Quantum Adiabatic Evolution Algorithms versus Simulated Annealing

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Abstract
We explain why quantum adiabatic evolution and simulated annealing perform similarly in certain examples of searching for the minimum of a cost function of \( n \) bits. In these examples each bit is treated symmetrically so the cost function depends only on the Hamming weight of the \( n \) bits. We also give two examples, closely related to these, where the similarity breaks down in that the quantum adiabatic algorithm succeeds in polynomial time whereas simulated annealing requires exponential time.

1 Introduction
Quantum adiabatic evolution algorithms \([1]\) are designed to minimize a (classical) cost function whose domain is the \( 2^n \) values taken by \( n \) bits. To test the algorithm it is natural to look at problems where classical local search algorithms, such as simulated annealing, have difficulty. It is easy to construct examples where both classical local search and quantum adiabatic evolution require time exponential in \( n \). An example is the Grover problem, where the function takes the value 0 at a single input and is 1 on the \( 2^n - 1 \) other inputs. A variant of this Grover example can be found in \([2]\).

More interesting examples arise when the cost function is local in the sense that it can be written as a sum of terms each of which involves only a few bits. A 3SAT example where both the classical local search and “standard” quantum adiabatic algorithms are exponentially slow has recently been given in \([3]\). In Section 3 below we analyze an example that is based on \([4]\) and give a quantum mechanical argument for why quantum adiabatic algorithms have trouble with these kinds of examples.

In Section 3 we give a nonlocal example where simulated annealing requires exponential time but quantum adiabatic evolution succeeds in polynomial time. In Section 3 we give a detailed analysis of a local (2SAT) example that first appeared in \([1]\). Here again a quantum adiabatic algorithm succeeds even though simulated annealing fails in polynomial time. These examples show that there is no general theorem that quantum adiabatic algorithms must fail if simulated annealing fails.

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2 Quantum adiabatic algorithms

Quantum adiabatic evolution algorithms offer a general approach to solving combinatorial search problems on a quantum computer. A local combinatorial search problem can be cast as the classical problem of finding the minimum of cost function $h(z_1, \ldots, z_n)$ where each $z_i = 0, 1$ and

$$h = \sum_C h_C \tag{1}$$

and each $h_C$ is a nonnegative integer-valued function that depends only on a few $z_i$. A quantum adiabatic algorithm converts this into the problem of producing the ground state of a quantum Hamiltonian $H_P$ given by

$$H_P |z_1, \ldots, z_n\rangle = h(z_1, \ldots, z_n) |z_1, \ldots, z_n\rangle \tag{2}$$

where $\{|z_1, \ldots, z_n\rangle\}$ is a basis for the $2^n$-dimensional Hilbert space of the quantum computer. Specifying the algorithm consists of choosing a smoothly varying Hamiltonian $\tilde{H}(s)$ for $0 \leq s \leq 1$ such that $\tilde{H}(1) = H_P$ and where $\tilde{H}(0)$ has a ground state $|\psi_0\rangle$ that is known and easily constructed. A run time $T$ must also be specified. The Hamiltonian that governs the evolution is given by

$$H(t) = \tilde{H}(t/T) \tag{3}$$

and the state of the quantum computer evolves according to the Schrödinger equation

$$i \frac{d}{dt} |\psi(t)\rangle = H(t) |\psi(t)\rangle \tag{4}$$

with the state at time $t = 0$ given by

$$|\psi(0)\rangle = |\psi_0\rangle \tag{5}.$$ 

Under conditions that generally apply in the cases of interest here, the quantum adiabatic theorem guarantees that for $T$ large enough the state of the quantum computer, $|\psi(t)\rangle$ for $0 \leq t \leq T$, will be close to the (instantaneous) ground state of $H(t)$, and in particular $|\psi(T)\rangle$ will be close to the ground state of $H_P$, encoding the solution to the problem at hand. When applied to a particular combinatorial search problem, the quantum algorithm is considered to be successful if the required running time grows polynomially in the number of bits $n$.

