Quantum algorithms (CO 781, Winter 2008)
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LECTURE 18: The quantum adiabatic theorem

In the last part of this course, we will discuss an approach to quantum computation based on the concept of *adiabatic evolution*. According to the quantum adiabatic theorem, a quantum system that begins in the nondegenerate ground state of a time-dependent Hamiltonian will remain in the instantaneous ground state provided the Hamiltonian changes sufficiently slowly. In this lecture we will prove the quantum adiabatic theorem, which quantifies this statement.

Adiabatic evolution When the Hamiltonian of a quantum system does not depend on time, the dynamics of that system are fairly straightforward. Given a time-independent Hamiltonian H, the solution of the Schrödinger equation

$$\mathrm{i}\frac{\mathrm{d}}{\mathrm{d}t}|\psi(t)\rangle = H|\psi(t)\rangle \tag{1}$$

with the initial quantum state $|\psi(0)\rangle$ is given by

$$|\psi(t)\rangle = \exp(-\mathrm{i}Ht)|\psi(0)\rangle. \tag{2}$$

So any eigenstate $|E\rangle$ of the Hamiltonian, with $H|E\rangle = E|E\rangle$, simply acquires a phase $\exp(-\mathrm{i}Et)$. In particular, there are no transitions between eigenstates.

If the Hamiltonian varies in time, the evolution it generates can be considerably more complicated. However, if the change in the Hamiltonian occurs sufficiently slowly, the dynamics remain relatively simple: roughly speaking, if the system begins close to an eigenstate, it remains close to an eigenstate. The *quantum adiabatic theorem* is a formal description of this phenomenon.

For a simple example of adiabatic evolution in action, consider a spin in a magnetic field that is rotated from the x direction to the z direction in a total time T:

$$H(t) = -\cos\left(\frac{\pi t}{2T}\right)\sigma_x - \sin\left(\frac{\pi t}{2T}\right)\sigma_z. \tag{3}$$

Suppose that initially, the spin points in the x direction: $|\psi(0)\rangle = (|0\rangle + |1\rangle)/\sqrt{2}$, the ground state of $H(0)$. As the magnetic field is slowly rotated toward the z direction, the spin begins to precess about the new direction of the field, moving it toward the z axis (and also producing a small component out of the xz plane). If T is made larger and larger, so that the rotation of the field direction happens more and more slowly (as compared to the speed of precession), the state will precess in a tighter and tighter orbit about the field direction. In the limit of arbitrarily slow rotation of the field, the state simply tracks the field, remaining in the instantaneous ground state of $H(t)$.

More generally, for $s \in [0,1]$, let $H(s)$ be a Hermitian operator that varies smoothly as a function of s. (The notion of smoothness will be made precise in the following section.) Let $s := t/T$. Then for T arbitrarily large, $H(t)$ varies arbitrarily slowly as a function of t. An initial quantum state $|\psi(0)\rangle$ evolves according to the Schrödinger equation,

$$\mathrm{i}\frac{\mathrm{d}}{\mathrm{d}t}|\psi(t)\rangle = H(t)|\psi(t)\rangle, \tag{4}$$

or equivalently,

$$\mathrm{i}\frac{\mathrm{d}}{\mathrm{d}s}|\psi(s)\rangle = TH(s)|\psi(s)\rangle. \tag{5}$$

Now suppose that $|\psi(0)\rangle$ is an eigenstate of $H(0)$, which we assume for simplicity is the ground state, and is nondegenerate. Furthermore, suppose that the ground state of $H(s)$ is nondegenerate for all values of $s \in [0,1]$. Then the adiabatic theorem says that in the limit $T \to \infty$, the final state $|\psi(T)\rangle$ obtained by the evolution (4) will be the ground state of $H(1)$.

Of course, evolution for an infinite time is rather impractical. For computational purposes, we need a quantitative version of the adiabatic theorem: we would like to understand how large T must be so that the final state is guaranteed to differ from the adiabatically evolved state by at most some fixed small amount. In particular, we would like to understand how the required evolution time depends on spectral properties of the interpolating Hamiltonian $H(s)$. We will see that the timescale for adiabaticity is intimately connected to the energy gap between the ground and first excited states.

Proof of the adiabatic theorem We would like to compare the evolution according to (5) to the corresponding *(exactly) adiabatic evolution*, in which the initial ground state $|\phi(0)\rangle = |\psi(0)\rangle$ evolves into the instantaneous ground state $|\phi(s)\rangle$ of $H(s)$ satisfying

$$H(s)|\phi(s)\rangle = E(s)|\phi(s)\rangle \tag{6}$$

where $E(s)$ is the instantaneous ground state energy. (We assume for simplicity that the ground state is unique.) Let

$$P(s) := |\phi(s)\rangle\langle\phi(s)| \tag{7}$$

denote the projector onto the ground state of $H(s)$. Then we claim that the Hamiltonian

$$H_a(s) := TH(s) + \mathrm{i}[\dot{P}(s), P(s)] \tag{8}$$

generates exactly adiabatic evolution, where we use a dot to denote differentiation with respect to s. In other words, we claim that the differential equation

