A new adiabatic quantum search algorithm

April 1, 2022

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Abstract

We present a new adiabatic quantum algorithm for searching over structured databases. The new algorithm is optimized using a simplified complexity analysis.

1 Introduction

Many computational search problems are surprisingly difficult to solve. Quantum computing is a promising candidate to tackle such difficult tasks. An important landmark was achieved by Grover: while an oracle search for a marked item out of $N$ classical unstructured items requires, on average, $O(N)$ steps, Grover [1] found a quantum algorithm that performs the oracle search in $\sqrt{N}$ steps. This quadratic speedup leads to the question of whether similar speedups can be achieved for other search problems.

Structured searches are natural extensions of the oracle search. They are used when the databases possess some structure. Exploiting the structure of the database will increase the performance of a search (classical or quantum). Cerf et al [2] were the first to study structured quantum search algorithms. Their work is based on quantum circuits. Recently Roland and Cerf [3] gave a quasi-adiabatic quantum version of the structured search.

To understand better the algorithm presented in [2, 3] we recall that Grover’s algorithm uses an iterative improvement strategy. It starts with an
equal superposition of all possible states representing items of the database, and by iterative application of unitary operations (gates) the initial state is rotated towards a state that encodes the solution of the search problem. However if the database has some structure of its own other strategies can be used. For example, one can use the divide-and-conquer strategy. In this strategy one divides the problem into subproblems of manageable size, then solves the subproblems. The solutions to the subproblems must then be patched back or nested together. For this method to produce good global solutions, the subproblems must naturally disjoint, and the division made must be an appropriate one (optimal). The optimization results in making the division such that the errors made in patching does not offset the gains obtained in applying more powerful methods to the subproblems. Roughly speaking, the algorithm of [2] uses a combination of the two outlined strategies. The problem is divided first into two oracle searches, then a third global search is used to patch back the two previous searches.

The present work gives an alternative scheme for dividing the original problem into subproblems. As will be seen later, our method allows one to relax some of the assumptions made in [2].

The paper is organized as follows: in section 2 we present the necessary tools for our algorithm, whereas the algorithm itself is presented in section 3. Using an average complexity analysis for our algorithm, we give in section 4 the running time for a variety of hard search problems. In the appendix we present a generalization of our algorithm to higher nesting levels.

2 Definitions

Search problems belong to the family of Constraint Satisfiability Problems (CSP). A search problem is defined as the problem of finding a satisfying assignment for a set (formula) of constraints acting on $n$ (qu)bits. In general, each constraint acts on a number of bits less than or equal to $n$. The search will terminate whenever the “program” finds an assignment, or assignments, that satisfy simultaneously all the constraints of the CSP formula. For example, the oracle search over an unstructured database corresponds to the problem of finding an assignment that satisfies all the constraints of the predefined formula, whose constraints are all $n$ bit constraints. Even though the number of qubits is fixed, by varying the length or the type of constraints the CSP can cover different types of problems.

For a structured database (problem) we can divide the initial search problem of $n$ qubits into subproblems with smaller number of variables.
One can choose to test first if an assignment to $n_A$ variables out of the $n$ variables satisfies all the constraints acting uniquely on this subset of variables, labeled $A$. The result of this test is kept in a register. A similar test is then applied to the remaining bits, that we label as subset $B$. And finally one must nest both tests to find a global solution for the initial search problem. This is what is meant by a structured or nested search.

More specifically, assume that the initial search problem admits a number $M_{AB}$ of solutions. In a quantum search problem, a solution or a satisfying assignment is a state in the Hilbert space of the $n$ qubits. The set of solutions we thereafter denote by

$$M_{AB} = \{ |m_i\rangle / i = 1, 2, \ldots, M_{AB} \}.$$ (1)

All elements of this set satisfy the predefined formula of constraints denoted generically by $\{ C_{AB} \}$. For our patching strategy, the constraints $\{ C_{AB} \}$ are classified as

- $\{ C_A \}$: the set of constraints acting only on the subset $A$. In general, there exist different solutions satisfying all the constraints of this set. The set of possible solutions is

$$M_A = \{ |m^A_i\rangle / i = 1, 2, \ldots, M_A \}.$$ (2)

- $\{ C_B \}$: the set of constraints acting only on the subset $B$. Again, different solutions can be found to satisfy all the constraints of this set. The set of possible solutions is

$$M_B = \{ |m^B_i\rangle / i = 1, 2, \ldots, M_B \}.$$ (3)

- $\{ C_{A/B} \} = \{ C_{AB} \} - \{ C_A \} - \{ C_B \}$ is the set of constraints acting simultaneously on $A$ and $B$.

