Turning States into Unitaries: Optimal Sample-Based Hamiltonian Simulation

Shelby Kimmel
Turning States Into Unitaries

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

(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

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

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

\[ \rho \]

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

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

Are global necessary or are local-sequential operations sufficient?

Local are sufficient!
Outline

1. Hamiltonian simulation
2. LMR (Lloyd, Mohseni, Rebentrost) Protocol & Optimality
3. Protocols & Applications of Sample-Based Hamiltonian Simulation
   a) Commutator and Anti-commutator simulation
   b) Jordan Lie Algebra simulation
4. Fun final application
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: \( i \to \) 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: \[ H = \rho \]

Cost: copies of \( \rho \)
## Sample-Based Hamiltonian Simulation

### Density Matrix Description:

<table>
<thead>
<tr>
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<th>$H = \rho$</th>
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<td>Cost:</td>
<td>$n$, (copies of $\rho$)</td>
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<tr>
<td>Output:</td>
<td>$e^{-i\rho t} \sigma e^{i\rho t}$ to error $\delta$ in trace distance</td>
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</table>

$\rho \otimes n \otimes \sigma, \; t, \; \delta$
Sample-Based Hamiltonian Simulation

Density Matrix Description:

Input: \( H = \rho \) 

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

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

- Most famous application: if \( \rho \) is mixed but has low rank, can produce pure state which is eigenvector of \( \rho \). (LMR 14)
Outline

1. Hamiltonian simulation
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3. Protocols & Applications of Sample-Based Hamiltonian Simulation
   a) Sum of states simulation
   b) Commutator simulation
   c) Lie Algebra simulation
4. Fun final application
LMR Protocol
LMR Protocol

$\rho$ source $\rightarrow \rho \sigma$
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

$\rho$

source

\[ \tilde{\sigma} \]

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

\( \rho \)

source

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

$\rho$ source $\rightarrow \rho \tilde{\sigma}$
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

\[ \rho \quad \text{source} \]

\[ \tilde{\sigma}' \]

\[ \tilde{\rho} \]
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

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

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

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

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

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

- Could we do better using global op?
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- 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

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)

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Lower Bound Sketch

I. Proof by Contradiction:

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

Task requires $n$ samples of $\rho$: $n = \Omega(\frac{1}{\epsilon^2})$. (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 $\rightarrow$ 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.

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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
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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 $mt$ to accuracy $m\delta$ by repeating $m \in \mathbb{Z}^+$ times:

$$f(mt, m\delta) \leq mf(t, \delta)$$
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.

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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:

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

\( m\delta \) 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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Outline

1. Hamiltonian simulation
2. LMR (Lloyd, Mohseni, Rebentrost) Protocol & Optimality
3. Protocols & Applications of Sample-Based Hamiltonian Simulation
   a) Useful tools
      i. Split Simulation Tool
      ii. Addition Tool
   b) Sum of states simulation
   c) Commutator & Anti-commutator simulation
   d) Jordan-Lie Algebra simulation
4. Fun final application
Split Simulation

Suppose can prepare the state

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

Where $\rho_+, \rho_- \succeq 0$ 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

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- Idea: Apply unitary

$$|0\rangle\langle 0| \otimes e^{-iSE} + |1\rangle\langle 1| \otimes e^{iSE}$$
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 \( O(\frac{t^2}{\delta}) \) 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 first qubit
Addition tool

If have sample access to $\rho_1$ and $\rho_2$, then can create by sampling

$$p\rho_1 + (1 - p)\rho_2$$

Can easily simulate $H = p\rho_1 + (1 - p)\rho_2$, even if $\rho_1$, $\rho_2$ don’t commute
Sum of States Simulation

Given: $\rho_1, \rho_2, ..., \rho_k$ and $a_1, a_2, ..., a_k \in \mathbb{R}$

Simulate: $H = \sum_i a_i \rho_i$ for time $t$, error $\delta$
Sum of States Simulation

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

Simulate: \( H = \sum_i a_i \rho_i \) for time \( t \), error \( \delta \)

- Sample \( \rho_i \) with prob. \( |a_i|/a \), where \( a = \sum_i |a_i| \)
  - if \( a_i > 0 \) append \( |0\rangle \langle 0| \)
  - if \( a_i < 0 \) append \( |1\rangle \langle 1| \):  

\[
|0\rangle \langle 0| \otimes \frac{1}{a} \sum_{i:a_i>0} a_i \rho_i + |1\rangle \langle 1| \otimes \frac{1}{a} \sum_{i:a_i<0} |a_i| \rho_i
\]
Sum of States Simulation

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

Simulate: $H = \sum_i a_i \rho_i$ for time $t$, error $\delta$

- Sample $\rho_i$ with prob. $|a_i|/a$, where $a = \sum_i |a_i|$
  - if $a_i > 0$ append $|0\rangle\langle 0|$, if $a_i < 0$ append $|1\rangle\langle 1|$

\[
|0\rangle\langle 0| \otimes \frac{1}{a} \sum_{i:a_i>0} a_i \rho_i + |1\rangle\langle 1| \otimes \frac{1}{a} \sum_{i:a_i<0} |a_i| \rho_i
\]

- Then use split simulation: $H = a \left( \frac{1}{a} \sum_{i:a_i>0} a_i \rho_i - \frac{1}{a} \sum_{i:a_i<0} |a_i| \rho_i \right)$

Requires $O(a^2 t^2 / \delta)$ samples, $\rho_j$ sampled $O\left(|a_j|a t^2 / \delta\right)$ times on average
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

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

- Claim output of circuit is:

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

where

\[ \rho_+ - \rho_- = \frac{1}{2} \left( e^{i\phi} \rho_1 \rho_2 + e^{-i\phi} \rho_2 \rho_1 \right) \]
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 \( O(t^2/\delta) \) samples
Applications of Commutator Simulation

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

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

* For \(\langle \psi_1 | \psi_2 \rangle = \lambda \neq 0\)
**Jordan-Lie Algebra Simulation**

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<td>Simulate:</td>
<td>$H = e^{i\phi} \rho_1 \rho_2 \ldots \rho_k + e^{-i\phi} \rho_k \rho_{k-1} \ldots \rho_1$</td>
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\[ \frac{1}{\sqrt{2}} |0\rangle + \frac{e^{i\phi}}{\sqrt{2}} |1\rangle \]

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

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

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

**Simulate:** 
\[
H = e^{i\phi} \rho_1 \rho_2 \cdots \rho_k + e^{-i\phi} \rho_k \rho_{k-1} \cdots \rho_1
\]

Uses \( O(kt^2/\delta) \) samples
Jordan-Lie Algebra Simulation

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

Simulate: \( H = \sum_j a_j (e^{i\phi_j} \rho_{j1} \rho_{j2} \cdots \rho_{jk} + e^{-i\phi_j} \rho_{jk} \rho_{jk-1} \cdots \rho_{j1}) \)
Jordan-Lie Algebra Simulation

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

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

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

- \( L = \max_j |j_k| \)
- \( a = \sum_j |a_j| \)
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 $\rho = |0\rangle \langle 0|$ 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 Multi-State Hamiltonian simulation optimal?
2. Is general Jordan Lie algebra simulation optimal?
3. Copyright protection?
4. Other applications?