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HARVARD UNIVERSITY
Department of Chemistry and Chemical Biology

Sombrero Adiabatic Quantum Computation: a heuristic strategy for quantum adiabatic evolution

UNIVERSITY OF OXFORD

Workshop on Complexity Resources in Physical Computation
Oxford University Computing Laboratory

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Agenda

1. Contribution.
2. Motivations.
3. NP-complete problems.
4. Basics of quantum adiabatic algorithms.
5. Results.

Contribution

A numerical study on the impact of initial condition heuristics in quantum adiabatic algorithms for NP-complete problems.

This presentation is based on:

Sombrero Adiabatic Quantum Computation… by
A.Perdomo, S.E. Venegas-Andraca, and A. Aspuru-Guzik
arXiv:0807.0354

Motivation (Perdomo, Venegas-Andraca and Aspuru-Guzik)

Computers play a key role in modern society for its potential usefulness in solving problems from different areas of science and engineering.

Initial conditions play a central role in algorithm development/execution. Whether we choose random initial conditions or not depends on our expertise on the particular application field.

Acquiring as much knowledge in advance as possible could be crucial in algorithm execution time.

Motivation (myself)

I am a computer scientist and an engineer. I am thus equally interested in theoretical and applied research, as well as in technology implementation.

My experience as engineer/computer practitioner is that wise (i.e. educated) choices on algorithm initial conditions usually leads to less computer power consumption.

Motivation (my group)

My research group in Mexico is focusing on quantum algorithms simulation on desktop and distributed computer platforms. The numerical simulation algorithms coded for this paper were a nice contribution to my group's expertise.

We are currently working with Google and IBM in order to simulate quantum algorithms in their computer cloud.

Examples of the importance of initial conditions in applied computer science follow:

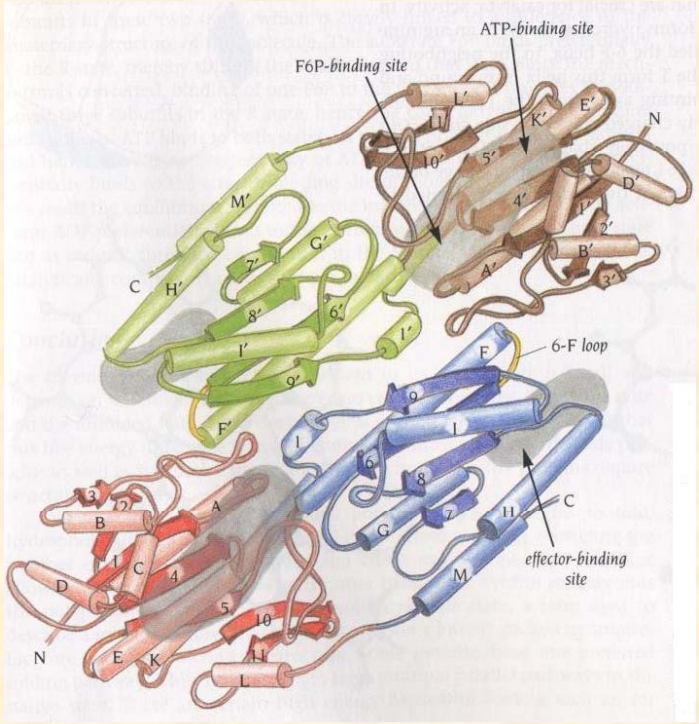
Image segmentation and Image recognition

Oh, Lenna, dear Lenna… ☺

http://computervision.wikia.com/wiki/Lenna

The Protein Folding Problem: Nature's lecture on Optimization methods

Given the amino acid sequence of a protein, predict its compact three-dimensional native state



Schematic diagram of a globular protein.
Introduction to Protein Structure.
C. Branden and J. Tooze.
Taylor and Francis (1999).

The Protein Folding problem is a key challenge in modern science, for both its intrinsic importance in the foundations of biological science and its applications in medicine, agriculture, and many other areas.

NP-complete problems

1. **Two equivalent ways** to define an NP-complete problem:

- A problem that can be solved in polynomial time in a nondeterministic Turing machine.

- A problem for which any proposed solution can be checked in polynomial time by a Turing machine.

2. **Solving NP-complete problems** is crucial for both theoretical and application purposes.

K-SAT, a most important NP-complete Problem

The K-SAT problem plays a most important role in the Theory of Computation (NP complete problem). The setup of the K-SAT problem is as follows

- Let B={x_1, x_2, …, x_n} be a set of Boolean variables.
- Let C_i be a disjunction of k elements of B
- Finally, let F be a conjunction of m clauses C_i.