Some elements of $M_A$ may not satisfy one or more constraints in $\{ C_{A/B} \}$, those elements can not give global solutions, so they are Not Solutions. The set of such elements is denoted by $M^S_A$. On the other hand, the set of elements of $M_A$ satisfying all the constraints in $\{ C_{A/B} \}$, and hence giving global solutions, will be denoted by $M^S_A$. Therefore

$$M_A = M^S_A \cup M^S_A.$$ (4)
Similarly we have
\[ \mathcal{M}_B = \mathcal{M}^S_B \cup \mathcal{M}^{NS}_B. \] (5)

So, an element \(|m_i\rangle \in \mathcal{M}_{AB}\) can be written as
\[ |m_i\rangle = |m^S_A\rangle \otimes |m^S_B\rangle, \] (6)

where \(|m^S_A\rangle\) and \(|m^S_B\rangle\) are elements of \(\mathcal{M}^S_A\) and \(\mathcal{M}^S_B\) respectively.

It is evident that for a given state \(|m^S_A\rangle\) there could be different states \(|m^S_B\rangle\) such that their product is an element of \(\mathcal{M}_{AB}\). At some stages, the authors of [2] and [3] made the assumption that for a given \(|m^S_A\rangle\) there is only one \(|m^S_B\rangle\) such that their product is a global solution. Although one may argue that such an assumption is justified for hard search problems, where there is just one global solution, it is unlikely that it holds for a generic search problem. This assumption is not needed for our algorithm, and hence our algorithm applies to a broader class of search problems.

3 Nested algorithm

The present algorithm consists of two stages. In the first stage (stage I) we evolve adiabatically the quantum system from a state which is the ground state of a Hamiltonian that can be easily obtained to a state which is a product of states of \(\mathcal{M}_A\) and states of \(\mathcal{M}_B\). As previously mentioned, this product is not yet a global solution. In stage II a global search, similar to what is labeled as stage C in [3], is applied to the output of stage I to rotate it towards an element of \(\mathcal{M}_{AB}\). The output of stage II is a global solution of the problem.

3.1 Stage I

In this stage we use the procedure defined in [5]. The Hamiltonian is split into two parts, each acting on one of the Hilbert spaces \(\mathcal{H}_A\), of dimension \(N_A = 2^n_A\), and \(\mathcal{H}_B\), of dimension \(N_B = 2^n_B\), spanned by subsets \(A\) and \(B\) respectively.

