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Quantum Annealing in Machine Learning: QBoost on D-Wave Quantum Annealer

Hadi Salloum[a,b,*], Ali Salloum[b], Manuel Mazzara[b], Sergey Zykov[c]

[a] *QDeep, Innpoolis, Russia*
[b] *Innopolis University, Innopolis, Russia*
[c] *HSE University, Moscow, Russia*

Abstract

Quantum computing (QC) has become a fascinating and popular topic due to its broad range of applications, particularly in machine learning (ML). The intersection of QC and ML is known as Quantum Machine Learning (QML). QML is a field that investigates how QC can enhance ML, making it one of the most exciting areas of research due to the potential of QC in solving complex problems. In this paper, we demonstrate the Quantum Annealing (QA) approach to improving ML in binary classification tasks. We implemented the QBoost algorithm on a few datasets using D-Wave's quantum computers, specifically the Advantage 1 and Advantage 2 prototypes, incorporating the new feature Fast Anneal.

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1. Introduction

Machine learning stands as a cornerstone in both research and industry, offering a plethora of applications ranging from drug discovery to financial modeling [1, 2, 3, 4, 5, 6]. However, the efficacy of classical computers is hindered by their limited processing power, especially when confronted with complex problems [7, 8]. As these problems grow in size and intricacy, classical computing demands exponentially increasing time and resources to provide solutions [9].

Enter quantum computing, heralding a new paradigm by harnessing the properties of quantum mechanics to execute massive calculations in significantly reduced time frames. This paradigm shift has introduced novel algorithms like

* Corresponding author. Tel.: +7 977 059 4392.
E-mail address: h.salloum@qdeep.net

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Shor's [10, 11, 12, 13] and Grover's [14], paving the way for Quantum Machine Learning (QML). Quantum computers come in two primary types: quantum gate-based systems and quantum annealers [15].

At the forefront of quantum annealer technology stands the D-Wave company, boasting the largest quantum computer, "Advantage1," with over 5000 qubits [16]. Recent advancements, exemplified by D-Wave's "Advantage2 prototype" featuring 1200+ qubits [17], showcase computational supremacy in quantum simulation [18]. This technological leap holds the promise of solving problems beyond classical computing's reach, such as simulating the non-equilibrium dynamics of complex systems like magnetic spin systems. Anticipated in 2025, the "Advantage2" is expected to be operational with 7000+ qubits [19], further enhancing its capabilities.

The release of user-accessible prototypes, like the Advantage1 and Advantage2 with fast anneal feature [20], signifies a significant step forward in achieving quantum computing's potential for practical applications and achievements.

This paper focuses on the QBoost algorithm, a binary classifier within the realm of QML. We will delve into its workings, conduct experiments, and assess its performance on both the Advantage1 and Advantage2 prototypes with fast anneal features. We aim to address several key questions:

1. How does quantum annealing compare to classical optimization methods in terms of accuracy and efficiency for binary classification?
2. What are the advantages and limitations of leveraging quantum computing for machine learning tasks?
3. How does the implementation on D-Wave's quantum computers impact the scalability and practicality of quantum-enhanced machine learning algorithms?

Through empirical evaluations of diverse datasets representative of real-world applications, we seek to provide empirical evidence of quantum annealing's capabilities and its potential contributions to advancing quantum-enhanced machine learning methodologies. This exploration is crucial for understanding the practical implications of quantum computing in the realm of data-driven decision-making and predictive modeling.

Paper's structure

The structure of this paper outlines an overview of quantum annealing in Section 2, explains the QBoost algorithm in Section 3, and presents experiments conducted on both the Advantage1 and Advantage2 prototypes in Section 4

2. Quantum Annealing

Quantum annealing, a distinctive facet of quantum adiabatic computing, diverges from gate-based quantum computing paradigms. It has evolved from classical simulated annealing algorithms, specifically designed to address optimization challenges classified as NP-hard. Quantum annealing uses quantum mechanical phenomena such as superposition, entanglement, and tunneling to navigate complex problem landscapes efficiently [21, 22].

At its core, quantum annealing relies on the adiabatic theorem [23], which governs the gradual evolution of a quantum system from an initial state to the ground state of a problem Hamiltonian. The adiabatic theorem ensures that the system remains in its instantaneous ground state throughout the evolution, given a sufficiently slow transition.

