Week 5: Hamiltonians and HHL

What is a Hamiltonian?

- The Hamiltonian **H** is the observable corresponding to the total energy of the system.

- The Hamiltonian is the sum of the kinetic energies of all the particles, plus the potential energy of the particles associated with the system.

$$\hat{H} = \hat{T} + \hat{V}$$

$$\implies \hat{H} = -\frac{\hbar}{2m}\nabla^2 + \hat{V}$$

What is a Hamiltonian?

- In reality, the Hamiltonian of an entire system is the sum of many operators which each act on only a part of the system.

$$H = \sum_{j=1}^{m} H_j$$

- **H** describes how a quantum state will evolve as a function of time and the initial state. This is given by the Schrodinger's equation.

$$i\hbar \frac{\partial}{\partial t}\left|\Psi(t)\right\rangle = \hat{H}\left|\Psi(t)\right\rangle$$

What is Hamiltonian simulation?

- The solution to the Schrodinger's equation has a solution describes the evolution of the state.

$$i\hbar\frac{\partial}{\partial t}\Big|\Psi(t)\Big\rangle = \hat{H}\Big|\Psi(t)\Big\rangle \qquad \Big|\Psi(t)\Big\rangle = exp\left(-\frac{i\hat{H}t}{\hbar}\right)\Big|\Psi(0)\Big\rangle$$

- U is an unitary operator, and hence can be used as a transformation in the quantum model.

$$U = exp\left(-\frac{iHt}{\hbar}\right)$$

What is Hamiltonian simulation?

- In his lecture "*Simulating Physics with Computers*", Feynman envisioned quantum computers as systems that could efficiently simulate every quantum process.

- In order to simulate a quantum process, we need to efficiently implement the unitary evolution induced by **H**.

- In our context, the t steps of evolution induced by **H**, corresponds to applying the unitary $U=\exp(-i\,\mathbf{H})$, t times.

- This process is called the Hamiltonian Simulation.

Hamiltonian simulation Technique: Lie Suzuki Trotter Decomposition

- The Lie Product Formula gives us

$$e^{X+Y} = \lim_{n\to\infty} \left(e^{\frac{X}{n}} e^{\frac{Y}{n}}\right)^n$$

- Also recall that the Hamiltonian of an entire system is the sum of many operators which each act on only a part of the system.

$$H = \sum_{j=1}^{m} H_j$$

Hamiltonian simulation Technique: Lie Suzuki Trotter Decomposition

- The **Lie-Suzuki-Trotter decomposition** uses this technique to give a unitary for the Hamiltonian form shown in the previous slide.

$$U = e^{iHt} = \left(e^{iHt/r}\right)^r = \left(e^{i\sum_j H_j t/r}\right)^r = \left(\prod_j e^{iH_j t/r} + E\right)^r$$

- E is the error term with respect to the Lie Product Formula. Our approximating Unitary is

$$\tilde{U} = \left(\prod_j e^{iH_j t/r}\right)^r$$

Harrow Hashimi Lloyd Algorithm (2009)

- The goal of this algorithm is to ***solve*** a ***well behaved*** linear system of equations.

- In the classical case, solving linear systems of equations Ax = b, meant finding the solution vector x and all it entries.

- In the quantum case, we get $|x\rangle$as a global state, and it is not possible to distinguish all the individual amplitudes of the basis states from it.

- In the quantum case, even estimating these values would mean producing many copies of$|x\rangle$, thereby increasing the running time significantly.

Harrow Hashimi Lloyd Algorithm (2009)

- On the other hand, the global state $|x\rangle$ can be used to estimate expressions which depend on all the basis states simultaneously.
- Classically, it is not clear how we would go about estimating expressions of this form without solving for the individual terms $x_1, \ldots, x_N$.
- The global state $|x\rangle$ is also handy when we want to test how similar the solutions of two systems of linear equations $Ax=b$ and $A'x'=b'$ are.
- Using HHL we simply generate $|x\rangle$ and $|x'\rangle$ and then compare them using the SWAP-test.

Harrow Hashimi Lloyd Algorithm (2009)

What do we mean by a "well behaved" system of equations?