The most convenient initial state is the equal superposition of all possible pure states of the system
\[ |\Psi(t = 0)\rangle = \frac{1}{\sqrt{N_A}} \sum_{i_A \in \mathcal{H}_A} |i_A\rangle \otimes \frac{1}{\sqrt{N_B}} \sum_{i_B \in \mathcal{H}_B} |i_B\rangle \]
\[ \equiv |\Psi_{0A}\rangle \otimes |\Psi_{0B}\rangle, \] (7)
where \( N = 2^n = N_A N_B \). \(|\Psi_0\rangle\) is the ground state of the Hamiltonian
\[
H_0 = (I_A - |\Psi_{0A}\rangle \langle \Psi_{0A}|) \otimes I_B + I_A \otimes (I_B - |\Psi_{0B}\rangle \langle \Psi_{0B}|). \tag{8}
\]
The initial Hamiltonian should evolve adiabatically into a final Hamiltonian which has the ground state
\[
\sqrt{M_A} \sum_{m_A \in M_A} |m_A\rangle \otimes \sqrt{M_B} \sum_{m_B \in M_B} |m_B\rangle \equiv |\Psi_{fA}\rangle \otimes |\Psi_{fB}\rangle. \tag{9}
\]
A possible final Hamiltonian is
\[
H_f^I = (I_A - |\Psi_{fA}\rangle \langle \Psi_{fA}|) \otimes I_B + I_A \otimes (I_B - |\Psi_{fB}\rangle \langle \Psi_{fB}|) \tag{10}
\]
We have chosen \( H_0 \) and \( H_f^I \) so that the evolution is decoupled in \( \mathcal{H}_A \) and \( \mathcal{H}_B \). The time dependent Hamiltonian evolving \( H_0 \) to \( H_f^I \) in a time \( T_I \) is the linear combination
\[
H(t) = (1 - s(t)) H_0 + s(t) H_f^I \equiv f(s) H_0 + g(s) H_f^I, \tag{11}
\]
where \( s(t) \) is chosen such that \( s(0) = 0 \) and \( s(T_I) = 1 \). When the adiabaticity condition holds, the initial ground state \(|\Psi_0\rangle\) will evolve slowly in time \( T_I \) to the ground state of the final Hamiltonian. The meaning of “slow” evolution is quantified by the adiabatic theorem \([6]\), which states that the accuracy with which the system remains in its instantaneous ground state is equal to the sum of the ratio of the transition matrix element from the ground state, with energy \( E_0 \), to any other state, with energy \( E_i \), over the fourth power of the “radiated” energy \( \omega_{0i} = E_0 - E_i \), i.e.
\[
\sum_i \frac{|\langle E_i | \frac{dH}{dt} | E_0 \rangle|^2}{\omega_{0i}^4} \leq \epsilon^2. \tag{12}
\]
This gives a lower bound on the evolution time \( T_I \).

The eigenvalues and eigenfunctions of the Hamiltonian \( H(t) \) can be calculated analytically. We find that the only nonvanishing transition probabilities from the ground state are to the two lowest energy levels:

- \( E_A = E_0^A + E_0^B \), i.e. the state where the subsystem \( A \) is in its first excited state, and the subsystem \( B \) is in its ground state

- \( E_B = E_0^A + E_1^B \), i.e. the state where the subsystem \( A \) is in its ground state, and \( B \) is in its first excited state.
The corresponding transition matrix elements are given by
\[ \left| \langle E_i \frac{dH}{dt} | E_0 \rangle \right|^2 = \left( \frac{ds}{dt} \right)^2 \frac{M_i^2 / N_i^2}{\omega_i^2} \left( \frac{N_i}{M_i} - 1 \right) \equiv \frac{\xi_i^2}{\omega_i^2} \left( \frac{ds}{dt} \right)^2, \quad i = A, B, \]
where
\[ \omega_i = \sqrt{(f - g)^2 + \frac{4M_i}{N_i}} fg = \sqrt{(1 - 2s)^2 + \frac{4M_i}{N_i}} s(1 - s) \]
is the gap (energy difference) between the first excited state and the ground state of the \( i \)-th subsystem.

By integrating eq. (12) over \( s \) using eq. (13) the lower bound, or the minimal time, will be
\[ T_I = \frac{1}{\epsilon} \int_0^1 ds \sqrt{\sum_{i=A,B} \frac{\xi_i^2}{\omega_i^2}}. \]

Note that the parallel evolution, in the two Hilbert spaces \( \mathcal{H}_A \) and \( \mathcal{H}_B \), of stage I is the major feature that distinguishes our algorithm from that of [2]. Stage I replaces the two-stages evolution (sequential evolution) used in [2]. A priori the sequential evolution seems more efficient, as one can use the result of the first stage to eliminate some of the no-good assignments in the second stage. However the algorithm used in [2] is not a tree-like search procedure, i.e. it does not pick an order in which it instantiates the variables. Hence the algorithm of [2] does not eliminate “bad” trees. Therefore replacing the sequential by the parallel evolution will not affect dramatically the time cost of the algorithm. On the other hand, as mentioned before, the symmetric parallel evolution allows one to analyse a broader set of structured search algorithms.