The required running time can be related to the spectrum of $\tilde{H}(s)$, in particular the difference between the two lowest eigenvalues $E_0(s)$ and $E_1(s)$. The required running time $T$ must obey

$$T \gg \frac{\mathcal{E}}{\text{gap}^2} \tag{6}$$

where

$$\text{gap} = \min_{0 \leq s \leq 1} \left( E_1(s) - E_0(s) \right) \tag{7}$$

and $\mathcal{E}$ is less than the largest eigenvalue of $H_P - \tilde{H}(0)$, always polynomial in $n$ in the examples here.
Simulated annealing

Simulated annealing is a classical local search strategy that can be used to find the global minimum of a function $h(z_1, \ldots, z_n)$ of the form (8). For any temperature $\tau$, $0 \leq \tau \leq \infty$, define the Boltzmann distribution by

$$P_{\tau}(z_1, \ldots, z_n) = c(\tau) \exp\left[{-h(z_1, \ldots, z_n)/\tau}\right]$$

(8)

where $c(\tau)$ is the normalizing constant such that

$$\sum_{z_1,\ldots,z_n} P_{\tau}(z_1, \ldots, z_n) = 1.$$

(9)

For $\tau = \infty$, all $2^n$ strings $z_1, \ldots, z_n$ are equally likely. For $\tau = 0$, the Boltzmann distribution concentrates on the global minimum (or minima) of $h$.

The idea is to construct a Markov chain that starts in the $\tau = \infty$ Boltzmann distribution and gradually moves through the Boltzmann distributions for decreasing $\tau$ down to $\tau$ near 0. If the process succeeds, the final distribution will be close to the zero temperature Boltzmann distribution, which means that the global minimum of $h$ has been found with high probability. More specifically, choose a sequence of temperatures $\infty \geq \tau_1 \geq \tau_2 \geq \cdots \tau_M \geq 0$ at which bit values may change. The $\tau_i$ can be chosen deterministically or randomly. Also choose a sequence of bits $i_1, i_2, \ldots, i_M$. Bit $i_k$ is the bit that might be changed (according to an acceptance rule to be given below in (10)) at step $k$. The sequence $i_1, i_2, \ldots, i_M$ can be deterministic or random.

The initial string is picked uniformly, i.e., all $2^n$ strings $z_1, \ldots, z_n$ have probability $2^{-n}$. At step $k$, if the current string is $z_1, \ldots, z_{i_k}, \ldots, z_n$ we flip bit $i_k$ and move to string $z_1, \ldots, (1 - z_{i_k}), \ldots, z_n$ with probability

$$\min\{1, \exp\left(-\Delta h/\tau_k\right)\}$$

where

$$\Delta h = h(z_1, \ldots, (1 - z_{i_k}), \ldots, z_n) - h(z_1, \ldots, z_{i_k}, \ldots, z_n).$$

(10)

(This is the Metropolis rule.) Otherwise the string remains unchanged. Note that bit $i_k$ is always flipped if the change decreases $h$, and is flipped with only small probability if the change would increase $h$ by a large amount relative to the current temperature.

The acceptance rule (10) guarantees that if many transitions are made at a single temperature $\tau$, the distribution of the string will converge to the Boltzmann distribution at temperature $\tau$. If the sequence $\tau_1, \tau_2, \ldots, \tau_M$ decreases slowly enough, the distribution, which starts in the $\tau = \infty$ Boltzmann distribution, will at step $k$ be close to the Boltzmann distribution for temperature $\tau_k$. The question is how many transitions must be made in order to stay near the Boltzmann distributions as the temperature is lowered down to near 0. If the total number of steps required grows only as a polynomial in $n$, we say that the simulated annealing algorithm succeeds.

Symmetrized cost functions

In this section we discuss cost functions of the form (8) that are functions only of the Hamming weight $w = z_1 + z_2 + \cdots + z_n$ as a result of all bits being treated symmetrically.
As an example, let $h_3$ depend on three bits $z, z', \text{ and } z''$ with the form

$$h_3(z, z', z'') = \begin{cases} 
0 & z + z' + z'' = 0 \\
q & z + z' + z'' = 1 \\
1 & z + z' + z'' = 2 \\
1 & z + z' + z'' = 3
\end{cases} \quad (11)$$

where $q$ is an integer greater than or equal to 3. Now let

$$h(z_1, \ldots, z_n) = \sum_{i<j<k} h_3(z_i, z_j, z_k) \quad (12)$$

which gives

$$h(w) \equiv h(z_1, \ldots, z_n) = \frac{q}{2} w(n - w)(n - w - 1) + \frac{1}{2} w(w - 1)(n - w) + \frac{1}{6} w(w - 1)(w - 2) \quad (13)$$

