Quantum Adiabatic Evolution Algorithms with Different Paths

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Abstract

In quantum adiabatic evolution algorithms, the quantum computer follows the ground state of a slowly varying Hamiltonian. The ground state of the initial Hamiltonian is easy to construct; the ground state of the final Hamiltonian encodes the solution of the computational problem. These algorithms have generally been studied in the case where the “straight line” path from initial to final Hamiltonian is taken. But there is no reason not to try paths involving terms that are not linear combinations of the initial and final Hamiltonians. We give several proposals for randomly generating new paths. Using one of these proposals, we convert an algorithmic failure into a success.

1 Introduction

Quantum adiabatic evolution algorithms [1] are designed to keep the quantum computer in the ground state of a slowly varying Hamiltonian $H(t)$. The initial Hamiltonian, $H_B = H(0)$, is chosen so that its ground state is easy to construct. The ground state of the final Hamiltonian $H_P = H(T)$, where $T$ is the running time of the algorithm, encodes the solution to the computational problem at hand. A simple way to construct the interpolating Hamiltonian is to define

$$H(t) = \tilde{H}(t/T) \quad 0 \leq t \leq T$$

where

$$\tilde{H}(s) = (1 - s)H_B + sH_P \quad 0 \leq s \leq 1.$$  \hfill (2)

But there is no reason to restrict attention to this path from $H_B$ to $H_P$. The possibility of varying the path was discussed in [2], [3], and [4]. The adiabatic algorithm will work taking any path $\tilde{H}(s)$ with $\tilde{H}(0) = H_B$ and $\tilde{H}(1) = H_P$ as long as $T$ is much larger than $1/gap^2$ where the $gap$ is the minimum energy difference, as $s$ varies.

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between the ground and first excited states of $\tilde{H}(s)$. In this paper we consider paths of the form

$$\tilde{H}(s) = (1 - s)H_B + sH_P + s(1 - s)H_E.$$  \hfill (3)

We view $H_E$ as an extra piece of the Hamiltonian that is turned off at the beginning and end of the evolution. For a given instance of a problem, that is, for a fixed $H_P$, we imagine running the algorithm repeatedly with different choices of $H_E$, possibly chosen randomly.

In this paper we propose some choices for $H_E$. We then apply one of these choices to a problem discussed in [5] and show that the addition of $H_E$ can change the performance of the algorithm from unsuccessful to successful.

## 2 Examples of different paths

We are most optimistic about the performance of quantum adiabatic algorithms when they are applied to the classical problem of finding the minimum of a “local” cost function. By this we mean a function $h(z_1, \ldots, z_n)$ where each $z_i = 0, 1$ and

$$h = \sum_C h_C$$  \hfill (4)

and each $h_C$ is a nonnegative integer-valued function that depends only on a few $z_i$.

The Hamiltonian that governs the quantum algorithm is constructed as follows. For each term $h_C$ we define an associated quantum operator $H_{P,C}$. Suppose, for example, that $h_C$ depends on three bits $i_C, j_C, k_C$. Then we have

$$H_{P,C}|z_1, \ldots, z_n\rangle = h_C(z_{i_C}, z_{j_C}, z_{k_C})|z_1, \ldots, z_n\rangle.$$  \hfill (5)

Accordingly we define the problem Hamiltonian

$$H_P = \sum_C H_{P,C}.$$  \hfill (6)

For the beginning Hamiltonian we define

$$H_{B,C} = \frac{1}{2}(1 - \sigma^{(i_C)}_x) + \frac{1}{2}(1 - \sigma^{(j_C)}_x) + \frac{1}{2}(1 - \sigma^{(k_C)}_x)$$  \hfill (7)

where (again) $i_C, j_C, k_C$ are the three bits appearing in $h_C$. Now

$$H_B = \sum_C H_{B,C}$$  \hfill (8)

and using (3) and (7) we see that $\tilde{H}(s)$ from (2) can be written

$$\tilde{H}(s) = \sum_C [(1 - s)H_{B,C} + sH_{P,C}].$$  \hfill (9)
This is the form of \( \tilde{H}(s) \) that was originally proposed in equations (2.26) and (2.28) in [1].