- A is Hermitian. If A is not Hermitian we convert it into Hermitian form (refer handout for details).
- A is **s-sparse** and we have sparse access to elements of A.
- The matrix Ais well conditioned. This means that all eigenvalues of A lie in the interval $[-1,-1/\kappa] \cup [1/\kappa,1]$, where κ is the ratio of its maximum singular value and minimum singular value.
- The state vector $|b\rangle$is provided to us from another subroutine, or we have a unitary that can efficiently produce this state.

Harrow Hashimi Lloyd Algorithm (2009)

Algorithm 1: HHL Algorithm

Input : A, $|b\rangle$, t_0, T, ϵ
output: $|x\rangle$

1. Start with two registers C(clock register) and I(input register). The clock register will be responsible for carrying out the Hamiltonian Simulation.

2. Prepare input state $|\Psi_0\rangle^C \otimes |b\rangle^I$. We have

$$|\Psi_0\rangle^C = \sqrt{\frac{2}{T}} \sum_{\tau=0}^{T-1} \sin \frac{\pi(\tau + 0.5)}{T} |\tau\rangle \quad , \text{and} \quad |b\rangle^I = \sum_{j=1}^{N} \beta_j |u_j\rangle$$

   Here T refers to the number of simulation steps for simulating e^{iAt}, where $0 \leq t_0 \leq t$. Hence t_0/T is the step size of the simulation. Note that $t_0 = O(\kappa/\epsilon)^a$ and $T = O((\log N)s^2 t_0)$.

3. Now we apply a conditional[b] Hamiltonian $\hat{H}$ on $|\Psi_0\rangle^C \otimes |b\rangle^I$.

$$\hat{H} = \left(\sum_{\tau=0}^{T-1} |\tau\rangle\langle\tau|^C \right) \otimes e^{iA\tau t_0/T}$$

Harrow Hashimi Lloyd Algorithm (2009)

After rearranging the terms we get,

$$|\Psi_0\rangle^C \otimes |b\rangle^I \overset{\hat{H}}{\mapsto} \sqrt{\frac{2}{T}} \sum_{j=1}^{N} \beta_j \left(\sum_{\tau=0}^{T-1} e^{i\lambda_j \tau t_0/T} \sin \frac{\pi(\tau+0.5)}{T} |\tau\rangle^C \right) |u_j\rangle^I$$

4. We now express the state of the clock register in the Fourier basis $|k\rangle^c$ to get

$$\overset{\text{QFT}}{\longmapsto} \sum_{j=1}^{N} \beta_j \sum_{k=0}^{T-1} \left(\frac{\sqrt{2}}{T} \sum_{\tau=0}^{T-1} e^{i\tau/T(\lambda_j t_0 - -2\pi k)} \sin \frac{\pi(\tau+0.5)}{T} \right) |k\rangle^C |u_j\rangle^I = \sum_{j=1}^{N} \beta_j \left(\sum_{k=0}^{T-1} \alpha_{k|j} \right) |k\rangle^C |u_j\rangle^I$$

