Adiabatic Quantum Computer Simulation

Pablo Xabier Arregui García
Alma Mater Studiorum - Università di Bologna

This pages will give the reader an introduction to the problem the simulation is trying to solve and the results that can be obtained from the execution of the code. However, although it is strongly suggested to read this document before running or trying to understand the code, it does not contain information about the algorithm and the functions used to solve the problem. It neither contains information about how to install and run the program. **To obtain an explanation of how to proceed with the execution of the code, go to the README file.**

I. Introduction to the Problem

A large part of computer science problems are based on optimization, and although we often have no choice but to develop complicated code to solve these problems, sometimes we have to look around, because nature itself is capable of giving us the solution. From the atomic structure of noble gases, to the minimization of the area of a soap film, nature always seeks stability, that is, the state of minimum energy.

An analog computer makes use of this property to solve optimization problems. However, these problems often present local minima, also known in physics as metastable states, and, if we are not careful, we may end up in one of these instead of the absolute minimum we are looking for. To avoid this, we use the method of "annealing", which consists of adding an element to a system that causes large fluctuations in energy (usually temperature) and slowly reducing it until the absolute minimum of energy is found. If during the "cooling" process the system is in a metastable state and the fluctuations are still large enough, it could overcome the barrier and continue towards the fundamental state.

Sometimes, however, the energy barriers, though fine, are too high and the method fails. We are forced to look for an alternative method that will allow us to break through these kinds of barriers. This is where quantum comes into play. Adiabatic quantum computing is the quantum analog of classical annealing and makes use of the tunnel effect to cross these high, narrow barriers. It operates as follows: Be an initial system, at low temperature (so that quantum effects are relevant), with a Hamiltonian H_0 whose fundamental state (GS) presents large quantum fluctuations due to an element external to the system. If we slowly reduce this element until it

disappears, it is to be expected that the hamiltonian will evolve into a target hamiltonian H_1 , whose GS is the solution to the problem. In fact, if the speed at which the system evolves is slow enough, the so called adiabatic theorem assures us that the GS of H_1 will be reached. This is where the difficulty of the problem lies: how fast should we proceed with annealing to ensure that we have reached the absolute minimum of energy?

According to the Landau-Zener formula, the speed is proportional to the square of the energy gap between the GS and the first excited state of the Hamiltonian at each instant. Taking this into account, our goal of using this simulation is to find the computation time that an AQC would need to solve the problem posed below, as well as to observe the variation of the hamiltonian GS and the energy gap as we proceed with the "annealing". A quantum system is established so that the energy is related to the function we want to minimize, that is, its base state will provide us with the solution we are looking for.

The quantum system of this specific simulation will be based on the spin glass problem. This problem considers a set of N spins with values $\uparrow$ and $\downarrow$, or numerically (1) and (0). These are considered to interact with each other, so that their interaction by pairs can be either ferromagnetic or anti-ferromagnetic, depending on whether the spins are parallel or anti-parallel. J_{ij} would represent the matching force between the spins s_i and s_j, i.e. the lower their absolute value, the lower the intensity of the interaction between that pair of spins. Furthermore, each spin can be affected by a magnetic field applied to it, which we designate as h_i. These local fields will give a different energy to each spin. So, the energy of the system will be:

$$E(s_1, ..., s_N) = \sum_{i,j} J_{ij} s_i s_j + \sum_i h_i s_i \tag{1}$$

This energy will be the function that we will minimize. We can write a Hamiltonian to represent this energy:

$$H_1 = \sum_{i,j} J_{ij} S_i^z S_j^z + \sum_i h_i S_i^z \tag{2}$$

As it can be seen, H_1 contains S^z operator, which acts multiplying by 1 if the corresponding qubit is 1 and multiplying by -1 if the qubit is 0. Therefore, H_1 will be a diagonal matrix. For example for a system of 2 particles with $h_1 = 1, h_2 = 2, J_{12} = J_{21} = 1$, then the H_1 matrix will be:

$$H_1 = \begin{pmatrix} -1 & 0 & 0 & 0 \\ 0 & -3 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 5 \end{pmatrix}$$

The ground state is the desired solution and as H_1 is a diagonal matrix, the energies of the different states are present in the diagonal. It can be easily seen that the ground state will be the one with the lowest energy, which in this case is -3. That is, the ground state is the one with the first spin down and the seccond up $|\downarrow\uparrow\rangle$.

