Quantum Discriminator for Binary Classification

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Abstract—Quantum computers operate in the highdimensional tensor product spaces and are known to outperform classical computers on many problems. They are poised to accelerate machine learning tasks in the future. In this work, we operate in the quantum machine learning (QML) regime where a QML model is trained using a quantum-classical hybrid algorithm and inferencing is performed using a quantum algorithm. We leverage the traditional two-step machine learning workflow, where features are extracted from the data in the first step and a discriminator acting on the extracted features is used to classify the data in the second step. Assuming that the binary features have been extracted from the data, we propose a quantum discriminator for binary classification. The quantum discriminator takes as input the binary features of a data point and a prediction qubit in the zero state, and outputs the correct class of the data point. The quantum discriminator is defined by a parameterized unitary matrix U_{Θ} containing $\mathcal{O}(N)$ parameters, where N is the number of data points in the training data set. Furthermore, we show that the quantum discriminator can be trained in $O(N \log N)$ time using $\mathcal{O}(N \log N)$ classical bits and $\mathcal{O}(\log N)$ qubits. We also show that inferencing for the quantum discriminator can be done in $\mathcal{O}(N)$ time using $\mathcal{O}(\log N)$ qubits. Finally, we use the quantum discriminator to classify the XOR problem on the IBM Q universal quantum computer with 100% accuracy.

Index Terms—Quantum Machine Learning, Quantum Artificial Intelligence, Quantum Computing, Supervised Learning, Binary Classification

I. INTRODUCTION

Machine learning models have been widely used for numerous scientific, business and consumer applications in the recent past with great success [1]. Presently, machine learning models are run on classical computing platforms containing CPUs, GPUs or FPGAs and trained using large amounts of data. However, this will not be sustainable in the future. In the future, while data available for training is expected to increase significantly and rapidly, the classical computing platforms are expected to stagnate in terms of speed and

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compute power owing to the inevitable end of Moore's law [2]. This will severely restrict our ability to build end-to-end machine learning applications. In order to continue developing machine learning applications in the post-Moore's law era, we must resort to non-conventional computing platforms like quantum computing and neuromorphic computing [3], [4].

Quantum computers operate in the high-dimensional tensor product spaces and possess the ability to perform several computationally difficult tasks faster than classical computers. Because of the exponential compression associated with these high-dimensional spaces, quantum computers are the ideal candidates to efficiently analyze large amounts of data for machine learning tasks beyond the Moore's law. While today's quantum computers are small, noisy and error-prone, future quantum computers are sought to be large, accurate and reliable. Therefore, it is important to develop efficient quantum machine learning approaches on today's quantum computers so that they can seamlessly transition onto the future machines.

In our previous work, we have developed quantum machine learning approaches for training deep belief network, restricted Boltzmann machine, k-means clustering, support vector machine and linear regression on adiabatic quantum computers [5]-[8]. In this work, we propose a quantum discriminator for binary classification that runs on universal quantum computers. We leverage the traditional two-step machine learning workflow, where features are extracted from the data in the first step and a discriminator acting on the extracted features is used to classify the data in the second step. We assume that binary features have been extracted from the data in the first step. The quantum discriminator takes as input the binary features of a given data point and a prediction qubit in the zero state, and outputs the correct class of the data point. We further show that the quantum discriminator can be trained in $\mathcal{O}(N \log N)$ time using $\mathcal{O}(N \log N)$ classical bits and $\mathcal{O}(\log N)$ qubits, where N is the number of points in the training data set. We also point out that inferencing with the quantum discriminator can be done in $\mathcal{O}(N)$ time using $\mathcal{O}(\log N)$ qubits. To demonstrate the proof of concept, we use the quantum discriminator to classify the two-dimensional XOR problem on the IBM Q universal quantum computer with 100% accuracy.

II. RELATED WORK

Several machine learning approaches that leverage universal quantum computers have been proposed in the literature [9]. Lloyd and Weedbrook as well as Dallaire-Demers and Killoran

derive the theoretical underpinnings of quantum generative adversarial networks [10], [11]. Many approaches to quantum machine learning leverage the two-step workflow followed by traditional machine learning models. Havlicek et al. propose a quantum variational classifier and a quantum kernel estimator for classification problems [12]. Schuld and Killoran propose a nonlinear feature map that maps data to a quantum feature space and discuss two discriminant models for classification [13]. Bergou and Hillery propose a quantum discriminator that can distinguish between two unknown quantum states [14]. The quantum discriminator proposed in this paper also aligns with this line of research leveraging the traditional two-step workflow of machine learning. It operates on a set of binary features extracted from the data and can classify its inputs into one of two classes correctly.