We now turn to \( H_E \). To preserve the \( \sum_C \) on the right-hand side of (9), we pick a term \( H_{E,C} \) for each term \( h_C \). This \( H_{E,C} \) will only depend on the bits involved in \( h_C \). We then have

\[
H_E = \sum_C H_{E,C} \tag{10}
\]

and \( \tilde{H}(s) \) from (3) is now

\[
\tilde{H}(s) = \sum_C \left[ (1 - s) H_{B,C} + s H_{P,C} + s(1 - s) H_{E,C} \right]. \tag{11}
\]

Note that for each clause the coefficients \((1 - s), s, \) and \( s(1 - s) \) could all be replaced by any three smooth functions with the same corresponding values at \( s = 0 \) and \( s = 1 \), but we make the clause-independent choices \((1 - s), s, \) and \( s(1 - s) \) for simplicity.

Finally we must choose \( H_{E,C} \). Here are three proposals.

P1. For each term \( h_C \) involving \( b_C \) bits let \( A_C \) be a randomly chosen Hermitian matrix of size \( 2^{b_C} \times 2^{b_C} \). We imagine that the distribution of \( A_C \) produces entries with magnitude of order unity. We also propose setting the diagonal entries in each \( A_C \) to 0. Now \( H_{E,C} \) is defined by letting the matrix \( A_C \) act on the \( b_C \) bits involved in \( h_C \). The 0 diagonal avoids confusing the effects of varying the path in the quantum algorithm with modifications of the classical cost function itself. See [4].

P2. For this proposal we specialize to the case where each term \( h_C \) has the same form independent of \( C \). For the case of three bits this means that there exists an \( h_3 \) such that

\[
h_C(z_{i_C}, z_{j_C}, z_{k_C}) = h_3(z_{i_C}, z_{j_C}, z_{k_C}) \tag{12}
\]

for each \( C \). (An example is the NP-complete problem Exact Cover where \( h_3(z, z', z'') = 1 \) if \( z + z' + z'' \neq 1 \) and 0 if \( z + z' + z'' = 1 \).) For simplicity we restrict to the case where each \( h_C \) depends on three bits. We propose generating a single (order unity) random \( 8 \times 8 \) Hermitian matrix \( A \) and then using this for each \( H_{E,C} \). Each \( H_{E,C} \) has the \( 8 \times 8 \) matrix \( A \) acting on bits \( i_C, j_C, \) and \( k_C \). Again, we propose choosing the diagonal entries of \( A \) to be 0.

P3. Here we make a proposal for 3-SAT. An \( n \)-bit instance of 3-SAT is a collection of clauses. Each clause specifies which three bits are in the clause. Each clause is True for seven of the eight assignments of the three bits and False on one assignment, so there are eight different types of clauses. Accordingly, \( h_C = 1 \) if \((z_{i_C}, z_{j_C}, z_{k_C})\) is the False assignment and \( h_C = 0 \) on the other seven assignments. Thus \( h(z_1, \ldots, z_n) \) is the number of clauses violated by the string \( z_1, \ldots, z_n \) and a satisfying assignment exists iff the minimum value of \( h \) is 0.
We can view the eight types of 3-SAT clauses as variants of a single basic clause, say the one for which \((0, 0, 0)\) is the False assignment. The other seven clauses are related to the basic clause by negation of some (or all) of the bits. For this proposal for \(H_E\) we start with a single \(8 \times 8\) matrix \(A\) and associate it with the basic clause. For the other seven clauses we have seven other \(8 \times 8\) matrices. Each is obtained from \(A\) by negating the same bits that are negated in the corresponding clause. (Bit negation of \(A\) is achieved by conjugating \(A\) with the \(\sigma_x\) matrix acting on the bit.) \(A\) might be chosen randomly but again we take the diagonal entries to be 0. This proposal has the invariance property that if an instance of 3-SAT is changed by replacing some bits by their negations in all clauses, the performance of the quantum algorithm is identical.

3 A different path can turn failure into success

Here we reexamine an example given in [5] where the quantum adiabatic evolution algorithm, evolving according to (2), without an \(H_E\), was shown to require a time exponential in the number of bits. We will now show that for \(H_E\) chosen randomly according to Proposal P2 above, the quantum adiabatic algorithm succeeds in polynomial time.