However, this ground state is difficult to obtain in practice, since if we establish in the laboratory a system of spins according to the Hamiltonian H_1, and we try to find the ground state by cooling the system, we obtain unsatisfactory results. This is due to the tendency of the system to remain anchored in metastable configurations. To avoid this, we use the adiabatic theorem. It states that given a H_0, whose ground state we can find, if we make the system evolve from H_0 to H_1 very slowly, the ground state of H_0 will evolve to the ground state of H_1. Consequently, we construct the hamiltonian H_0, which in our problem will correspond to a transverse magnetic field:

$$H_0 = -\sum_i S_i^x \tag{3}$$

applied on the N-spin system. H_0 Hamiltonian contains S^x operator, which changes the value of the qubit $0 \leftrightarrow 1$. For a system of 2 particles H_0 will look like this:

$$H_0 = -\begin{pmatrix} 0 & 1 & 1 & 0 \\ 1 & 0 & 0 & 1 \\ 1 & 0 & 0 & 1 \\ 0 & 1 & 1 & 0 \end{pmatrix}$$

The Hamiltonian H_0's ground state, is easy to find, as it will correspond to the state in which all spins are pointing to the right. Applying the recently mentioned theorem, we make an interpolation between these two Hamiltonians:

$$H(\lambda) = \lambda H_1 + (1-\lambda)H_0 = \lambda\left(\sum_{i,j} J_{ij} S_i^z S_j^z + \sum_i h_i Si^z\right) - (1-\lambda)\sum_i S_i^x \tag{4}$$

so that H(λ) slowly evolves from H_0 (for λ=0) to H_1 (for $lambda$=1).

The program must calculate the energy of the ground state and the energy of the first excited state of H(λ) for each λ, to establish the evolution of the energy gap from λ=0 to λ=1. The speed at which the Hamiltonian should vary is given by the Landau-Zener formula:

$$v(\lambda) \propto \Delta E(\lambda)^2 \tag{5}$$

We can calculate the total time needed by the adiabatic quantum computer by performing the integral:

$$T_{AQC} \sim \int_0^1 \frac{d\lambda}{v(\lambda)} \tag{6}$$

The $H(\lambda)$ autovector corresponding to the ground state is a combination of the 2^N settings of the N-spin system:

$$|\phi\rangle = \alpha_1 |00\ldots00\rangle + \alpha_2 |00\ldots01\rangle + \ldots + \alpha_{2^N} |11\ldots.11\rangle \tag{7}$$

Now, if we interpret the inside of each of the kets as binary numbers, we can rewrite the autovector as:

$$|\phi\rangle = \alpha_1 |0\rangle + \alpha_2 |1\rangle + \ldots + \alpha_{2^N} |2^N - 1\rangle \tag{8}$$

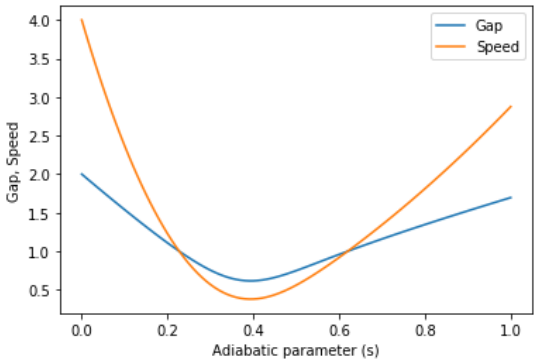
We can represent the evolution of the probability of each of the 2^N configurations. At the end of the process the probability of all of them will tend to 0, except one that will take the value of 1. At this moment $\lambda = 1$ and $H(\lambda) = H_1$. Therefore, the ground state, will be one of the 2^N configurations of the spin system:

$$|\phi\rangle = \alpha_{2^i} |2^i - 1\rangle \tag{9}$$

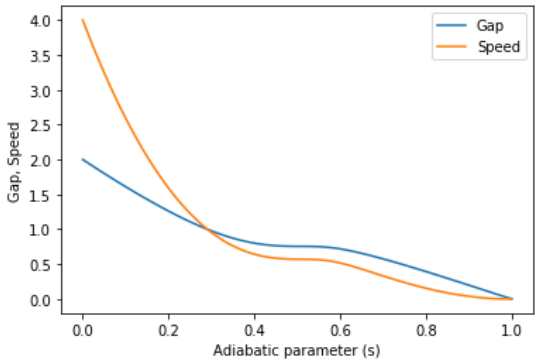
II. Results of the Simulation

The main goal of the simulation is to determine the minimum time needed for the real quantum system to find the fundamental state. This time, as discussed above, is limited by the energy gap between the fundamental state and the first excited state of the system for any instant of time.

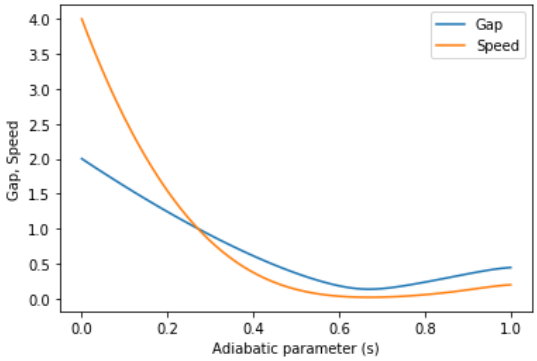
From the execution of the simulation the graphs shown in Figure 1 are obtained. In those graphs we can see how the Gap and Speed evolve with the adiabatic parameter λ for different simulations. There are some common characteristics in all four graphs. They all start with the same gap and speed. That's because we've started in every case with the same system with the same energies. It's important to note that, in most cases, the gap, and therefore the speed, presents a minimum for a finite value of λ. That would be the interval in which the evolution should be slower. And why is this magnitude important? We're trying to evolve the system adiabatically. To do this we have to meet two conditions (ideally): that the gap is strictly greater than 0 for all λ and that evolution is infinitely slow. If we want to perform the evolution in a finite time we run the risk of losing the adiabaticity and not finding the fundamental state of the system but a metastable state. This probability increases the lower is the gap and therefore in those areas we will have to be very careful not to lose the adiabaticity, and the speed of evolution will be lower.