III. NOTATION

We use the following notation throughout this paper:

- ℝ, ℕ, ℍ: Set of real numbers, natural numbers and binary numbers (𝔻 = {0, 1}) respectively.
- N: Number of data points in training data set $(N \in \mathbb{N})$.
- d: Dimension of each data point in the training data set $(d \in \mathbb{N})$.
- b: Dimension of each feature in the binary feature set of the training data set (b ∈ N).
- B: Number of unique states that can be attained using b bits or qubits $(B = 2^b)$.
- X: Training data set $(X \in \mathbb{R}^{N \times d})$.
- Y: Training labels $(Y \in \mathbb{B}^N)$. If the i^{th} data point belongs to class 0 (class 1), then $y_i = 0$ ($y_i = 1$).
- \hat{X} : The binary feature set of the training data set X ($\hat{X} \in \mathbb{B}^{N \times b}$). $\hat{x}_i \in \hat{X}$ contains the features corresponding to the i^{th} data point $x_i \in X$.
- P: The labels predicted by the quantum binary classification model $(P \in \mathbb{B}^N)$. Ideally, the predicted labels should be identical to the training labels (Y).
- Θ : Model parameters of the quantum discriminator ($\Theta = \{\theta_1, \theta_2, \dots, \theta_B\}, \ \theta_i \in \mathbb{B}, \ \forall i = 1, 2, \dots, B$).

IV. THE QUANTUM DISCRIMINATOR

Given a data point x belonging to one of two classes (Class 0 or Class 1), the goal of a binary classification model is to predict the correct class for x. The binary classification model is characterized by a set of model parameters Θ . Traditionally, the workflow governing any classification model comprises of two steps: (i) Feature extraction from the data; and (ii) Class determination by application of a discriminant function.

The feature space associated with data is domain-specific usually, and not necessarily binary. For example, Histogram of Oriented Gradients (HOG) [15] and Scale-Invariant Feature Transform (SIFT) [16] are widely used features in computer vision. The feature space could also originate from dimensionality reduction techniques like Principal Component Analysis (PCA) [17]. In this work, we assume that a set of binary features (\hat{X}) has been extracted as a result of the feature extraction process. Each point in this feature space $(\hat{x} \in \hat{X})$ is

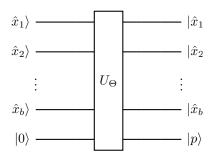


Fig. 1: The quantum discriminator

one of B such points on a b-dimensional unit hypercube. The quantum feature state associated with \hat{x} is denoted by $|\hat{x}\rangle$.

The quantum feature state $|\hat{x}\rangle = |\hat{x}_1 \dots \hat{x}_b\rangle$, along with the prediction qubit in the $|0\rangle$ state serve as inputs to the quantum discriminator as shown in Figure 1. The quantum discriminator (U_Θ) is a $2B \times 2B$ matrix, which acts on these inputs and produces $|\hat{x}\rangle$ and the prediction qubit $|p\rangle$ as the outputs. The matrix U_Θ is parameterized by Θ , and described as follows:

$$U_{\Theta} = \begin{bmatrix} 1 - \theta_1 & \theta_1 & 0 & 0 & \dots & 0 & 0 \\ \theta_1 & 1 - \theta_1 & 0 & 0 & \dots & 0 & 0 \\ 0 & 0 & 1 - \theta_2 & \theta_2 & \dots & 0 & 0 \\ 0 & 0 & \theta_2 & 1 - \theta_2 & \dots & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & \dots & 1 - \theta_B & \theta_B \\ 0 & 0 & 0 & 0 & \dots & \theta_B & 1 - \theta_B \end{bmatrix}$$

$$(1)$$

We now show that U_Θ is a unitary matrix by showing that $U_\Theta^\dagger U_\Theta = U_\Theta U_\Theta^\dagger = I$. Since U_Θ is symmetric, $U_\Theta^\dagger = U_\Theta$. Because $\theta_i \in \mathbb{B}$, the off-diagonal elements in $U_\Theta^\dagger U_\Theta$ and $U_\Theta U_\Theta^\dagger$ are zeros. The diagonal elements of $U_\Theta^\dagger U_\Theta$ and $U_\Theta U_\Theta^\dagger$ are of the form $(1-\theta_i)^2+\theta_i^2$, which always equals unity. So, $U_\Theta^\dagger U_\Theta = U_\Theta U_\Theta^\dagger = I$. Thus, U_Θ is a unitary matrix.

