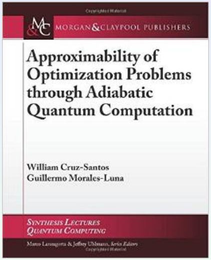
Solving NP-hard combinatorial optimization problems with adiabatic quantum computing

Guillermo Morales Luna

Departamento de Computación, Cinvestav-IPN, México, D. F.



January 13, 2015

1. INTRODUCTION
2. AQC
   - Adiabatic evolution
   - QC by adiabatic evolution
3. SOLVING NP-HARD OPTIMIZATION PROBLEMS
   - The classical Ising model
   - Reduction to quadratic pseudo-Boolean maps
4. AQ FORMULATION OF GRAPH PROBLEMS
   - Construction of the ending Hamiltonian
   - Construction of the initial Hamiltonian

Abstract

A construction of a Hamiltonian path that allows the treatment of quadratic pseudo-Boolean optimization with Adiabatic Quantum Computing is introduced.

Any NP-hard optimization problem can be solved by reducing it to the *Maximum Independent Set* problem, then through the equivalent formulation of quadratic Boolean maps optimization by slowly evolving the corresponding quantum system in an adiabatic processing.

Adiabatic Quantum Computing (AQC) was introduced to solve optimization problems based on the Adiabatic Theorem.

Two Hamiltonian operators are constructed: an initial Hamiltonian H_0 and an ending Hamiltonian H_1, such that the ground states of H_0 are easily calculated, and the ground states of H_1 codify solutions of the given optimization problem.

If the time evolution of the quantum system is large enough, then the system remains close to its instantaneous ground state.

The ending Hamiltonian H_1 is prepared so that its energy function corresponds to the goal objective function.

DECISION PROBLEM

Consists of a domain set and a partition of this set into two subsets, the Yes-instances and the No-instances: Given an instance, it is required to decide whether it is a Yes-instance.

SEARCH PROBLEM

Consists of a domain set and a solution set: Given a domain instance it is required to find, to locate or to build a corresponding companion in the solution set.

Each search problem has a decision version: Given a pair

(instance , possible_solution)

it is required to decide whether the possible_solution is indeed a solution.

OPTIMIZATION PROBLEM

Consists of a domain set, a feasible solution set, an objective map and a goal which is either maximization or minimization: Given a domain instance it is required to find the corresponding feasible solution that maximizes or minimizes (according to the goal) the objective map.

Without loss of generality, it can be assumed that the goal is always to minimize.

Each optimization problem poses a corresponding search problem: Given a domain instance and a threshold, it is required to find a corresponding feasible solution whose value at the objective map is below the given threshold.

Let $\mathbb{H}_1 = \mathbb{C}^2$ be the 2-dimensional complex Hilbert space.

Let, for each $n > 1$, $\mathbb{H}_n = \mathbb{H}_{n-1} \otimes \mathbb{H}_1$. It is the 2^n-dimensional complex Hilbert space.

Let $H : \mathbb{R} \to \mathrm{GL}(\mathbb{H}_n)$ be a time dependent Hamiltonian operator.

The differentiable transformation $\mathbf{x} : \mathbb{R} \to \mathbb{H}_n$ is a solution of the Schrödinger equation in the interval $I \subset \mathbb{R}$ if

$$\forall t \in I : i\frac{d}{dt}\mathbf{x}(t) = H(t)\mathbf{x}(t). \tag{1}$$

Let $J \subset \mathbb{R}$ be an interval and let $\tau : J \to I$, $s \mapsto t = as + b$.

Let $G : J \to \mathrm{GL}(\mathbb{H}_n)$, $s \mapsto G(s) = aH(\tau(s))$.

If $\mathbf{x} : \mathbb{R} \to \mathbb{H}_n$ is a solution of (1),

$$\forall s \in J : i\frac{d}{dt}\mathbf{x}(\tau(s)) = G(s)\mathbf{x}(\tau(s))$$

hence $\mathbf{x} \circ \tau$ is a solution of the Schrödinger equation in J for the Hamiltonian $G = a\,H \circ \tau$.

G: continuous path in the space of Hermitian operators on $\mathbb{H}_n$.

Suppose $J_{t_0} = [0, t_0]$ and $I = [0, 1]$.

