Randomized Algorithms for Hamiltonian Simulation

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Outline

- Problem: Simulation of Hamiltonian H,

$$H = H_1 + H_2 + \cdots + H_m,$$

  where $e^{-iH_j\tau}$ can be implemented efficiently for any evolution time τ for $j = 1, \cdots, m$.
- For a given error bound ε, the cost is measured by the number of exponentials of $H_1, \cdots, H_m$.

Outline

- Trotter Formula:

$$\|e^{-iH\Delta t} - \prod_{j=1}^{m} e^{-iH_j\Delta t}\| = O(\Delta t^2).$$

- Strang Splitting Formula

$$\|e^{-iH\Delta t} - \prod_{j=1}^{m} e^{-iH_j\Delta t/2} \prod_{j=m}^{1} e^{-iH_j\Delta t/2}\| = O(\Delta t^3).$$

- High-Order Suzuki's Decomposition:

$$S_2 = \prod_{j=1}^{m} e^{-iH_j \Delta t/2} \prod_{j=m}^{1} e^{-iH_j \Delta t/2},$$

$$S_{2k} = [S_{2k-2}(p_k \Delta t)]^2 S_{2k-2}((1-4p_k)\Delta t)[S_{2k-2}(p_k \Delta t)]^2,$$

where $p_k = (4 - 4^{1/(2k-1)})^{-1}$.

- Error Bound of Suzuki's Decomposition:

$$\left\| e^{-iH\Delta t} - S_{2k}(\Delta t) \right\| = O(\Delta t^{2k+1}).$$

Let $\|H_1\| \geq \|H_2\| \geq \cdots \geq \|H_m\|$. Then

- In Suzuki's decomposition, for error bound ε, the number of exponentials is

$$O\left(\|H_1\| t 10^{k-1} \left(\frac{t\|H_2\|}{\varepsilon} \right)^{1/(2k)} \right).$$

- Problems for Suzuki's decomposition
  - The number of const factors grows exponentially in k.
  - The factors in S_{2k} are irrational when $k \geq 2$.

Outline

Simulation of Hamiltonian H, where $H = \sum_{j=1}^{m} H_j$.

- The evolution is simulated by a product of exponentials for some random sequence

$$\rho = \sum_{\omega} p_{\omega} U_{\omega} |\psi_0\rangle\langle\psi_0| U_{\omega}^{\dagger},$$

where

$$U_{\omega} = \prod_{s=1}^{N_{\omega}} e^{-iH_{j_{s,\omega}} t_{s,\omega}}$$

Error bounds for randomized simulation

- The error bound is measured by the trace distance of output states

$$D(\rho, \sigma) = \frac{1}{2}(\mathrm{Tr}|\rho - \sigma|),$$

where $|A| = \sqrt{A^\dagger A}$.

- An upper bound for the error of randomized simulation

$$2\|E(U_\omega) - U_0\| + E(\|U_\omega - U_0\|^2).$$

Outline

Algorithm 1 :

- Select a unitary operator uniformly and independently at random from
$$\{e^{-iH_1\Delta t}, \ldots, e^{-iH_m\Delta t}\}.$$
- $e^{-iH\Delta t}$ is simulated by
$$\rho \to \frac{1}{m}\sum_{j=1}^{m} e^{-iH_j\Delta t}\rho e^{iH_j\Delta t}.$$

The cost of Algorithm 1:

- Local error rate: $O(\Delta t^2)$.
- Total cost for error bound ε:

$$O(\Delta t^2) \to O(t^2/\varepsilon).$$

- Algorithm 1 has the same cost as the Trotter's Formula.

Algorithm 2 :

- Select a unitary operator uniformly and independently at random from

$$\{U_1 = \prod_{j=1}^{m} e^{-iH_j\Delta t}, U_2 = \prod_{j=m}^{1} e^{-iH_j\Delta t}\}.$$

- $e^{-iH\Delta t}$ is simulated by

$$\rho \to \frac{1}{2}\left(U_1 \rho U_1^{\dagger} + U_2 \rho U_2^{\dagger}\right).$$

The cost of Algorithm 2:

- Local error rate: $O(\Delta t^3)$.
- Total cost for error bound ε:

$$O(\Delta t^3) \to O(t^{3/2}/\varepsilon^{1/2}).$$

- Algorithm 2 has the same cost as the Strang Splitting Formula.

Algorithm 3:

- Algorithm 3 is applied for the simulation of $e^{-i(H_1+H_2)t}$.
- Select

$$
\begin{array}{ll}
e^{-i\frac{1}{2}H_1\Delta t}e^{-i\frac{1}{2}H_2\Delta t}e^{-i\frac{1}{2}H_1\Delta t}e^{-i\frac{1}{2}H_2\Delta t} & \text{with prob } \frac{5}{12}, \\
e^{-i\frac{1}{2}H_2\Delta t}e^{-i\frac{1}{2}H_1\Delta t}e^{-i\frac{1}{2}H_2\Delta t}e^{-i\frac{1}{2}H_1\Delta t} & \text{with prob } \frac{5}{12}, \\
e^{-i\frac{3}{2}H_1\Delta t}e^{i\frac{1}{2}H_2\Delta t}e^{i\frac{1}{2}H_1\Delta t}e^{-i\frac{3}{2}H_2\Delta t} & \text{with prob } \frac{1}{12}, \\
e^{-i\frac{3}{2}H_2\Delta t}e^{i\frac{1}{2}H_1\Delta t}e^{i\frac{1}{2}H_2\Delta t}e^{-i\frac{3}{2}H_1\Delta t} & \text{with prob } \frac{1}{12}.
\end{array}
$$

The cost of Algorithm 3:

- Local error rate: $O(\Delta t^4)$.
- Total cost for error bound ε:

$$O(\Delta t^4) \to O(t^{4/3}/\varepsilon^{1/3}).$$

Outline

- In certain problems the evolution time is required to be positive, i.e., $t_j > 0$ for any j. For instance, the diffusion operator [1].
- We show that any deterministic or randomized algorithm simulating e^{-iHt} requires at least

$$\Omega(t^{3/2}\varepsilon^{-1/2})$$

exponentials.

Summary

- We proposed the randomized model for Hamiltonian Simulation.
- There are randomized algorithms which has the same efficiency as certain deterministic algorithms, but much easier to implement.

- Future Work
  - How to derive randomized algorithms for higher orders?

For Further Reading

- M. Suzuki
  Fractal decomposition of exponential operators with applications to many-body theories and Monte Carlo simulations,
  Phys. Lett. A 146, 319-323 (1990)
- Anargyros Papageorgiou, Chi Zhang
  On the Efficiency of Quantum Algorithms for Hamiltonian Simulation,
  quant-ph 1005.1318, 2010