Lecture 18: Quantum annealing and Adiabatic quantum computation

1 Introduction

Another model of quantum computation that has also received a lot of attention, partly due to the D-Wave machines. We will not go into substantial detail for this alternate model of quantum computation but for completeness it is useful to give the basics.

The generic problem to be solved is finding the ground state of a classical Ising model, which is specified as a quadratic function of a set of N spins $s_i = \pm 1$:

$$H = -\sum_{i<j} J_{ij} s_i s_j - \sum_{i=1}^{N} h_i s_i \tag{1.1}$$

The decision problem associated with determining the ground state energy of H (e.g. does the ground state have energy ≤ 0?) is NP-complete. Therefore, there exists an efficient mapping between the Ising model and other combinatorial optimization problems such as the traveling salesman, graph partitioning, exact cover, 3SAT, etc. These mappings are explicitly given in Ref. [1].

Therefore, solving for the ground state of an Ising spin glass can encode solutions of combinatorial optimization problems, and hence finding ways to find these ground states is of interest. In general, of course, an efficient solution does not exist. However, there may be instances that can be solved by different algorithms.

A class of algorithms that aim to solve such problems are annealing. A motivation for these types of algorithms is as follows. Consider a liquid that undergoes a phase transition to a solid. We can imagine this process as a type of analog computation in which the atoms identify the lowest energy state given the external thermodynamic constraints (e.g. the crystalline phase). However, the crystalline state is not necessarily realized if the path from the liquid to solid phase is not favorable. For instance, if a liquid is quenched too rapidly the system will end up in a metastable state that is not the ground state. However, if it is cooled sufficiently slowly it will end up in the global minimum.

By analogy, simulated annealing mimics the annealing process to eventually settle into the ground state of a cost function. The simulations generally start at high temperature so that all the phase space is explored. The system temperature is gradually decreased, decreasing the transition probabilities to transition to energetically unfavorable states. Gradually, the system will (ideally) settle into the ground state of the energy landscape described by the cost function.

Classical simulated annealing works quite well for certain instances of hard problems. However, a theorem exists known as the "No Free Lunch" theorem, which states that every optimization method that works for certain classes of problems fails for other classes. For classical simulated annealing, a class of problems for which it fails is that containing cost functions with tall, thin barriers as occurs with spin glasses. This failure motivates a search for alternate types of annealing methods.

Quantum annealing is an alternate annealing method that many hope can solve certain instances of these problems. The quantum version of this Ising model above is the quantum transverse Ising model, obtained from above by adding a transverse field and Pauli operators:

$$H = -\Gamma(t)\sum_i X_i - \left(\sum_i h_i Z_i + \sum_{i>j} J_{ij} Z_i Z_j\right) \equiv -\Gamma(t)\sum_i X_i - H_1 \tag{1.2}$$

Quantum annealing is a type of analog quantum computation. The actual device consists of spins that can be subjected to biases and couplers, representing the h_i and J_{ij} terms in the Hamiltonian, respectively. Just as in classical annealing, if we simply apply the terms corresponding to our desired Hamiltonian to the device, we will generally end up in a metastable state that is not the ground state. What we do instead is analogous to classical annealing: we start at a high "temperature" that allows to explore all states, then gradually decrease the temperature to settle into the ground state.

In the quantum case, a transverse field is used to place the system in a superposition of all states, corresponding to high temperature in the classical simulation. We apply a field, corresponding to a Hamiltonian for which the ground state is easily found and for which the operator does not commute with the rest of the system Hamiltonian, and the system then enters that ground state. We gradually decrease the external field and add in our desired Hamiltonian, and (hopefully) we eventually end up in the ground state of our desired Hamiltonian. Quantum fluctuations due to the non-commuting nature of the different operators takes the place of thermal excitations in classical annealing. We can then perform measurements on this state to get desired quantities.

You may hear thtat the advantage of quantum annealing relates to the ability to tunnel through tall, thin barriers. However, the actual mechanism of any possible speedup for quantum annealing over classical methods is rather subtle. [2] It is known that tunneling is not required for speedup. Further, tunneling generally refers to the energy landscape of the final cost function corresponding to the Hamiltonian of interest. But, this landscape is actually not present at all during the calculation since the Hamiltonian is continuously changing during the anneal! Overall, the mechanism of a possible speedup is not clear at present.