A. Bound on Number of Binary Features (b)

We would like to extract b binary features so that the N points in the feature set span as much of the feature space as possible. This would ensure that the trained quantum discriminator would be generalizable to any test data point that follows the same distribution as the training data set. Since the size of the feature space is $B=2^b$, we want $N\approx B$, i.e. $N\approx 2^b$. This implies $b\approx \mathcal{O}(\log N)$ and $B\approx \mathcal{O}(N)$.

B. Training the Quantum Discriminator

Given the binary feature set \hat{X} and the training labels Y, we first prepare the quantum feature states $|\hat{x}_1\rangle\dots|\hat{x}_N\rangle$, along with the $|0\rangle$ state. Algorithm 1 presents the training algorithm for the quantum discriminator. The inputs to the model are the feature vectors $\hat{x}_1, \hat{x}_2, \dots \hat{x}_N$, and the training labels y_1, y_2, \dots, y_N . b and b are initialized on lines 1 and 2 respectively. The length(b) function on line 1 computes the length of b. Next, the vector b0 is set

Algorithm 1: Training the quantum discriminator.

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Input: \hat{x}_1, \hat{x}_2, \dots, \hat{x}_N, y_1, y_2, \dots, y_N

1 Set b = \text{length}(\hat{x}_1);

2 Set B = 2^b;

3 Set \tau = [2^{b-1}, 2^{b-2}, \dots, 2^1, 2^0]^T;

4 Initialize \theta_j = 0 \quad \forall j = 1, 2, \dots, B;

5 for i = 1, 2, \dots, N do

6 | if y_i == 1 then

7 | j = 1 + \tau \cdot \hat{x}_i;

8 | Set \theta_j = 1;

9 | end

10 end
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on line 3. Next, we setup the quantum circuit shown in Figure 1, where $U_\Theta=I$, by initializing all the model parameters θ_j to zero on line 4. We then look at each feature vector \hat{x}_i on line 6. If \hat{x}_i belongs to Class 1, then we compute the index $j=1+\tau\cdot\hat{x}_i$ on line 7, and set $\theta_j=1$ on line 8. We repeat this process for all N points in the training feature set \hat{X} . When Algorithm 1 terminates, it assigns all points in \hat{X} to their respective correct classes.

We now shed some light on why Algorithm 1 works. The input state to the quantum discriminator, $|\hat{x}| = 0$, exists in (b+1)dimensional Hilbert space and is in a superposition of all 2B possible states. As such, each of the B quantum feature states $|\hat{x}\rangle$, occurs twice: as $|\hat{x}| 0\rangle$ and $|\hat{x}| 1\rangle$. These two states can be interpreted as $|\hat{x}\rangle$ belonging to Class 0 or Class 1 respectively. When training the quantum discriminator, we select the correct class for each $|\hat{x}\rangle$. The rows and columns of U_{Θ} that correspond to \hat{x} can be found at indices $j = 1 + \tau \cdot \hat{x}$ and j + 1, which can be leveraged to assign \hat{x} to Class 0 or Class 1 respectively. Initially, the 2×2 sub-matrix at j^{th} row and j^{th} column of U_{Θ} is an identity matrix because θ_i is initialized to 0. If \hat{x} belongs to Class 0, then this sub-matrix outputs $|\hat{x}| = 0$ for the input $|\hat{x}| = 0$, which can be interpreted as \hat{x} being assigned to Class 0. If \hat{x} belongs to Class 1, then this sub-matrix must be changed to the Pauli-X gate (also called the bit-flip gate or the NOT gate), which is done by setting θ_i to 1. The Pauli-X gate at j^{th} row and j^{th} column of U_Θ outputs $|\hat{x}|$ 1 for the input $|\hat{x}|$ 0, which can be interpreted as \hat{x} being assigned to Class 1.

C. Computational Complexity of Training and Inferencing

We analyze the time and space complexity for training the quantum discriminator here. In Algorithm 1, lines 1 and 2 require $\mathcal{O}(1)$ time and line 3 requires $\mathcal{O}(b)$ time. Initializing θ_j to 0 on line 4 essentially refers to setting up the quantum circuit with $U_\Theta = I$ and takes $\mathcal{O}(b)$ time. Computing the dot product on line 7 takes $\mathcal{O}(b)$ time and setting θ_j to unity on line 8 takes $\mathcal{O}(1)$ time. Since we repeat lines 7 and 8 N-times in the worst case, the time complexity of Algorithm 1 is $\mathcal{O}(Nb)$, which is the same as the size of the feature set \hat{X} . Since b is $\mathcal{O}(\log N)$ from Section IV-A, the time complexity is $\mathcal{O}(N\log N)$. Since we use $\mathcal{O}(Nb)$ classical bits for storing \hat{X} ,