$$\mathrm{i}\frac{\mathrm{d}}{\mathrm{d}s}|\xi(s)\rangle = H_a(s)|\xi(s)\rangle \tag{9}$$

with $|\xi(0)\rangle = |\phi(0)\rangle$ has the solution $|\xi(s)\rangle = e^{\mathrm{i}\theta(s)}|\phi(s)\rangle$ for some time-dependent phase $\theta(s)$. Equivalently, the density matrix $P(s) = |\phi(s)\rangle\langle\phi(s)| = |\xi(s)\rangle\langle\xi(s)|$ satisfies the differential equation

$$\mathrm{i}\dot{P}(s) = \mathrm{i}\left[\left(\frac{\mathrm{d}}{\mathrm{d}s}|\xi(s)\rangle\right)\langle\xi(s)| + |\xi(s)\rangle\left(\frac{\mathrm{d}}{\mathrm{d}s}\langle\xi(s)|\right)\right] \tag{10}$$

$$= [H_a(s), P(s)]. \tag{11}$$

To see this, we compute

$$[H_a, P] = T[H, P] + \mathrm{i}[[\dot{P}, P], P] \tag{12}$$

$$= \mathrm{i}(\dot{P}P - 2P\dot{P}P + P\dot{P}) \tag{13}$$

(dropping the argument s when it is clear from context). Differentiating the identity $P^2 = P$ gives

$$\dot{P} = \dot{P}P + P\dot{P}, \tag{14}$$

and multiplying this identity by P on both sides gives

$$P\dot{P}P = 0. \tag{15}$$

Thus we see that $[H_a, P] = \mathrm{i}\dot{P}$ as claimed.

Recall that our goal is to understand the evolution according to (5), which can be written as

$$|\psi(s)\rangle = U(s)|\psi(0)\rangle \tag{16}$$

for some unitary operator $U(s)$. It is helpful to write the evolution in terms of a differential equation for $U(s)$. We have

$$\begin{aligned}
\frac{\mathrm{d}}{\mathrm{d}s}U(s)|\psi(0)\rangle &= \frac{\mathrm{d}}{\mathrm{d}s}|\psi(s)\rangle && (17)\\
&= -\mathrm{i}TH(s)|\psi(s)\rangle && (18)\\
&= -\mathrm{i}TH(s)U(s)|\psi(0)\rangle, && (19)
\end{aligned}$$

and since this holds for any initial state $|\psi(0)\rangle$, we see that $U(s)$ satisfies the differential equation

$$\mathrm{i}\dot{U}(s) = TH(s)U(s). \tag{20}$$

Similarly, we have

$$\mathrm{i}\dot{U}_a(s) = TH_a(s)U_a(s) \tag{21}$$

for the corresponding adiabatic evolution.

We would like to show that the difference between U and U_a is small. Thus we consider

$$\begin{aligned}
U(1) - U_a(1) &= -U(1)\int_0^1 \frac{\mathrm{d}}{\mathrm{d}s}(U^\dagger U_a)\,\mathrm{d}s && (22)\\
&= -\mathrm{i}U(1)\int_0^1 U^\dagger[H_a - TH]U_a\,\mathrm{d}s && (23)\\
&= U(1)\int_0^1 U^\dagger[\dot{P}, P]U_a\,\mathrm{d}s && (24)
\end{aligned}$$

where the first line follows from the fundamental theorem of calculus, the second from (20) and (21), and the third from the definition of H_a.

It turns out that the expression $[\dot{P}, P]$ can be written as a commutator with the Hamiltonian, $[\dot{P}, P] = [H, F]$, where

$$F := R\dot{P}P + P\dot{P}R \tag{25}$$

where we have defined the *resolvent*

$$R := \frac{1}{H - E}. \tag{26}$$

This can be seen as follows: noting that $(H - E)R = 1$ so that $HR = 1 + ER$, and $PH = EP$, we have

$$\begin{aligned}
[H, F] &= HR\dot{P}P + HP\dot{P}R - R\dot{P}PH - P\dot{P}RH && (27)\\
&= \dot{P}P + ER\dot{P}P + EP\dot{P}R - ER\dot{P}P - P\dot{P} - EP\dot{P}R && (28)\\
&= [\dot{P}, P] && (29)
\end{aligned}$$

as claimed.

Now let us define

$$\tilde{F} := U^\dagger F U. \tag{30}$$

Using (20), we have

$$\dot{\tilde{F}} = \mathrm{i}TU^\dagger[H,F]U + U^\dagger \dot{F} U; \tag{31}$$

therefore

$$U^\dagger[\dot{P},P]U = U^\dagger[H,F]U \tag{32}$$

$$= \frac{1}{\mathrm{i}T}(\dot{\tilde{F}} - U^\dagger \dot{F} U). \tag{33}$$

Now we insert this into (24) and integrate the first term by parts:

$$U(1) - U_a(1) = \frac{1}{\mathrm{i}T}U(1)\int_0^1 [(\dot{\tilde{F}} - U^\dagger \dot{F} U)U^\dagger U_a]\,\mathrm{d}s \tag{34}$$