The problem Hamiltonian (H_p) is typically represented as a weighted sum of terms, each corresponding to a component of the optimization objective:

$$H_p = \sum_i w_i \sigma_i^z$$

Here, w_i are the weights associated with each term, and σ_i^z are the Pauli-Z operators acting on qubits. The primary goal of quantum annealing is to determine the ground state of H_p, which represents the optimal solution to the optimization problem. This process involves initializing the system in the ground state of an initial Hamiltonian (H_0) and gradually transitioning towards the ground state of H_p using the adiabatic theorem.

Mathematically, the time-dependent Schrödinger equation [24] governing the evolution of the quantum system during annealing can be written as:

$$i\hbar\frac{\partial}{\partial t}|\psi(t)\rangle = H(t)|\psi(t)\rangle \tag{1}$$

where $|\psi(t)\rangle$ is the state vector of the quantum system at time t, $\hbar$ is the reduced Planck constant, and $H(t)$ is the time-dependent Hamiltonian. In the context of quantum annealing, the Hamiltonian is often expressed as a linear interpolation between H_0 and H_p over a total evolution time T [25]:

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

This equation describes how the Hamiltonian evolves from the easy-to-solve initial problem to the target problem during the annealing process.

Quantum annealing systems, such as those developed by D-Wave, employ qubits as the fundamental units of computation. Unlike classical bits, which can only be in states 0 or 1, qubits utilize quantum superposition to exist in multiple states simultaneously. The dynamics of qubits during annealing are governed by the time-dependent Hamiltonian [26]:

$$H(t) = \sum_i \left[w_i(t)\sigma_i^z + A(t)\sigma_i^x\right] + \sum_{i,j} J_{i,j}(t)\sigma_i^z\sigma_j^z \tag{3}$$

Here, $w_i(t)$ represents time-varying biases, $A(t)$ is the annealing function controlling the qubit transitions, and $J_{i,j}(t)$ are time-dependent couplings between qubits. This comprehensive Hamiltonian captures the interplay of qubit states, biases, and couplings throughout the annealing process.

The physical interpretation of quantum annealing involves energy landscapes and transitions between quantum states. Initially, the system resides in a low-energy state resembling a single valley. As annealing progresses, the energy landscape transforms into a multi-valley structure, with each valley representing a potential solution to the optimization problem. External biases, akin to magnetic fields, guide the system's evolution towards lower energy states corresponding to optimal solutions. Entanglement plays a crucial role in quantum annealing, where qubits become correlated and exhibit joint quantum states. This correlation allows qubits to explore solution spaces collectively, contributing to the computational power of quantum annealing systems.

As the number of qubits increases, system complexity escalates exponentially, posing computational challenges. To implement quantum annealing effectively, crucial steps include system description and initialization, energy scale determination, freezeout point estimation, anneal offset calculation, and global anneal schedule parameterization [27]. These steps ensure optimized quantum annealing processes, crucial for tackling complex optimization tasks in diverse domains.

3. QBoost: Quantum-Inspired Boosting Algorithm

QBoost [28] operates through an iterative process that combines quantum selection and classical adaptation to refine the ensemble of weak classifiers into a robust strong classifier. This algorithmic framework represents a significant advancement in machine learning methodologies, offering improved performance and efficiency in constructing accurate classifiers.

The algorithm begins by initializing an ensemble of weak classifiers and a labeled training dataset. In the quantum selection phase, Adiabatic Quantum Optimization (AQO) [29] facilitates efficient exploration of the classifier space by leveraging quantum tunneling effects, allowing QBoost to focus on configurations that offer the most significant performance improvements compared to classical selection methods. This quantum-inspired approach allows for efficient exploration of the classifier space, focusing on configurations that offer the most significant performance improvements. The quantum selection process involves encoding the weak classifiers and training data into a quantum representation suitable for optimization. By leveraging quantum annealing or other quantum-inspired techniques, QBoost explores different combinations of weak classifiers to identify those that contribute most effectively to the strong classifier's accuracy. This phase emphasizes the algorithm's ability to leverage quantum computing principles for efficient selection and optimization, contributing to its overall effectiveness.

Following the quantum selection phase, QBoost adapts its dictionary of weak classifiers based on the errors identified by the strong classifier constructed in the previous step. This adaptation process is crucial for fine-tuning the ensemble, incorporating new classifiers that address specific error patterns and enhance overall classification accuracy.