The affine transformation is $s \mapsto as + b = \frac{s}{t_0}$ and the Hamiltonian on J_{t_0} is $H_{t_0}(s) = \frac{1}{t_0} H(\frac{s}{t_0})$.

Let $\mathbf{x}_{t_0} : J_{t_0} \to \mathbb{H}_n$ be a solution of

$$\forall s \in J_{t_0} : i \frac{d}{dt} \mathbf{x}_{t_0}(s) = H_{t_0}(s) \mathbf{x}_{t_0}(s). \tag{2}$$

Let $\{\lambda_0, \ldots, \lambda_{2^n-1}\} \subset \mathbb{R}^I$ be the spectrum of the Hamiltonian H. Then $\forall j \in [\![0, 2^n - 1]\!]$

$$\exists \mathbf{y}_j \in \mathbb{H}_n^I \, \forall t \in I : \; H(t)\mathbf{y}_j(t) = \lambda_j \mathbf{y}_j(t) \text{ with } \|\mathbf{y}_j(t)\| = 1.$$

Each $\mathbf{y}_j(t)$ is an instantaneous eigenstate of $H(t)$ with corresponding energy λ_j.

Let us enumerate the eigenvalues paths

$$\forall t \in I: \; \lambda_0(t) \leq \cdots \leq \lambda_{2^n-1}(t).$$

The path $(\mathbf{y}_0(t))_{t\in[0,1]}$ has extreme points $\mathbf{y}_0(0), \mathbf{y}_0(1)$.

Let us consider $\mathbb{H}_n \to \mathbb{C}$, $\mathbf{z} \mapsto \langle \mathbf{y}_0(1)|\mathbf{z}\rangle$.

If $\lambda_1(t) - \lambda_0(t) > 0$ for all $t \in [0,1]$ then, the Adiabatic Theorem asserts:

$$\lim_{t_0 \to +\infty} |\langle \mathbf{y}_0(1)|\mathbf{x}_{t_0}(t_0)\rangle| = 1.$$

Indeed, an upper-bound for the required time to satisfy the Adiabatic Theorem is:

$$T \geq \frac{\Delta_{\max}}{\epsilon \delta_{\min}^2}$$

where

$$\delta_{\min} = \min_{0 \leq t \leq 1} (\lambda_1(t) - \lambda_0(t))$$

$$\Delta_{\max} = \max \| \frac{d}{dt} H(t) \|$$

and $\epsilon \in [0, 1]$ is the approximation ratio to the ground state of H.

The steps of an AQC algorithm are the following:

1. Prepare the quantum system in the ground state (which is known and easy to prepare) of the initial Hamiltonian H_0.
2. Encode the solution of the posed optimization problem into the ground state of an ending Hamiltonian H_1.
3. Evolve slowly enough satisfying the Adiabatic Theorem with $H(t) = (1 - \frac{t}{T})H_0 + \frac{t}{T}H_1$ for a total time T. The final state $\mathbf{x}(t)$ at time $t = T$ will be (very close) to the ground state of H_1.
4. Perform a measurement of the state $\mathbf{x}(t)$ at time $t = T$. With high probability the optimal solution of the optimization problem will be found.

Let $G = (V, E)$ be a graph, $E \subset V^{(2)}$.

Let $\mathbb{S} = \{-1, +1\}$ be the set of signs.

An assignment is a map $\sigma : V \to \mathbb{S}$.

An edge weight map is of the form $e : E \to \mathbb{R}$ and a vertex weight map is of the form $w : V \to \mathbb{R}$.

Let us enumerate $V = (v_i)_{i=0}^{n-1}$, thus there are 2^n assignments.

For respective edge and vertex weight e, w, let $e_{ij} = e(v_i, v_j)$ and $w_i = w(v_i)$.

For an assignment σ, its energy is

$$\eta(e, w; \sigma) = -\sum_{\{v_i, v_j\} \in E} e_{ij}\sigma(v_i)\sigma(v_j) - \sum_{v_k \in V} w_k \sigma(v_k). \tag{3}$$

An assignment with minimum energy is a ground state.

