Lecture 9: Adiabatic Quantum Computation

Computational Aspects of Quantum Simulation
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Abstract

In the last lecture we explored the class QMA and looked into the proof of the quantum Cook-Levin theorem. In today's lecture we will get acquainted with adiabatic quantum computation, which proves to be a potent link between time and ground state simulation.

All exercises are optional unless stated otherwise.

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1 Adiabatic quantum computation

So far we have considered Hamiltonians that are fixed in time. Adiabatic quantum computation instead uses a continuous path of Hamiltonians $H(s)$, $s \in [0,1]$, that interpolates between an initial Hamiltonian $H(0)$, whose ground state is easy to prepare, and a final Hamiltonian $H(1)$, whose ground state encodes the solution to a computational problem.

Definition 1.1 (Adiabatic path and spectral gap)**.** An *adiabatic path* is a sufficiently smooth family of Hermitian operators $H(s)$, $0 \le s \le 1$, with eigenvalues $E_0(s) \le E_1(s) \le \cdots$ and a nondegenerate instantaneous ground state $|\psi_0(s)\rangle$ for every s, i.e. $H(s)\,|\psi_0(s)\rangle = E_0(s)\,|\psi_0(s)\rangle$. The *spectral gap* of the path is

$$\Delta(s) := E_1(s) - E_0(s), \qquad \Delta := \min_{s\in[0,1]} \Delta(s).$$

The minimum gap Δ controls how slowly the path must be traversed. To traverse it in total time T, set $s = t/T$ and evolve according to the Schrödinger equation

$$i\frac{d}{dt}\,|\psi(t)\rangle = H\left(\frac{t}{T}\right)|\psi(t)\rangle\,, \qquad |\psi(0)\rangle = |\psi_0(0)\rangle\,, \qquad 0 \le t \le T. \tag{1}$$

Increasing T makes the Hamiltonian change more slowly. The adiabatic theorem says that if the gap stays open and T is large enough, the state remains close to the instantaneous ground state, and hence ends close to $|\psi_0(1)\rangle$.

For a path-dependent operator $A(s)$, let $\|A\| := \max_{s\in[0,1]} \|A(s)\|$, with the operator norm on the right.

Theorem 1.2 (Adiabatic theorem)**.** *Let $H(s)$, $0 \le s \le 1$, be a twice-differentiable Hamiltonian path with a unique ground state for every s and minimum gap $\Delta > 0$. Let $|\psi(t)\rangle$ solve (1). Then for any $\epsilon > 0$ it suffices to take*

$$T \ge \frac{10^5}{\epsilon^2} \max\left\{ \frac{\|H'\|^3}{\Delta^4}, \frac{\|H'\|\,\|H''\|}{\Delta^3} \right\}$$

to guarantee

$$\min_{\theta\in\mathbb{R}} \left\| |\psi(T)\rangle - e^{i\theta} |\psi_0(1)\rangle \right\| \le \epsilon.$$

Here H' and H'' are derivatives with respect to s.

(See [2] for a statement and proof of this form.) In particular, an inverse-polynomial minimum gap together with polynomially bounded derivatives of $H(s)$ gives polynomial-time adiabatic evolution.

1.1 Ground-state preparation

The adiabatic theorem yields a simple algorithm for preparing ground states. Take an initial Hamiltonian with an easily prepared ground state, for concreteness

$$H_0 = -\sum_{i\in[n]} X_i, \qquad |\psi_0\rangle = \bigotimes_{i\in[n]} |+\rangle,$$

and, for a target Hamiltonian H_F, the linear interpolation

$$H(s) = (1-s)H_0 + sH_F.$$

The procedure is:

1. Prepare $|\psi_0\rangle$, the ground state of H_0.
2. Evolve under $H(t/T)$ as in (1) for a sufficiently large time T.
3. Output the final state, which approximates the ground state of H_F.

For the linear path, $H' = H_F - H_0$ and $H'' = 0$, so the adiabatic theorem gives the sufficient scaling

$$T = O\left(\frac{\|H_F - H_0\|^3}{\epsilon^2 \Delta^4}\right).$$

Hence if $\Delta \ge 1/\operatorname{poly}(n)$ and $\|H_F - H_0\| \le \operatorname{poly}(n)$, the ground state is prepared in polynomial time.

The subtlety is that Δ is the minimum gap along the *entire* path, not just at its endpoints. Even if H_0 and H_F both have large gaps, the gap can become very small, or close entirely, at an intermediate s. Different interpolations between the same endpoints can have very different minimum gaps, so designing a good adiabatic algorithm largely amounts to designing a path that avoids small gaps.

1.2 Adiabatic simulation of quantum circuits

Adiabatic quantum computation connects circuit simulation and ground-state preparation. Recall that if the spectral gap along a path $H(s)$ is sufficiently large, the adiabatic theorem lets us prepare the ground state of $H(1)$, provided the ground state of $H(0)$ is easy to prepare. We now show how to choose such a path so that its final ground state encodes the entire history of an arbitrary quantum circuit. To keep the argument transparent we do *not* impose locality on the Hamiltonians (local constructions are given in [2]).

