheap” unitary operators
- A realistic case is the set S consists of
- each unitary touches only a few qubits

$V = \bigotimes_j U_j$



$$\text{Depth}(U) = \min\{l \geqslant 1 : U = V_1 \cdots V_l, V_i = \bigotimes_j U_j, U_j \text{ is } k-\text{local}\}.$$

Lower bound on quantum simulation: a summary

- Commutator (Triangle inequality) bound
- Geometric (Nielsen) approach: Geodesic length.
- Volume and covering arguments
- Schmidt-rank: lower bound on depth
- Lieb-Robinson velocity(continuous setting) and light cone argument(discrete setting)

Lower bound on quantum simulation: a summary

- Commutator (Triangle inequality) bound
- Geometric (Nielsen) approach: Geodesic length.
- Volume and covering arguments
- Schmidt-rank: lower bound on depth
- Lieb-Robinson velocity(continuous setting) and light cone argument(discrete setting)

This work!

Connection

- We show that the minimal number of gates or depth for a quantum simulation task can be lower bounded by the transportation cost, with the dual picture given by Connes 1989, Rieffel 2003.

The key ingredient is the commutator $[A, B] := AB - BA$, and the Lipschitz semi-norm

$$|||A|||_S := \sup_{s \in S} \|[s, A]\|_{op}. \tag{1}$$

The transportation cost from ρ to σ is defined by

$$W_S(\rho, \sigma) = \sup_{|||A|||_S \leqslant 1, A = A^\dagger} \mathrm{Tr}(\rho A) - \mathrm{Tr}(\sigma A) \tag{2}$$

Exercise 1

$$\mathrm{Count}(U) := \min\{l \geqslant 1 : U = u_1 u_2 \cdots u_l, u_i \in S\}.$$

$$\mathrm{Count}(U) \geqslant \frac{\|[U, x]\|_{op}}{\sup_{u \in S} \|[u, x]\|_{op}}, \quad x \in \mathcal{B}(\mathcal{H}).$$

It is a well-known commutator triangle inequality. Suppose $U = u_1 \cdots u_l$, using the Leibniz rule for commutators, $[AB, C] = A[B, C] + [A, C]B$, and triangle inequalities,

$$\begin{aligned}
\|[u_1 \cdots u_l, x]\|_{op} &\leqslant \|u_l[u_{l-1} \cdots u_1, x]\|_{op} + \|[u_l, x]u_{l-1} \cdots u_1\|_{op} \\
&\leqslant \|[u_{l-1} \cdots u_1, x]\|_{op} + \|[u_l, x]\|_{op} \\
&\leqslant \sum_{i=1}^{l} \|[u_i, x]\|_{op} \leqslant l \sup_i \|[u_i, x]\|_{op}.
\end{aligned}$$

Exercise 2

$$\mathrm{Depth}(U) = \min\{l \geqslant 1 : U = V_1 \cdots V_l, V_i = \bigotimes_j U_j, U_j \text{ is } k-\text{local}\}.$$

Suppose S is the set of 1-local Pauli operators.

$$(2k)^{\mathrm{Depth}(U)} \geqslant \frac{\sup_{P\in S} \|[P, U^\dagger x U]\|_{op}}{\sup_{P\in S} \|[P, x]\|_{op}}, \forall x \in \mathcal{B}(\mathcal{H}).$$

For any $P \in S$, $V = \bigotimes_j U_j$, we have

$$\begin{aligned}
\|[P, V^\dagger x V]\|_{op} &= \|[VPV^\dagger, x]\|_{op} \\
&= \|[U_j P U_j^\dagger, x]\|_{op}, \ U_j \text{ is } k-\text{local} \\
&= \|[U_j P U_j^\dagger, x - \mathrm{tr}_k(x) \otimes \mathbb{I}_k/2^k]\|_{op} \\
&= \|[P, U_j^\dagger (x - \mathrm{tr}_k(x) \otimes \mathbb{I}_k/2^k) U_j]\|_{op} \\
&\leqslant 2\|P U_j^\dagger (x - \mathrm{tr}_k(x) \otimes \mathbb{I}_k/2^k) U_j\|_{op} \\
&= 2\|x - \mathrm{tr}_k(x) \otimes \mathbb{I}_k/2^k\|_{op} \\
&= 2\|\frac{1}{2^k} \sum_{P_k \in S_k} (x - P_k x P_k)\|_{op} \\
&\leqslant 2 \sup_{P_k \in S_k} \|[P_k, x]\|_{op} \leqslant 2k \sup_{P\in S} \|[P, x]\|_{op}
\end{aligned}$$

S_k is the set of k-local Pauli operators.

$$\|[P_k, x]\|_{op} \leqslant k \sup_{P\in S} \|[P, x]\|_{op}.$$

Apply the inequality l times,

$$\begin{aligned}
&\|[P, (V_1 \cdots V_l)^\dagger x (V_1 \cdots V_l)]\|_{op} \\
&\leqslant (2k)^l \sup_{P\in S} \|[P, x]\|_{op}.
\end{aligned}$$

