UCSD Spring School lecture notes: Continuous-time quantum computing

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1 Efficient simulation of quantum dynamics

Quantum mechanics is described mathematically using linear algebra, so at some level is very simple. On the other hand to simulate a quantum system using a classical computer seems to require storing and manipulating exponentially large vectors (in the size of the quantum system). Motivated by this apparent difficulty, in 1982 Richard Feynman suggested that a quantum computer could be used for simulating other quantum systems [Fey82].

Consider a quantum spin system composed of n qubits, which is described by a normalized vector $|\psi\rangle \in (\mathbb{C}^2)^{\otimes n}$. The Schrodinger equation

$$\frac{d|\psi\rangle}{dt} = -iH|\psi\rangle \tag{1}$$

describes the time evolution of such a quantum system with a Hamiltonian H. The Hamiltonian H may itself depend on time and later we will see an example of this. For now, let us specialize to the case in which H is time-independent, and the solution to Eq. (1) is easily seen to be

$$|\psi(t)\rangle = e^{-iHt}|\psi(0)\rangle. \tag{2}$$

Following Lloyd [Llo96], we now describe a simple method whereby a universal quantum computer can efficiently simulate time evolution Eq. (2) (below we aim for simplicity; later we summarize more recent methods which improve the efficiency of the simulation). Quantum simulation remains one of the most compelling applications in which quantum computers achieve an exponential speedup over the best known classical algorithm.

Theorem 1 ([Llo96]). *There is an efficient classical algorithm which takes as input a precision $\epsilon \in (0,1)$, a time $t > 0$, and a k-local Hamiltonian*

$$H = \sum_{j=1}^{m} h_j.$$

The algorithm computes a quantum circuit composed of $\mathrm{poly}(m, t, \epsilon^{-1})$ *gates such that the unitary U implemented by the circuit satisfies*

$$\|U - e^{-iHt}\| \leq \epsilon. \tag{3}$$

Exercise 2. Let A, B be n-qubit operators and $\delta \in (0,1)$ such that $\|A\| \leq \delta$ and $\|B\| \leq \delta$. Then

$$\|e^A e^B - e^{A+B}\| \leq O(\delta^2).$$

Exercise 3. Suppose $V_1, V_2, \ldots, V_M$ and $W_1, W_2, \ldots, W_M$ are unitary operators. Then

$$\|V_1 V_2 \ldots V_M - W_1 W_2 \ldots W_M\| \leq \sum_{j=1}^{M} \|W_j - V_j\|.$$

Proof of Theorem 1. Let R be a positive integer satisfying $R \geq mt$ (recall m is the number of local terms in H and t is the evolution time). We start by dividing up the evolution time into small segments of length t/R:

$$e^{-iHt} = \left(e^{-iHt/R}\right)^R \tag{4}$$

Now let us consider one segment. Below we will show

$$\|e^{-iHt/R} - e^{-ih_1 t/R} e^{-ih_2 t/R} \ldots e^{-ih_m t/R}\| \leq O(m^3 t^2 R^{-2}). \tag{5}$$

Using this fact and Exercise 3 we get

$$\|e^{-iHt} - \left(e^{-ih_1 t/R} e^{-ih_2 t/R} \ldots e^{-ih_m t/R}\right)^R \| \leq O(m^3 t^2 R^{-1}).$$

and so we can make the RHS at most ϵ by taking $R = \Theta(m^3 t^2 \epsilon^{-1})$. With this choice of R the quantum circuit

$$U = \left(e^{-ih_1 t/R} e^{-ih_2 t/R} \ldots e^{-ih_m t/R}\right)^R$$

satisfies Eq. (3) and the above is a decomposition into $Rm = \text{poly}(t, m, \epsilon^{-1})$ k-local gates. This establishes the theorem since these k-local gates can be further decomposed into a universal set of 1- and 2-local gates while incurring only polylogarithmic overhead in the size of the circuit.

It remains to show Eq.(5). For each $0 \leq L \leq m$ define

$$U_L = e^{-i \sum_{j=1}^{L} h_L t/R} e^{-ih_{L+1} t/R} e^{-ih_{L+2} t/R} \ldots e^{-ih_m t/R}.$$

Then

$$\|U_L - U_{L-1}\| = \|e^{-i \sum_{j=1}^{L} h_L t/R} - e^{-i \sum_{j=1}^{L-1} h_j t/R} e^{-ih_L t/R}\| \leq O(L^2 t^2 R^{-2}). \tag{6}$$

where we used Exercise 2. Since $U_m = e^{-iHt/R}$ and $U_0 = e^{-ih_1 t/R} e^{-ih_2 t/R} \ldots e^{-ih_m t/R}$ we get

$$\|e^{-iHt/R} - e^{-ih_1 t/R} e^{-ih_2 t/R} \ldots e^{-ih_m t/R}\| = \| \sum_{L=1}^{m} (U_L - U_{L-1})\| \leq O(m^3 t^2 R^{-2}).$$