The example has a cost function \(h\), of the form (4), where each \(h_C\) depends on three bits and is of the same form for each \(C\), that is, equation (12) holds. In this example

\[
h_3(z, z', z'') = \begin{cases} 
0 & z + z' + z'' = 0 \\
3 & z + z' + z'' = 1 \\
1 & z + z' + z'' = 2 \\
1 & z + z' + z'' = 3
\end{cases} .
\] (13)

The cost function includes a term for each set of three bits giving

\[
h(z_1, \ldots, z_n) = \sum_{i<j<k} h_3(z_i, z_j, z_k) .
\] (14)

Note that the global minimum of \(h\) occurs at \(z_1 = 0, z_2 = 0, \ldots, z_n = 0\) where \(h\) is 0.

The performance of the quantum adiabatic algorithm on this highly symmetrized problem can be analyzed asymptotically in the number of bits \(n\). Using the symmetry and equations (5), (6), (13), and (14) we can write

\[
H_P = \frac{3}{2} \left( \frac{n}{2} - S_z \right) \left( \frac{n}{2} + S_z \right) \left( \frac{n}{2} + S_z - 1 \right) + \frac{1}{2} \left( \frac{n}{2} - S_z \right) \left( \frac{n}{2} - S_z - 1 \right) \left( \frac{n}{2} + S_z \right) + \frac{1}{6} \left( \frac{n}{2} - S_z \right) \left( \frac{n}{2} - S_z - 1 \right) \left( \frac{n}{2} - S_z - 2 \right) .
\] (15)
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where $S_z$ is the $z$-component of the total spin:

$$S_z = \frac{1}{2} \sum_{i=1}^{n} \sigma_z^{(i)}.$$  \hfill (16)

For $H_B$ we use (7) and (8) to obtain

$$H_B = \left( \frac{n-1}{2} \right) \left( \frac{n}{2} - S_x \right)$$  \hfill (17)

where

$$S_x = \frac{1}{2} \sum_{i=1}^{n} \sigma_x^{(i)} \tag{18}$$

and for later use

$$S_y = \frac{1}{2} \sum_{i=1}^{n} \sigma_y^{(i)}.$$ \hfill (19)

We now turn to $H_E$ generated by Proposal P2, from a single $8 \times 8$ matrix $A$ with 0’s on the diagonal. By (10) and the fact that all sets of three bits are included in the sum we find that $H_E$ is a cubic function of $S_x$, $S_y$, and $S_z$ whose coefficients are linear combinations of the entries of $A$. The choice that $A$ is 0 on the diagonal implies that there are no $S_z$, $S_z^2$, and $S_z^3$ terms in $H_E$ whereas these are the only terms in $H_P$.

In this symmetric case the total Hamiltonian $\tilde{H}(s)$ given by (11) is a function of the total spin operators $S_x$, $S_y$, and $S_z$. For $n$ large, we make the ansatz that for each $s$ the ground state of $\tilde{H}(s)$ is a state $|\theta, \varphi\rangle$ that is an eigenstate of the total spin in the $(\theta, \varphi)$ direction

$$(\sin \theta \cos \varphi \ S_x + \sin \theta \sin \varphi \ S_y + \cos \theta \ S_z) |\theta, \varphi\rangle = \frac{n}{2} |\theta, \varphi\rangle.$$ \hfill (20)

With this ansatz finding the ground state of $\tilde{H}(s)$ is reduced to finding the minimum over $(\theta, \varphi)$ of

$$\langle \theta, \varphi | \tilde{H}(s) | \theta, \varphi \rangle.$$ \hfill (21)

To evaluate (21) in the large-$n$ limit we use relations such as
\[ \langle \theta, \varphi | S_x | \theta, \varphi \rangle = \frac{n}{2} \sin \theta \cos \varphi \]
\[ \langle \theta, \varphi | S_y | \theta, \varphi \rangle = \frac{n}{2} \sin \theta \sin \varphi \]
\[ \langle \theta, \varphi | S_z | \theta, \varphi \rangle = \frac{n}{2} \cos \theta \]
\[ \langle \theta, \varphi | S_x^2 | \theta, \varphi \rangle = \left( \frac{n}{2} \right)^2 \sin^2 \theta \cos^2 \varphi + O(n) \]
\[ \langle \theta, \varphi | S_x S_y | \theta, \varphi \rangle = \left( \frac{n}{2} \right)^2 \sin^2 \theta \cos \varphi \sin \varphi + O(n) \]
\[ \langle \theta, \varphi | S_x S_z | \theta, \varphi \rangle = \left( \frac{n}{2} \right)^2 \sin \theta \cos \theta \cos \varphi + O(n) \]