Question: Is there an assignment of Boolean variables in F that satisfies all clauses simultaneously, i.e. F=1?

Example. Instance of 3-SAT

$$F = (x_1 \vee \bar{x}_2 \vee \bar{x}_3) \wedge (\bar{x}_1 \vee \bar{x}_4 \vee \bar{x}_2) \wedge (x_3 \vee x_4 \vee x_7) \wedge (x_3 \vee \bar{x}_5 \vee \bar{x}_6)$$

Quantum Adiabatic Algorithms

Quantum adiabatic algorithms (1/6)

The quantum adiabatic model of computation was originally proposed by E. Farhi, J. Goldstone, S. Gutmann and M. Sipser, and has the following characteristics:

Quantum adiabatic algorithms (2/6)

The main idea behind quantum adiabatic algorithms is to employ the Schrödinger equation:

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

with a specific structure for the Hamiltonian.

Quantum adiabatic algorithms (3/6)

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

where

$$\hat{H}(t) = \left(1 - \frac{t}{T}\right)\hat{H}_b + \frac{t}{T}\hat{H}_p$$

T is the total running time of the quantum algorithm

This is the initial Hamiltonian, which has a **unique and easy to prepare** ground state.

This is the final Hamiltonian, which **encodes** in its ground state the solution to the problem under study.

Quantum adiabatic algorithms (4/6)

The rationale behind an adiabatic quantum algorithm is:

1. Start with an initial Hamiltonian $\hat{H}_b$ that has

   i) an <u>easy to prepare</u> and <u>unique</u> ground state $|\psi(0)\rangle$

   ii) Different eigenvalues $E_o < E_1 < \ldots < E_n$

2. Evolve the system slowly.
   By doing this evolution **<u>sufficiently slowly</u>**, the quantum adiabatic theorem allows us to predict that the system will stay in the ground state of its Hamiltonian

$$\hat{H}(t)$$

for all the computing time $t \in [0,T]$

Quantum adiabatic algorithms (5/6)

3. If we let the system run for sufficiently long time T, the quantum adiabatic algorithm allows us to predict that, when measuring the state of the system described by

$$\hat{H}(t)$$

We shall be very close to the ground state of the Hamiltonian

$$\hat{H}_p$$

which, by definition, has the solution to the problem encoded in its ground state!

Quantum adiabatic algorithms (6/6)

For how long should we run the quantum adiabatic computer?

$$T >> \frac{\varepsilon}{g_{\min}^2}$$

where

$$g_{\min}^2 = \min_{0 \le t/T \le 1} \left(E_1(t/T) - E_0(t/T) \right)^2$$

Sombrero Adiabatic Quantum Computation (1/7)

A. Perdomo, S.E. Venegas-Andraca and A. Aspuru-Guzik (2008)

We diverge from the conventional idea of starting quantum adiabatic algorithms with a uniform superposition state.

Instead, our proposed algorithm, named Sombrero Adiabatic Quantum Computation (sombrero-AQC) **starts with an initial guess that can be chosen at will or following intuition about the problem**.

We provide a proof of concept for sombrero-AQC and the potential usefulness of starting with a guess state for the adiabatic evolution by performing an exhaustive numerical study on hard-to-satisfy six and seven variable instances of the 3-SAT problem, and comparing our results with the conventional AQC approach.

Sombrero Adiabatic Quantum Computation (2/7)

Why starting with an initial guess instead of uniform superposition?

In addition to random choices for the initial guess (a good idea if less computational power is to be invested), there are many ways to make an educated guess of a solution:

1) One could use physical intuition or constraints imposed in the problem, e. g., in a lattice model for protein folding an educated guess would be to start with an amino acid configuration such that there are not two amino acids on top of each other and that they are connected according to the primary amino acid sequence that defines the protein.