Let $V = V_L \cdots V_2 V_1$ be a quantum circuit acting on a work register $\mathcal{H}_w$ of n qubits, initialized in $|0^n\rangle$. Let $\mathcal{H}_c = \operatorname{span}\{|0\rangle, \ldots, |L\rangle\}$ be an $(L+1)$-dimensional clock register, and define the uniform clock state

$$|u\rangle := \frac{1}{\sqrt{L+1}} \sum_{t=0}^{L} |t\rangle.$$

Define the *trivial propagation Hamiltonian*, which acts only on the clock:

$$H^0_{\text{prop}} := \frac{1}{2} \sum_{t=0}^{L-1} \mathbb{I}_w \otimes \Big(|t\rangle\langle t| + |t+1\rangle\langle t+1| - |t+1\rangle\langle t| - |t\rangle\langle t+1| \Big).$$

For each gate V_j, choose a Hermitian operator K_j with $V_j = e^{iK_j}$ (for instance via the principal logarithm, so that $\|K_j\| \le \pi$), and for $s \in [0,1]$ set $C_j(s) = e^{isK_j}$. Define the unitary

$$U(s) = \sum_{t=0}^{L} C_t(s) \cdots C_1(s) \otimes |t\rangle\langle t|_c \,,$$

where the $t = 0$ term is the identity on $\mathcal{H}_w$.

Exercise 1.3. Show that $U(1) H^0_{\text{prop}} U(1)^\dagger$ is the operator H_{prop} from the quantum Cook–Levin proof (with the ancillas absorbed into the work register), and that

$$U(1)\big(|0^n\rangle \otimes |u\rangle\big) = \frac{1}{\sqrt{L+1}} \sum_{t=0}^{L} V_t \cdots V_1 \, |0^n\rangle \otimes |t\rangle \,.$$

Next define

$$H_{\text{init}} := \big(\mathbb{I} - |0^n\rangle\langle 0^n|\big)_w \otimes |0\rangle\langle 0|_c \,.$$

Exercise 1.4. Show that $U(s) H_{\text{init}} U(s)^\dagger = H_{\text{init}}$.

We thus define our adiabatic path as

$$H(s) = U(s) H^0_{\text{prop}} U(s)^\dagger + H_{\text{init}}.$$

Exercise 1.5. Show that $H(s)$ has $|\psi_0(s)\rangle = U(s)\big(|0^n\rangle \otimes |u\rangle\big)$ as its instantaneous ground state. (Bonus: argue that it is the *unique* ground state. The Perron–Frobenius theorem may be helpful.)

The spectral gap. Because $H(s)$ is obtained from $H(0) = H^0_{\text{prop}} + H_{\text{init}}$ by the unitary similarity $U(s)$, the eigenvalues, and hence the spectral gap, are independent of s and equal those of $H(0)$. The two terms of $H(0)$ do not commute, but we can analyze their sum by decomposing the work space as

$$\mathcal{H}_w = \text{span}\{|0^n\rangle\} \oplus \text{span}\{|0^n\rangle\}^\perp.$$

Since H^0_{prop} acts only on the clock and H_{init} is block diagonal in this decomposition, $H(0)$ is block diagonal too.

Sector 1: $\text{span}\{|0^n\rangle\} \otimes \mathcal{H}_c$. Here $H_{\text{init}} = 0$, so $H(0) = H^0_{\text{prop}}$.

Exercise 1.6. Show that the eigenvalues of H^0_{prop} are $\lambda_k = 1 - \cos\big(\pi k/(L+1)\big)$ for $k = 0, \ldots, L$, and that its spectral gap is $\Theta(L^{-2})$.

The ground energy is 0, attained by $|u\rangle$, and by the exercise the gap in this sector is $\Theta(L^{-2})$.

Sector 2: $\text{span}\{|0^n\rangle\}^\perp \otimes \mathcal{H}_c$. Here $H_{\text{init}} = \mathbb{I} \otimes |0\rangle\langle 0|_c$, so $H(0)$ acts as $H^0_{\text{prop}} + |0\rangle\langle 0|$ on the clock. For a normalized clock state $|x\rangle = \sum_{t=0}^{L} x_t \, |t\rangle$, its energy is

$$\langle x| \left(H^0_{\text{prop}} + |0\rangle\langle 0|\right) |x\rangle = |x_0|^2 + \frac{1}{2} \sum_{t=0}^{L-1} |x_{t+1} - x_t|^2.$$

Writing $x_t = x_0 + \sum_{j=0}^{t-1} (x_{j+1} - x_j)$ and applying $|\alpha + \beta|^2 \le 2|\alpha|^2 + 2|\beta|^2$ together with Cauchy–Schwarz,

$$|x_t|^2 \;\le\; 2|x_0|^2 + 2t \sum_{j=0}^{L-1} |x_{j+1} - x_j|^2.$$

Summing over t gives

$$1 = \sum_{t=0}^{L} |x_t|^2 \le 4(L+1)^2 \left(|x_0|^2 + \frac{1}{2} \sum_{t=0}^{L-1} |x_{t+1} - x_t|^2 \right).$$

Hence every state in this sector has energy at least $1/\big(4(L+1)^2\big)$.