For $\beta > 0$, let

$$\phi(e, w, \beta; \cdot) : \sigma \mapsto \phi(e, w, \beta; \sigma) = \exp\left(-\beta\, \eta(e, w; \sigma)\right).$$

Let $\Phi(e, w, \beta) = \sum\{\phi(e, w, \beta; \sigma) |\ \sigma$ is an assignment$\}$.

A probability density results:

$$\pi(e, w, \beta; \cdot) : \sigma \mapsto \frac{\phi(e, w, \beta; \sigma)}{\Phi(e, w, \beta)}.$$

From (3), if the vertex weight w is null then the energy map is "even":

$$\forall \text{ assignment } \sigma : \quad \eta(e, 0; \sigma) = \eta(e, 0; -\sigma).$$

For an assignment σ let $\mathrm{Spt}\,(\sigma) = \{v \in V \mid \sigma(v) = +1\}$.

A 2-partition of V is a collection $\{U, V - U\}$ such that $U \subseteq V$.

Clearly $\sigma \leftrightarrow \{\mathrm{Spt}\,(\sigma)\,, V - \mathrm{Spt}\,(\sigma)\}$ is a bijective correspondence among assignments and 2-partitions of V.

For any set $U \subseteq V$, let

$$c(U) = \{e \in E | \ \mathrm{card}\,(e \cap U) = 1 \ \& \ \mathrm{card}\,(e \cap (V - U)) = 1\} \quad (4)$$

be the collection of edges with an extreme in U and the other in its complement. Since an assignment is an $\mathbb{S}$-valued map:

$$\begin{aligned} \forall \text{ assignment } \sigma : \quad \eta(e, 0; \sigma) &= -\sum_{\{v_i, v_j\} \in E} e_{ij} + 2 \sum_{\{v_i, v_j\} \in c(\mathrm{Spt}(\sigma))} e_{ij} \\ &=: \eta_s(e; \mathrm{Spt}\,(\sigma)). \end{aligned} \quad (5)$$

Let us introduce the following problem:

MINIMUM WEIGHT CUT

Instance: A graph $G = (V, E)$ and an edge weighting map $e : E \to \mathbb{R}^+$.
Solution: A partition $\{U, V - U\}$ of the vertex set V such that $c(U)$, as defined by (4), is minimum.

Clearly, this problem is equivalent to minimize the energy operator $\eta(e, 0; \cdot)$ as defined by (3), or equivalently to find a vertex set U which minimizes $\eta_s(e; U)$ as defined by (5).

Let $X = \{x_i : 0 \leq i \leq n-1\}$ be a set of n Boolean variables.

Let $Q = \{0, 1\}$ be the set of the integer values 0 and 1.

A Boolean function on n variables is a map from Q^n into Q^n, where n is a positive integer and Q^n denotes the n-fold Cartesian product of Q with itself.

A pseudo-Boolean map of n variables is a function $f : Q^n \to \mathbb{R}$, where n is a positive integer.

The pseudo-Boolean maps are expressed as multilinear polynomials.

Of particular interest are the quadratic pseudo-Boolean maps $f_{ue} : Q^n \to \mathbb{R}$ (i.e., $\deg(f_{ue}) \leq 2$) expressed as

$$f_{ue}(X) = \sum_{i \in [\![0,n-1]\!]} u_j x_j + \sum_{\{i,j\} \in [\![0,n-1]\!]^{(2)}} e_{ij} x_i x_j,$$

for some $u \in \mathbb{R}^n$ and $e \in \mathbb{R}^{\frac{n(n-1)}{2}}$.

For instance, given a graph $G = (V, E)$, with $V = [\![0, n-1]\!]$ and $E \subseteq [\![0, n-1]\!]^{(2)}$, let

$$f_G = \sum_{j \in [\![0,n-1]\!]} x_j - \sum_{\{i,j\} \in E} x_i x_j. \tag{6}$$

An independent vertex subset of a graph G is a subset of V such that no two vertexes in the subset represent an edge of G.

The optimization version of the Maximum Independent vertex Subset (MIS) problem consists in finding an independent vertex subset of maximal cardinality.

It is an NP-hard optimization problem.

REMARK

Finding a maximal independent vertex subset in G is equivalent to maximize the map $f_G(X)$ over the hypercube Q^n.

