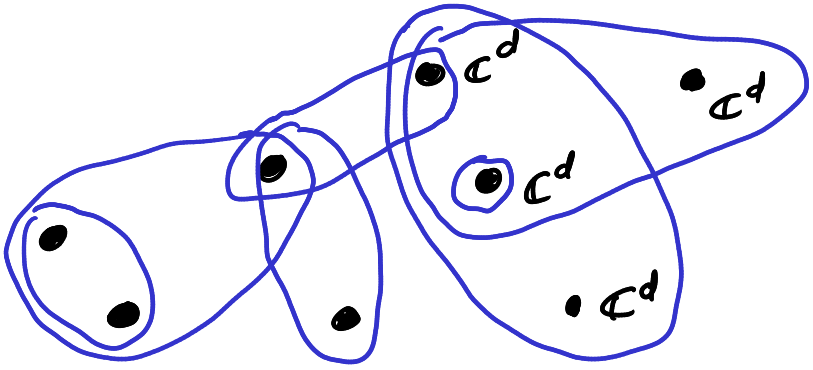
# Lecture 6: Hamiltonian Simulation

So far, we've seen two important classes of quantum algorithm: QFT-based, & amplitude-amplification-based. The former give large speedups over (known) classical algorithms, but applications seem to limited to certain types of problems that have important applications in cryptography, but not much else. (Of course, this could be due to a lack of imagination so far!).

The other class (Grover etc.) can be applied more broadly to many types of abstract search problem (and more besides which we haven't covered — see literature). But only offers a modest (though still potentially useful) quadratic speedup over classical.

However, there is another application of quantum computing which promises exponential speedups over (known) classical algorithms for a large class of practically important problems (and the algorithm is simpler than Grover & Shor to boot!): simulating quantum dynamics.

# 1. Hamiltonian Simulation




Many-body quantum system:

- Multipartite Hilbert space $\mathcal{H} = (\mathbb{C}^d)^{\otimes n}$
  e.g. particles with spin-$s$ ($d = \frac{s(s+1)}{2}$)

- Local interaction Hamiltonian:
  $h = h_S \otimes \mathbb{1}_{[n]\setminus S}$, $S \subset [n]$

  i.e. $h$ acts "non-trivially" only on subset $S$ of the particles

  We say that interaction $h$ is <u>$k$-local</u> if $|S| = k$ (i.e. $h$ acts non-trivially on $k$ particles).

<u>Notation</u>: Often write "$h_S$" $\equiv h_S \otimes \mathbb{1}_{[n]\setminus S}$, i.e. subscript indicates indices of particles acted on, $\mathbb{1}$ on rest is implicit.

**Def** (k-local Hamiltonian)

$H = \sum_j h_j$ on $n$ qudits $(\mathbb{C}^d)^{\otimes n}$

We say that $H$ is a **k-local Hamiltonian** (or "$H$ is k-local") if $\forall j$ $h_j$ is $\leq$ k-local.

I.e. k-local many-body Hamiltonian made of many interactions each involving at most k particles.

Examples:

- spins on line with nearest-neighbour interactions: $H = \sum_{i=1}^{n-1} h_{i,i+1}$
- spins on lattice —— " —— " ——: $H = \sum_{\langle i,j \rangle} h_{ij}$

  ↖ neighbours

Note: In general, no underlying geometry
⇒ no requirement that local interactions are geometrically local.

Physics terminology: "k-local" = "k-body"
but stuck with "k-local" now in QIT.

$H = \sum_{j=1}^{m} h_j$ k-local

⇒ at most $m = \binom{n}{k} = O(n^k)$ local terms $h_j$.

**Problem** (Hamiltonian simulation)

Input: $k$-local $H$, $|\psi_0\rangle$, $t$, $\delta$

Output: $|\tilde{\psi}_t\rangle$ s.t. $\langle\tilde{\psi}_t|\psi(t)\rangle \geq 1-\delta$

where $|\psi(t)\rangle = e^{-iHt}|\psi_0\rangle$

As stated, this problem is inherently quantum: it takes quantum input $|\psi\rangle$ and produces quantum output $|\psi(t)\rangle$.

However, if $|\psi\rangle$ has an efficient classical description (e.g. product state; output of poly-sized $\Rightarrow$ efficiently classically describable quantum circuit), & we ask for outcome of some efficiently describable measurement on $|\psi(t)\rangle$ (e.g. local observable; computational basis), then this becomes a bona-fide computational problem.

Simulating the dynamics of a quantum many-body system on classical computers is notoriously hard. Best algorithms known for general $H$ are exponential-time.

Except for some particular classes of Hamiltonian, even heuristic algorithms (i.e. algorithms with no rigorous performance or correctness guarantees) perform poorly in practice on general H.

Feynman [1982; 1985] suggested quantum systems may require quantum computers to simulate them effectively.

[Lloyd 1996] made this idea rigorous. There have been many important developments since then, & state-of-the-art simulation algorithms with optimal run-time are based on very different ideas to Lloyd's original algorithm (see [Aharanov & Tash-ma 2003], [Berry, Cleve, Ahokav, Sanders 2007], [Childs et al. 2012-present], [Low & Chuang 2017], [Haah, Hastings, Kothari, Low 2018]), unfortunately beyond the scope of this course.)