Combining the two sectors, the ground state is unique with energy 0, and

$$\Delta(H(s)) = \Theta(L^{-2}).$$

Running time. Since $\|K_j\| \le \pi$ and $\|H^0_{\text{prop}}\| \le 2$, we have $\|H'(s)\| = O(L)$ and $\|H''(s)\| = O(L^2)$, so these norms are polynomial in L. Theorem 1.2 therefore implies that the history state $|\eta(1)\rangle = U(1)(|0^n\rangle \otimes |u\rangle)$ can be prepared in time $T = \text{poly}(L, 1/\epsilon)$; crudely, $T = O(L^{11}/\epsilon^2)$.

Remark 1.7. The final ground state is a history state, not just the final circuit state. Measuring the clock and obtaining $t = L$ leaves the work register in $V_L \cdots V_1 |0^n\rangle$. This happens with probability only $1/(L+1)$, but the probability can be boosted to a constant by padding the circuit with polynomially many identity gates.

2 Assigned exercise

Recall the Quantum Approximate Optimization Algorithm (QAOA). Given a classical Hamiltonian H_C, let $H_X = -\sum_{k=1}^n X_k$ and define the parameterized circuit

$$U_p(\vec{\gamma}, \vec{\alpha}) := \prod_{j=1}^{p} e^{-i\gamma_j H_X} e^{-i\alpha_j H_C},$$

where the factor with $j = 1$ acts first (i.e. the product is ordered with j increasing from right to left). Recall also the first-order Lie–Trotter formula and the bounds for discretization of time dependent Hamiltonian evolutions.

Theorem 2.1 (First-order Lie–Trotter formula)**.** *For Hermitian $h_1, \ldots, h_\ell$, real t, and integer $r \ge 1$,*

$$\left\| e^{-it\sum_{a=1}^{\ell} h_a} - \left(e^{-ith_1/r} \cdots e^{-ith_\ell/r} \right)^r \right\| \le \frac{t^2}{2r} \sum_{a<b} \|[h_a, h_b]\| .$$

In particular, this error tends to zero as $r \to \infty$.

Theorem 2.2 (Discretization of time dependent evolutions.)**.** *Let $U(T)$ be the solution to the time dependent Schrödinger equation:*

$$i\frac{d}{dt}|\psi(t)\rangle = H(t)|\psi(t)\rangle$$

with initial state $|\psi(0)\rangle$, in the sense that $U(T)|\psi(0)\rangle = |\psi(T)\rangle$. Then:

$$\left\| U(T) - \prod_{j=1}^{M} e^{-i\frac{T}{M}H\left(\frac{jT}{M}\right)} \right\| \le \frac{T^2}{2M} \max_{t\in[0,T]} \|H'(t)\|$$

Exercise 2.3 (Assigned)**.** Assume that the linear path $H(s) = (1-s)H_X + sH_C$ satisfies the hypotheses of the adiabatic theorem (Theorem 1.2) with spectral gap Δ; in particular, H_C has a unique ground state $|\psi_0\rangle$. Show that for p large enough there exist angles $(\vec{\gamma}, \vec{\alpha})$ such that

$$\left\| U_p(\vec{\gamma}, \vec{\alpha})|+\rangle^{\otimes n} - |\psi_0\rangle \right\| \le \epsilon$$

up to a global phase. Obtain an upper bound on p in terms of ϵ, $\|H_C\|$, $\|H_X\|$, and Δ. What are these angles? (Hint: combine the adiabatic theorem with the Lie–Trotter formula and the discretization bounds.)

You may find the following useful:

Lemma 2.4. *For unitaries V_i, U_i*

$$\|U_1U_2\cdots U_N - V_1V_2\cdots V_N\| \le \sum_{i=1}^{N} \|U_i - V_i\|$$

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References

[1] S. Gharibian, *Approximation, Proof Systems, and Correlations in a Quantum World*, arXiv:1301.2632 (2013).

[2] D. Aharonov, W. van Dam, J. Kempe, Z. Landau, S. Lloyd, and O. Regev, *Adiabatic quantum computation is equivalent to standard quantum computation*, SIAM J. Comput. **37**(1), 166–194 (2007); arXiv:quant-ph/0405098.

[3] A. Yu. Kitaev, A. H. Shen, and M. N. Vyalyi, *Classical and Quantum Computation*, Graduate Studies in Mathematics **47**, American Mathematical Society (2002).

[4] J. Kempe, A. Kitaev, and O. Regev, *The complexity of the local Hamiltonian problem*, SIAM J. Comput. **35**(5), 1070–1097 (2006).