3.2 Stage II

The output state of stage I can be written as the sum of a state encoding the solution to the search problem and a residual part, which is not a solution:
\[ |\Psi_{fA} \rangle \otimes |\Psi_{fB} \rangle = \sqrt{\frac{M_A M_B - M_{AB}}{M_A M_B}} |\Psi^{NS} \rangle + \sqrt{\frac{M_{AB}}{M_A M_B}} |\Psi^S \rangle, \]
where the “solution state” is
\[ |\Psi^S \rangle = \frac{1}{\sqrt{M_A^S M_B^S}} \sum_{m_A^S \in M_A^S} |m_A^S \rangle \otimes \sum_{m_B^S \in M_B^S} |m_B^S \rangle = \frac{1}{\sqrt{M_{AB}}} \sum_{m_i \in M_{AB}} |m_i \rangle \]

(17)
and we have used the fact that \( M_A^S M_B^S = M_{AB} \).

At this stage one is inclined to start again an adiabatic evolution from a Hamiltonian whose ground state is \( |\Psi_{fA}\rangle \otimes |\Psi_{fB}\rangle \), e.g.

\[
H_i = 1 - |\Psi_{fA}\rangle\langle \Psi_{fA}| \otimes |\Psi_{fB}\rangle\langle \Psi_{fB}|
\]

(18)

to a final Hamiltonian whose ground state is \( |\Psi^S\rangle \), e.g.

\[
H_f = 1 - |\Psi^S\rangle\langle \Psi^S|
\]

(19)
in time \( O(\sqrt{M_A M_B / M_{AB}}) \). Unfortunately, this is not possible since the initial Hamiltonian \( H_i \) is not accessible. Following \[3\] a global search can be applied to nest between the two subsets \( A \) and \( B \). The global search is achieved through the following procedure:

- Stage I is approximated by an evolution operator \( U \) such that \( |\Psi_{fA}\rangle \otimes |\Psi_{fB}\rangle \approx U |\Psi_{0A}\rangle \otimes |\Psi_{0B}\rangle \).

- Hence \( H_i \approx U H_0 U^\dagger \), note that \( H_i \) is “replaced” by \( H_0 \) which is easily accessible.

- The adiabatic evolution from \( H_i \) to \( H_f \) is implemented on quantum circuits. The continuous evolution is replaced by a “step evolution” over intervals of time. In each step, at a given time \( t \), we use the approximation

\[
e^{-iH_i t} \approx U e^{-iH_0 t} U^\dagger
\]

i.e. a backward evolution in time \( T_I \), an application of \( \exp(-iH_0 t) \), then a forward evolution in time \( T_I \). This step requires a time \( O(T_I) \).

The number of steps is chosen to minimize the error involved in the discretization needed during the global evolution. The number of iteration is at least (see \[3\]) of the order of \( \sqrt{M_A M_B / M_{AB}} \). So that the total running time needed to get a global solution, is proportional to

\[
T = T_I \sqrt{M_A M_B / M_{AB}} = T(M_A, M_B, M_{AB}, n, n_A/n).
\]

(21)

This expression is not yet the final answer, since there is still the problem of determining the values of \( M_{A,B,AB} \). This will be discussed in the next section.
4 Complexity analysis

The total running time $T$ is a function of $M_A, M_B, M_{AB}, n$ and $x = n_A/n$, among which $n$ is the only input parameter, and $x$ will be chosen to minimize $T$. Hence we are left with the three parameters $M_A, M_B$ and $M_{AB}$. A pri- ori, these parameters are problem dependent and are difficult to determine. However, since we are interested in getting general results which depend as little as possible on the details of the problem, we can approximate these quantities using a complexity analysis.

Computational complexity theory studies the quantitative laws which govern computing. It seeks a comprehensive classification of problems by their intrinsic difficulty and an understanding of what makes these problems hard to compute. The simplified average complexity analysis derived in [7, 2] can be adapted for our generic algorithm. The major simplification made in [2] is the approximation of independent no-good assignments\(^2\). This allows for a relatively easy combinatorial analysis. Following [2] the unknown parameters are estimated by

$$M_j \approx 2^{n_j - n\alpha(n_j/n)^k} \quad \text{for} \quad j = A, B, AB \quad \text{with} \quad n_{AB} = n ,$$  \hspace{1cm} (22)

where $k$ is the number of variables per constraint, assuming a constant length constraint. $\alpha$ represents the average difficulty of the problem, it characterizes the average number of no-good ground instances per variable. Hardest problems are found near a critical\(^3\) value $\alpha = \alpha_c = 1$. The critical $\alpha$ is obtained from the number of solutions

$$M_{AB} \approx N^{1-\alpha}$$

for $\alpha < 1$, $M_{AB}$ is large, i.e. the problem is under-constrained and easy to solve, while for $\alpha > 1$, $M_{AB} < 1$, i.e. the problem is over-constrained and probably has no solution. Finally for $\alpha = 1$ we have one solution, this is the definition of the critical value.