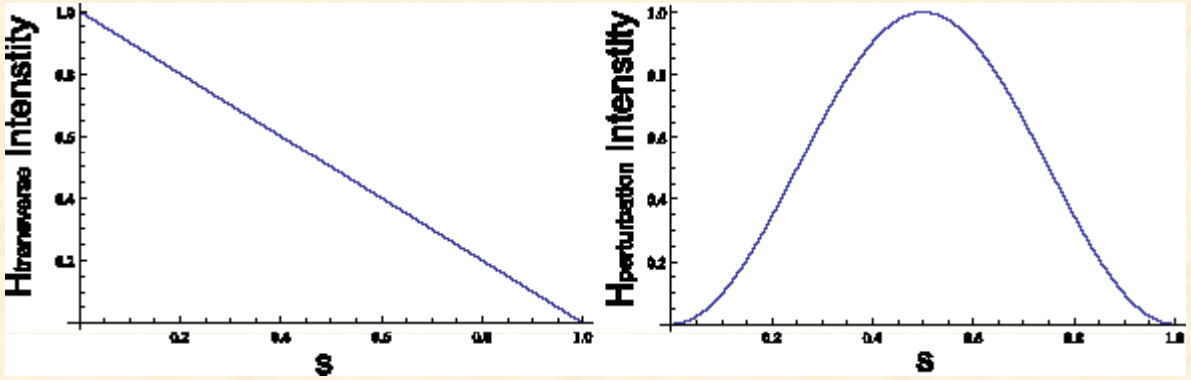
2) One might use classical methods to estimate an approximate solution or use for example a mean field approach to find an approximate solution to be used as the educated guess.

Sombrero Adiabatic Quantum Computation (3/7)

For the adiabatic evolution in a conventional-AQC algorithm, one connects through a linear ramp an initial Hamiltonian with the final Hamiltonian whose ground state encodes the solution to the problem. For sombrero AQC, the time-dependent Hamiltonian can be written as

$$\hat{H}_{sombrero}(t) = \left(1 - \frac{t}{T}\right)\hat{H}_i + hat\left(\frac{t}{T}\right)\hat{H}\ perturbation + \frac{t}{T}\hat{H}_f$$

Where the hat function may have the form:



1-t/T

t/T(1-t/T)

The hat function must turn off the perturbation Hamiltonian at t=0 and t=T.

Sombrero Adiabatic Quantum Computation (4/7)

$$\hat{H}_{sombrero}(t) = \left(1 - \frac{t}{T}\right)\hat{H}_i + \delta \; hat\left(\frac{t}{T}\right)\hat{H}\; perturbation + \frac{t}{T}\hat{H}_f$$

Intensity transverse field

Built using operators of the form $\hat{\sigma}_x$

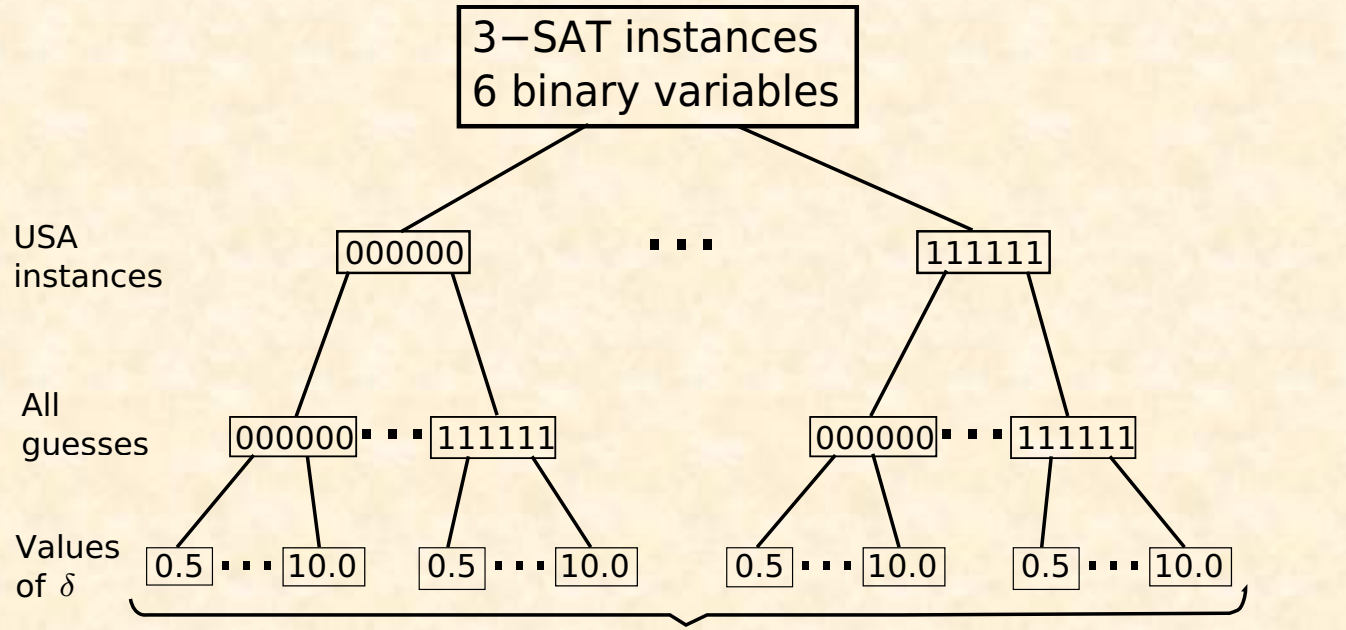
Built using operators of the form

$$\frac{1}{2}(\hat{I} - \hat{\sigma}_x)$$

Built using operators of the form

$$\frac{1}{2}(\hat{I} - \hat{\sigma}_z)$$

Sombrero Adiabatic Quantum Computation (5/7)



