Turning States into Unitaries: Optimal Sample-Based Hamiltonian Simulation

Shelby Kimmel

Cedric Lin (QuICS)
Guang Hao Low (MIT)
Maris Ozols (Cambridge)
Ted Yoder (MIT)
Turning States Into Unitaries

\[ \rho \rightarrow e^{-i\rho t}\sigma e^{i\rho t} \]

(normally \( e^{-iHt} \), for \( H \) Hermitian, but density matrices are Hermitian!)
Turning States Into Unitaries

\[ e^{-i\rho t} \sigma e^{i\rho t} \]
Turning States Into Unitaries

\[ \rho \]

\[ e^{-i\rho t} \sigma e^{i\rho t} \]
Turning States Into Unitaries

\[ \rho \]

\[ e^{-i\rho t} \sigma e^{i\rho t} \]
Turning States Into Unitaries

\[ e^{-i\rho t} \sigma e^{i\rho t} \]
Question

Are global necessary or are local-sequential operations sufficient?
Answer

Are global necessary or are local-sequential operations sufficient?

Local are sufficient!
Are global necessary or are local-sequential operations sufficient?

Local are sufficient!

Applications:
• Quantum software
• Tomographic applications (e.g. anti-swap test)
• Decomposing mixed state into component pure states
Outline

1. Hamiltonian simulation
2. LMR (Lloyd, Mohseni, Rebentrost) Protocol & Optimality
3. Protocols & Applications of Sample-Based Hamiltonian Simulation
Hamiltonian Simulation

Classical Description:

- Input: \( H = V(x) + \frac{\hat{p}^2}{2m} \)
- Cost: time, gates
- Method: e.g. Trotter-Suzuki

Black Box Description:

- Input: \( i \rightarrow \) non-zero elements of \( i^{th} \) row of \( H \)
- Cost: uses of box
- Method: (sparse) Low, Chuang / Berry, Childs, Kothari,
Sample-Based Hamiltonian Simulation

Density Matrix Description:

Input: Quantum states: $\rho^\otimes n \otimes \sigma$, Parameters: $t, \delta \in \mathbb{R}$

Cost: $n$, (copies of $\rho$)

Output: $e^{-i\rho t} \sigma e^{i\rho t}$ to error $\delta$ in trace distance
Outline

1. Hamiltonian simulation
2. LMR (Lloyd, Mohseni, Rebentrost ‘14) Protocol & Optimality
3. Protocols & Applications of Sample-Based Hamiltonian Simulation
LMR Protocol

$\rho$

source

$\sigma$
LMR Protocol

ρ

source

ρ σ
Partial SWAP: \[ e^{i\epsilon S} = \cos(\epsilon)\mathbb{I} - i \sin(\epsilon) S \]

\[ S = SWAP \]
LMR Protocol

\[ \tilde{\rho} \leftrightarrow \tilde{\sigma} \]

\( \rho \) source
LMR Protocol

\[ \rho \]

source

\[ \tilde{\rho} \]

\[ \tilde{\sigma} \]
LMR Protocol
LMR Protocol

\[ \rho \rightarrow \rho \tilde{\sigma} \]
LMR Protocol

Partial SWAP: $e^{i\epsilon S} = \cos(\epsilon)\mathbb{I} - i \sin(\epsilon) S$

$S = \text{SWAP}$
LMR Protocol

\( \rho \)

source

\( \tilde{\rho} \leftrightarrow \tilde{\sigma}' \)
LMR Protocol

ρ

source

ρ'
LMR Protocol

\[ tr_B \left[ e^{-i\epsilon S} (\sigma_A \otimes \rho_B) e^{i\epsilon S} \right] = e^{-i\rho \epsilon} \sigma e^{i\rho \epsilon} + O(\epsilon^2) \]
LMR Protocol

\[
tr_B \left[ e^{-i\epsilon S} (\sigma_A \otimes \rho_B) e^{i\epsilon S} \right] = e^{-i\rho \epsilon} \sigma e^{i\rho \epsilon} + O(\epsilon^2)
\]

\[
\epsilon = \delta / t, \text{ repeat } t^2 / \delta \text{ times: } e^{-i\rho t} \sigma e^{i\rho t} + O(\delta)
\]
LMR Protocol

\[ tr_B \left[ e^{-i\varepsilon S} (\sigma_A \otimes \rho_B) e^{i\varepsilon S} \right] = e^{-i\rho \varepsilon} \sigma e^{i\rho \varepsilon} + O(\varepsilon^2) \]

\[ \varepsilon = \delta/t, \text{ repeat } t^2/\delta \text{ times: } e^{-i\rho t} \sigma e^{i\rho t} + O(\delta) \]

Uses \( O(t^2/\delta) \) samples
LMR Seems Too Simple

- Could we do better using global op?

\[ \rho \quad \sigma \]

\( \rho \) source
LMR Seems Too Simple

- Could we do better using global op?
LMR Seems Too Simple

- Could we do better using global op?

