

Lecture 3: Adiabatic quantum computation and QAOA

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1 Adiabatic quantum computation

The quantum circuit model is a discrete model of quantum computation, and it has much appeal to computer scientists. Physicists however are more inclined to think about quantum dynamics as following Schrödinger's equation

$$\partial_t |\psi_t\rangle = -iH_t |\psi_t\rangle,$$

where H_t is the (potentially time-dependent) *Hamiltonian* of the quantum system. In the time-independent case ($H_t = H$), this solves to $|\psi_t\rangle = e^{-iHt} |\psi_0\rangle$. In physics, an important role is played by the ground state of the Hamiltonian H , corresponding to the eigenvector with the smallest eigenvalue.

The idea of adiabatic quantum computation is to (i) encode (the solution of) a quantum computation in the ground state of a Hamiltonian (see Section 1.2), and (ii) use adiabatic evolution to prepare that ground state (see Section 1.1).

1.1 Quantum adiabatic algorithm

In its simplest form, the quantum adiabatic algorithm takes the following form:

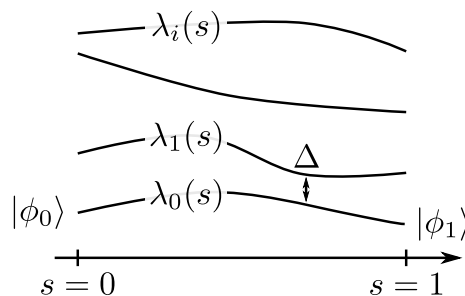
- **Input:** initial Hamiltonian H_0 with an easy-to-prepare ground state $|\phi_0\rangle$, final Hamiltonian H_1 whose ground state $|\phi_1\rangle$ we wish to prepare
- **Evolution:** Prepare $|\psi_0\rangle = |\phi_0\rangle$, and let it evolve according to the Schrödinger equation

$$\partial_t |\psi_t\rangle = -iH(t/T) |\psi_t\rangle,$$

where $H(s) = (1 - s)H_0 + sH_1$ for $0 \leq s \leq 1$.

- **Output:** state $|\psi_T\rangle$

The algorithm succeeds if $|\psi_T\rangle \approx |\phi_1\rangle$. The reason why this algorithm could succeed at all is called the *quantum adiabatic theorem*. It says that if we start in the ground state of a “slowly-varying” Hamiltonian, then we stay in the ground state of that Hamiltonian. Clearly, as $T \rightarrow \infty$ then our Hamiltonian $H(t/T)$ will be slowly varying, and so the output state $|\psi_T\rangle$ should equal $|\phi_1\rangle$, the ground state of the final Hamiltonian.



A more quantitative statement is given by the following theorem. Let $\lambda_0(s) \leq \lambda_1(s) \leq \dots \leq \lambda_{N-1}(s)$ denote the eigenvalues of $H(s)$. The theorem states that the evolution time depends on the *spectral gap* of $H(s)$, which is the distance between the ground energy $\lambda_0(s)$ and the energy $\lambda_1(s)$ of the first excited state (see figure above).

Theorem 1 (Quantum adiabatic theorem). *Let the spectral gap of $H(s)$ be at least Δ for all $0 \leq s \leq 1$. For any $\epsilon > 0$, there exists*

$$T = \text{poly} \left(\frac{1}{\Delta}, \frac{1}{\epsilon}, \|H_0\| + \|H_1\| \right)$$

such that $|\psi_T\rangle$ will be ϵ -close to $|\phi_1\rangle$.

1.2 Feynman Hamiltonian

Now that we defined the quantum adiabatic algorithm, how do we actually do a computation with it? A closely related problem was considered a long time ago by Feynman.¹

Consider a general quantum circuit applying some T gates U_1, U_2, \dots, U_T to an n -qubit system. The Feynman Hamiltonian is defined as

$$H_F = \sum_{t=1}^T H_t, \quad H_t = I \otimes |t\rangle\langle t| - U_t \otimes |t\rangle\langle t-1| + I \otimes |t-1\rangle\langle t-1| - U_t^\dagger \otimes |t-1\rangle\langle t|,$$

where the H_t 's are positive semi-definite.