We now define the effective potential

\[ V(\theta, \varphi, s) = \lim_{n \to \infty} \left( \frac{2}{n} \right)^3 \langle \theta, \varphi | \tilde{H}(s) | \theta, \varphi \rangle \]

which we break into two parts:

\[ V_0(\theta, \varphi, s) = \lim_{n \to \infty} \left( \frac{2}{n} \right)^3 \langle \theta, \varphi | \{(1 - s)H_B + sH_P\} | \theta, \varphi \rangle \]

and

\[ V_E(\theta, \varphi, s) = \lim_{n \to \infty} \left( \frac{2}{n} \right)^3 \langle \theta, \varphi | s(1 - s)H_E | \theta, \varphi \rangle \]

so that

\[ V = V_0 + V_E. \]

We now review what happens without \( H_E \). We have

\[ V_0(\theta, \varphi, s) = 2(1 - s)(1 - \sin \theta \cos \varphi) + \frac{1}{6} s(13 + 3 \cos \theta - 9 \cos^2 \theta - 7 \cos^3 \theta). \]

The minimum of \( V_0 \) for any \( s \) is at \( \varphi = 0 \). In Figure we plot \( V_0(\theta, 0, s) \) for six values of \( s \). In the first panel \( s = 0 \) and the effective potential is minimized at \( \theta = \pi/2 \), which corresponds to the ground state of \( H_B \). As \( s \) increases the minimum moves to the right (see \( s = .2 \)). Continuously following this local minimum leads to the local minimum at \( \theta = \pi \) when \( s = 1 \). A quantum computer running the adiabatic algorithm for a time only polynomial in \( n \) will evolve close to the state \( |\theta = \pi, \varphi = 0\rangle \) at the end of the run. This state \( |\theta = \pi, \varphi = 0\rangle = |z_1 = 1, z_2 = 1, \ldots, z_n = 1\rangle \) does not correspond to the ground state of \( H_P \), which is at \( |\theta = 0, \varphi = 0\rangle = |z_1 = 0, z_2 = 0, \ldots, z_n = 0\rangle \).

The failure of the quantum adiabatic algorithm on this highly symmetrical problem with \( n^3 \) clauses may not be a good test of the effectiveness of the algorithm on
Figure 1: The diamond continuously tracks a local minimum of the effective potential, corresponding to the behavior of the quantum adiabatic algorithm run for polynomial time. The final point reached is not the global minimum of the effective potential at $s = 1$ and the algorithm fails. Here $H_E$ is absent.

computationally interesting problems. But in any event this failure can be turned to success with the addition of $H_E$.

Although Proposal P2 uses a random $8 \times 8$ matrix $A$, we begin by studying the effects of $H_E$ arising from a carefully chosen $A$:

$$A = \begin{bmatrix} 0 & -2 & -2 & 0 & -2 & 0 & 0 & 0 \\ -2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ -2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 2 \\ -2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 2 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 2 \\ 0 & 0 & 0 & 2 & 0 & 2 & 2 & 0 \end{bmatrix} \quad (28)$$

which gives rise to

$$H_E = -2n(S_zS_x + S_xS_z) + O(n^2) \quad (29)$$
from which we get
\[ V_E(\theta, \varphi, s) = -8s(1 - s) \cos \theta \sin \theta \cos \varphi . \] (30)

The full effective potential \( V(\theta, \varphi, s) \) given by (26) with (27) and (30) can only be extremized at \( \varphi = 0 \) and \( \pi \). In Figure 2 we show \( V(\theta, 0, s) \) as a solid line and

Figure 2: The diamond continuously tracks a local minimum of the effective potential for the Hamiltonian including a particular \( H_E \). (The solid line corresponds to \( \varphi = 0 \); the dotted line to \( \varphi = \pi \).) The final point reached is the global minimum of the effective potential at \( s = 1 \), and the algorithm succeeds in polynomial time.

