Hybrid quantum-classical algorithms for solving optimization problems

Davide Pastorello

Department of Mathematics, University of Trento

Workshop *Quantum Computing and High Performance Computing*
CINECA, 19 Dec 2019

Premise

A general goal to reach

Given an optimization problem, we need to represent it into a quantum hardware in order to efficiently solve it.

A general issue to face

The problem encoding can be computationally hard with deleterious effects on efficiency.

Premise

A general goal to reach

Given an optimization problem, we need to represent it into a quantum hardware in order to efficiently solve it.

A general issue to face

The problem encoding can be computationally hard with deleterious effects on efficiency.

A hybrid quantum-classical approach

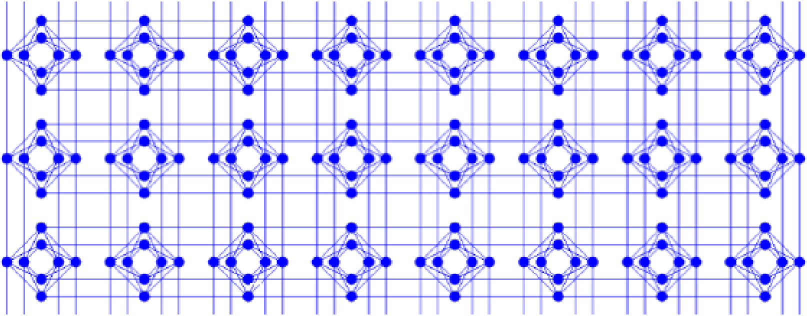
Repeated calls of the quantum machine within a classical iterative structure to represent optimization problems into a quantum hardware exploiting the quantum resource itself.

Quantum Annealing

Quantum Annealers

The hardware is a *quantum spin glass*, i.e. a collection of qubits arranged in the vertices of a graph (V, E) where edges represent the interactions between neighbors.

Example: *D-Wave Chimera topology*



Quantum Annealing

Annealing process (annealing time $20\mu s$)

By energy dissipation the quantum system evolves in the **ground state** (the less energetic state) corresponding to the **solution** of a given optimization problem.

Ising Hamiltonian

$$H(\theta) = \theta_0 + \sum_{i \in V} \theta_i \sigma_z^{(i)} + \sum_{(i,j) \in E} \theta_{ij} \sigma_z^{(i)} \sigma_z^{(j)}$$

where $\sigma_z^{(i)} = \mathbb{I} \otimes \cdots \otimes \sigma_z \otimes \cdots \otimes \mathbb{I}$ and $\theta_0, \theta_i, \theta_{ij} \in \mathbb{R}$ (the **weights**)

Minimization (w.r.t. $\boldsymbol{z}$) of the function:

$$E(\theta, \boldsymbol{z}) = \theta_0 + \sum_{i \in V} \theta_i \sigma_z^{(i)} + \sum_{(i,j) \in E} \theta_{ij} \sigma_z^{(i)} \sigma_z^{(j)} \qquad \boldsymbol{z} \in \{-1, 1\}^{|V|}\ ,\ \theta_0, \theta_i, \theta_{ij} \in \mathbb{R}$$

Quantum Annealing

Main limitation of quantum annealers?

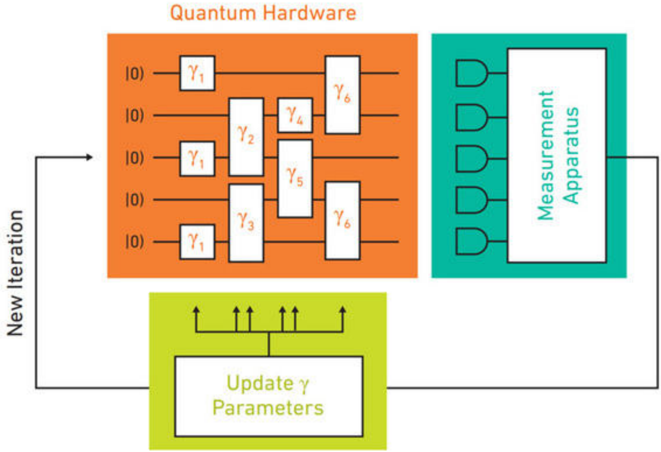
The cost of the problem embedding into a graph with low connectivity may destroy the computational speed up!

The quality of the embedding has strong effects on performances...

Possible solutions

- Improvement of the hardware;
- Formulation of efficient problem encodings;
- Hybrid quantum/classical algorithms.

The hybrid paradigm of QC



Hybrid approach to QA

[D.P., E. Blanzieri. *Quantum Information Processing* 18: 303 (2019)]

Tabu search

A local search in the solution space where worse candidate solutions can be sometimes accepted and already-visited solutions are penalized.

Tabu search with a quantum annealer

- Generation of candidate solutions by quantum annealing;
- Energetic penalization of a set of quantum states:

Let $\{\mathbf{z}^{(\alpha)}\}_{\alpha \in I} \subset \{-1, 1\}^n$ be the set of solutions to be penalized.
Corresponding weights assignment:

$$\begin{cases} \theta_i = b \sum_{\alpha \in I} z_i^{(\alpha)} \\ \theta_{ij} = c \sum_{\alpha \in I} z_i^{(\alpha)} z_j^{(\alpha)} \quad \text{for } (i,j) \in E \end{cases}$$

$b, c > 0$

Hybrid approach to QA

Tabu matrix penalizing $\{\boldsymbol{z}^{(\alpha)}\}_{\alpha \in I} \subset \{-1,1\}^n$

$$S := \sum_{\alpha \in I} [\boldsymbol{z}^{(\alpha)} \otimes \boldsymbol{z}^{(\alpha)} - \mathbb{I}_n + \mathrm{diag}(\boldsymbol{z}^{(\alpha)})]$$

Tabu-implementing encoding of a binary optimization problem

Let $f : \{-1,1\}^n \to \mathbb{R}$ be a function to be minimized.

$$\mu[f](\boldsymbol{z}) := E(\theta_\mu[f] + P_\pi S P_\pi \circ A, \pi(\boldsymbol{z}))$$

where:

$\theta_\mu[f]$ is the matrix of weights reproducing some properties of f

π is a permutation and P_π the permutation matrix.