Exercise 1. *Check that the following family of states are ground states of H_F , for any $|\psi\rangle$:*

$$\frac{1}{\sqrt{T+1}} \sum_{t=0}^T U_t \dots U_1 |\psi\rangle |t\rangle. \quad (1)$$

Argue that these are the only ground states.

We call a state of the form Eq. (1) a “clock state”, as it encodes (in superposition) the different timesteps of the quantum computation applied to an initial state $|\psi\rangle$. As we are typically only interested in the computation applied to the initial state $|\psi\rangle = |0^n\rangle$, we add an extra penalty term

$$H_{\text{init}} = (I - |0^n\rangle\langle 0^n|) \otimes |0\rangle\langle 0|.$$

The only ground state of H_F that also satisfies this penalty term is the state

$$|\phi_1\rangle = \frac{1}{\sqrt{T+1}} \sum_{t=0}^T U_t \dots U_1 |0^n\rangle |t\rangle,$$

and hence this is the unique ground state of the combined Hamiltonian $H_1 = H_F + H_{\text{init}}$. If we measure the last register and retrieve T (which happens with probability $1/(T+1)$), then we know the resulting quantum state is $U_T \dots U_1 |0^n\rangle$, which corresponds to the output of the quantum computation. As a consequence, if we can efficiently prepare the ground state of $H_F + H_{\text{init}}$, then we can efficiently simulate a computation in the quantum circuit model.

¹See [Fey86]. Interestingly, Feynman only showed how to do *classical* computation with the quantum adiabatic algorithm, but it equally works for quantum computation.

To actually prepare the ground state of H_1 we use the quantum adiabatic algorithm. As the final Hamiltonian we pick H_1 , and as initial Hamiltonian H_0 we pick the trivial (diagonal) Hamiltonian

$$H_0 = I \otimes (I - |0\rangle\langle 0|) + H_{\text{init}},$$

whose ground state is $|\phi_0\rangle = |0^n\rangle |0\rangle$. By the quantum adiabatic theorem, we can efficiently traverse from $|\phi_0\rangle$ to the clock state $|\phi_1\rangle$ if the gap Δ of $H(s) = (1-s)H_0 + sH_1$ is not too small. One can show that $\Delta \in \Omega(1/T^2)$ (see e.g. [Chi17, Lemma 30.1]), and this yields (half of) the following theorem.

Theorem 2 ([AVDK⁺08]). *Adiabatic quantum computation is polynomially equivalent to the quantum circuit model.*

The second half of the theorem states that quantum adiabatic computation is not more powerful than the circuit model. This follows from the fact that we can do Hamiltonian simulation in the circuit model (see exercises).

2 Quantum adiabatic optimization algorithm

While quantum adiabatic computation is polynomially equivalent to the quantum circuit model, there are still algorithms that are much more natural to implement in the adiabatic model. One such algorithm is called the *quantum adiabatic optimization algorithm*, proposed by Farhi, Goldstone, Gutman and Sipser [FGGS00].

Consider a classical optimization problem over n -bit strings, encoded by a function

$$h : \{0,1\}^n \mapsto \mathbb{R}.$$

Our goal is to find a string x that minimizes $h(x)$. We can easily frame this as a ground state problem. Indeed, such a minimizer x would correspond to a ground state $|x\rangle$ of the (diagonal) Hamiltonian

$$H_1 = \sum_{z \in \{0,1\}^n} h(z) |z\rangle\langle z|. \quad (2)$$

We then use the quantum adiabatic algorithm to try and prepare a ground state $|\phi_1\rangle$ of H_1 . Such a state must be a linear combination of minimizers of h , and so measuring the state must return a minimizer of h .

It remains to specify the initial Hamiltonian H_0 . A naive approach is to pick again a diagonal Hamiltonian such as $H_0 = I - |0^n\rangle\langle 0^n|$ or $H_0 = -\sum_j Z_j$, where Z_j is shorthand for applying the Pauli Z -gate to the j -th qubit while leaving the other qubits invariant. Both Hamiltonians have a unique (and trivial to prepare) ground state $|0^n\rangle$.