- E.g, near optimal tomography of $\rho$ requires global operation (1,2)

1. Haah et al., 2015
2. O’Donnell, Wright 2015
LMR Seems Too Simple

- Could we do better using global op?

- Suppose use tomography to get estimate $\tilde{\rho}$ of $\rho$, then implement $H = \tilde{\rho}$
  - Worse Scaling!
    - Tomography scales with dimension and rank of $\rho$
    - For constant dimension, scaling with precision is worse by square root factor!
LMR Seems Too Simple

- Change tactics: instead of trying to improve on LMR by using global operations, can we prove LMR is optimal!
Lower Bound Sketch

I. Proof by Contradiction:

Task:

Task requires $n$ samples

If could do sample-based Hamiltonian simulation better than LMR, could do task with fewer than $n$ samples
Lower Bound Sketch

I. Proof by Contradiction:

Task: Decide if $\rho$ is $\begin{bmatrix} 1/2 & 0 \\ 0 & 1/2 \end{bmatrix}$ or $\begin{bmatrix} 1/2 + \epsilon & 0 \\ 0 & 1/2 - \epsilon \end{bmatrix}$, with probability $\geq 2/3$

Task requires $n$ samples of $\rho$: $n = \Omega \left( \frac{1}{\epsilon^2} \right)$. (Bound uses trace distance)

If could do sample-based Hamiltonian simulation better than LMR, could do task with fewer than $n$ samples
Lower Bound Sketch

I. Proof by Contradiction:

Task: Decide if $\rho$ is $\begin{bmatrix} 1/2 & 0 \\ 0 & 1/2 \end{bmatrix}$ or $\begin{bmatrix} 1/2 + \epsilon & 0 \\ 0 & 1/2 - \epsilon \end{bmatrix}$, with probability $\geq 2/3$

Task requires $n$ samples of $\rho$: $n = \Omega \left( \frac{1}{\epsilon^2} \right)$. (Bound uses trace distance)

- $\exp[-i\rho t] = \begin{cases} 
\mathbb{I} & \text{when } \rho \text{ is max. mixed} \\
Z & \text{when } \rho \text{ is not max. mixed and } t = \frac{\pi}{2\epsilon} 
\end{cases}$

If could do sample-based Hamiltonian simulation for time $t$ and accuracy $1/3$ with fewer than $\Omega(t^2)$ samples $\rightarrow$ contradiction
Lower Bound Sketch

Let $f(t, \delta)$ be the number of samples required to simulate $H = \rho$ for time $t$ to accuracy $\delta$ using an optimal protocol.

Part I $\Rightarrow f\left(t, \frac{1}{3}\right) = \Omega(t^2)$
Lower Bound Sketch

Let \( f(t, \delta) \) be the number of samples required to simulate \( H = \rho \) for time \( t \) to accuracy \( \delta \) using an optimal protocol.

Part I \( \Rightarrow f\left(t, \frac{1}{3}\right) = \Omega(t^2) \)

II. Concatenation

Suppose can simulate \( H = \rho \) for time \( \tau \) to accuracy \( \delta \)
Then can simulate \( H = \rho \) for time \( m\tau \) to accuracy \( m\delta \) by repeating \( m \in \mathbb{Z}^+ \) times
Lower Bound Sketch

Let $f(t, \delta)$ be the number of samples required to simulate $H = \rho$ for time $t$ to accuracy $\delta$ using an optimal protocol.

Part I $\Rightarrow f\left(t, \frac{1}{3}\right) = \Omega(t^2)$

II. Concatenation

Suppose can simulate $H = \rho$ for time $\tau$ to accuracy $\delta$ Then can simulate $H = \rho$ for time $m\tau$ to accuracy $m\delta$ by repeating $m \in \mathbb{Z}^+$ times:

$$f(m\tau, m\delta) \leq mf(\tau, \delta)$$
Lower Bound Sketch

Let $f(t, \delta)$ be the number of samples required to simulate $H = \rho$ for time $t$ to accuracy $\delta$ using an optimal protocol.