We will restrict our attention to the original Lie-Trotter-Suziki-based approach...

**Theorem** (Lie-Trotter error bound)

For $A, B$ Hermitian,

$$\| e^{i(A+B)} - e^{iA} e^{iB} \| \leq 2 \|A\| \cdot \|B\|$$

**Proof**

Note

$$\frac{d}{ds}\left(e^{-iAs} e^{i(A+B)s}\right)$$

$$= -iA e^{-iAs} e^{i(A+B)s} + i e^{-iAs}(A+B) e^{i(A+B)s}$$

$$= i e^{-iAs} B e^{i(A+B)s}.$$

Similarly

$$\frac{d}{ds}\left(e^{i(A+B)s} e^{-iBs}\right)$$

$$= i e^{i(A+B)s}(A+B) e^{-iBs} - i e^{i(A+B)s} B e^{-iBs}$$

$X$, $e^X$ commute

$$= i e^{i(A+B)s} A e^{-iBs}.$$

Using these,

$$\frac{d^2}{ds^2}\left(e^{-iAs} e^{i(A+B)s} e^{-iBs}\right)$$

$$= \frac{d}{ds}\left(i e^{-iAs} B e^{i(A+B)s} e^{-iBs} - i e^{-iAs} e^{i(A+B)s} e^{-iBs} B\right)$$

$$= A e^{-iAs} B e^{i(A+B)s} e^{-iBs}$$
$$- e^{-iAs} B e^{i(A+B)s} A e^{-iBs}$$
$$+ A e^{-iAs} e^{i(A+B)s} e^{-iBs} B$$
$$- e^{-iAs} e^{i(A+B)s} A e^{-iBs} B$$

So

$$\left\| \frac{d^2}{ds^2} \left( e^{-iAs} e^{i(A+B)s} e^{-iBs} \right) \right\| \leq 4 \|A\| \|B\|$$

$\|\cdot\|$ unitarily invariant $\Rightarrow \|e^{iH}\| = 1$

Thus

$$\| e^{i(A+B)} - e^{iA} e^{iB} \|$$
$$= \| e^{-iA} e^{i(A+B)} e^{-iB} - \mathbb{1} \| \quad \text{unitary invariance}$$
$$= \left\| \int_0^1 \int_0^{s'} \frac{d^2}{ds^2} \left( e^{-iAs} e^{i(A+B)s} e^{-iBs} \right) ds\, ds' \right\|$$
$$\leq \int_0^1 ds' \int_0^{s'} ds \left\| \frac{d^2}{ds^2} \left( e^{-iAs} e^{i(A+B)s} e^{-iBs} \right) \right\|$$
$$\leq \int_0^1 ds' \int_0^{s'} ds\, 4 \|A\| \cdot \|B\| = 2 \|A\| \cdot \|B\| \quad \square$$

Usual proof of Lie-Trotter error bound is by Taylor expanding $e^A$, $e^B$, $e^{A+B}$ and bounding terms of order $\geq 2$ by $e^{\|A\|}$ etc. Works for any $A, B$, not just Hermitian, but only gives right scaling for $\|A\|, \|B\| \leq 1$.

**Corollary** (Lie-Trotter formula)

$$\lim_{N\to\infty} \left( e^{iA/N} e^{iB/N} \right)^N = e^{i(A+B)}$$

**Proof**

$$\left\| \left( e^{iA/N} e^{iB/N} \right)^N - e^{i(A+B)} \right\|$$

$$\leq \left\| e^{i(A+B)/N} \left( e^{iA/N} e^{iB/N} \right)^{N-1} - e^{i(A+B)} \right\|$$

$$+ 2 \cdot \left\| A/N \right\| \cdot \left\| B/N \right\|$$

Applying this recursively $n$ times, we obtain

$$\left\| \left( e^{iA/n} e^{iB/n} \right)^n - e^{i(A+B)} \right\|$$

$$\leq \left\| \left( e^{i(A+B)/N} \right)^N - e^{i(A+B)N} \right\| + N \cdot \frac{2}{N^2} \|A\| \cdot \|B\|$$

$$= \frac{2}{N} \|A\| \cdot \|B\| \longrightarrow 0 \quad \text{as } N \to \infty. \quad \square$$

Lie-Trotter formula actually holds for any $A, B$, not just Hermitian (see above).

Lie-Trotter formula shows we can approximate time-evolution $e^{-iHt}$ under local Hamiltonian $H = \sum_{j=1}^{m} h_j$ by a sequence of small "Trotter steps": $\left( \prod_{j=1}^{m} e^{-ih_j t/N} \right)^N$.

We know this converges to the exact time-evolution $e^{-iHt}$ in the limit $n \to \infty$.