Two quantities

- Motivated by the previous calculations, we introdu the following quantities for quantum circuits, or m generally, quantum channels.

$$\mathrm{Cost}_S(\Phi) := \sup_{x=x^\dagger, |||x|||_S \leqslant 1} \|\Phi^*(x) - x\|_{op}, \tag{1}$$

$$\mathrm{Lip}_S(\Phi) := \sup_{x=x^\dagger, |||x|||_S \leqslant 1} |||\Phi^*(x)|||_S. \tag{2}$$

The first quantity, called transportation cost of channels(also named as Lipschitz cost), provides a lower bound on the volume(number of unitary operators). The second quantity, called Lipschitz constant, provides a lower bound on the depth.

Wasserstein metric

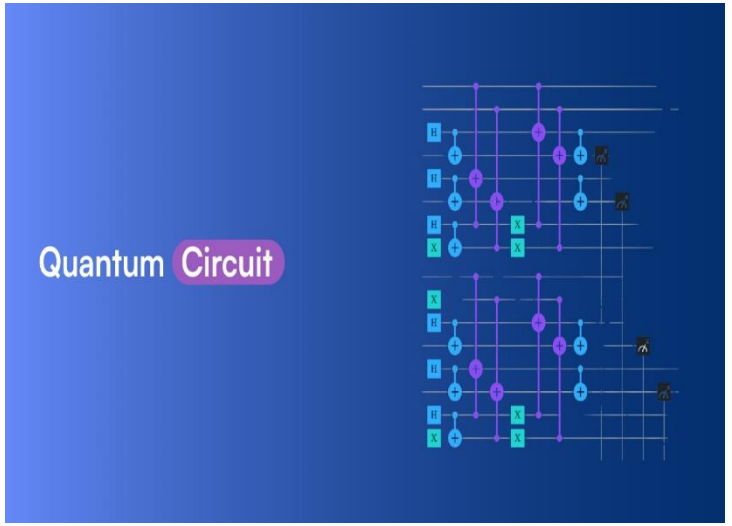
The first quantity is the maximal cost from any state to Φ. The second quantity is the contraction coefficient under the Wasserstein metric.

$$\mathrm{Cost}_S(\Phi) := \sup_{\rho} W_S(\rho, \Phi(\rho)), \tag{1}$$

$$\mathrm{Lip}_S(\Phi) := \sup_{\rho \neq \sigma} \frac{W_S(\Phi(\rho), \Phi(\sigma))}{W_S(\rho, \sigma)}. \tag{2}$$

Limitations on simulation of Lindblad dynamics

Strong quantum Church-Turing thesis:
Every quantum mechanical computational process can be simulated efficiently in the unitary circuit model of quantum computation.



Lindbladian generator:

$$L(\rho) = \underbrace{-i[H,\rho]}_{\text{coherent part}} + \sum_{j=1}^{m} \underbrace{L_{V_j}(\rho)}_{\text{dissipative part}} \quad , \quad L_V(\rho) = \underbrace{V\rho V^\dagger}_{\text{Jump}} - \frac{1}{2}\underbrace{(V^\dagger V\rho + \rho V^\dagger V)}_{\text{No jump}}.$$

Q: Given a set of accessible unitary circuits (gates), what is the minimum number of gates (simulation cost) required to approximate an open quantum system at a target time T?

Preparing Gibbs state via Lindbladians

Given a Hamiltonian on n-qubit system, how do we design a Lindbladian such that it converges to the Gibbs state

$$\rho_\beta = \frac{\exp(-\beta H)}{\mathrm{Tr}(\exp(-\beta H))}, \beta \in (0, \infty)$$

Idea: design a Lindbladian admitting the Gibbs state as the unique fixed state. To ensure mixing fast, we assume symmetry property.

Gibbs state sampler: KMS and GNS symmetry

- There are two typical choices for the Gibbs sampler:
- GNS symmetry:

$$\mathrm{Tr}(\rho_\beta \mathcal{L}_\beta(X)Y) = \mathrm{Tr}(\rho_\beta X \mathcal{L}_\beta(Y)).$$

- KMS symmetry:

$$\mathrm{Tr}\left(\rho_\beta^{1/2} \mathcal{L}_\beta(X) \rho_\beta^{1/2} Y\right) = \mathrm{Tr}\left(\rho_\beta^{1/2} X \rho_\beta^{1/2} \mathcal{L}_\beta(Y)\right).$$

The issue with GNS Gibbs sampler

- GNS detailed balance is equivalent to the Lindbladian generator commuting with the modular automorphism group:

$$\sigma_t^{\rho_\beta}(X) := \rho_\beta^{it} X \rho_\beta^{-it}.$$

- The jump operators must be the eigen-operators of the modular automorphism group (see the remark in Carlen-Maas).
- Physically, it means the dissipation channel must “know about” the entire spectrum of the Hamiltonian.
- By energy-time uncertainty principle, it requires exponential time to implement.

