The efficiency the Quantum Adiabatic Algorithm

A.P. Young

Talk at MIT, November 1, 2010.

Work supported by
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- QAA study of the hardest problem for WALKSAT: p=3 spin model (XORSAT)
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• Conclusions
Complexity Classes

- **NP**: set of problems which can be verified in polynomial time.
- **P**: set of problems which can be solved in polynomial time on a classical computer.
- **NP-complete**: a set of hard problems. All problems in NP can be mapped into an NP-complete one in polynomial time. Takes an exponentially large time on a classical computer, for worst (and typical?) case.
- **BQP**: set of problems that can be solved in polynomial time on a quantum computer. Integer factoring is in BQP (Shor’s algorithm) but (probably) not in P.
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- **BQP**: set of problems that can be solved in polynomial time on a quantum computer. Integer factoring is in BQP (Shor’s algorithm) but (probably) not in P.

Could a quantum computer solve NP-complete problems in polynomial time (i.e. does BQP contain NP-complete)? If so, would increase importance of building a quantum computer.
The Quantum Adiabatic Algorithm I

Proposed by Farhi et. al to solve hard optimization problems on a quantum computer.

\[ \mathcal{H}(t) = \left[ 1 - \lambda(t) \right] \mathcal{H}_D + \lambda(t) \mathcal{H}_P \]

\( \mathcal{H}_D \) (g.s.) adiabatic? \( \mathcal{H}_P \) (g.s.?)

0 \leq \lambda(t) \leq 1, \quad \lambda(0) = 0, \quad \lambda(\mathcal{T}) = 1

\( \mathcal{T} \) is the running time.
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\( \mathcal{H}_P \) is the problem Hamiltonian, depends on the \( \sigma_i^z \)
\( \mathcal{H}_D \) is the driver Hamiltonian \( = -\hbar \sum \sigma_i^x \)

\( 0 \leq \lambda(t) \leq 1, \quad \lambda(0) = 0, \quad \lambda(T) = 1 \)

\( T \) is the running time
The Quantum Adiabatic Algorithm II

System starts in ground state of driver Hamiltonian. If process is adiabatic (and \( T \to 0 \)), it ends in g.s. of problem Hamiltonian, and problem is solved.

Minimum \( \mathcal{T} \) is the “complexity”.
The Quantum Adiabatic Algorithm II

System starts in ground state of driver Hamiltonian. If process is adiabatic (and $T \to 0$), it ends in g.s. of problem Hamiltonian, and problem is solved.

Minimum $\mathcal{T}$ is the “complexity”.

Is $\mathcal{T}$ exponential or polynomial in the problem size $N$?
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Landau Zener Theory: To stay in the ground state the time needed is proportional to $\Delta E_{\text{min}}^{-2}$.

Using QMC, compute $\Delta E$ for different $\lambda$: $\Delta E_{\text{min}}$.
The Exact Cover Problem

Studied in early numerics and our recent Quantum Monte Carlo simulations. An NP-complete “constraint satisfaction problem”

**N** Ising spins, ±1, pick **M** triplets (“clauses”) at random. A clause is “satisfied” (has zero energy) if two of the spins are up and one is down. Otherwise is “unsatisfied” (has positive energy, “cost”).

Is there an assignment of the bits which satisfies **all** the clauses?

Small **M/N**, (exponentially) many satisfying assignments, Large **M/N**, no satisfying assignments.
The Exact Cover Problem II

Satisfiability transition at (Smelyanskiy et al., Zdeborova et al.)

\[(M/N)_c \approx 0.626 \quad (N \to \infty)\]

For finite \(N\), work close to the “transition”, i.e. point where number of satisfying assignments (SA) drops to 0.

Reasons:

(i) Problem is hard near the transition (Kirkpatrick et al)

(ii) Convenient to study instances with a “unique satisfying assignment” (USA).

(For finite \(N\), the “transition”, and hence the greatest probability of a USA, occurs at \(M/N\) a little above the infinite-\(N\) critical value)

Example of a USA with \(N=7, M=5\) (V. Choi)
Early Simulations

The simplest model for the energy costs:
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\[
\mathcal{H}_P = \sum_{\alpha=1}^{M} \frac{1}{4} \left( \sigma_{\alpha,1}^{z} + \sigma_{\alpha,2}^{z} + \sigma_{\alpha,3}^{z} - 1 \right)^2
\]
Early Simulations

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This is the problem Hamiltonian

Early numerical work (enumerate all states) (Farhi et al.) found

$$T \propto N^2$$

but only for $N \leq 20$
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Polynomial complexity!

