

Different Strategies for Optimization Using the Quantum Adiabatic Algorithm

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We present the results of a numerical study, with 20 qubits, of the performance of the Quantum Adiabatic Algorithm (QAA) on randomly generated instances of MAX 2-SAT with a unique assignment that maximizes the number of satisfied clauses. The probability of obtaining this assignment at the end of the quantum evolution measures the success of the algorithm. Here we report three strategies which consistently increase the success probability for the hardest instances in our ensemble: decreasing the overall evolution time, initializing the system in excited states, and adding a random local Hamiltonian to the middle of the evolution.

To use the Quantum Adiabatic Algorithm as an optimization method [1] for maximizing the number of satisfied clauses we first prepare the quantum system to be in the ground state of a transverse field, which is the uniform superposition of computational basis states, and slowly change the system Hamiltonian to one which is diagonal in the computational basis and assigns to each computational basis state an energy corresponding to the number of clauses which are violated by that bit assignment. By the adiabatic theorem, if this transformation of the system is done over a sufficiently long time then the state of the system at the end of the evolution will have a large overlap with the string that satisfies the maximum number of clauses.

The time scale needed for the adiabatic theorem to be applicable is polynomially related to the inverse of the minimum energy gap in the spectrum of the interpolating Hamiltonian. For some families of problem instances, this spectral gap may be decreasing exponentially in the size of the problem, which implies that the system would need to evolve exponentially slowly in order for the adiabatic theorem to be satisfied. In this work we explore strategies that do not necessarily require the adiabatic condition to hold, and we sidestep the usual question of determining how the run time needed to achieve a certain success probability scales with the problem size. Instead we work at a fixed number of bits, and look at strategies for improving the success probability for hard instances at this number of bits.

To accumulate an ensemble of MAX 2-SAT instances that are hard for the standard version of the QAA, we randomly generated over 200,000 instances and used over 20,000 hours of CPU time to select those which have the lowest success probability (after some fixed evolution time) according

to a numerical integration of the Schrodinger equation. At the chosen time scale over half of our random instances have a success probability above 0.95, and so we focus on the ensemble of 137 hard instances which have a final success probability below 10^{-4} .

Our first strategy for increasing the success probability is counterintuitive: by evolving the system more rapidly, with a 10 fold decrease in the overall evolution time, we find a dramatic increase in the final success probability (typically 2 to 3 orders of magnitude) for *all* of the 137 hard instances in our ensemble. This result is contrary to the usual strategy suggested by the adiabatic theorem, so it must be that non-adiabatic effects contribute to the increased success probability.

We were able to understand this phenomenon by numerically analyzing the energy spectra for these instances. All of these instances have a tiny minimum energy gap. This corresponds to an avoided crossing between the ground state and first excited state, which means that the ground state just before the minimum gap is similar to the first excited state just after it. If the system is evolving slowly enough to remain close to the ground state prior to the avoided crossing, but too quickly compared to the minimum gap, then it will jump to the first excited state after the avoided crossing and eventually arrive almost entirely in the first excited subspace of the final Hamiltonian. In contrast, when the system is evolved more rapidly it leaks substantial amplitude into the first excited state prior to the avoided crossing, which increases the probability of finding the system in the ground state immediately after the avoided crossing and therefore at the end of the evolution.

This explanation leads to our next strategy for improving the success probability of QAA on hard instances. If we expect an avoided crossing between the ground state and first excited state, we can attempt to directly exploit the phenomenon described above by initializing the system in the first excited state of the beginning Hamiltonian. We simulated this strategy for each of the 20 first excited states for each of our 137 hard instances and find that it produces an average success probability near $1/20$ for nearly all of our hard instances. This saturates the upper bound given by probability conservation and affirms the utility of this alternate strategy.

The final alternative strategy we apply to our ensemble of instances follows a previous proposal [2] to alter the Hamiltonian evolution path by the insertion of a random local Hamiltonian which has the same interaction graph as the clause structure of the 2-SAT instance, but otherwise does not use any information specific to the particular instance. We apply this path change strategy with random local Hamiltonians of three types: purely diagonal (representing an essentially classical path change strategy), stoquastic Hamiltonians [3] (i.e. Hamiltonians which have all non-negative off-diagonal entries and therefore do not have a sign problem, for which the local Hamiltonian

problem has computational complexity which is intermediate between quantum and classical), and finally general complex Hamiltonians. For each of our 137 hard instances we simulate 25 random path changes of each of the three types. The effective success probability for this strategy is determined by the geometric mean of the failure probabilities for the 25 trials, and according to this measure all three types of path change increase the average success probabilities for our ensemble of hard instances by 2 to 3 orders of magnitude. We contrast the three types of path change, and among other things we find that the complex path changes produce the largest average increase in the effective success probability. We confirm the hypothesis that the higher success probabilities from the path change strategy are correlated with larger spectral gaps in path-changed Hamiltonian evolutions.

The fact that our strategies improve the success probability for all 137 hard instances may be a consequence of those instances having the most room for improvement. The majority of instances we generated at 20 bits are far easier than the ones we selected. It may be the case that at higher bit number most instances have very low success probability when the traditional QAA is run for a time that scales polynomially in the number of bits. Therefore in future analytical or numerical work at higher bit number it will be important to determine whether these strategies can increase the success probability of difficult instances beyond that of typical instances.

The surprising result of this large computational study, which used in total over 45,000 hours of CPU time, is to demonstrate that non-adiabatic strategies and alternative Hamiltonian paths may dramatically improve the success probabilities when the QAA is applied to random instances of optimization. To our knowledge this is the first time that non-adiabatic strategies have been applied to a large ensemble of randomly generated instances and shown to consistently improve the success probabilities compared to the traditional QAA. We hope that one day these strategies will be tested on a quantum computer running the Quantum Adiabatic Algorithm at high bit number where classical simulations are not available.

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