Therefore, the optimization procedure reduces to a minimization of the running time as a function of the ratio $x$ for different values of $\alpha$ and $k$.

\(^2\)For most CSP there are classes of no-good assignments that can be deduced from each other. For example, one can use propositional reasoning to generate some no-goods from others, see for example chapter two of [5].

\(^3\)This critical behavior is similar to a phase transition in condensed matter physics. Similar phase transition features were observed for random K-SAT problems [9, 10].
4.1 Approximate and exact scalings

The running time $T$ can not be calculated analytically. However by the following simple arguments it is possible to give an estimate for $T$:

- We first recognize that our algorithm is inefficient if $M_i/N_i \sim 1$. This can be easily seen by remembering that $N_i$ is the number of possible assignments in space $A$ or $B$ and $M_i$ is the number of solution in that space. For $M_i \sim N_i$ any assignment will become a solution, then, one step (picking up any state) is sufficient to find a solution in the subspace $i$. This is reflected through the limit

$$\xi_i = \frac{M_i}{N_i} \sqrt{\frac{N_i}{M_i}} - 1 \rightarrow 0 \text{ when } M_i \rightarrow N_i.$$ 

Therefore, the first stage does not eliminate any no-good assignment and consequently the second stage will take $\sqrt{N}$ steps to give a solution, i.e. as if the search is an oracle search. But what does this means?

Using the average complexity analysis of the previous section we write:

$$M_A/N_A = 2^{-n\alpha x^k}.$$ 

Taking $M_A/N_A \sim 1$ implies that $n\alpha x^k \sim 1$ or $k \sim \ln(n\alpha)/\ln(1/x)$, on the other hand we expect\(^4\) that optimization will give a value of $x$ not far from 1/2, hence for large values of $n$ and near the critical $\alpha = 1$ our algorithm breaks down for $k \sim \ln(n)$. But the larger the $k$ is, the closer we are to the unstructured search where each constraint is an $n$ qubit constraint.

- From the previous remark we deduce that our algorithm is effective as long as $M_i/N_i \ll 1$.

- The running time of stage $I$, given in eq. (15), exhibits a near singular behavior for $M_i/N_i \ll 1$. This near singularity occurs when the integration variable $s$ is close to the value for which $f(s) = g(s)$, i.e. $s = 1/2$.

These remarks imply that, for a given $x$, $T_I$ can be approximated using the near singular behavior to obtain

$$T_I(x) \sim \sqrt{\text{Max} \left( \frac{N_A}{M_A}, \frac{N_B}{M_B} \right)}.$$  

\(^4\)If $x = 0$ or 1, the first stage is again useless as there is no division of the initial space.
Figure 1: The numerical value of the running time $T$ as a function of $x$, for $(k = 2, \alpha = \alpha_c = 1, n = 32)$, compared to the analytical estimate of $T$. Similar results are obtained for different values of $k$.

In other words, the time $T_I$ scales with the square root of the largest value of the dimension of each Hilbert space divided by the number of possible solutions in that space. Multiplying by the number of iterations of stage $II$, the total running time reads

$$T(x) \sim \sqrt{\text{Max} \left( \frac{N_A M_B}{M_{AB}}, \frac{N_B M_A}{M_{AB}} \right)}.$$  

(24)

Using the average complexity analysis we get

$$T(x) \sim \sqrt{\text{Max} \left( N^{\alpha - \alpha(1-x)} k, N^{\alpha - \alpha x} k \right)}.$$  

(25)

In figure 1 we compare this approximate formula with the time calculated numerically. The two results match extremely well for all values of $x$.