We generated 2^6 3-SAT unique satisfying assignment instances, each having as its only solution one of the 2^6 possible assignments. All 2^6 instances have a different state as solution. The same applies to our study on 2^7 3-SAT unique satisfying assignment instances.

Sombrero Adiabatic Quantum Computation (6/7)

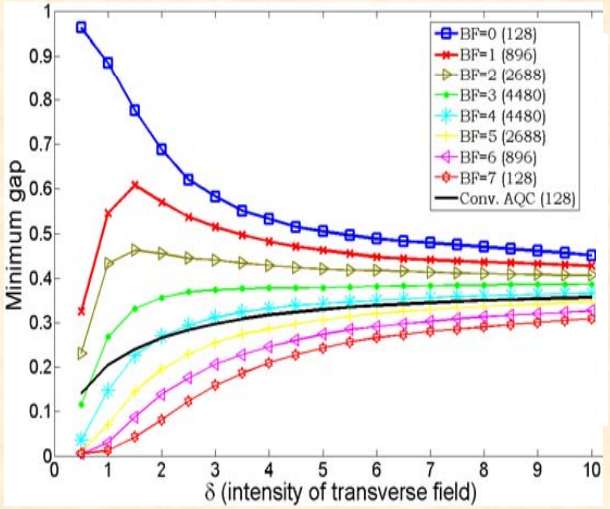
$$\hat{H}_{sombrero}(t) = \left(1 - \frac{t}{T}\right)\hat{H}_i + \delta \quad hat\left(\frac{t}{T}\right)\hat{H}\ perturbation + \frac{t}{T}\hat{H}_f$$

We then built 2^6 different sombrero Hamiltonians, one for each possible initial condition, per 3-SAT clause, and executed a simulation of a quantum adiabatic algorithm.

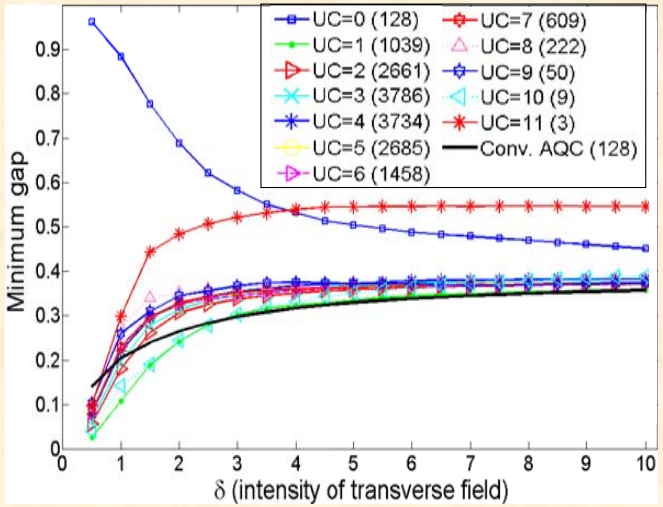
We focused on the numerical values of the gap between the ground state and the first excited state. Results follow.

Sombrero Adiabatic Quantum Computation (7/7)

Mind the gap!



(a)



(b)

Summary of the 327,680 calculations for 7 variable 3SAT instances of minimum-gap median values as function of the transverse field intensity within groups sorted by number of bit ips (BF) [(a)] and number of unsatised clauses (UC) [(b)]. Plots include the 128 calculations using conventional-AQC (Eq. 2).

Focus on:

- Better values than Conventional OAC.
- Random initial conditions.
- Role of transverse field intensity.

Self-criticism and future research directions

1. 3-SAT is not the best choice for a study on initial conditions. We chose 3SAT because this is one of the most studied NP-complete problems. Farhi et al and Van Dam et al have studied it under the light of quantum adiabatic algorithms.

   Thus, next steps include research on TSP and protein Folding.

2. Sufficient conditions for full adiabaticity are still under study. We only focused on minimum gap.

3. In future research efforts, we shall study other adiabaticity conditions (for example, whether epsilon truly scales polinomially wrt input size).