Quantum Machine Learning and Optimization

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1 Introduction

.Quantum machine learning (QML) is an emerging field that integrates quantum computing with machine learning algorithms to process information in fundamentally new ways, aiming to outperform traditional computational methods on specific tasks. At the core of QML lies the use of quantum algorithms such as the Quantum Approximate Optimization Algorithm (QAOA), Quantum Annealing, Grover's algorithm for search optimization, and quantum versions of classical machine learning algorithms, including quantum neural networks and quantum support vector machines. These algorithms take advantage of quantum superposition and entanglement. Quantum optimization, a critical application of QML, focuses on solving complex optimization problems more efficiently than classical approaches. Quantum annealing and the QUBO framework are specifically pivotal in this aspect, enabling the tackling of NP-Hard problems by finding optimal or near-optimal solutions through a process that mirrors natural quantum systems' evolution. By exploiting these quantum properties, QML aims to revolutionize fields ranging from drug discovery to financial modeling. In the following section, I will explain one particular quantum optimization algorithm called quantum annealing.

1.1 Quantum Annealing

Quantum annealers are special type of quantum computers which use adiabatic theorem to solve the combinatorial optimization problems and find the optimal or sub-optimal solutions. The idea behind adiabatic quantum computing is to start with a simple Hamiltonian, one for which we can easily prepare the ground state and evolve it. We then slowly change the hamiltonain to problem hamiltoian whose ground state solution is of our interest. Let, H_1 is the Hamiltonian whose ground state encodes the result that we want to find and the system is in ground state of some hamiltonian H_0. Suppose, we run this process for time T which is known as anneal time. Then, the time-dependent hamiltonian becomes,

$$H(t) = A(t)H_0 + B(t)H_1 \tag{1}$$

We choose $A(0) = B(T) = 1$ and $A(T) = B(0) = 0$.
A natural choice of A and B becomes, $A(t) = 1 - \frac{t}{T}$ and $B(t) = t/T$
The final expression becomes,

$$H(t) = (1 - \frac{t}{T})H_0 + (\frac{t}{T})H_1 \tag{2}$$

Quantum annealing is based on the same principle of adiabatic quantum computing but it differs in two ways. In quantum hamiltonian, the problem hamiltonian H_1 cannot be chosen at will but has to be selected from a restricted class. The following form can be utilized in quantum annealing.

$$-\sum_{j,k} J_{jk} Z_j Z_k - \sum_{j} h_j Z_j \tag{3}$$

The used has the freedom of J_{jk} and h_j coefficients within certain ranges. Due to this restriction in the choice of the final hamiltonian, quantum annealing, unlike adiabatic quantum computing is not universal and can be used to solve specific type of problems only.

2 QUBO framework

We need a language in which we can state problem in a manner that makes it possible for a quantum computer to solve them. In this regard, with the Quadratic Unconstrained Binary Optimization (QUBO) framework we can formulate many different optimization problems in a way that maps directly into the quantum setting, allowing us a plethora of quantum algorithms to try to find solutions that are optimal or at least close to optimal. The QUBO model [1] is expressed by the optimization problem, to maximize or minimize,

$$y = X^T Q X \tag{4}$$

where X is a vector of binary decision variables and Q is a square matrix of constants. It is common to assume that the Q matrix is symmetric or in upper triangular form, which can be achieve without loss of generality simply as follows,
Symmetric form: For all i and j except i=j, replace by $(q_{ij} + q_{ji})/2$
Upper triangular form: For all i and j with $j > i$, replace q_{ij} by $(q_{ij} + q_{ji})$. Then replace all q_{ij} for $j < i$ by 0.

3 Examples

NP-Hard problems like maxcut problem, maxclique, graph coloring problem, number partition, SAT problems, nurse scheduling, etc. are explicitly studied using quantum annealing approach. A detailed list of problems can be found in [2], [3].

References

[1] Elias F Combarro, Samuel González-Castillo, and Alberto Di Meglio. *A Practical Guide to Quantum Machine Learning and Quantum Optimization: Hands-on Approach to Modern Quantum Algorithms*. Packt Publishing Ltd, 2023.

[2] Andrew Lucas. Ising formulations of many np problems. *Frontiers in physics*, 2:74887, 2014.

[3] Anuradha Mahasinghe, Vishmi Fernando, and Paduma Samarawickrama. Qubo formulations of three np problems. *Journal of Information and Optimization Sciences*, 42(7):1625–1648, 2021.