The time $T$ is then optimal for $N^{\alpha - \alpha(1-x)} k = N^{\alpha - \alpha x} k$, i.e. $x = 1/2$, which is compatible with the symmetric nature of the algorithm. This result agrees with the numerical results presented in figure 2, where $x = 1/2$ is found to give the optimal time for different values of $k$. The plot also illustrates that the larger $k$ is the closer we are to an oracle type search, which is what we predicted before. Hence the optimal time is given by

$$T_{\text{min}} = T(x = 1/2) \sim N^{\alpha/2 - \alpha/2^{k+1}} \sim 2^{\alpha(1/2 - 1/2^{k+1})}.$$  

(26)

We conclude that the parameter of interest in these considerations is $n$. In figure 3 we plot the running time as a function of $x$ for different values of $n$. 

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{figure1.png}
\caption{The numerical value of the running time $T$ as a function of $x$, for $(k = 2, \alpha = \alpha_c = 1, n = 32)$, compared to the analytical estimate of $T$. Similar results are obtained for different values of $k$.}
\end{figure}
Figure 2: The running time $T$ as a function of $x$, for $(k = 2, 3, 5, \alpha = \alpha_c = 1, n = 32)$. The optimal time is attained at $x = 1/2$. The horizontal line is the $\sqrt{N}$ scaling. It is evident that the larger $k$ is the closer we are to the horizontal line, i.e. to the oracle search.

$\alpha$ and $n$ keeping their product constant. The fact that the different plots coincide strongly supports the scaling obtained from the analytical estimate.

Another important aspect is the (sub)-exponential growth of $T$ as a function of $\alpha$. This can be seen either from eq. (26) or from the “critical” behavior depicted in figure 4.

Finally we consider the special case $(k = 2, \alpha = 1)$. In this case the running time is $O(N^{3/8})$, which is better than the classical running time $O(N^{0.5})$ but less efficient than the result obtained using the algorithm of Cerf et al. which gives $O(N^{0.31})$. The $O(N^{0.375})$ scaling is compared with the numerical result in figure 5.

5 Conclusions

We have presented a new adiabatic quantum algorithm for searches over structured databases. Our algorithm is constructed with minimum assumptions about the nature of the database and the specificity of the search problem. Moreover, it results in a significant potential speedup over its classical counterpart.

The new algorithm is in fact “quasi”-adiabatic, it requires the use of quantum circuits at some stages. An interesting topic for future work would be to construct a “pure” adiabatic quantum algorithm. Another important issue is to explore the possibility of using smart classical strategies such
Figure 3: The running time $T$ as a function of $x$, for $(k = 3, \alpha = 1.054, n = 32), (k = 3, \alpha = 1.25, n = 27)$, such that $n\alpha$ is approximately constant. This supports the effective parameterization in terms of $n\alpha$.

Figure 4: The running time $T$ as a function of $x$, for $(k = 5, \alpha = 0.9, 1, 1.054, n = 32)$. The slightest variation of $\alpha$ affects dramatically the running time, which reflects the critical behavior predicted by the complexity analysis.
Figure 5: The running time $T$ as a function of $N$, for $(k = 2, x = 0.5)$. The numerical result matches the approximate analytical scaling: $T \sim O(N^{0.375})$.

as back tracking and constraint propagation, and to see the effect of such strategies on quantum interference and coherence. These and other related issues will be addressed elsewhere.

A Multi-nesting verses multi-partition

The nesting procedure can be applied to subsets $A$ and $B$, resulting in higher level nesting or multi-nesting [2]. In multi-nesting stages I and II are applied to subsets $A$ and $B$ separately. Then stage II is applied to nest $A$ and $B$. Then the time $T_I$ is replaced by a shorter time. More nesting can be used to enhance the effectiveness of the structured search. Another alternative is to modify stage I by splitting the $n$ variables into more than two subset then

$$T_I = \frac{1}{\epsilon} \int_0^1 ds \sqrt{\sum_{i=A,B,C,D,...} \frac{\xi_i^2}{\omega_i}}$$

(27)

and hence applying the procedure of stage II we get

$$T = T_I \left[ \prod_{i=A,B,C,D,...} \frac{M_i}{M_{AB}} \right] = T(M_A, M_B, M_C, ..., M_{AB}, n, n_A/n).$$

(28)

An average complexity analysis can then be applied to obtain an estimate for $T$. 

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