Metrics such as error rates, validation accuracy, and convergence criteria guide the adaptation process, ensuring that weak classifiers contributing positively to error reduction are given higher importance while those causing significant errors are downgraded or replaced. Weak classifiers that contribute positively to reducing errors are given higher importance, while those causing significant errors are downgraded or replaced. This adaptive dictionary ensures that the ensemble evolves dynamically, optimizing its composition to handle complex classification tasks effectively. The inner loop of QBoost involves the dynamic refinement of the strong classifier. Through iterative training and evaluation, the algorithm continuously assesses and updates the composition of the strong classifier based on error analysis and convergence criteria. This dynamic approach ensures that the final classifier achieves optimal performance while minimizing computational overhead.

During the refinement process, QBoost evaluates the performance of the strong classifier on both training and validation datasets. It monitors changes in error rates, convergence of optimization objectives, and the stability of the classifier's predictions. If the validation error decreases or converges within predefined thresholds, the algorithm updates the strong classifier with new weak classifiers or modified weights. Conversely, if the validation error stagnates or increases, indicating potential overfitting or lack of improvement, the algorithm adjusts its strategies, such as freezing the current classifier and exploring alternative configurations. The dynamic refinement phase of QBoost ensures that the strong classifier evolves iteratively, adapting to changing data patterns, minimizing errors, and improving generalization capabilities. The following pseudocode outlines the core steps of QBoost algorithm, highlighting its quantum-inspired selection, dictionary adaptation, and dynamic refinement processes.

Algorithm 1 QBoost Algorithm

Require: Training dataset D, number of weak classifiers Q, number of iterations T
Ensure: Trained strong classifier C
Initialize ensemble of weak classifiers Q_{weak} and strong classifier C (initially empty)
for $t = 1$ **to** T **do**
    Select T_{inner} weak classifiers W_{inner} using AQO minimizing validation error
    Update Q_{weak} with modified dictionary based on errors of C using W_{inner}
    while validation error decreases **do**
        Train C using W_{inner}
        if validation error decreases **then**
            Update C with new classifiers
        else
            Freeze C and add another partial classifier
        end if
    end while
end for
return Trained strong classifier C

This structured pseudocode encapsulates the iterative brilliance of QBoost, showcasing its quantum-inspired selection mechanisms, adaptive dictionary refinement, and dynamic training regimen.

4. Experiments

For our experiments, we selected two datasets from the field of Health and Medicine [30, 31], specifically focusing on classification tasks related to cancer prediction:

4.1. Data

4.1.1. Differentiated Thyroid Cancer Recurrence Dataset

Dataset Description:

- Name: Differentiated Thyroid Cancer Recurrence
- Donation Date: 10/30/2023
- Characteristics: Tabular data with 13 clinicopathologic features
- Purpose: Predicting recurrence of well-differentiated thyroid cancer
- Data Collection Duration: 15 years
- Follow-Up Period: At least 10 years for each patient
- Number of Instances: 383
- Number of Features: 16 (Real, Categorical, Integer)

Dataset Creation Purpose:

- Part of research in the field of AI and Medicine

4.1.2. Glioma Grading Clinical and Mutation Features Dataset

Dataset Description:

- Name: Glioma Grading Clinical and Mutation Features
- Donation Date: 12/13/2022
- Characteristics: Tabular data with clinical and molecular/mutation features
- Purpose: Grading gliomas as Lower-Grade Glioma (LGG) or Glioblastoma Multiforme (GBM)
- Data Source: TCGA-LGG and TCGA-GBM brain glioma projects
- Key Features: 20 most frequently mutated genes and 3 clinical features
- Number of Instances: 839
- Number of Features: 23 (Real, Categorical, Integer)

Dataset Creation Purpose:

- To determine an optimal subset of mutation genes and clinical features for glioma grading process
- Objective: Improve grading performance and reduce diagnostic costs

4.2. Results

User conducted experiments using the 'Advantage_System2 prototype' , 'Advantage_System4.1', and 'Advantage_System6.4' Quantum Annealers. Two datasets were used: the Differentiated Thyroid Cancer Recurrence Dataset and the Glioma Grading Clinical and Mutation Features Dataset.