We can also write

$$h(w) = \left(\frac{n}{2}\right)^3 g(w/n) + O(n^2) \quad (14)$$

where

$$g(u) = 4qu(1 - u)^2 + 4u^2(1 - u) + \frac{4}{3}u^3. \quad (15)$$

For $n$ large the form of $g(u)$ determines the behavior of the classical and quantum algorithms. In Figure 1 we plot $g(u)$ for $q = 3$. Note that the global minimum of $g$ is at $u = 0$ corresponding to the unique input $z_1, \ldots, z_n = 0, \ldots, 0$. The derivative $g'(1/2)$ is negative and there is a local minimum at $u = 1$ corresponding to $z_1, \ldots, z_n = 1, \ldots, 1$.

We now look at the quantum algorithm applied to this problem. The cost function (13) corresponds to the Hamiltonian

$$H_P = \frac{q}{2} \left( \frac{n}{2} - S_z \right) \left( \frac{n}{2} + S_z \right) \left( \frac{n}{2} + S_z - 1 \right) + \frac{1}{2} \left( \frac{n}{2} - S_z \right) \left( \frac{n}{2} - S_z - 1 \right) \left( \frac{n}{2} + S_z \right) + \frac{1}{6} \left( \frac{n}{2} - S_z \right) \left( \frac{n}{2} - S_z - 1 \right) \left( \frac{n}{2} - S_z - 2 \right) \quad (16)$$

where

$$S_z |z_1, \ldots, z_n\rangle = \left( \frac{n}{2} - w \right) |z_1, \ldots, z_n\rangle. \quad (17)$$

We choose for the initial Hamiltonian (following [1], formula 2.28)

$$\tilde{H}(0) = \left( \frac{n}{2} - S_z \right) \quad (18)$$
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Figure 1: The leading term in the scaled cost as a function of the scaled Hamming weight \( u = w/n \).

where

\[
S_x = \frac{1}{2} \sum_{i=1}^{n} \sigma_x^{(i)} .
\]  

Choosing a linear interpolation between \( \tilde{H}(0) \) and \( H_P \) gives

\[
\tilde{H}(s) = (1-s)\tilde{H}(0) + sH_P \quad \text{for } 0 \leq s \leq 1.
\]  

Since \( \tilde{H}(s) \) depends only on the two operators \( S_x \) and \( S_z \), we start our analysis by considering the states \( |\theta\rangle \) defined by

\[
\langle \theta | S_x + \cos \theta S_z | \theta \rangle = \frac{n}{2} |\theta\rangle .
\]  

Note that

\[
\langle \theta | S_x | \theta \rangle = \frac{n}{2} \sin \theta
\]  

\[
\langle \theta | S_x^2 | \theta \rangle = \left( \frac{n}{2} \sin \theta \right)^2 + O(n)
\]  

\[
\langle \theta | S_z | \theta \rangle = \frac{n}{2} \cos \theta
\]  

\[
\langle \theta | S_z^2 | \theta \rangle = \left( \frac{n}{2} \cos \theta \right)^2 + O(n)
\]  

\[
\langle \theta | S_z^3 | \theta \rangle = \left( \frac{n}{2} \cos \theta \right)^3 + O(n^2)
\]

Now define

\[
V(\theta, s) = 2(1-s)(1-\sin \theta) + sg\left(\frac{1}{2}(1-\cos \theta)\right)
\]
where \( g \) is given in (13). Using (16), (18), (20), and (22) we have
\[
V(\theta, s) = \left( \frac{2}{n} \right)^3 \langle \theta | \tilde{H}(s) | \theta \rangle + O(1/n)
\] (24)
where we have also used the operator relation \( w = \frac{n}{2} - S_z \). The function \( V(\theta, s) \), for each \( s \), represents a large-\( n \) “effective potential”. For \( n \) large, for each \( s \), the ground state of \( \tilde{H}(s) \) is well approximated by \( | \theta_m \rangle \) where \( \theta_m \) minimizes \( V(\theta, s) \).