Exercise 2. *What goes wrong if we try to apply the adiabatic theorem to the resulting Hamiltonian $H(s) = (1-s)(I - |0^n\rangle\langle 0^n|) + sH_1$?*

Surprisingly, this problem can be easily avoided by picking an initial Hamiltonian that does not commute with H_1 (equivalently, H_1 is not diagonal in the same basis as H_0). A phenomenon called “avoided crossing” then ensures that no energy levels $\lambda_i(s)$ and $\lambda_j(s)$ will cross for $i \neq j$. This ensures a nonzero gap $\Delta > 0$ throughout the evolution. A typical choice is the Hamiltonian

$$H_0 = -\sum_j X_j, \quad (3)$$

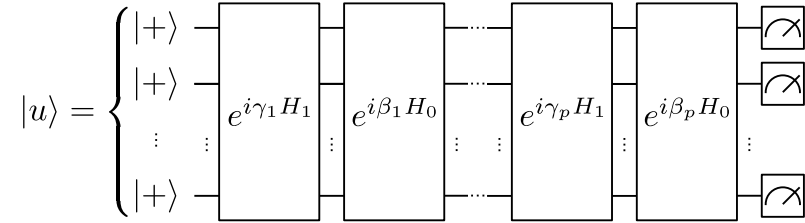
where X_j is shorthand for applying the Pauli X -gate to the j -th qubit while leaving the other qubits invariant. The unique ground state of H_0 is $|\phi_0\rangle = |+\rangle^{\otimes n} = \frac{1}{\sqrt{2^n}} \sum_{z \in \{0,1\}^n} |z\rangle$.

The resulting quantum adiabatic optimization algorithm will succeed if run for a time $T \geq \text{poly}(1/\Delta)$, with Δ the gap of the intermediate Hamiltonian $H(s)$. The algorithm will hence be efficient precisely when $H(s)$ has a large gap (at least inversely polynomial with n). Unfortunately, as is the case with classical variants of this algorithm (e.g., simulated annealing), this is generally hard to verify. This makes the quantum adiabatic optimization algorithm mostly a heuristic.

3 Quantum approximate optimization algorithm (QAOA)

As there was excitement around the quantum adiabatic optimization algorithm around the year 2000, there is currently excitement around the quantum *approximate* optimization algorithm (QAOA). This is a variation on the adiabatic algorithm, and was proposed in 2014 by the same Farhi, Goldstone and Gutmann. QAOA is a so-called “variational” quantum algorithm, and it lies between the quantum adiabatic model and the quantum circuit model.

Similar to the adiabatic algorithm, the purpose is to minimize some cost function $h : \{0, 1\}^n \mapsto \mathbb{R}$. We again define the cost Hamiltonian $H_1 = \sum_z h(z) |z\rangle \langle z|$, as well as a second (noncommuting) “mixer” Hamiltonian H_0 (e.g., $H_0 = -\sum_j X_j$). The quantum approximate optimization algorithm is then described by the following circuit, parameterized by a depth parameter $p \in \mathbb{N}$ and reals $\gamma = (\gamma_1, \dots, \gamma_p)$ and $\beta = (\beta_1, \dots, \beta_p)$:



The circuit corresponds to alternatingly letting the system evolve according to the Hamiltonians H_0 and H_1 , for times given by the parameters γ and β . The performance of the algorithm is measured by the expected cost $E(\gamma, \beta)$ of the output, which is

$$E(\gamma, \beta) = \langle \psi(\gamma, \beta) | H_1 | \psi(\gamma, \beta) \rangle = \sum_z |\langle \psi(\gamma, \beta) | z \rangle|^2 h(z).$$

We can estimate $E(\gamma, \beta)$ for fixed γ and β by repeatedly running the QAOA circuit and measuring the output. The parameters are then tuned via a classical algorithm (typically in a variational manner) with the purpose of minimizing $E(\gamma, \beta)$.

Similar to the adiabatic optimization algorithm, QAOA is mostly a heuristic algorithm, in that it has proven difficult to show rigorous bounds on its performance. Nevertheless, there have been some (recent) promising studies, such as [BM22], showing that it can outperform brute force algorithms such as Grover’s algorithm.

References

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