$\square$

While the above algorithm establishes that efficient simulation of Hamiltonian dynamics is possible, the circuit produced by the above algorithm consists of $O(m^4 t^2 \epsilon^{-1})$ gates which is far from optimal. In the roughly 20 years since Lloyd's paper there have been many new quantum algorithms for Hamiltonian simulation which achieve better scaling in various parameters. For example it is known that one can simultaneously achieve linear scaling in the evolution time t (improving the above by a quadratic factor) and a logarithmic dependence on ϵ^{-1} (an exponential improvement) [BCC$^+$17, BCK15, LC17].

2 Adiabatic Quantum Computation

In this section we are going to imagine that we have a system of qubits that evolves according to the Schrodinger equation with a local time-dependent Hamiltonian H which we get to choose. We will be interested in the case where the Hamiltonian changes very slowly.

Motivating example

Adiabatic quantum computing is a model of computation based on the adiabatic theorem of quantum mechanics. Roughly speaking, the adiabatic theorem states that if a quantum system is prepared in its ground state and then the Hamiltonian is changed very slowly then the state of the system will be well approximated by the ground state of the instantaneous Hamiltonian at all times.

To understand how adiabatic quantum computation can be used to solve computational problems, let's begin with a motivating example which was proposed in Ref. [FGGS00]. In that paper the authors introduced the adiabatic model of quantum computation and proposed the following quantum algorithm for 3-satisfiability.

Suppose we are given a 3-satisfiability instance on n bits with m clauses. Define $h(z)$ to be the function that computes the number of clauses violated by a given bit string $z \in \{0,1\}^n$. We can write

$$h(z) = \sum_{c=1}^{m} h_c(z) \qquad h_c(z) = \begin{cases} 0 & \text{if } z \text{ satisfies clause } c \\ 1 & \text{otherwise.} \end{cases}$$

Clearly we can solve 3-SAT if we can find the bit string z_0 such that $h(z_0)$ is minimal. Now define a Hamiltonian H_P which is diagonal in the computational basis

$$H_P|z\rangle = h(z)|z\rangle \qquad z \in \{0,1\}^n.$$

It is not hard to see that H_P can be expressed as a 3-local Hamiltonian:

Exercise 4. Show that H_P can be expressed as a 3-local Hamiltonian.

Its ground state is the computational basis state $|z_0\rangle$ and if we could prepare this state then we can solve the given 3-SAT instance. So our goal in the following will be to prepare the ground state of H_P using a quantum algorithm.

Farhi et. al consider a one-parameter family of Hamiltonians that interpolates between a "beginning Hamiltonian" H_B whose ground state is easy to prepare and the "problem Hamiltonian" H_P whose ground state provides the solution to the 3-SAT instance.

$$H(s) = (1 - s)H_B + sH_P \qquad 0 \le s \le 1$$

One possible choice for the beginning Hamiltonian is

$$H_B = \sum_{j=1}^{n}(1 - X_j)/2$$

which describes a system of non-interacting spins. The ground state of this Hamiltonian is the product state $|+\rangle^{\otimes n}$ where $|+\rangle = \sqrt{2}^{-1}(|0\rangle + |1\rangle)$.

An adiabatic quantum algorithm for 3-satisfiability is as follows:

1. Prepare the ground state $|+\rangle^{\otimes n}$ of $H(0) = H_B$.

2. Slowly change the Hamiltonian $H(s)$ from $H(0)$ to $H(1)$. In particular change the parameter $s(t) = t/T$ where t is time and T is the total time.

3. Measure all qubits in the computational basis to obtain a bit string $z \in \{0, 1\}^n$

The adiabatic theorem (desribed below) guarantees that if the total time T is large enough then the final quantum state after step 2 will be well approximated by the ground state $|z_0\rangle$ of $H(1)$ and the result of the final measurement will be $z = z_0$ which provides the solution to the given 3-SAT instance.

The runtime of the above algorithm using our adiabatic quantum computer (which is capable of implementing Schrodinger time evolution with a slowly varying Hamiltonian) is equal to the total evolution time T. To understand the efficiency of this algorithm we need to understand how big T needs to be as a function of n in order to ensure that the state of the system after step 2 is well approximated by the ground state $|z_0\rangle$ of $H(1)$. A partial answer to this question is provided by the adiabatic theorem which we describe in the next section. Before proceeding we make two remarks.