Figure 2: The effective potential versus \( \theta \) changes shape as \( s \) increases.

In Figure 2 we plot \( V(\theta, s) \) versus \( \theta \) for \( s = 0, 0.2, 0.4, 0.4341, 0.46 \), and 1. At \( s = 0 \) the minimum is at \( \theta = \pi/2 \) corresponding to Hamming weight \( n/2 \). Because \( g'(1/2) < 0 \), this minimum moves to \( \theta \) bigger than \( \pi/2 \) for small \( s \) as can be seen in the \( s = 0.2 \) panel. As \( s \) increases, a local minimum forms at values of \( \theta \) less than \( \pi/2 \). There is a critical value of \( s \), \( s^* = 0.4341 \), at which the two minima occurring at \( \theta_1 < \pi/2 \) and at \( \theta_2 > \pi/2 \) are degenerate; that is, \( V(\theta_1, s^*) = V(\theta_2, s^*) \). For \( s > s^* \) the global minimum is always at a value of \( \theta \) less than \( \pi/2 \). For \( s = 1 \) this global minimum is at \( \theta_1 = 0 \).

For the quantum adiabatic evolution algorithm to work, the quantum state of the system should remain in (or very near) the instantaneous ground state of \( \tilde{H}(s) \) with \( s = t/T \). For \( s < s^* \) the ground state is smoothly varying. However, at \( s = s^* \) the ground state changes from \( \approx | \theta_2 \rangle \) to \( \approx | \theta_1 \rangle \). For the quantum system to go from \( | \theta_2 \rangle \) to \( | \theta_1 \rangle \) requires quantum tunneling through the barrier separating the minima at \( \theta_1 \) and \( \theta_2 \). This takes a time exponential in \( n \) and implies that the gap of \( \tilde{H}(s^*) \) is exponentially small. Using a combination of standard large spin and instanton methods [4] we can estimate the dominant exponentially small term. We obtain
\[
\text{gap} \sim \text{poly}(n)e^{-S_0n}
\] (25)
Figure 3: The log of the gap plotted versus $n$. The straight line behavior indicates that the gap is decreasing exponentially in $n$.

where

$$S_0 = \frac{1}{2} \int_{\theta_1}^{\theta_2} \varphi(\theta) \sin \theta \, d\theta$$  \hspace{1cm} (26a)$$

and

$$\varphi(\theta) = \cosh^{-1}\left[1 + \frac{V(\theta, s^*) - V(\theta_1, s^*)}{2(1 - s^*) \sin \theta}\right].$$  \hspace{1cm} (26b)$$

For $q = 3$, we find $s^* = 0.4341$ and $S_0 = 0.2015$. We can also determine the minimum gap of $\tilde{H}(s)$ by numerical diagonalization. Because of the symmetry of $\tilde{H}$ and the initial state, although the full Hilbert space is $2^n$ dimensional, the evolution takes place in the $(n + 1)$-dimensional subspace of total spin $n/2$. In Figure 3 we show the log of the gap versus $n$ for $n$ between 60 and 100. At $n = 100$ the minimum gap occurs at $s = 0.4338$. Fitting the gap to the functional form $An^p e^{-cn}$ and finding the best values of $A$, $p$, and $c$ gives $c = 0.2021$, which certainly supports our approach. For $q = 5$ we have $S_0 = 0.4946$ and $c = 0.4966$, and for $q = 7$ we have $S_0 = 0.7008$ and $c = 0.6930$.

Formula (23) is valid for any example where the cost function depends only on the Hamming weight $w$ and we can write

$$h(w) = n^r g(w/n) + O(n^{r-1})$$  \hspace{1cm} (27)$$

where the global minimum of $g(u)$ occurs at $u < 1/2$ and $g'(1/2) < 0$. This guarantees that there is a value $s^*$ such that $V(\theta, s^*)$ given by (23) has degenerate minima at $\theta_1 < \pi/2$ and $\theta_2 > \pi/2$. Then (23) can be used to calculate the coefficient of $n$ in the exponent of (23).
We now study the performance of simulated annealing for this kind of problem. Again we start with a cost function \( h(z_1, \ldots, z_n) \), which is a sum of local terms but because of symmetry only depends on the Hamming weight, so we can write the cost function as \( h(w) \). Now for any temperature \( \tau \), the Boltzmann distribution (8) depends only on the Hamming weight of the string \( w = z_1 + z_2 + \cdots + z_n \). The number of strings with Hamming weight \( w \) is \( \binom{n}{w} \). We can define the (unnormalized) probability

\[
p_\tau(w) = \binom{n}{w} \exp(-h(w)/\tau) \tag{28}\]

which gives the probability of finding a string with Hamming weight \( w \) at temperature \( \tau \) in the Boltzmann distribution.