$$= \frac{1}{\mathrm{i}T}U(1)\left(\left[\tilde{F}U^\dagger U_a\right]_0^1 - \int_0^1 \left(\tilde{F}\frac{\mathrm{d}}{\mathrm{d}s}(U^\dagger U_a) - U^\dagger \dot{F} U_a\right)\mathrm{d}s\right) \tag{35}$$

$$= \frac{1}{\mathrm{i}T}U(1)\left(\left[\tilde{F}U^\dagger U_a\right]_0^1 - \int_0^1 \left(\tilde{F}U^\dagger[\dot{P},P]U_a - U^\dagger \dot{F} U_a\right)\mathrm{d}s\right) \tag{36}$$

where we compute the derivative of $U^\dagger U_a$ as in (24). Thus we have

$$T\|U(1) - U_a(1)\| \le \|F(0)\| + \|F(1)\| + \int_0^1 \mathrm{d}s\,\left(2\|F\|\cdot\|\dot{P}\| + \|\dot{F}\|\right). \tag{37}$$

Now

$$\|F\| \le 2\|R\dot{P}P\| \tag{38}$$

$$= 2\|R(1-P)\dot{P}\| \tag{39}$$

$$\le 2\|R(1-P)\|\cdot\|\dot{P}\| \tag{40}$$

$$\le \frac{2\|\dot{P}\|}{\Delta} \tag{41}$$

where we have used (14) to see that $\dot{P}P = (1-P)\dot{P}$, and where $\Delta(s)$ is the gap between the smallest eigenvalue $E(s)$ of $H(s)$ and the nearest distinct eigenvalue of $H(s)$. Also,

$$\dot{F} = \dot{R}\dot{P}P + R\ddot{P}P + R\dot{P}^2 + P\dot{P}\dot{R} + P\ddot{P}R + \dot{P}^2R \tag{42}$$

and

$$\dot{R} = -\frac{1}{(H-E)}\dot{H}\frac{1}{(H-E)} \tag{43}$$

(to see this, differentiate the identity $(H-E)R = 1$), so (by similar calculations as above)

$$\|\dot{F}\| \le 2\left(\frac{\|\dot{H}\|\cdot\|\dot{P}\|}{\Delta^2} + \frac{\|\ddot{P}\|}{\Delta} + \frac{\|\dot{P}\|^2}{\Delta}\right). \tag{44}$$

Thus we have

$$\frac{T}{2}\|U(1) - U_a(1)\| \le \frac{\|\dot{P}(0)\|}{\Delta(0)} + \frac{\|\dot{P}(1)\|}{\Delta(1)} + \int_0^1 \mathrm{d}s \left(3\frac{\|\dot{P}\|^2}{\Delta} + \frac{\|\dot{H}\| \cdot \|\dot{P}\|}{\Delta^2} + \frac{\|\ddot{P}\|}{\Delta}\right). \tag{45}$$

Finally, we would like to express $\|\dot{P}\|$ and $\|\ddot{P}\|$ in terms of H. We can obtain upper bounds for these quantities using first and second order perturbation theory. Intuitively, if the Hamiltonian changes slowly, and if its eigenvalues are not close to degenerate, then its eigenvectors should also change slowly. At first order, we have

$$\|\dot{P}\| \le c_1 \frac{\|\dot{H}\|}{\Delta} \tag{46}$$

for some constant c_1, and at second order,

$$\|\ddot{P}\| \le c_2 \frac{\|\ddot{H}\|}{\Delta} + c_3 \frac{\|\dot{H}\|^2}{\Delta^2} \tag{47}$$

for some constants c_2, c_3. Plugging these estimates into (45), we have

$$\frac{T}{2}\|U(1) - U_a(1)\| \le c_1 \frac{\|\dot{H}(0)\|}{\Delta(0)^2} + c_1 \frac{\|\dot{H}(1)\|}{\Delta(1)^2} + \int_0^1 \mathrm{d}s \left((3c_1^2 + c_1 + c_3)\frac{\|\dot{H}\|^2}{\Delta^3} + c_2 \frac{\|\ddot{H}\|}{\Delta^2}\right). \tag{48}$$

Overall, we have proved the following quantitative version of the adiabatic theorem:

Theorem. *Suppose $H(s)$ has a nondegenerate ground state for all $s \in [0,1]$, and suppose that the total evolution time satisfies*

$$T \ge \frac{2}{\epsilon}\left[c_1 \frac{\|\dot{H}(0)\|}{\Delta(0)^2} + c_1 \frac{\|\dot{H}(1)\|}{\Delta(1)^2} + \int_0^1 \mathrm{d}s \left((3c_1^2 + c_1 + c_3)\frac{\|\dot{H}\|^2}{\Delta^3} + c_2 \frac{\|\ddot{H}\|}{\Delta^2}\right)\right]. \tag{49}$$

Then evolution of the initial state $|\psi(0)\rangle = |\phi(0)\rangle$ under the Schrödinger equation (5) produces a final state $|\psi(1)\rangle$ satisfying

$$\||\psi(1)\rangle - |\phi(1)\rangle\| \le \epsilon. \tag{50}$$