Firstly, time evolution with a local Hamiltonian can be simulated efficiently on a universal quantum computer. In the previous section we describe a simple simulation algorithm for the case of time-independent Hamiltonians but one can straightforwardly extend these methods to the time-dependent case. This implies that any algorithm developed using adiabatic time evolution can be implemented with only polynomial overhead using a standard quantum computer.

Secondly, note that we don't expect quantum computers to be able to solve NP-complete problems such as 3-SAT in polynomial time. We expect that the run time T of the above algorithm must scale exponentially with n in the worst case.

The adiabatic theorem and the runtime of adiabatic algorithms

Let

$$H(s) \qquad 0 \le s \le 1$$

be a smooth 1-parameter family of local Hamiltonians. Suppose for simplicity that the ground state of $H(s)$ is unique for all $s \in [0, 1]$, and denote this ground state by $|\phi(s)\rangle$. Imagine initializing the system in the ground state $|\phi(0)\rangle$ of $H(0)$, and then evolving with a time-varying Hamiltonian $H(s = t/T)$ where t is time and T is the total evolution time. The time-evolved state $|\psi(t)\rangle$ is defined by

$$\frac{d|\psi\rangle}{dt} = -iH(t/T)|\psi\rangle \qquad 0 \le t \le T.$$

The adiabatic theorem states that as $T \to \infty$ the time-evolved state $|\psi(t = sT)\rangle$ approximates the ground state $|\phi(s)\rangle$ of $H(s)$. Below we quote a rigorous version of this statement from Ref. [JRS07] which provides an error bound for finite T.

Write the eigenvalues of $H(s)$ as

$$E_0(s) < E_1(s) \le E_2(s) \le \ldots \le E_{2^n}(s) \qquad 0 \le s \le 1,$$

where the leftmost inequality is strict because we assume the ground state is unique. Define the minimum spectral gap

$$g_{\min} = \min_{0 \le s \le 1} \left(E_1(s) - E_0(s) \right).$$

Also define

$$C = \max \left\{ 1, \max_{0 \le s \le 1} \|\frac{dH}{ds}\|, \max_{0 \le s \le 1} \|\frac{d^2H}{ds^2}\| \right\}. \tag{7}$$

Theorem 5 (Special case of Theorem 3 from Ref. [JRS07])**.** *Suppose $H(s)$ is smooth one-parameter family of local Hamiltonians with a unique ground state for all $0 \le s \le 1$ as described above. Then for all $0 \le s \le 1$ we have*

$$|\langle \psi(t = sT)|\phi(s)\rangle|^2 \ge 1 - O\left(\frac{C^4}{T^2 g_{\min}^6} \right)$$

where the big-O hides a universal constant which in particular does not depend on s.

From the above we see that by choosing a total running time

$$T = \Theta(C^2 g_{\min}^{-3}) \tag{8}$$

we can ensure that at all intermediate times t there is a high overlap between the state of the system and the ground state $|\phi(t/T)\rangle$ of the instantaneous Hamiltonian.

Can we use Eq. (8) in practice to bound the runtime of quantum adiabatic algorithms (such as the one considered in the previous section)? Let us suppose we are interested only in whether a particular quantum adiabatic algorithm is efficient, that is, we aim to understand whether or not Eq. (8) scales polynomially with n. In most cases of interest including the example from the

previous section one can easily upper bound $C = O(\text{poly}(n))$ and so the efficiency of the quantum adiabatic algorithm is determined by the minimum spectral gap $g_{\min}$. The algorithm is efficient if $g_{\min}$ is lower bounded by an inverse polynomial function of n and inefficient otherwise.

Unfortunately, lower bounding the minimum spectral gap $g_{\min}$ is a notoriously difficult problem and there are few examples of nontrivial Hamiltonians $H(s)$ for which useful estimates have been obtained.

Equivalence between adiabatic quantum computation and the circuit model

We have discussed how, at least in principle, adiabatic evolution can be used to solve certain computational problems. Moreover, such quantum computations can be efficiently simulated by a universal quantum computer. It was shown by Aharanov et al. [AVDK$^+$08] that any quantum circuit can also be efficiently simulated by adiabatic evolution. This establishes that the two models are in fact equivalent.