\( V(\theta, \pi, s) \) as a dashed line for six values of \( s \). At \( s = 0 \) the ground state of \( \tilde{H}(0) \) is \( |\theta = \pi/2, \varphi = 0\rangle \). In the first panel we see that \( \theta = \pi/2, \varphi = 0 \) is the global minimum of \( V(\theta, \varphi, 0) \). As \( s \) increases, the global minimum moves continuously to \( \theta = 0, \varphi = 0 \). The state \( |\theta = 0, \varphi = 0\rangle = |z_1 = 0, z_2 = 0, \ldots, z_n = 0\rangle \) is the ground state of \( H_P \) and corresponds to the minimum of the cost function given by (13) and (14). Running the quantum adiabatic evolution algorithm for a time polynomial in \( n \) will bring the quantum computer close to the state \( |\theta = 0, \varphi = 0\rangle \), solving the problem of finding the minimum of \( h \).

The example just given is not an isolated success. Clearly the same behavior will be seen for \( A \)'s close to (28). Moreover, we performed the following experiment. We
toss a random real symmetric $8 \times 8$ matrix $A$ with nondiagonal elements independently and uniformly distributed between $-3$ and 3 and with the diagonal set to 0. We use $A$ to construct $H_E$ and the corresponding $V_E$. We then continuously track a local minimum of $V(\theta, \varphi, s)$ as $s$ varies from 0 to 1, starting at $\theta = \pi/2$, $\varphi = 0$ when $s = 0$. In 351 out of 1000 tries, this local minimum moves to $\theta = 0$, $\varphi = 0$, which is the global minimum of the effective potential at $s = 1$. Thus, in these tries, the adiabatic algorithm run for polynomial time will end up close to the ground state of $H_P$. This shows that a large “volume” of the space of possible $A$’s leads to an $H_E$ that ensures finding the global minimum of $h$ in polynomial time.

(It is conceivable that in some of these tries the continuously tracked local minimum, which coincides with the global minimum at $s = 0$ and $s = 1$, does not coincide with the global minimum for all intermediate $s$. If this happens, the algorithm run for polynomial time will still succeed in finding the global minimum of $h$, because the probability of leaving the state corresponding to the local minimum is exponentially small.)

Our analysis, via the effective potential, of the quantum algorithm with an $H_E$ chosen according to Proposal P2 gives the asymptotic (large $n$) behavior of the algorithm. This analysis is only possible because of the symmetry: the same terms are included in the Hamiltonian for each set of three bits. The function $h_3$ in (13) could also be viewed as arising from a sum of terms corresponding to thirteen 3-SAT clauses. We could then use Proposal P3, which is designed for 3-SAT. Here one could apply the effective potential analysis and determine the asymptotic behavior of the algorithm with random choices of $A$. Presumably the behavior is similar to what we found using proposal P2, but we have not done the analysis.

Proposal P1 could be used instead in this problem, but choosing a different $A_C$ for each $C$ breaks the symmetry and we don’t know how to determine the large $n$ performance of the algorithm in this case. In [4] a study of random 9-bit 3-SAT instances was performed using proposal P1. The gaps were compared with and without $H_E$. Overall the gaps with $H_E$ were smaller than without $H_E$. However, the gaps that were smallest without $H_E$ often increased after the addition of $H_E$ and were no longer small compared to the other gaps. This argues for running the quantum adiabatic algorithm on each instance with a variety of randomly chosen paths.

4 Conclusion

Previous work on quantum adiabatic evolution algorithms has assumed a “straight line” path in Hamiltonian space from the beginning Hamiltonian $H_B$ to the problem Hamiltonian $H_P$ as in (2). This path is simple but arbitrary. The idea of trying to remain close to the ground state of a time-varying Hamiltonian is equally applicable to other paths from $H_B$ to $H_P$, such as (3). The quantum adiabatic algorithm is guaranteed to give a 100% probability of success only as the run time goes to infinity, so a finite run time requires repetition. We suggest that repetitions be carried out with different paths. In cases where the gap in $\tilde{H}(s)$ given by (3) happens to be small, the required run time is correspondingly long. Adding $H_E$ as in (3) may avoid the region in Hamiltonian space where the gap is small and be computationally advantageous.
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