Why KMS Gibbs sampler is a remedy

- Recall that a Lindbladian generator satisfies KMS-symmetry, if and only if

$$\mathcal{L}(X) = i[G, X] + \sum_j L_{V_j},$$

$$\Delta_\sigma^{1/2}(V_j) = V_j^\dagger \text{ and}$$

$$G = -i \tanh\left(\log\left(\Delta_\sigma^{1/4}\right)\right)\left(\frac{1}{2}\sum_j V_j^\dagger V_j\right).$$

KMS Gibbs sampler

- To design a KMS Gibbs sampler, we choose the jump operator as

$$V_j = \int_0^\infty f_\beta(t) \exp(iHt)\sigma_j \exp(-iHt)dt, \tag{1}$$

here σ_j is the set of single Pauli gates

- The function is a nicely chosen function, usually Gaussian type.
- We choose the Hamiltonian part to make sure the Lindbladian is KMS symmetric. Implementing this Lindbladian only needs Hamiltonian evolution + energy-gap filters which have polynomially many circuits.

Theorem(Ding, Junge, Schleich, W.): Limitations of this simulation algorithm

- Using the Hamiltonian and energy-gap filters, when the temperature is very high, any simulation algorithm must incur a simulation cost satisfying

$$\mathrm{Cost}(T_t) \geqslant c \cdot t \left(\lambda_{\max}(H) - \lambda_{\min}(H)\right)$$

  for small constant time t and universal constant $c > 0$.

- Our method is restrictive to rapid mixing dynamics.
- When the temperature is very low, B. Kiani's talk in workshop I showed that the mixing time is slow.
- Modified Log-Sobolev inequality is completely open: find a non-GNS and KMS-symmetric Lindbladian admitting the Gibbs state of a non-commuting Hamiltonian as the fixed state, such that MLSI fails.
- An alternative approach for mixing time is

$$\mathrm{Lip}(T_t) \leqslant c \exp(-\lambda t)$$

lower bound on the depth of a quantum channel

Suppose Φ is a quantum channel on $\mathcal{B}\left(\bigotimes_{i=1}^{n}\mathcal{H}_i\right)$ of layer L

$$\Phi=\prod_{\ell=1}^{L}\Phi_\ell.$$

Then for any resource set,

$$S^n\subseteq\mathcal{B}\left(\bigotimes_{i=1}^{n}\mathcal{H}_i\right)$$

we have

$$L\geqslant\frac{\log\left(\mathrm{Lip}_{S^n}(\Phi)\right)}{\log\left(\max_{1\leqslant\ell\leqslant L}\mathrm{Lip}_{S^n}(\Phi_\ell)\right)}.$$

A concrete lower bound on the Lipschitz constant by measurement on the output state

- In n-qubit system with orthonormal basis

$$\{|\psi_x\rangle\}_{x\in\mathcal{X}}, \text{ where } \mathcal{X} = \{0,1\}^n \text{ and } S^n \subseteq \mathcal{B}(\mathcal{H}).$$

- $\text{Initial state: } \rho_{in}\text{; output state: } \sigma = \Phi(\rho_{in}).$

- Define $\mu_\sigma(x) = \langle\psi_x|\,\sigma\,|\psi_x\rangle, \quad x \in \mathcal{X}. \qquad (1)$

- Note that in the literature, the orthonormal basis is chosen as the computational basis. Here we do not assume that.

Main result(DJSW25+)

- If Φ is a circuit, then the Lipschitz constant of Φ must satisfy

$$\mathrm{Lip}_{S^n}(\Phi) \geqslant \frac{\min_{x\in A, y\in B} |f(x)-f(y)|}{|||O_f|||_{S^n}} \times \frac{1}{\left(\mu_\sigma(A)^{-\frac{1}{2}} + \mu_\sigma(B)^{-\frac{1}{2}}\right)\sqrt{Poinc_2(\rho_{in})}},$$

  for any A, B *and* f. $Poinc_2(\rho) = \sup_{|||O|||_{S^n}\leqslant 1} \mathrm{tr}\left(\rho O^2 - \mathrm{tr}(\rho O)^2\right)$

- Note that if we choose the orthonormal basis as the computational basis, it recovers the well-known Harrow-Lidar argument (well-spread property for the output state).
- Answering a question during M. Marvian's talk.

Reference

- Araiza, R., Chen, Y., Junge, M., and Wu, P. (2023). Resource-dependent complexity of quantum channels. arXiv preprint arXiv:2303.11304
- Araiza, R., Junge, M., and Wu, P. (2023). Transportation cost and Contraction coefficient for channels on von Neumann algebras, 2025, preprint
- Ding, Z., Junge, M., Schleich, P., and Wu, P. (2025). Lower bound for simulation cost of open quantum systems: Lipschitz continuity approach. Communications in Mathematical Physics, 406(3), 60
- Ding, Z., Junge, M., Schleich, P., and Wu, P. (2025). Quantifying simulation depth and volume of quantum channels via their Lipschitz constant, 2025, preprint.