But perhaps crossover to exponential at larger $$N$$?

$$2^N$$ basis states. So how can we do much larger sizes?

⇒ Quantum Monte Simulations (classical algorithm; do a **sampling** of the states)
Quantum Monte Carlo: I
(with V. Smelyanskiy and S. Knysh)

In Quantum Monte Carlo (QMC) simulations we can only study equilibrium (possibly time-dependent) quantities.

**Reason:** QMC depends on the correspondence between the time evolution operator in quantum mechanics, $e^{-iHt}$, and the Boltzmann operator in (equilibrium) statistical mechanics, $e^{-\beta H}$. We see that $\beta \equiv 1/T$ is like imaginary time.

One ends up simulating an effective classical Hamiltonian (really an action) in space and imaginary time $\tau$, where $0 \leq \tau < \beta$.

Simplest is to discretize imaginary time into $L_\tau$ “time slices” each of width $\Delta \tau$ where $T^{-1} \equiv \beta = L_\tau / \Delta \tau$.

There are also continuous imaginary time algorithms (Gosset et al., Krzakala et al.).
Time Dependence

We assume that $T$ is sufficiently low that the system is in its ground state, i.e. $T \ll \Delta E \equiv E_1 - E_0$.

In quantum mechanics, correlations between spins at an initial (real) time $t_0$ and a later time $t_0 + t$ have the form

$$C(t) \equiv \frac{1}{N} \sum_{i=1}^{N} \langle \sigma^z_i(t_0) \sigma^z_i(t_0 + t) \rangle = \frac{1}{N} \sum_{i=1}^{N} \left[ \sum_{n} |\langle 0 | \sigma^z_i | n \rangle|^2 \right] e^{i(E_n - E_0)t}.$$ 

In imaginary time, complex exponentials are replaced by real, decaying exponentials

$$C(\tau) = \frac{1}{N} \sum_{i=1}^{N} \left[ \sum_{n} |\langle 0 | \sigma^z_i | n \rangle|^2 \right] e^{-(E_n - E_0)\tau}.$$ 

Hence, at large $\tau$, we have

$$C(\tau) = q + \frac{1}{N} \sum_{i=1}^{N} |\langle 0 | \sigma^z_i | 1 \rangle|^2 e^{-(E_1 - E_0)\tau},$$

where

$$q = \frac{1}{N} \sum_{i=1}^{N} \langle 0 | \sigma^z_i | 0 \rangle^2 = \frac{1}{N} \sum_{i=1}^{N} \langle \sigma^z_i \rangle^2.$$
Sample results for $C(\tau)$

Results for the time dependent correlation function for one instance of Exact Cover with $N = 128$, near the location of the minimum gap. (Vertical axis is logarithmic.) Fitting to the straight line region gives the slope $\Delta E = 0.0354$.

We took $L_\tau = 300$, $\Delta \tau = 1$, so $T^{-1} \equiv \beta = 300$ so $T \ll \Delta E$, as required.

Use “parallel tempering” to speed up equilibration. Simulation is run many times to reduce the noise and get error bars.
Dependence of gap on $\lambda$

Results for the gap to the first excited state $\Delta E$ as a function of the control parameter $\lambda$ for one instance with $N = 64$. The gap has value $2$ ($= 2 \times$ transverse field) for $\lambda = 0$, and value $1$ for $\lambda \to 1$ (lowest excited state has one clause not satisfied). Remember this has a USA so the ground state at $\lambda = 1$ is unique.

There is a minimum gap at an intermediate value of $\lambda$. Compute $\Delta E_{\text{min}}$ for 50 instances for $N = 16, 32, 64, 128, 192, 256$
Size Dependence

We take the median value of the minimum gap among different instances of a given size \( N \) as a measure of the “typical” gap.

A log-log lot of the median minimum gap as a function of \( N \) up to \( N = 64 \), In this range we have a power law variation:

\[
\text{median } \Delta E_{\text{min}} \propto N^{-\mu},
\]

where \( \mu = 0.94 \pm 0.13 \).

Complexity \( \propto N^{2\mu} \) (neglect matrix element effects), so consistent with \( N^2 \) behavior found in early work.