Part I $\Rightarrow f\left(t, \frac{1}{3}\right) = \Omega(t^2)$

II. Concatenation

Suppose can simulate $H = \rho$ for time $\tau$ to accuracy $\delta$
Then can simulate $H = \rho$ for time $m\tau$ to accuracy $m\delta$ by repeating $m \in \mathbb{Z}^+$ times:

$$f(m\tau, m\delta) \leq mf(\tau, \delta)$$

- $m\delta$ can be $1/3$
- $\delta$ can be small!

$f(t, \delta) = \Omega(t^2/\delta)$
Lower Bound Sketch

Proof sketch used mixed states, but using similar ideas, can prove also optimal for pure states.
Application of Lower Bound Technique

State-based Grover Search:

Given:

- \( O_S \) s.t. \( O_S |\psi\rangle|b\rangle = \begin{cases} 
|\psi\rangle|b \oplus 1\rangle & \text{if } |\psi\rangle \in S, \text{ for } S \text{ a subspace of } \mathbb{C}^{2^n} \\
|\psi\rangle|b\rangle & \text{otherwise} 
\end{cases} 

- Sample access to an unknown state \( |\phi\rangle \)

Decide: Is overlap of \( |\phi\rangle \) with \( S \) zero or \( \lambda \), promised one is the case, using as few copies of \( |\phi\rangle \) possible.
Application of Lower Bound Technique

State-based Grover Search:

Normally: $O\left(\frac{1}{\sqrt{\lambda}}\right)$ uses of $O_S$

In our case: We show require $\Omega\left(\frac{1}{\lambda}\right)$ copies of $|\phi\rangle$

Why:
- In Grover’s algorithm, need to reflect about $|\phi\rangle$, but given only sample access to $|\phi\rangle$, this is difficult!
- Can use Hamiltonian simulation, but not very efficient.
Outline

1. Hamiltonian simulation
2. LMR (Lloyd, Mohseni, Rebentrost) Protocol & Optimality
3. Protocols & Applications of Sample-Based Hamiltonian Simulation
Split Simulation

Suppose can prepare the state

$$\rho' = |0\rangle\langle 0| \otimes \rho_+ + |1\rangle\langle 1| \otimes \rho_-$$

Where $\rho_+, \rho_- \geq 0$ are subnormalized states, but $\rho_+ + \rho_-$ is a normalized state. Then can simulate

$$H = \rho_+ - \rho_-$$

for time $t$, accuracy $\delta$, using $O\left(\frac{t^2}{\delta}\right)$ copies of $\rho'$
Split Simulation

Suppose can prepare the state

\[ \rho' = |0\rangle\langle 0| \otimes \rho_+ + |1\rangle\langle 1| \otimes \rho_- \]

Where \( \rho_+, \rho_- \geq 0 \) are subnormalized states, but \( \rho_+ + \rho_- \) is a normalized state. Then can simulate

\[ H = \rho_+ - \rho_- \]

for time \( t \), accuracy \( \delta \), using \( O\left(\frac{t^2}{\delta}\right) \) copies of \( \rho' \)

- Idea: Apply unitary

\[ |0\rangle\langle 0| \otimes e^{-iS\epsilon} + |1\rangle\langle 1| \otimes e^{iS\epsilon} \]
Split Simulation

Suppose can prepare the state

\[ \rho' = |0\rangle \langle 0| \otimes \rho_+ + |1\rangle \langle 1| \otimes \rho_- \]

Where \( \rho_+, \rho_- \gtrsim 0 \) are subnormalized states, but \( \rho_+ + \rho_- \) is a normalized state. Then can simulate

\[ H = \rho_+ - \rho_- \]

for time \( t \), accuracy \( \delta \), using \( O \left( \frac{t^2}{\delta^2} \right) \) copies of \( \rho' \)

- Idea: Apply unitary

\[ |0\rangle \langle 0| \otimes e^{-iS\epsilon} + |1\rangle \langle 1| \otimes e^{iS\epsilon} \]

to state

\[ (|0\rangle \langle 0| \otimes \rho_+ + |1\rangle \langle 1| \otimes \rho_-) \otimes \sigma \]

then discard system
Commutator/Anti-commutator Simulation

Given: \( \rho_1, \rho_2 \)