4.2.1. Differentiated Thyroid Cancer Recurrence Dataset

Interpretation: - Advantage2 prototype shows the highest F1 score of 0.827 on the test set (see Fig. 1.), outperforming both Advantage1 4.1 (F1 score of 0.824) and Advantage1 6.4 (F1 score of 0.818). This indicates that Advantage2 prototype achieves a better balance between precision and recall for predicting cancer recurrence on this dataset.

System	Advantage1 4.1		Advantage1 6.4		Advantage2 prototype	
	Train	Test	Train	Test	Train	Test
Accuracy	0.855	0.839	0.855	0.833	0.857	0.845
Precision	0.794	0.778	0.789	0.768	0.805	0.795
Recall	0.882	0.875	0.893	0.875	0.868	0.861
F1 Score	0.836	0.824	0.838	0.818	0.835	0.827

Table 1. Comparison of metrics for Advantage1 4.1, Advantage1 6.4, and Advantage2 prototype for Differentiated Thyroid Cancer Recurrence Dataset

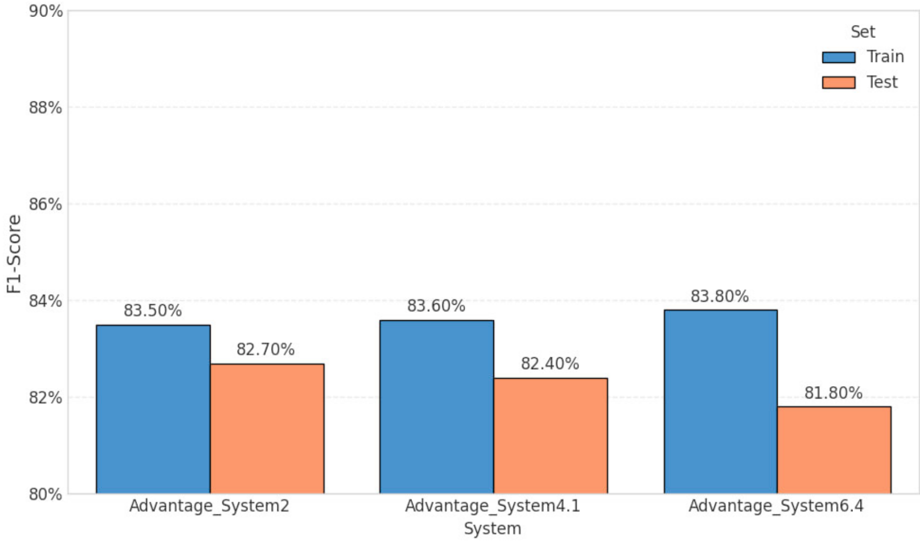

Fig. 1. F1-Score for the Differentiated Thyroid Cancer Recurrence Dataset

4.2.2. Glioma Grading Clinical and Mutation Features Dataset

System	Advantage1 4.1		Advantage1 6.4		Advantage2 prototype	
	Train	Test	Train	Test	Train	Test
Accuracy	0.882	0.896	0.873	0.857	0.886	0.870
Precision	0.736	0.769	0.701	0.690	0.743	0.731
Recall	0.907	0.909	0.953	0.909	0.907	0.864
F1 Score	0.812	0.833	0.808	0.784	0.817	0.792

Table 2. Performance metrics comparison for Advantage1 4.1, Advantage1 6.4, and Advantage2 (prototype) on Glioma Grading Clinical and Mutation Features Dataset

Interpretation: - Advantage1 4.1 achieved the highest F1 score of 0.833 on the test set, followed by Advantage2 with an F1 score of 0.792 and Advantage1 6.4 with an F1 score of 0.784 (See Fig. 2). This suggests that Advantage1 4.1 performs slightly better in terms of overall classification performance on this dataset. It's expected that the future release of Advantage2 with over 7000 qubits in 2025 will give even better results, given the anticipated increase in computational power.

