Turning States into Unitaries: Optimal Sample-Based Hamiltonian Simulation

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Turning States Into Unitaries

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

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

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Turning States Into Unitaries

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

$$e^{-i\rho t} \sigma e^{i\rho t}$$
Answer

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

1. Hamiltonian simulation
2. LMR (Lloyd, Mohseni, Rebentrost) Protocol & Optimality
3. Protocols & Applications of Sample-Based Hamiltonian Simulation
   a) Sum of states simulation
   b) Commutator simulation
   c) Lie Algebra simulation
4. Fun final application
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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: $i \rightarrow \text{non-zero elements of } i^{th} \text{ row of } H$
- Cost: uses of box
- Method: (sparse) Low, Chuang / Berry, Childs, Kothari,
Sample-Based Hamiltonian Simulation

Density Matrix Description:

Input: \[ H = \rho \]
Cost: copies of \( \rho \)
Sample-Based Hamiltonian Simulation

Density Matrix Description:

Input: \( H = \rho \) \((\rho^\otimes n \otimes \sigma, \ t)\)

Cost: copies of \( \rho \)

Output: \( e^{-i\rho t} \sigma e^{i\rho t} \) (to error \( \delta \) in trace distance)
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LMR Protocol
LMR Protocol

ρ
source

ρ σ
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

\[ \rho \text{ source} \]
LMR Protocol

ρ
source

→

ρ   ~σ
LMR Protocol

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LMR Protocol

\(\rho\) source

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

\( \rho \) source

\( \tilde{\rho} \)

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

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

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

\( \epsilon = \delta/t, \) repeat \( t^2/\delta \) times: \( e^{-i\rho t} \sigma e^{i\rho t} + O(\delta) \)
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Uses \( O(t^2/\delta) \) samples
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- LMR Application: Quantum Machine Learning
LMR Protocol

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

- LMR Application: Quantum Machine Learning
  - Generate quantum descriptions of eigenstates of low rank density matrices (modulo errors in protocol that we can fix)
LMR Seems Too Simple

- Could we do better using global op?
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\[ \rho \text{ source} \rightarrow \rho, \sigma \]
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?

- How about tomography? 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

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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.
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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 $O(t^2)$ samples → 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 $\Rightarrow f\left(t, \frac{1}{3}\right) = \Omega(t^2)$
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II. Concatenation

If 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:

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

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\[
f(m\tau, m\delta) \leq mf(t, \delta)
\]

\( m\delta \) 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

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

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.
Application of Lower Bound

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Sum of States Simulation

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

Simulate: \( H = \sum_i a_i \rho_i \)
# Sum of States Simulation

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Create: \( e^{-iHt} \sigma e^{-iHt} \) (to error \( \delta \) in trace distance)

Our Protocol: uses \( n_j = O \left( \frac{|a_j|a t^2}{\delta} \right) \), where \( a = \sum_i |a_i| \)
Commutator Simulation

Given: \( \rho_1, \rho_2 \)
Simulate: \( H = i[\rho_1, \rho_2] \)

Given: \( \rho_1 \otimes^n \otimes \rho_2 \otimes^n \otimes \sigma \) (\( \rho, \sigma \) arbitrary states)
Create: \( e^{[\rho_1, \rho_2]t} \sigma e^{[\rho_1, \rho_2]t} \) (to error \( \delta \) in trace distance)
Commutator Simulation

\[ \rho_1 \] source

\[ \rho_2 \] source

\[ \rho_1 \]

\[ \rho_2 \]

\[ e^{-iS\pi/4} \]

\[ \frac{1}{2} (\rho_1 + \rho_2 + i[\rho_1, \rho_2]) \]
Commutator Simulation

\[ i[\rho_1, \rho_2] = 2 \rho_{12} - \rho_1 - \rho_2 \]

- Use Sum of State Simulation!
- Uses \( O \left( \frac{t^2}{\delta} \right) \) copies each of \( \rho_1 \) and \( \rho_2 \)
- Can prove optimal using similar approach as before
Applications of Commutator Simulation

• **State Addition:**
  
  \[ e^{[|\psi_1\rangle\langle\psi_1|,|\psi_2\rangle\langle\psi_2|]t} \] 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 \(\langle\psi_1|\psi_2\rangle = \lambda \neq 0\)
Lie Algebra Simulation

**Given:** \( \rho_1, \rho_2, \ldots, \rho_k \)

**Simulate:** Any element of Lie algebra generated by \( \{\rho_1, \rho_2, \ldots, \rho_k\} \)

That is, any linear combination of nested commutators of \( \rho_1, \rho_2, \ldots, \rho_k \), e.g. \( H = \rho_1 + [\rho_2, [\rho_3, \rho_5]] \)

**Our Protocol:** exponential samples in \# of \( \rho_i \) in a single term

- Idea: use \( \pi/4 \) swaps to create states with nested commutator components, then use state addition simulation to get rid of unwanted terms.
Fun Side-bar: 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 $\rho = |0\rangle\langle0|$ 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 Multi-State Hamiltonian simulation optimal?
2. Is general Lie algebra simulation optimal?
3. Copyright protection?
4. Other applications?