We also define the “Free energy”, \( F(w, \tau) \), by

\[
\exp(-F(w, \tau)/\tau) = \binom{n}{w} \exp(-h(w)/\tau). \tag{29}\]

Note that for any \( \tau \), the most likely value of the Hamming weight occurs at the value of \( w \) that minimizes \( F(w, \tau) \). Now we further specialize to the case (13) so that (14) and (15) apply. If we rescale the temperature and let \( a = 8\tau/n^2 \) then we can write

\[
F(w, an^2/8) = \left(\frac{n}{2}\right)^3 F(u, a) + O(n^2) \tag{30}\]

where

\[
F(u, a) = a \left[ (1 - u) \log(1 - u) + u \log u \right] + g(u) \tag{31}\]

and again \( u = w/n \).

For \( n \) large, for any value of the temperature \( \tau = an^2/8 \), the Boltzmann distribution is peaked on those strings with Hamming weight \( nu \) where \( u \) minimizes (31). At infinite temperature, the first term in (31) dominates and is minimized at \( u = 1/2 \). As \( a \) is decreased the minimum moves to a value of \( u \) above \( 1/2 \). In Figure 4 we show \( F(u, a)/a \) versus \( u \) for \( a = 100, 10, 3.4, 3.0574, 2.8, \) and \( 0.01 \). The similarity with Figure 2 is apparent. The critical value of \( a, a^* = 3.0574 \), is where the global minimum switches from a value of \( u \) above \( 1/2 \) to a value below. To follow the Boltzmann distribution, in the simulated annealing Markov chain, the Hamming weight, \( nu \), must change from the value corresponding to the larger local minimum to the smaller while \( \tau \) is approximately \( a^*n^2/8 \).

This order-\( n \) change in the Hamming weight requires exponentially many steps: The sign of the derivative \( \frac{\partial}{\partial u} F(u, a^*) \) determines whether the Markov chain is more likely to move left or right. For large \( n \), if in the steps of the annealing process the bits are chosen uniformly at random, \( w \) is more likely to move to \( w + 1 \) than to \( w - 1 \) if \( \frac{\partial}{\partial u} F(u, a^*) < 0 \). This means that climbing the hill separating the local minima is exponentially unlikely in polynomially many steps.

As long as \( g(u) \) has a global minimum at \( u < 1/2 \) and \( g'(1/2) < 0 \) simulated annealing, like quantum adiabatic evolution, will require a time exponential in \( n \) to succeed. The method used in this section, tracking the local minima of the effective potential and the free energy, can be used to show the similarity of the performance of quantum adiabatic evolution and simulated annealing for many examples with a cost that depends on the Hamming weight alone.
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Figure 4: The scaled free energy $F/a$ plotted as a function of the scaled Hamming weight changes shape as the temperature decreases. Compare to Figure 3.

5 The Hamming weight with a spike

Here we consider the cost function

$$h(w) = \begin{cases} 
  w, & w \neq n/4 \\
  n, & w = n/4 \end{cases}$$

where again $w$ is the Hamming weight of $n$ bits and also $n$ is taken to be a multiple of 4. Note that this cost function cannot be written as a sum of terms each of which involves only a few bits. The global minimum of $h(w)$ is at $w = 0$ and there is a local minimum at $w = (n/4) + 1$.

It is easy to see that simulated annealing fails to find the global minimum in polynomial time. For $\tau > 1/\log 3$, the Boltzmann distribution concentrates at Hamming weights larger than $n/4$. For $\tau < 1/\log 3$ the Boltzmann distribution concentrates at Hamming weights smaller than $n/4$. At temperatures $\sim 1/\log 3$, according to the acceptance rule (10), a string with Hamming weight $(n/4) + 1$ will only flip to a string with Hamming weight $n/4$ with a probability that is exponentially small in $n$. Thus a simulated annealing algorithm running for only polynomial time gets hung up in the false minimum of $h$.