To analyse the error for finite $n$, we need one more Lemma, which shows that errors only accumulate linearly in quantum circuits:

## Lemma

Let $\| U_i - V_i \| \leq \varepsilon$. Then

$$\| U_1 U_2 \cdots U_n - V_1 V_2 \cdots V_n \| \leq n\varepsilon.$$

## Proof

$$\| U_1 U - V_1 V \| = \| (U_1 - V_1) U - V_1 (V - U) \|$$

$$\leq \| U_1 - V_1 \| + \| U - V \| \quad \text{unitary invariance}$$

$$= \varepsilon + \| U - V \|.$$

Applying this inductively with $U = U_2 U_3 \cdots U_n$ $V = V_2 V_3 \cdots V_n$ gives the result. □

We can now prove an error bound for approximating time-evolution by finite Trotter steps:

**Theorem**

Let $H = \sum_{j=1}^{m} h_j$, with $\|h_j\| \leq k$.

$$\left\| e^{-iHt} - \left( \prod_{j=1}^{m} e^{-ih_j t/N} \right)^N \right\| = O\left(\frac{m^2 k^2 t^2}{n}\right)$$

**Proof**

$$\left\| e^{-iH\tau} - \prod_{j=1}^{m} e^{-ih_j\tau} \right\|$$

$$\leq \left\| e^{-iH\tau} - e^{-i(h_1+h_2)\tau} \prod_{j\geq 3} e^{-ih_j\tau} \right\|$$

$$+ 2(k\tau)^2 \quad \text{by Lie-Trotter error bound}$$

$$\leq \left\| e^{-iH\tau} - e^{-i(h_1+h_2+h_3)\tau} \prod_{j\geq 4} e^{-ih_j\tau} \right\|$$

$$+ 2k^2\tau^2 + 2\cdot(2k\tau)(k\tau)$$

$\uparrow \|h_1+h_2\| \leq 2k$

$$\leq \cdots$$

$$\leq \left\| e^{-iH\tau} - e^{-i\sum_j h_j \tau} \right\| + 2k^2\tau^2 \sum_{j=1}^{m} j$$

$$\leq 2m^2k^2\tau^2.$$

$$\left\| e^{-iHt} - \left( \prod_{j=1}^{m} e^{-ih_j t/N} \right)^N \right\|$$

$$= \left\| \left( e^{-iHt/N} \right)^N - \left( \prod_{j=1}^{m} e^{-ih_j t/N} \right)^N \right\|$$

$$\leq N \left\| e^{-iHt/N} - \prod_{j=1}^{m} e^{-ih_j t/N} \right\|$$ by error accumulation Lemma

$$\leq N \cdot 2m^2 k^2 \left(\frac{t}{N}\right)^2$$ by above

$$= \frac{2m^2 k^2 t^2}{N}.$$ □

## Hamiltonian Simulation Algorithm + Analysis

Approximate time-evolution under $H$ using Trotterization.

→ error $O\left(\frac{m^2 k^2 t^2}{N}\right)$ by above Thm.

Each Trotter step $e^{-ih_j t/n}$ is a unitary acting on at most $k$ qudits ($H$ $k$-local).

We can approximate each $e^{-ih_j t/n}$ to error $\varepsilon$ using $O(\log^c \frac{1}{\varepsilon})$ gates, by Solovay-Kitaev Theorem.

→ additional error $O(N \log^c \frac{1}{\varepsilon})$, by error accumulation Lemma.

Total error $= O\left(\frac{m^2 k^2 t^2}{N} + N\varepsilon\right)$

To achieve overall error $\delta$, take

$n = \frac{m^2 k^2 t^2}{\delta}$ , $\varepsilon = \frac{\delta}{N}$

Recall $m = O(N^k)$ for $k$-local $H$ on $n$ qudits

$\longrightarrow$ Overall run-time $O(N \cdot \log \frac{1}{\varepsilon})$

$= O\left(\frac{k\, n^{2k} t^2 k^2 \log^2(ntk)}{\delta}\right)$.

## Improvements

By using higher order Lie-Trotter-Suzuki formulae, scaling can be improved to $O(t^{1+o(1)})$ in $t$. E.g.

Exercise:

Prove

$$\| e^{-iA/2} e^{-iB} e^{-iA/2} - e^{-i(A+B)} \| \leq \|A\|^2 \cdot \|B\|$$

and use this to obtain a Hamiltonian simulation algorithm that improves on $t^2$.

Note: cannot do better than $O(t)$ or we would be able to "fast-forward" any quantum evolution $\rightarrow$ contradictions.

State-of-the-art algorithms are based on different & much more sophisticated techniques, which achieve scaling in all parameters that is essentially asymptotically optimal. However, constant factors are very large.

Modern algorithms also generalise beyond k-local H to sparse Hamiltonians:

**Def** (s-sparse)

Matrix $M$ is s-sparse if it has $\leq s$ non-zero entries in any row or col.

**Problem** (Sparse Hamiltonian simulation)

Input: $H$ $N \times N$, poly$(\log N)$-sparse; $|\psi_0\rangle$, $t$, $\delta$

Output: $|\psi_t\rangle$ s.t. $\| |\psi_t\rangle - e^{-iHt} |\psi_0\rangle \| \leq \delta$.