But this behavior does NOT continue for larger sizes because ....
First order Quantum Phase Transition

... the transition becomes discontinuous (1st order).

e.g. the spin glass order parameter

\[ q = \frac{1}{N} \sum_{i=1}^{N} \langle \sigma_i^z \rangle^2 \]

Figure shows one instance for \( N = 128 \).
Note: big jump in ordering, transition far from \( \lambda = 1 \).
We averaged over 50 instances at each size for sizes between 16 and 256.
Sometimes, multiple first order transitions
Fraction First Order

Fraction first order seems to tend to 1 as $N$ tends to infinity.

Instances with a first order transition are expected to have a minimum gap which is exponentially small in $N$ (Amin and Choi, Jörg et al, Altshuler et al).
Can we avoid a 1st order transition?

Path changes (make transverse fields random) (Farhi et al)

Can also make “costs” random.

Work in progress. By taking of order N random fields and costs the probability of a first order transition is reduced. To systematically determine how this varies with N for large N is computationally challenging.

Hence, look for other models, where the crossover to a first order transition occurs for smaller sizes.

Guided by results from a classical, heuristic, algorithm WALKSAT. This is similar in spirit to “simulated annealing”, it flips a bit in an unsatisfied clause, either the one that minimizes the number of unsatisfied clauses, or by choosing one at random, with some relative probability.
WALKSAT (with M. Guidetti)

A classical, heuristic, local-search algorithm.

For all models, the instances have a USA.

“unlocked” 1-in-3 SAT is exact cover, (previous model).

In “locked” instances (Mézard and Zdeborova) each bit is each at least two clauses. As they claimed, these are harder.

But the hardest is 3-regular XORSAT. What is this?
The Hamiltonian of each clause involves the product of \( p \) spins, where we take \( p = 3 \). A clause is satisfied if the product of the spins has a specified value (\(+1\) or \(-1\))

\[
\mathcal{H}_P = \sum_{\alpha=1}^{M} \left( 1 - J_\alpha \sigma_{\alpha,1}^z \sigma_{\alpha,2}^z \sigma_{\alpha,3}^z \right), \quad \text{where} \quad J_\alpha = \pm 1.
\]

We take \( M \) (no. of clauses) = \( N \) (no. of bits).

Also each bit is in exactly three clauses (3-reg. XORSAT).

This is precisely at the satisfiability threshold (Jörg et al. 2009).

There is a finite probability (28\%) of a unique satisfying assignment (USA). We take these instances.

For USA instances, the sign of the \( J_\alpha \) can be “gauged away” so we take all \( J_\alpha = 1 \). The USA then has all \( \sigma_i^z = 1 \) (ferromagnet).
XORSAT II

In terms of bits \( z_i = (1 - \sigma_i^2)/2 \),

\[ z_{\alpha,1} + z_{\alpha,2} + z_{\alpha,3} = v_\alpha \pmod{2} \]

where \( v_\alpha = 1 \) or 0

i.e.

\[ A z = v, \pmod{2} \]

where \( A_{\alpha i} = 1 \) if bit \( i \) is in clause \( \alpha \) and is 0 otherwise.

Here all the \( v_\alpha = 0 \), and the USA is all \( z_i = 0 \).

This is “trivial” and yet it is very hard for WALKSAT to find it.

Even for non-zero \( v_\alpha \), the linear equations can be solved in polynomial time using Gaussian elimination to see whether there is a solution. Hence the satisfiability problem is in \( P \) but this doesn’t help the algorithms, which find this problem very hard.

Now let’s see how the QAA fares (Jörg et al, 2009)

\[ \mathcal{H}(s) = (1 - s) \sum_{i=1}^{N} \left( 1 - \sigma_i^{z_1} \right) + s \sum_{\alpha=1}^{M} \left( 1 - \sigma_{\alpha,1}^{z} \sigma_{\alpha,2}^{z} \sigma_{\alpha,3}^{z} \right) \]
Curves are very close to symmetric about $s = 1/2$. There is an exact duality $\mathcal{H}(s) = \mathcal{H}^{\text{Dual}}(1 - s)$ where the dual lattice interchanges the clauses and bits (is a different member of the ensemble), see the “factor graph” above.
XORSAT Results II (diagonalization)

3-reg XORSAT

Red triangles: minimum gap decreases exponentially. (Agrees with Jörg et al.)

In the other data: Green: make fields, and Brown: make fields and costs, ...

Random.

Doesn’t seem to help.

With diagonalization one can include terms which would give minus sign problems in QMC, “non-stoquastic” (Bravyi et al.)

So far, not found an escape from the 1st order transition.
Conclusions

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Thank You