In quantum mechanics, it is well known that a low-energy particle can penetrate a high potential barrier. If the barrier is thin, the penetration probability need not be small. This turns out to be the case here. As in the examples of Section 4, since the cost is a function only of the Hamming weight, the quantum evolution takes place in an $(n + 1)$-dimensional subspace. The gap can be calculated by explicit diagonalization (using a technique similar
to the one in [1], section 4.2). The result is that

$$\text{gap}(n) \approx 1.35 n^{-1/2}$$

and, for $n$ large, occurs at $s = 0.366$. We can also find the gap by numerical diagonalization; see Figure 5, which plots $\log \text{gap}(n)$ versus $\log(n)$ for $500 \leq n \leq 848$. The straight line fit has slope $-0.474$, consistent with the predicted $-0.5$ in (33). For $n = 848$, the gap occurs at 0.3675, close to the predicted 0.366.

6 The bush of implications

In the previous section we discussed an example with a cost function that treats all bits symmetrically and depends only on the Hamming weight of the $n$ bits. Here we describe an example where the cost function depends on the Hamming weight of $n$ bits, but also on the value of a single additional bit. As in Section 4, we consider the effective potential and free energy. In the example in this section, quantum adiabatic evolution succeeds in polynomial time while simulated annealing does not.

We label the $n + 1$ bits 0, 1, 2, ..., $n$. The cost function is given by

$$h(z_0, z_1, \ldots, z_n) = \sum_{i=1}^{n} z_0(1 - z_i) + (1 - z_0) .$$

The terms $z_0(1 - z_i)$ can be viewed as “imply” clauses, since they are 0 unless $z_0 = 1$ and $z_i = 0$. The unique string with $h = 0$ has $z_0 = 1$ and all $z_i = 1$. If $z_0 = 0$, then $h = 1$ no matter what the values of $z_1, \ldots, z_n$ are. If $z_0 = 1$, then $h$ equals $n - w$ where
\[ w = z_1 + z_2 + \cdots + z_n \] is the Hamming weight of the string \( z_1, \ldots, z_n \). We can rewrite (34) as

\[ h(z_0, w) = z_0(n - w) + 1 - z_0 \]  

(35)

and as before

\[ h(z_0, w) = ng(z_0, \frac{w}{n}) + O(1) \]

(36)

with

\[ g(0, u) = 0 \]  

(37a)

and

\[ g(1, u) = 1 - u . \]  

(37b)

Note the degeneracy of the minima of \( g \); this is removed by including the lower order term \((1 - z_0)\).

As before, to determine the performance of annealing, we calculate the free energy \( F \), defined by

\[
\exp\left(-F_{z_0}(w, t)/\tau\right) = \left(\frac{n}{w}\right) \exp\left(-h(z_0, w)/\tau\right)
\]

(38)

and

\[
F_{z_0}(w, \tau) = nF_{z_0}\left(\frac{w}{n}, \tau\right) + O(1) .
\]

(39)

We get

\[
F_0(u, \tau) = \tau\left[(1 - u) \log(1 - u) + u \log u\right]
\]

(40a)

and

\[
F_1(u, \tau) = \tau\left[(1 - u) \log(1 - u) + u \log u\right] + (1 - u) .
\]

(40b)

In Figure 7 we plot \( F_{z_0}(w, \tau)/\tau \), \( \tau = 100, 5, 1, \) and 0.05. We see that with the \( O(1) \) terms neglected, the value \( z_0 = 0, w = \frac{n}{2} \) minimizes the free energy for all \( \tau, 0 < \tau < \infty \).
Figure 7: The bush of implications. The scaled free energy plotted versus the scaled Hamming weight as the temperature changes. In each panel the top curve corresponds to \( z_0 = 1 \) and the lower corresponds to \( z_0 = 0 \). The global minimum never moves from \( z_0 = 0, u = 1/2 \).