2 Adiabatic quantum computation

Quantum annealing does have a firm theoretical foundation, however, in the ideal limit of adiabatic quantum computation (AQC). In the limit of adiabaticity, we have the well-known adiabatic theorem which states that a system that starts in a given eigenstate of a Hamiltonian will remain in that position in the eigenspectrum as the Hamiltonian is evolved, if the evolution happens sufficiently slowly. Of relevance for us, the eigenstate can be the ground state.

Let's formally define what we mean by AQC [2]. Let $H = \sum_{i=1}^{n} H_i$ where H_i is k-local. k-local AQC is defined by H_0 and H_1 acting on a total of n sites, each with $p \geq 2$ states. The ground state of H_0 is a unique product state. The output is a state that is ϵ close to the ground state of H_1. The procedure follows a path $s(t) : [0, t_f) \rightarrow [0, 1]$, known as the schedule, where t_f is the smallest time such that the adiabatic evolution generated by

$$H(s) = (1 - s)H_0 + sH_1 \tag{2.1}$$

at t_f is ϵ close to H_1.

The reason that this procedure can work is due to the Adiabatic Theorem, which is formally stated as:

If a system is initially in an eigenstate (e.g. the ground state) $|\epsilon_0(0)\rangle$ of $H(t)$, then time evolution will keep the actual state in the instantaneous eigenstate of $H(t)$ if $H(t)$ varies sufficiently slowly.

The mathematical requirement of slowly enough is a bit subtle to define.[2] One specification is this one: let $s = t/t_f$, $H = H(s)$, indicating that H only depends on time through s rather than on the absolute time. Define the instantaneous eigenstates and energies of $H(s)$ as

$$H(s) \left|\epsilon_j(s)\right\rangle = \epsilon_j(s) \left|\epsilon_j(s)\right\rangle \tag{2.2}$$

where h indexes the eigenstate in the spectrum. The Schrodinger equation for such a Hamiltonian is:

$$\frac{\partial |\psi_{t_f}(s)\rangle}{\partial t} = \frac{1}{t_f}\frac{\partial |\psi_{t_f}(s)\rangle}{\partial s} = -iH(s)|\psi_{t_f}(s)\rangle \tag{2.3}$$

Then the requirement for adiabaticity is:

$$\frac{1}{t_f}\max_{s\in[0,1]}\frac{\langle\epsilon_i(s)|\partial_s H(s)|\epsilon_j(s)\rangle}{|\epsilon_i(s)-\epsilon_j(s)|^2} \ll 1 \tag{2.4}$$

for all $j \neq i$. Therefore, this equation is the origin the often-quoted result that the required t_f is set by the inverse square of the minimum energy gap along the path. For a ground state, $\Delta = \min_s \epsilon_1(s) - \epsilon_0(s)$.

Ref. [3] says that AQC is reasonably robust against external perturbation and noise in the likely situation that the device is not perfectly adiabatic.

3 Results from complexity theory

What types of problems can this form of quantum computation handle, and will it yield a quantum speedup? Complexity analysis helps us answer these questions. First, we have the following extremely important result [4]: the adiabatic computation model and the standard quantum circuit model are polynomially equivalent. What this means is that if we can consider any type of Hamiltonian to evolve in AQC, we can find one that will reproduce the result of applying unitary gates, and in the other direction we can apply gates to mimic the evolution of the Hamiltonian in AQC.

However, problems considered by present quantum annealing devices are typically stoquastic, which are defined as Hamiltonians with real, non-positive off-diagonal matrix elements in some basis such as the computational basis.[5] Such Hamiltonians are often found in optimization problems and have a number of very favorable properties that make achieving quantum speedups difficult. First, consider the following result:

The ground state $|\psi\rangle$ of a stoquastic Hamiltonian H can always be expressed using only real nonnegative amplitudes:

$$|\psi\rangle = \sum_{x\in\{0,1\}^n} a_x |x\rangle \tag{3.1}$$

with $a_x \geq 0$.