Y and τ , and computing the dot product on line 7, the classical space complexity of Algorithm 1 is also $\mathcal{O}(N\log N)$. The qubit footprint of Algorithm 1 is $\mathcal{O}(b)$ because we use b+1 qubits. Thus, it is possible to train the quantum discriminator shown in Figure 1 in $\mathcal{O}(N\log N)$ time, using $\mathcal{O}(N\log N)$ classical bits and $\mathcal{O}(b)$ qubits.

For inferencing, the binary feature state for each data point as well as the $|0\rangle$ qubit is fed into the quantum circuit of the quantum discriminator, characterized by U_{Θ} . The circuit outputs the prediction made by the model in the prediction qubit. This process takes $\mathcal{O}(N)$ time for getting through all data points in the test data set and uses $\mathcal{O}(\log N)$ qubits.

D. Generalizability

Generalizability refers to the ability of a machine learning model to make predictions on data points not encountered during training. An estimator for generalizability is the performance of the model on the test data set. If a machine learning model is too complex (has a large number of model parameters), it may perform well on the training data set (high accuracy, low error), but fare poorly on the test data set. This is called overfitting.

The quantum discriminator has an exponential number of model parameters $(\theta_1,\theta_2,\ldots,\theta_B)$, is highly complex, and highly susceptible to overfitting the training data. This affinity to overfit is kept in check by the feature extraction process. If the extracted binary features are good and small in number $(b \approx \mathcal{O}(\log N))$, the number of model parameters are also small $(B \approx \mathcal{O}(N))$. The subsequent quantum discriminator would have a lower tendency of overfitting and would be generalizable. On the other hand, if the number of binary features are large in number, the quantum discriminator will have a tendency to overfit the training data. Also, if the training data set does not span the entire binary feature space or is not representative of the binary feature space, then the quantum discriminator might fare poorly on the test data set.

If the points in the feature space of the training data set are separable, i.e. identical points in the feature space do not have different ground truth labels in the training data set, the quantum discriminator can theoretically achieve 100% accuracy on the training data set. In such a scenario, if the test data set follows the same distribution as the training data set, then the quantum discriminator can potentially attain 100% accuracy on the test data set as well.

V. PRELIMINARY RESULTS

As a proof of concept for the quantum discriminator, we use it to classify two-dimensional binary data shown in Figure 2. The classification problem in Figure 2 is an XOR problem, where the data points (0,0) and (1,1) belong to Class 0 and the points (0,1) and (1,0) belong to Class 1. Since the data is binary in this case, we skip the binary feature extraction step and work with the data directly. An example of a quantum circuit that can be used to correctly classify this data is shown in Figure 3. We use Algorithm 1 to train a quantum discriminator on the IBM Q universal quantum computer. The

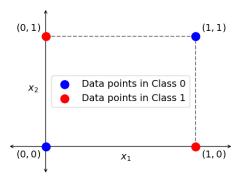


Fig. 2: 2-bit binary classification problem

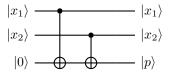


Fig. 3: Quantum circuit for classification problem in Figure 2

unitary matrix representing the circuit of the trained quantum discriminator (as shown in Figure 1) is as follows:

Note that the 2×2 submatrices corresponding to the points (0,0) (i.e. submatrix starting at $1^{\rm st}$ row and column) and (1,1) (i.e. submatrix starting at $7^{\rm th}$ row and column) are identity matrices, which assign these points to the Class 0. On the other hand, the submatrices corresponding to the points (0,1) and (1,0) are Pauli-X gates, which assign these points to Class 1. We obtain 100% classification accuracy on the XOR problem.

VI. CONCLUSION

Machine learning beyond the Moore's law requires use of non-conventional computing platforms like quantum computing. In this work, we presented the quantum discriminator, which acts on binary features extracted from the data and assigns them to the correct class. We obtained bounds on the number of binary features ($b \approx \mathcal{O}(\log N)$), proposed a training algorithm, performed computational complexity analysis of the training algorithm and shed some light on the generalizability of the proposed model. Our preliminary results on the XOR problem achieve 100% classification accuracy. In the future we would like to test the quantum discriminator on other quantum computing platforms such as Google, Rigetti etc. using benchmark data sets like Iris and MNIST.

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