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
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 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 20µs)
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 $$\sigma_z^{(i)} = I \otimes \cdots \otimes \sigma_z \otimes \cdots \otimes I$$ and $$\theta_0, \theta_i, \theta_{ij} \in \mathbb{R}$$ (the weights)

Minimization (w.r.t. $$z$$) of the function:

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


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

\[
\begin{align*}
\theta_i &= b \sum_{\alpha \in I} z_i^{(\alpha)} \\
\theta_{ij} &= c \sum_{\alpha \in I} z_i^{(\alpha)} z_j^{(\alpha)} \quad \text{for } (i, j) \in E
\end{align*}
\]

\( b, c > 0 \)
Hybrid approach to QA

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

\[
S := \sum_{\alpha \in I} [z^{(\alpha)} \otimes z^{(\alpha)} - I_n + \text{diag}(z^{(\alpha)})]
\]

Tabu-implementing encoding of a binary optimization problem

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

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

where:

\( \theta_{\mu}[f] \) is the matrix of weights reproducing some properties of \( f \)

\( \pi \) is a permutation and \( P_{\pi} \) 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 $\mu$-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: $f(z)$ to be minimized w.r.t. $z \in \{-1, 1\}^n$

Result: $z^*$ minimum of $f$

1. randomly generate: $\mu_j[f](z) := E_A(\theta_j[f], \pi_j(z))$, $j = 1, 2$;
2. find $z_1$ and $z_2$ s.t. $\pi_1(z_1), \pi_2(z_2)$ minimize $E_A(\theta_1, \cdot)$ and $E_A(\theta_2, \cdot)$;
3. evaluate $f(z_1)$ and $f(z_2)$;
4. use the best to initialize $z^*$ and the encoding $\mu^*$;
5. use the worst to initialize $z'$;
6. initialize the tabu matrix: $S \leftarrow z' \otimes z' - I_n + \text{diag}(z')$;
7. repeat
8. from $\mu^*$ generate $\mu[f](z) := E_A(\theta[f] + P^T \pi S \pi \circ A, \pi(z))$;
9. find $z'$ whose image $\pi(z')$ minimize $E_A(\theta, \cdot)$ in the annealer;
10. if $z' \neq z^*$ then
11. evaluate $f(z')$;
12. if $z'$ is better of $z^*$ then
13. swap($z', z^*$); $\mu^* \leftarrow \mu$;
14. end
15. use $z'$ to update the tabu matrix $S$;
16. $S \leftarrow S + z' \otimes z' - I_n + \text{diag}(z')$;
17. end
18. until convergence or maximum number of iterations conditions;
19. return $z^*$;
Convergence for QUBO problems

Quadratic Unconstrained Binary Optimization (QUBO)

Minimize \( f(z) = z^T Q z \)

\( z \in \{-1, 1\}^n \), \( Q \) is a real symmetric matrix.
Convergence for QUBO problems

Quadratic Unconstrained Binary Optimization (QUBO)

Minimize \( f(z) = z^T Q z \)

\( z \in \{-1, 1\}^n, \) \( Q \) 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 \( \Pi_k \) of \( M(k) \) for any \( k \).

2. it converges and its limit distribution is

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

3. \( \Pi^* \) is non-zero only on the solutions of the QUBO problem.
Hybrid approach to Adiabatic Quantum Computing


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