Simulate: \( H = i[\rho_1, \rho_2] \) or \( H = \{\rho_1, \rho_2\} \) for time \( t \), error \( \delta \)
Commutator/Anti-commutator Simulation

\[ \frac{1}{\sqrt{2}} |0\rangle + \frac{e^{i\phi}}{\sqrt{2}} |1\rangle \]

\[ \rho_1 \]

\[ \rho_2 \]

- Claim output of circuit is:

\[ |0\rangle\langle 0| \otimes \rho_+ + |1\rangle\langle 1| \otimes \rho_- \]

where

\[ \rho_+ - \rho_- = \frac{1}{2} (e^{i\phi} \rho_1 \rho_2 + e^{-i\phi} \rho_2 \rho_1) \]
Commutator/Anti-commutator Simulation

Given: $\rho_1, \rho_2$

Simulate: $H = i[\rho_1, \rho_2]$ or $H = \{\rho_1, \rho_2\}$ for time $t$, error $\delta$

Uses $\Theta(t^2/\delta)$ samples
Applications of Commutator Simulation

- **State Addition:**
  \[ e^{i [\psi_1 \langle \psi_1 | \psi_2 \langle \psi_2 ]} t \] is a rotation of the 2-D subspace spanned by \( |\psi_1\rangle \) and \( |\psi_2\rangle \).* Can rotate \( |\psi_1\rangle \) to \( \alpha |\psi_1\rangle + \beta |\psi_2\rangle \).

- **Orthogonality Testing:**
  Commutator of two orthogonal states is 0. Commutator simulation gives optimal strategy to test orthogonality (square root improvement over swap test).

* For \( \langle \psi_1 | \psi_2 \rangle = \lambda \neq 0 \)
| Given:       | $\rho_1, \rho_2, \ldots, \rho_k$ |
| Simulate:    | $H = e^{i\phi} \rho_1 \rho_2 \ldots \rho_k + e^{-i\phi} \rho_k \rho_{k-1} \ldots \rho_1$ |
Jordan-Lie Algebra Simulation

\[
\frac{1}{\sqrt{2}} |0\rangle + \frac{e^{i\phi}}{\sqrt{2}} |1\rangle
\]

\[S: (1 \rightarrow 2, 2 \rightarrow 3 \ldots k \rightarrow 1)\]

\[\rho_+ - \rho_- = \frac{1}{2} (e^{i\phi} \rho_1 \rho_2 \ldots \rho_k + e^{-i\phi} \rho_k \ldots \rho_2 \rho_1)\]
Jordan-Lie Algebra Simulation

Given: \( \rho_1, \rho_2, \ldots, \rho_k \), and \( a_1, a_2, \ldots, a_k \in \mathbb{R} \)

Simulate: \( H = \sum_j a_j (e^{i\phi j} \rho_{r_1} \rho_{r_2} \ldots \rho_{r_{|j|}} + e^{-i\phi j} \rho_{r_{|j|}} \rho_{r_{|j|-1}} \ldots \rho_{r_1}) \)
Jordan-Lie Algebra Simulation

Given: \( \rho_1, \rho_2, \ldots, \rho_k, \) and \( a_1, a_2, \ldots, a_k \in \mathbb{R} \)

Simulate: \( H = \sum_j a_j (e^{i\phi_j} \rho_{r_1} \rho_{r_2} \ldots \rho_{r_{|j|}} + e^{-i\phi_j} \rho_{|j|} \rho_{|j|-1} \ldots \rho_{r_1}) \)

Uses \( O(La^2t^2/\delta) \) samples total

- \( L = \max_j |j_k| \)
- \( a = \sum_j |a_j| \)
Final application: Universal Model of QC

• **Fact 1:**
  Partial SWAP (Heisenberg exchange) + single qubit gates are universal for quantum computing. [3] (In particular, arbitrary single qubit X and Z rotations).

• **Fact 2:**
  - $e^{-i\rho t}$ with $\rho = |+\rangle\langle +|$ give arbitrary X rotations
  - $e^{-i\rho t}$ with $\rho = |0\rangle\langle 0|$ give arbitrary Z rotations

• **Consequence:**
  Heisenberg exchange plus source of $|+\rangle$ and $|0\rangle$ states is universal for quantum computing (with polynomial overhead.)

Open Questions

1. Is general Jordan Lie algebra simulation optimal?
2. Copyright protection?
3. Other applications?