5. Discussion

The results presented in the previous section provide insights into the performance of different quantum annealing systems, specifically Advantage1 4.1, Advantage1 6.4, and the Advantage2 prototype, across two distinct datasets

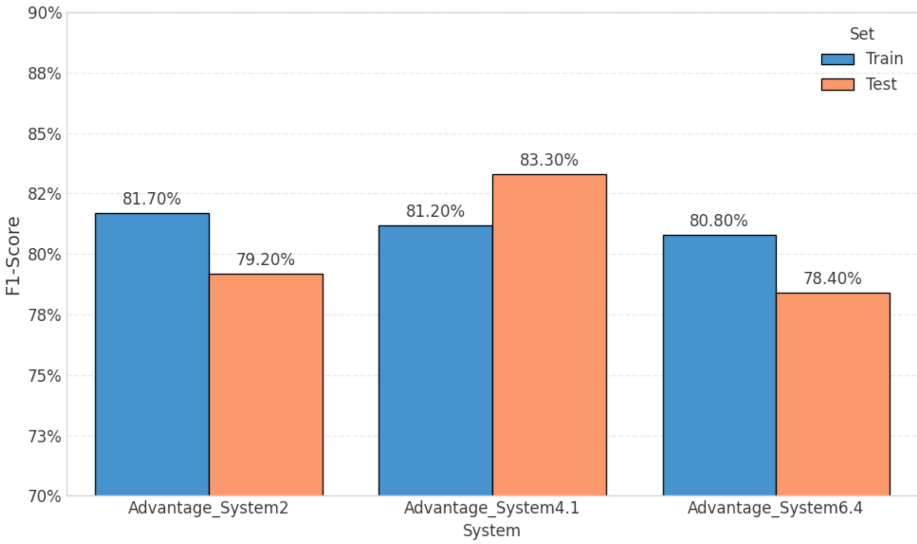

Fig. 2. F1-Score for the Glioma Grading Clinical and Mutation Features Dataset

related to cancer recurrence and glioma grading. These discussions aim to interpret the findings, discuss their implications, and highlight areas for further research.

The results on the Differentiated Thyroid Cancer Recurrence Dataset reveal interesting trends. The Advantage2 prototype demonstrated the highest F1 score on the test set, indicating its efficacy in achieving a balance between precision and recall in predicting cancer recurrence. This finding suggests that the increased qubit count in Advantage2 plays a significant role in improving classification performance compared to Advantage1 4.1 and Advantage1 6.4.

However, it's important to note that the difference in F1 scores between the Advantage2 prototype and the other systems is relatively small. This could imply that while the higher qubit count offers advantages, the fundamental algorithms and methodologies used across these systems may have a more substantial impact on classification performance. On the Glioma Grading Clinical and Mutation Features Dataset, Advantage1 4.1 achieved the highest F1 score on the test set, followed closely by Advantage2 with 1200 qubits. This suggests that Advantage1 4.1 excels in classifying glioma grading cases, showcasing its effectiveness in this specific domain. However, Advantage2 with its increased qubit count also performs admirably, indicating its potential for broader applications beyond the current dataset.

The differences in performance across the systems on this dataset highlight the importance of dataset characteristics and the need for tailored approaches in quantum machine learning. Factors such as data complexity, feature representation, and algorithmic optimizations may influence the performance of quantum annealers differently, necessitating careful consideration in system selection for specific tasks.

The results presented in this study offer valuable insights into the capabilities of quantum annealing systems for classification tasks related to medical diagnostics. The observed improvements with higher qubit counts, as seen in Advantage2, suggest a promising trajectory for the field of quantum machine learning.

Future research directions could explore:

- Further scaling up quantum annealers to assess the impact of even larger qubit counts on classification performance.
- Investigating the transferability of quantum models trained on one dataset to similar but distinct datasets, evaluating the generalization capabilities of quantum algorithms.
- Exploring hybrid quantum-classical approaches to leverage the strengths of both quantum and classical computing paradigms for enhanced performance and scalability.

Overall, this study contributes to the growing body of research in quantum machine learning and underscores the potential of quantum annealing systems in addressing complex real-world problems in healthcare and beyond.

6. Conclusion

This study delves into the performance evaluation of quantum annealing systems, focusing on their efficacy in binary classification tasks related to medical diagnostics using the QBoost Algorithm. The findings illuminate the impact of increased qubit counts, as seen in the Advantage2 prototype, on classification performance, highlighting promising advancements in quantum machine learning. Moreover, the nuanced performance variations across different datasets underscore the importance of tailored approaches and dataset characteristics in quantum algorithm selection. These insights contribute to the evolving landscape of quantum machine learning, paving the way for further exploration into hybrid quantum-classical methodologies and larger-scale quantum annealers for enhanced problem-solving capabilities in diverse domains.

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