Also, quadratic maps can be considered over the *n*-fold Cartesian power of the set $\mathbb{S} = \{-1, +1\}$. In fact

PROPOSITION

Any maximization problem of a quadratic pseudo-Boolean map over the hypercube Q^n is equivalent to a minimization problem of a quadratic map over the power $\mathbb{S}^n$. In symbols:

$\forall e \in \mathbb{R}^{\frac{n(n-1)}{2}}, u \in \mathbb{R}^n \ \exists \varepsilon \in Q^n :$

$$\varepsilon = \arg\max_{Q^n} f_{ue}(X) \ \Leftrightarrow \ \theta(\varepsilon) = \arg\min_{Q^n} f_{ue}(X).$$

Proposition (Boros & Hammer)

Every pseudo-Boolean function f over n Boolean variables can be reduced in linear time, w.r.t. size(f), to a quadratic pseudo-Boolean function f_{ue} in m variables, with size polynomially bounded w.r.t. size(f), and such that

$$\min_{y \in Q^n} f_{ue}(y) = \min_{x \in Q^m} f(x).$$

In this section we show the construction of the ending and initial Hamiltonian operators for AQC.

The ending Hamiltonian is constructed such that it is diagonal in the computational basis, and whose energy function corresponds to a quadratic pseudo-Boolean function.

On the other hand, the initial Hamiltonian is constructed such that it is diagonal in the Hadamard basis, and whose ground state is a uniform superposition of all basis vectors.

Finally, the Hamiltonian path for AQC is stated.

The Pauli transforms $\sigma_x, \sigma_z : \mathbb{H}_1 \to \mathbb{H}_1$, with respect to the canonical basis, are

$$\sigma_x = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \quad , \quad \sigma_z = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}.$$

For any bit $\delta \in \{0, 1\}$, let $\tau_{\delta z} = \frac{1}{2}(I_2 - (-1)^\delta \sigma_z)$.

Independently of δ, the characteristic polynomial of $\tau_{\delta z}$ is $p_z(\lambda) = (\lambda - 1)\lambda$ and its eigenvalues are 0 and 1 with unit eigenvectors $|0\rangle$ and $|1\rangle$, respectively.

The correspondence among eigenvalues and eigenvector is:

$$\forall \varepsilon \in Q : \quad \tau_{\delta z} \left| \varepsilon \right\rangle = (\delta \oplus \varepsilon) \left| \varepsilon \right\rangle .$$

For any $\delta \in \{0, 1\}$ and $j \in [\![0, n-1]\!]$ let

$$R_{E\delta jn} = \bigotimes_{\nu=0}^{n-1} s_\nu : \mathbb{H}_n \to \mathbb{H}_n,$$

where $s_\nu = \tau_{\delta z}$ if $\nu = j$ and $s_\nu = I_2$ otherwise. In other words, $R_{E\delta jn}$ applies the transform $\tau_{\delta z}$ at the j-th qubit of any n-quregister in $\mathbb{H}_n$. Consequently,

$$\forall \varepsilon \in Q^n \ : \ R_{E\delta jn} \left| \varepsilon \right\rangle = (\delta \oplus \varepsilon_j) \left| \varepsilon \right\rangle . \tag{7}$$

Let $G = (V, E)$ be a graph with vertex set $V = [\![0, n-1]\!]$ and edge set $E \subseteq [\![0, n-1]\!]^{(2)}$.

Given a vertex weight map $w : V \to \mathbb{R}$ and $\delta \in \{0, 1\}$, let:

$$H_w : \mathbb{H}_n \to \mathbb{H}_n \ , \ H_w = \sum_{j \in [\![0,n-1]\!]} w_j R_{E\delta jn}, \tag{8}$$

such that

$$\forall \varepsilon \in Q^n \ : \ H_w \left|\varepsilon\right\rangle = \left(\sum_{j \in [\![0,n-1]\!]} w_j (\delta \oplus \varepsilon_j) \right) \left|\varepsilon\right\rangle . \tag{9}$$

Similarly, given an edge weight map $e : E \to \mathbb{R}$, let us consider

$$H_e : \mathbb{H}_n \to \mathbb{H}_n \ , \ H_e = \sum_{\{i,j\} \in E} e_{ij} R_{E\delta in} \circ R_{E\delta jn}. \tag{10}$$