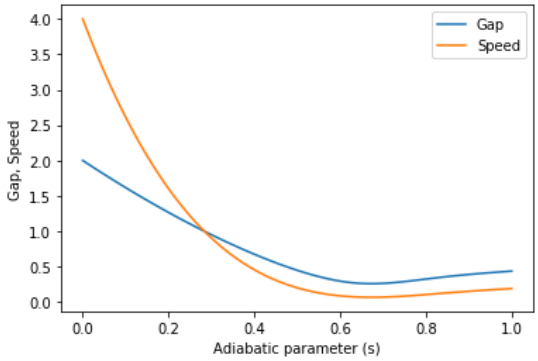
(a) Simulation 1



(b) Simulation 2



(c) Simulation 3

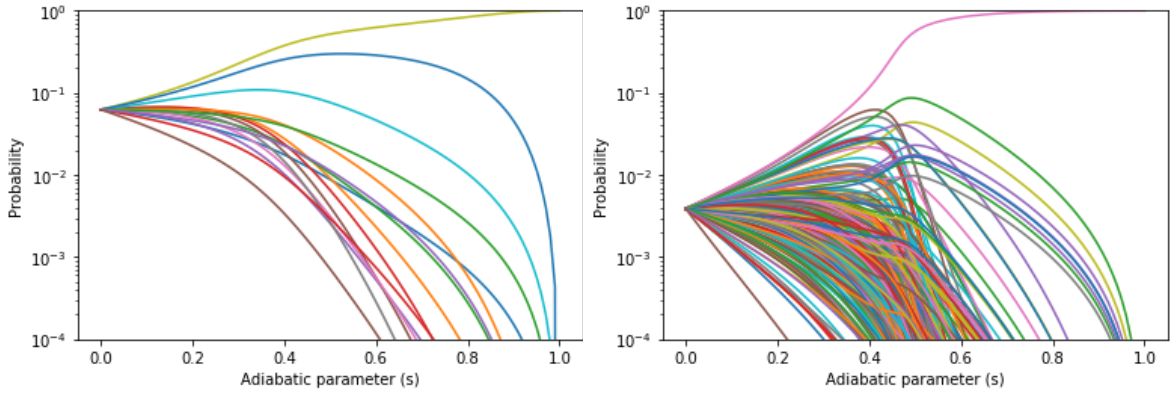


(d) Simulation 4

Figure 1: Evolution of the Gap and speed for different simulations using random values of J_{ij} and h_i and a system of 4 particles.

The execution of the code also yields the evolution of the probability of each one of the spin configurations. To represent what happens to the probability of each configuration 2 systems are shown in Figure 2, one with 4 qubit (or particles) and another one with 8.

We can see how the initial probability (when λ=0) is the same for all states. This is because of the choice we have made of the initial Hamiltonian H0, which is a transverse field. It depends on the x-components of the spins, when we are measuring the z-components of them. That is, to look a spin pointing in the x-axis from the z-axis gives the impression of a spin along the z-axis but fluctuating indifferently between $|\uparrow\rangle$ and $|\downarrow\rangle$. All spins fluctuate independently and therefore all are equally likely.



(a) System of 4 particles.

(b) System of 8 particles.

Figure 2: Evolution of the probability of each one of the spin system configurations with respect to the adiabatic parameter λ. In both cases random values of J_{ij} and h_i have been used.

In a more rigorous way, we can write the state of a spin pointing to the x-axis as a combination of the eigenstates of the base of S^z. Performing this for the 2^N spins present on the system, the initial state of the system would be the following:

$$|\rightarrow ... \rightarrow\rangle = \frac{1}{2^N}\left(|0\rangle + |1\rangle + ... + |2^N - 1\rangle\right) \tag{10}$$

At the end of the simulation, when λ =1, all probabilities are 0 except to one, whose probability is 1. The state corresponding to that probability is the solution to our problem: the ground state.

The last thing that the execution of the program gives is the total time required for the adiabatic quantum computation. The time is not given in any unit, because what is known is that it is the integral of the inverse of the speed, which is proportional to the square of the Gap, but the dimension of this speed is unknown (at least to the author of this text). However, what is interesting is to compare the growth of the time with the input size of the problem or for different problems.

It must be said that to obtain concluding results of the growth of the time with the increasing of the input size of the problem, a high computing power is required. This is due to the fact that the dimension of the matrices used in the simulation grows according to 2^N, so a system of 20 particles would require operating with $2^{20} \times 2^{20}$ matrices, which, unless you are using a supercomputer, is not bearable for your device.

III. Conclusions

All things considered, it is clear that this code is not useful in terms of calculating the ground state of the system, as it is known from the beginning in the simulation (H_1 is a diagonal matrix, so the energy of the ground state is one of its diagonal components). Thus, the purpose of the code is to understand how an Adiabatic Quantum Computer should operate in a real situation, evolving slowly from an initial induced state into the final ground state. The simulation helps to visualize the evolution of the probability of the states and how in the end the mentioned ground state is reached. Furthermore, it allows to visualize the evolution of the Gap and its consequences on the speed at which a Quantum Computer should operate, showing that when the Gap tends to 0, the speed of the computation must be quasi-infinitely slow. The code also provides an approximation of the time required for the AQC, which can give us an idea of how the initial parameters affect the performance and speed of the computation.

IV. Acknowledgements

The author wants to acknowledge Javier Rodriguez-Laguna and Silvia N. Santalla, as this project is based on the text they wrote about adiabatic quantum computing, used for a seminar at Universidad Complutense de Madrid (UCM).

V. References

- Rodriguez-Laguna, Javier and N. Santalla, Silvia. "My Computer wants to be quantum when it grows up". March 31, 2016.