Theorem 6 ([AVDK$^+$08]). *A quantum circuit can be simulated efficiently by an adiabatic quantum computation.*

Proof sketch. Suppose we are given a quantum circuit $U = U(m)U(m-1)\dots U(1)$ where each $U(j)$ is a 1- or 2-qubit gate. The adiabatic quantum computer will have two registers–a data register with n qubits and a clock register with m qubits. Define a 5-local Hamiltonian

$$H(s) = H_{input} + I \otimes H_{clock} + (1-s)(I \otimes |1\rangle\langle 1|_1) + s \sum_{j=1}^{m} H_j$$

where

$$H_{input} = \sum_{i=1}^{n} |1\rangle\langle 1|_i \otimes |0\rangle\langle 0|_1 \tag{9}$$

$$H_{clock} = \sum_{i=1}^{n} |01\rangle\langle 01|_{i,i+1} \tag{10}$$

$$H_j = \frac{1}{2}\big(I \otimes |100\rangle\langle 100|_{j-1,j,j+1} + I \otimes |110\rangle\langle 110|_{j-1,j,j+1}$$
$$- U(j) \otimes |110\rangle\langle 100|_{j-1,j,j+1} - U(j)^\dagger \otimes |100\rangle\langle 110|_{j-1,j,j+1}\big) \tag{11}$$

Eq. (11) should be modified when $j = 1$ or $j = m$ in the obvious way (by removing operators which act on qubits $j-1$ and $j+1$ respectively).

Define states

$$|\widehat{j}\rangle = (U(j)U(j-1)\dots U(1)|0^n\rangle) \otimes |1^j 0^{m-j}\rangle \qquad j = 0, 1, \dots, m.$$

When $s = 0$ the Hamiltonian is diagonal in the computational basis and its unique ground state is

$$|\widehat{0}\rangle = |0^n\rangle^{data} \otimes |0^m\rangle^{clock}. \tag{12}$$

When $s = 1$ the Hamiltonian is the Feynman-Kitaev construction encountered earlier and its unique ground state is

$$\frac{1}{\sqrt{m+1}} \sum_{j=0}^{m} |\hat{j}\rangle. \tag{13}$$

To simulate the given quantum circuit by adiabatic evolution one prepares the initial product state $|\hat{0}\rangle$, and then slowly changes the Hamiltonian as a function of time as $H(t/T)$ for $0 \le t \le T$. Here T is chosen large enough so that at the end of the evolution the state is well approximated by the history state Eq. (13). A final measurement of all qubits of the clock register in the computational basis gives outcomes 1^m with probability $1/(m+1)$ in which case the state of the data register contains the output of the quantum computation $U(m)U(m-1)\ldots U(1)|0^n\rangle$.

It remains to show that T can be chosen to scale polynomially with n and m. It is convenient to use the fact that for all $0 \le s \le 1$ the Hamiltonian $H(s)$ preserves the subspace

$$\mathcal{A} = \text{span}\{|\hat{0}\rangle, \ldots, |\hat{m}\rangle\}. \tag{14}$$

Since the state of our adiabatic quantum computer is initialized in $|\hat{0}\rangle \in \mathcal{A}$, and since $H(s)$ preserves $\mathcal{A}$, the entire computation proceeds within this subspace. We can therefore consider $\mathcal{A}$ to be the whole Hilbert space and apply the adiabatic theorem to the restricted Hamiltonian $H(s)|_{\mathcal{A}}$. This restricted Hamiltonian is an $m+1 \times m+1$ matrix with a simple one dimensional structure:

$$H(s)|_{\mathcal{A}} = (1-s)\text{diag}(0,1,1,\ldots 1) + s \begin{bmatrix} \frac{1}{2} & -\frac{1}{2} & 0 & 0 & 0 \ldots & 0 \\ -\frac{1}{2} & 1 & -\frac{1}{2} & 0 & 0 \ldots & 0 \\ 0 & -\frac{1}{2} & 1 & -\frac{1}{2} & 0 \ldots & 0 \\ \vdots & \vdots & \vdots & \ddots & & \vdots \\ 0 & 0 & 0 & \cdots -\frac{1}{2} & 1 & -\frac{1}{2} \\ 0 & 0 & 0 & \ldots 0 & -\frac{1}{2} & \frac{1}{2} \end{bmatrix} \tag{15}$$

Note that the above matrix does not depend on the quantum circuit at all. Its minimum spectral gap on the interval $s \in [0,1]$ can be bounded as $g_{\min} \ge \Omega(m^{-2})$ (see Ref. [AVDK$^+$08] for details). We may also straightforwardly upper bound the parameter C since

$$\frac{d^2}{ds^2}\left(H(s)|_{\mathcal{A}}\right) = 0$$

and

$$\|\frac{d}{ds}\left(H(s)|_{\mathcal{A}}\right)\| \le 1 + (m+1)$$

where we used the triangle inequality and Eq. (15). Plugging $C = O(m)$ and $g_{\min} \ge \Omega(m^{-2})$ into Eq. (8) we see that a total evolution time $T = O(\text{poly}(m))$ suffices to simulate the quantum circuit using an adiabatic quantum computer. $\square$

References

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