A is the adjacency matrix of the annealer graph.

$\circ$ is the Hadamard product.

The quantum-classical algorithm

Quantum Annealing Learning Search

Tabu search in the solution space and a **guided evolution in the space of encodings** toward a faithful representation of the objective function f into the quantum annealer architecture.

The quantum-classical algorithm

Quantum Annealing Learning Search

Tabu search in the solution space and a **guided evolution in the space of encodings** toward a faithful representation of the objective function f into the quantum annealer architecture.

The hybrid scheme

Definition of a **sequence of μ-encodings** such that:

- Already rejected solutions are (energetically) penalized;
- The representation of f gets better during the search;
- Convergence to a faithful encoding of the problem (i.e. the limit annealing process produces one of the global optima)

Repeated calls of the quantum annealer within an **iterative structure**.

Data: Annealer graph matrix A of order n
Input: $f(\boldsymbol{z})$ to be minimized w.r.t. $\boldsymbol{z} \in \{-1, 1\}^n$
Result: $\boldsymbol{z}^*$ minimum of f

randomly generate: $\mu_j[f](\boldsymbol{z}) := E_A(\theta_j[f], \pi_j(\boldsymbol{z}))$, $j = 1, 2$;
find $\boldsymbol{z}_1$ and $\boldsymbol{z}_2$ s.t. $\pi_1(\boldsymbol{z}_1)$, $\pi_2(\boldsymbol{z}_2)$ minimize $E_A(\theta_1, \cdot)$ and $E_A(\theta_2, \cdot)$;
evaluate $f(\boldsymbol{z}_1)$ and $f(\boldsymbol{z}_2)$;
use the best to initialize $\boldsymbol{z}^*$ and the encoding μ^*;
use the worst to initialize $\boldsymbol{z}'$;
initialize the tabu matrix: $S \leftarrow \boldsymbol{z}' \otimes \boldsymbol{z}' - \mathbb{I}_n + \mathrm{diag}(\boldsymbol{z}')$;
repeat
    from μ^* generate $\mu[f](\boldsymbol{z}) := E_A(\theta[f] + P_\pi^T S P_\pi \circ A, \pi(\boldsymbol{z}))$;
    find $\boldsymbol{z}'$ whose image $\pi(\boldsymbol{z}')$ minimize $E_A(\theta, \cdot)$ in the annealer;
    if $\boldsymbol{z}' \neq \boldsymbol{z}^*$ **then**
        evaluate $f(\boldsymbol{z}')$;
        if *$\boldsymbol{z}'$ is better of $\boldsymbol{z}^*$* **then**
            swap$(\boldsymbol{z}', \boldsymbol{z}^*)$; $\mu^* \leftarrow \mu$;
        end
        use $\boldsymbol{z}'$ to update the tabu matrix S;
        $S \leftarrow S + \boldsymbol{z}' \otimes \boldsymbol{z}' - \mathbb{I}_n + \mathrm{diag}(\boldsymbol{z}')$;
    end
until *convergence or maximum number of iterations conditions*;
return $\boldsymbol{z}^*$;

Convergence for QUBO problems

Quadratic Unconstrained Binary Optimization (QUBO)

$$\text{Minimize} \quad f(\boldsymbol{z}) = \boldsymbol{z}^T Q \boldsymbol{z}$$

$\boldsymbol{z} \in \{-1, 1\}^n$, Q is a real symmetric matrix.

Convergence for QUBO problems

Quadratic Unconstrained Binary Optimization (QUBO)

$$\text{Minimize} \quad f(\boldsymbol{z}) = \boldsymbol{z}^T Q \boldsymbol{z}$$

$\boldsymbol{z} \in \{-1, 1\}^n$, Q is a real symmetric matrix.

Proposition [D.P., E. Blanzieri, 2019]

The hybrid search can be modeled by an inhomogeneous Markov chain.

Let $\{M(k)\}_{k>0}$ be the transition matrix.
(k is related to the counter of iterations)

1. $\exists!$ stationary distribution Π_k of $M(k)$ for any k.
2. it converges and its limit distribution is

$$\Pi^* = \lim_{k \to +\infty} \Pi_k$$

3. Π^* is non-zero only on the solutions of the QUBO problem.

Hybrid approach to Adiabatic Quantum Computing

[D. P., E. Blanzieri. **Learning adiabatic quantum algorithms for solving optimization problems.** Submitted (2019)]

Adiabatic Quantum Computing

It is a model of computation based on adiabatic evolution of quantum systems. AQC is a universal model of quantum computing.

Goal

Given an optimization problem.
Find an adiabatic quantum algorithm to (efficiently) solve it.

The hybrid algorithm

A convergent tabu-inspired search finds an encoding of the problem into an adiabatic quantum architecture providing an adiabatic quantum algorithm and its run time.

Work in progress

Collaborations: Quantum Informatics Laboratory (University of Verona);

Center of high-performance computing (German Aerospace Agency)

- Implementation of the presented hybrid algorithm into the real D-Wave machine.
- Application of the Quantum Annealer tabu technique to represent data into quantum Ising model:
  - Quantum data compression.
  - Quantum machine learning.
- Learning quantum algorithms beyond optimization problems.

Thank you for your attention