Can the addition of the correction, which adds 1 to \( F_0(w, \tau) \) for all \((w, \tau)\), make any difference in a simulated annealing process? For \( \tau = 0 \), the \(1 - z_0\) term means that the global minimum of \( h \) occurs at \( z_0 = 1, w = n \). For \( \tau \approx 1 \), a simulated annealing process that is following the Boltzmann distribution will be concentrated at \( z_0 = 0, w = n/2 \). There are two routes from \( z_0 = 0, w = n/2 \) to \( z_0 = 1, w = n \). One route is to jump from \( z_0 = 0 \) to \( z_0 = 1 \) while \( w \approx n/2 \). But the probability of accepting this change is exponentially small in \( n \) for \( \tau < 1 \), so this route is exponentially unlikely in polynomially many steps. (Note that changing the rate at which bit 0 is flipped does not help.) The other route is to maintain \( z_0 = 0 \) while \( w \) increases. But this is exactly the kind of hill climbing in free energy \([this time \( F_0(u, \tau) \)]\) that cannot occur in polynomial time as in the example in the previous section. In conclusion, simulated annealing fails to reach the true minimum of \( h \) at \( z_0 = 1, w = n \) in polynomial time.

We now turn to the behavior of a quantum adiabatic algorithm for the bush of implications. Using spin operators we write the quantum Hamiltonian corresponding to \( h \) of (34) as

\[
H_P = \frac{1}{2}(1 - \sigma_z^{(0)})(\frac{n}{2} + S_z) + \frac{1}{2}(1 + \sigma_z^{(0)})
\]

where \( S_z \) is the z component of the total spin for bits 1 through \( n \), whereas \( \frac{1}{2}\sigma_z^{(0)} \) is the spin component of the spin of bit 0. Now bits 1 through \( n \) are each involved in one term in (34) whereas bit 0 is in \( n + 1 \) terms. Accordingly, we get for \( \tilde{H}(0) \) [see \([1]\), formula (2.22)]

\[
\tilde{H}(0) = (n + 1)\frac{1}{2}(1 - \sigma_x^{(0)}) + \left(\frac{n}{2} - S_x\right).
\]
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1.6
1.8
2
2.2
2.4
2.6
2.8
3

$\alpha$

Figure 8: The bush of implications. The global minimum of the effective potential plotted as a function of $s$.

For the interpolating Hamiltonian we take

$$\tilde{H}(s) = (1 - s)\tilde{H}(0) + sH_p.$$  \hfill (43)

Consider the states $|\alpha, \theta\rangle = |\alpha\rangle \otimes |\theta\rangle$ where $|\alpha\rangle$ is the bit 0 state

$$|\alpha\rangle = (\sin \alpha/2)|z_0 = 0\rangle + (\cos \alpha/2)|z_0 = 1\rangle$$  \hfill (44)

and $|\theta\rangle$ is made of bits 1 through $n$ and is defined by (21). For the effective potential we set

$$V(\alpha, \theta, s) = (1 - s)[2 - \sin \alpha - \sin \theta] + 2s \cos^2 \alpha/2 \cos^2 \theta/2$$  \hfill (45)

which gives

$$V(\alpha, \theta, s) = \frac{2}{n} \langle \alpha, \theta | \tilde{H}(s) | \alpha, \theta \rangle + O\left(\frac{1}{n^2}\right).$$  \hfill (46)

Note that $V(\alpha, \theta, s) = V(\theta, \alpha, s)$ for all $s$.

In Figure 8 we plot $(\alpha(s), \theta(s))$, the global minimum of $V(\alpha, \theta, s)$, as a parameterized curve for $0 \leq s \leq 1$. At $s = 0$ the global minimum occurs at $\alpha = \pi/2$, $\theta = \pi/2$, which corresponds to a uniform superposition for bit 0 and a Hamming weight concentrated at $n/2$ for bits 1 through $n$. As $s$ increases the minimum is at $\alpha(s) = \theta(s)$ until a critical value $s = s^* = 0.805$. For $s > s^*$ there are two global minima symmetric under interchange of $\alpha$.
and $\theta$. We go beyond the effective potential and analyze the quantum corrections for $s = s^*$, using a representation in terms of a 2-component (to represent the state of bit 0) anharmonic oscillator (to represent the fluctuations about the state $|\theta(s^*)\rangle$). We find an expansion in powers of $n^{-1/3}$. The symmetry under interchange of $\alpha$ and $\theta$ is broken by the quantum corrections, and the branch heading towards $\alpha = \pi/2$, $\theta = \pi$ has the lower energy. The adiabatic evolution is therefore heading towards the state that is a uniform superposition for bit 0 and has Hamming weight $n$ for bits 1 through $n$. This analysis so far has neglected the $1/2 (1 + \sigma^z(s))$ term in $H_P$ because it is lower order in $n$. For $(1 - s)$ of order $1/n$, the effect of this term in $\tilde{H}(s)$ is of the same order as $\tilde{H}(0)$. The net effect of this term is to rotate bit 0 to $|z_0 = 1\rangle$ in an $n$-independent fashion.