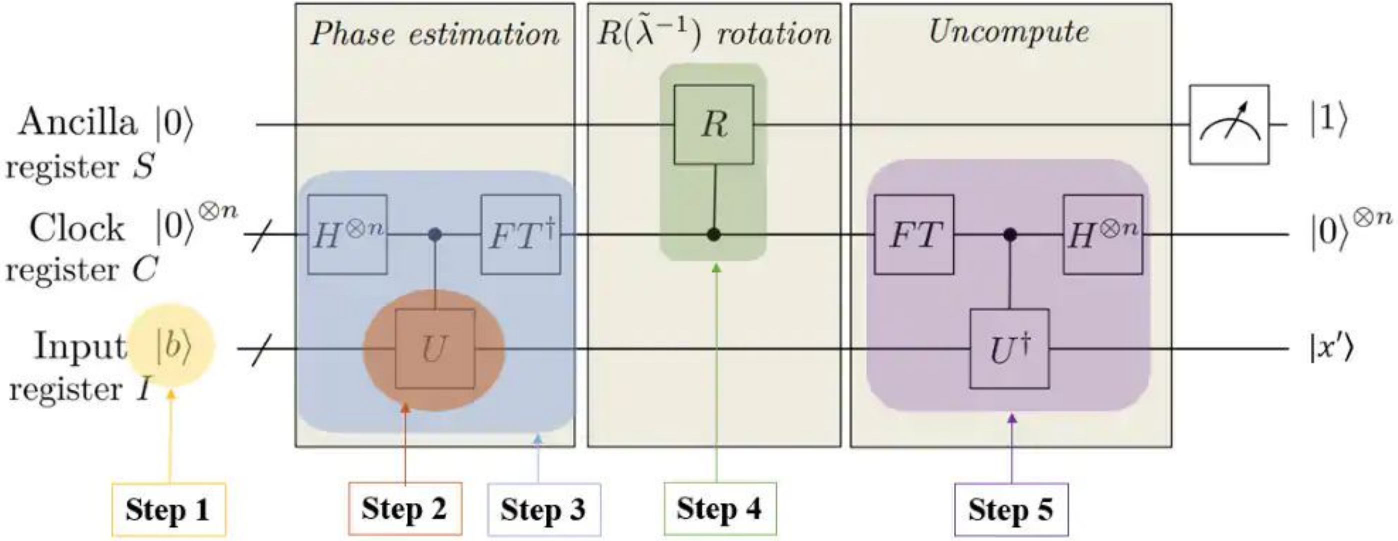
We can show that $\alpha_{k|j}$ is large if and only if $\lambda_j \approx 2\pi k/t_0$. Since only these eigenvalues are of interest[d], let us relabel the basis states $|k\rangle$ by defining $\hat{\lambda}_k = 2\pi k/t_0$.

Harrow Hashimi Lloyd Algorithm (2009)

5. An ancilla qubit S is added to our current state, and then rotated conditioned on our clock register to obtain
$$\sum_{j=1}^{N}\beta_j\left(\sum_{k=0}^{T-1}\alpha_{k|j}\right)|\hat{\lambda}_k\rangle^C|u_j\rangle^I\left(\sqrt{1-\frac{C^2}{\hat{\lambda}_k^2}}|0\rangle+\frac{C}{\hat{\lambda}_k}|1\rangle\right)^S$$
C is chosen to be $O(1/\kappa)$. We now undo the phase estimation to uncompute the $|\hat{\lambda}_k\rangle^C$ and assume the phase estimation to be perfect[e].

6. Conditioned on seeing $|1\rangle$, we measure the last register to get $c\sum_{j=1}^{N}\beta_j\frac{C}{\lambda_j}|u_j\rangle$, where c is the normalizing constant. This state corresponds to $|x\rangle=\sum_{j=1}^{N}\beta_j\lambda_j^{-1}|u_j\rangle$.

Harrow Hashimi Lloyd Algorithm (2009)



<u>The Circuit for HHL</u>

Harrow Hashimi Lloyd Algorithm (2009)

The runtime of HHL can be calculated as follows

- Each run of HHL concludes in T steps.
- The success probability of the post-selection process is at-least O(1/κ2) since C is chosen to beO(1/κ).

Hence to get a good success probability we need to perform O(κ) amplifications.

Putting both of these points together we see that the runtime of HHL is

$$O(\kappa T) = O(\kappa(\log N)s^2 t_0) = O\left(\frac{(\log N)s^2\kappa^2}{\epsilon}\right)$$

Variable Time Amplitude Amplification (2010)

Andris Ambainis came up with an improvement to the HHL algorithm by carefully analysing the dependence on the condition number. He improved the running time to

$$O\left(\frac{(\log N)s^2\kappa\log^3\kappa}{\epsilon}\right)$$

Refer to the handout for details. Further improvements were made to HHL over the years. One recent improvement was by Childs et.al in 2017, which focused on the sparsity factor. Combined with VTAA, we get pretty decent theoretical bounds on QLSP problems nowadays.

Detailed Description given in Handouts
References for further study in Handouts