We can prove it with the following argument. If H is stoquastic, then the Gibbs matrix $\rho = \exp(-\beta H)/Tr(\exp(-\beta H))$ has all positive matrix elements. This follows because $-\beta H$ is non-negative (remember we can choose the diagonal entries by a suitable choice of energy offset) and hence powers of $-\beta H$ are non-negative, hence $e^{-\beta H}$ is non-negative. For small β, $\rho \approx I - \beta H$ is also non-negative. The largest eigenvalue of $I - \beta H$ corresponds to the smallest eigenvalue of H, or the ground state energy. By the Perron-Frobenius theorem, this eigenvalue is unique and the eigenvector $|\psi\rangle$ can be chosen with real non-negative amplitudes: Therefore, we can assign a probability distribution to the eigenvector amplitudes that can be classically sampled. That means that the problem can in fact be tractable with a classical probabilistic algorithm.

There are other results that imply classical tractability of stoquastic problems:

- The ground state energy of the ferromagnetic Ising model can be found in polynomial time classically, even including a transverse field.

- The stoquastic k-local H is in the complexity class AM. Since it is not believed that QMA $\subseteq$ AM, stoquastic problems are likely not QMA-complete, meaning they cannot be reduced to all other problems in QMA.
- For various reasons, stoquastic problems are unlikely to be universal for quantum computation (otherwise the polynomial hierarchy of complexity classes would collapse).
- Adiabatic evolution for stoquastic, frustration free H is in BPP, meaning it can be efficiently simulated probabilistically on a classical computer.

There are cases where a quantum speedup might happen. But there are other challenges too. For instance, in an adiabatic quantum computation, the speed of evolution is limited by the minimum gap along the path which is not known in advance. Further, in actual quantum annealers, the machine is not in fact adiabatic - it does interact with the environment causing decoherence and violating the assumptions of the adiabatic theorem.

4 The D-Wave machine

D-Wave has received a lot of attention so we should discuss it in light of all the material above. The D-Wave machine is a quantum annealer consisting of superconducting qubits. The D-Wave QPU consists of interconnected qubits arranged in a Chimera architecture, meaning that connected unit cells are themselves connected in some way. The machine is able to bias and couple qubits using external controls that are programmable. The Hamiltonian implemented by the machine is the quantum transverse Ising model:

$$H = -\frac{A(s)}{2}\sum_i X_i + \frac{B(s)}{2}\left(\sum_i h_i Z_i + \sum_{i>j} J_{ij} Z_i Z_j\right) \tag{4.1}$$

The first term is the initial state, having a ground state of a superposition of all states as expressed in the computational basis (somewhat analogous to high temperature in classical annealing). The second term is the Hamiltonian for which we want the ground state. $A(s)$ and $B(s)$ define the schedule, or the evolution path. The simulation starts with $A(s) \gg B(s)$ and ends with $A(s) \ll B(s)$. Regardless of sign of $A(s)$ it is stoquastic as local unitaries can be applied to change the basis such that the overall sign of the transverse field term is negative.

Due to limitations in the hardware, the Hamiltonian (transverse Ising model) for the D-Wave system is stoquastic. Making it non-stoquastic would require additional couplings, e.g. XX that are difficult to implement experimentally, although a very recent report claims to have done so [**ozfidan_2019**]. Despite this advance, it does not provide arbitrary control over non-stoquastic interactions between qubits and thus is still limited in what types of non-stoquastic couplings can be performed.

In sum, finding unambiguous quantum speedup with quantum annealers is challenging, and the latest results of which I am aware show that they are still not better than the best classical algorithms.

References

[1]A. Lucas, "Ising formulations of many NP problems", Frontiers in physics **2** (2014) 10.3389/fphy.2014.00005.

[2]T. Albash and D. A. Lidar, "Adiabatic quantum computation", Reviews of Modern Physics **90**, 015002 (2018).

[3]A. M. Childs, E. Farhi, and J. Preskill, "Robustness of adiabatic quantum computation", Physical Review A **65**, 012322 (2001).

[4]D. Aharonov, W. van Dam, J. Kempe, Z. Landau, S. Lloyd, and O. Regev, "Adiabatic quantum computation is equivalent to standard quantum computation", in 45th annual IEEE symposium on foundations of computer science (2004), pp. 42–51.

[5]S. Bravyi, D. P. DiVincenzo, R. I. Oliveira, and B. M. Terhal, "The complexity of stoquastic local hamiltonian problems", arXiv (2006).