According to this analysis the minimum gap appears at $s = s^* + O(n^{-2/3})$, where $s^*$ is the bifurcation point in Figure 8. We calculate

$$\text{gap}(n) = \frac{0.5782}{n^{1/3}} + \frac{B}{n^{2/3}} + O(n^{-1}).$$

(47)

We can confirm this analysis numerically because the Hamiltonian $\tilde{H}(s)$ acts in a reduced Hilbert space of dimension $2(n + 1)$. In Figure 9 we show the difference between the lowest two eigenvalues $E_1(s) - E_0(s)$ for $0 \leq s \leq 1$ at $n = 300$. Note that the minimum difference occurs at $s = 0.800$. In Figure 10 we plot $n^{1/3} \cdot \text{gap}(n)$ versus $n^{-1/3}$ for $300 \leq n \leq 1540$. According to prediction (47) this should be a straight line (with corrections of order $n^{-2/3}$).
with an intercept of 0.5782. A straight-line fit to the data in Figure 10 has an intercept of 0.5812.

It is worth noting that the choice of $\tilde{H}(0)$ in (42) was made so that $\tilde{H}(s)$ would be the sum of terms

$$\tilde{H}(s) = \sum_C \tilde{H}_C(s)$$

where each $\tilde{H}_C(s)$ depends only on clause $C$ (see [1], formula 2.28). Suppose instead, for the bush of implications, we write

$$\tilde{H}(0) = \lambda (n+1)\frac{1}{2}(1 - \sigma_x^{(0)}) + \left(\frac{n}{2} - S_x\right)$$

with $\lambda$ a parameter. We can recalculate the effective potential and draw the picture analogous to Figure 8. If $\lambda > 1$, the gap for $n$ large is a positive constant. If $\lambda < 1$, the gap is exponentially small. Note that the choice $\lambda = 1/(n+1)$ corresponds to a magnetic field in the $x$-direction with the same strength for each bit. This case, mentioned in [1], is an example of a local problem with a choice for a quantum adiabatic algorithm that requires exponential time. This illustrates that the cost function alone does not determine the performance of the quantum algorithm but rather that the choice of the path to $H_P$ is sometimes crucial.
7 Conclusion

In this paper we first compared the behavior of quantum adiabatic evolution and classical simulated annealing in searching for the global minima of cost functions that depend on $n$ bits symmetrically. When the cost depends smoothly on the Hamming weight of the $n$ bits, quantum adiabatic evolution and simulated annealing typically perform similarly.

We have also shown, however, that there are examples where this similarity breaks down. In the spike example, the cost function has a barrier that can be penetrated quantum mechanically but not classically, so the quantum algorithm succeeds in polynomial time whereas annealing does not. In the bush example, the addition of a single spin-1/2 leads to quantum behavior with no classical analogue. These examples suffice to show that there is no theorem that says quantum adiabatic evolution will fail when simulated annealing fails. It remains an open question whether they also indicate that quantum adiabatic evolution algorithms will succeed on problems of computational interest that cannot be solved efficiently by classical local search.

Acknowledgments

This work was supported in part by the Department of Energy under cooperative agreement DE–FC02–94ER40818 and by the National Security Agency (NSA) and Advanced Research and Development Activity (ARDA) under Army Research Office (ARO) contract DAAD19-01-1-0656. We thank Andrew Childs and John Preskill for helpful discussions and Umesh Vazirani for sharing some of his group’s results prior to posting. We also thank Martin Stock for his help preparing this manuscript.

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