From equation (7) it is satisfied that

$$\forall \varepsilon \in Q^n \ : \ H_e \left| \varepsilon \right\rangle = \left(\sum_{\{i,j\} \in E} e_{ij} (\delta \oplus \varepsilon_i)(\delta \oplus \varepsilon_j) \right) \left| \varepsilon \right\rangle \tag{11}$$

Using (8) and (10), let us define the operator

$$H_{we} : \mathbb{H}_n \to \mathbb{H}_n \ , \ H_{we} = H_w + H_e \tag{12}$$

and from equation (9) and (11) it follows that $\forall\varepsilon \in Q^n$:

$$H_{we}\left|\varepsilon\right\rangle = \left(\sum_{j\in[\![0,n-1]\!]} w_j(\delta\oplus\varepsilon_j) + \sum_{\{i,j\}\in E} e_{ij}(\delta\oplus\varepsilon_i)(\delta\oplus\varepsilon_j)\right)\left|\varepsilon\right\rangle \tag{13}$$

The expression enclosed by the greatest parentheses at (13) corresponds to a quadratic pseudo-Boolean map, and the ground states of the Hamiltonian H_{we} correspond to those points at Q^n minimizing the former quadratic form.

The Pauli transform σ_x has eigenvalues $+1, -1$ with respective eigenvectors $c_0 = W|0\rangle$ and $c_1 = W|1\rangle$, where W is the Hadamard transform:

$$W = \frac{1}{\sqrt{2}}\begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}.$$

Let $(c_\varepsilon)_{\varepsilon\in Q^n}$ be the Hadamard basis, $\forall\varepsilon \in Q^n : c_\varepsilon = \bigotimes_{j=1}^n c_{\varepsilon_j}$.

For any bit $\delta \in \{0, 1\}$, let $\tau_{\delta x} = \frac{1}{2}(I_2 - (-1)^\delta \sigma_x)$.

Independently of δ, the characteristic polynomial of $\tau_{\delta x}$ is $p_x(\lambda) = \lambda(\lambda - 1)$ and its eigenvalues are 0 and 1 with respective eigenvectors c_0 and c_1.

The correspondence among eigenvalues and eigenvectors is determined by δ:

$$\forall \varepsilon \in Q,\ \tau_{\delta x} c_\varepsilon = ((1 - \delta) \oplus \varepsilon) c_\varepsilon.$$

For any index $j \in [\![0, n-1]\!]$ and $\delta \in \{0, 1\}$ let

$$R_{Z\delta jn} = \bigotimes_{\nu=0}^{n-1} r_\nu : \mathbb{H}_n \to \mathbb{H}_n,$$

where $r_\nu = \tau_{\delta x}$ if $\nu = j$ and $r_\nu = I_2$ otherwise. In other words, $R_{Z\delta jn}$ applies the transform $\tau_{\delta x}$ at the j-th qubit of any n-quregister in $\mathbb{H}_n$.

Consequently,

$$\forall \varepsilon \in Q^n \ : \ R_{Z\delta jn} c_\varepsilon = ((1-\delta) \oplus \varepsilon_j) c_\varepsilon. \tag{14}$$

Given a vertex weighting map $h : V \to \mathbb{R}$, let us introduce the operator

$$H_h : \mathbb{H}_n \to \mathbb{H}_n \;,\; H_h = \sum_{j \in [\![0,n-1]\!]} h_j R_{Z\delta jn}.$$

From eq. (14), $\forall \varepsilon \in Q^n$:

$$H_h c_\varepsilon = \left(\sum_{j \in [\![0,n-1]\!]} ((1-\delta) \oplus \varepsilon_j) h_j \right) c_\varepsilon .$$

The ground state of H_h is $x_0 = \frac{1}{2^{\frac{n}{2}}} \sum_{\varepsilon \in Q^n} |\varepsilon\rangle$ with corresponding eigenvalue equal to 0.

The problem of finding the ground state of the operator H_{we} given at eq. (12) can be approximated by adiabatic evolution with the following path operator:

$$H_t = \left(1 - \frac{t}{T}\right) H_h + \frac{t}{T} H_{we}$$

for some large enough $T \in \mathbb{R}^+$.

Thanks for your kind attention!!

Questions?

gmorales@cs.cinvestav.mx
http://delta.cs.cinvestav.mx/~gmorales