Multi-objective Quantum-inspired Genetic Algorithm for Supervised Learning of Deep Classification Models

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Abstract. Quantum decision making is an emerging field that explores how quantum computing can be used to make decisions more efficiently and effectively than classical computing. The main advantage of quantum decision making is the ability to explore multiple possible solutions to a problem simultaneously, using the principles of superposition and entanglement. A quantum-inspired genetic algorithm can improve a quality of a multi-criteria supervised learning of deep classification models. Designed classifiers can be trained by a quantum simulator with Hadamard, CNOT and rotation gates. To demonstrate advantages of the new algorithm, we analyze the Pareto-optimal classifiers for an efficient diagnosis of SARS-CoV-2 infection based on remote analysis of X-rays images with the quantum computing platform QI.

Keywords: Deep Learning Models, Genetic Algorithms, Quantum Gates.

1 Introduction

The power of quantum computing comes from its ability to perform many computations in parallel. Quantum genetic algorithms leverage this capability by representing the search space in a quantum superposition of states, which allows for exploration of multiple potential solutions at once. These properties make quantum genetic algorithms a promising area of research for solving complex optimization problems, such as those encountered in machine learning. For the above reasons, we propose a quantum-inspired genetic algorithm to train deep neural networks for diagnosis of Covid-19 cases using chest radiography X-rays images. Obtained results of numerical experiments with the quantum simulator QuTech confirmed the great potential of quantum algorithms [24].

To order many important issues in this paper, related work is described in Section II. Then, the issues related to using deep learning in SARS-CoV-2 are characterized in Section III. Next, Section IV presents some studies under quantum encoding and an evolution device for evolutionary algorithms. Finally, some experimental results are presented in Section V.

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To cite this paper please use the final published version:
DOI: 10.1007/978-3-031-36030-5_20

2 Related Work

Richard Feynman introduced hypothesis that a classical computer is not able to simulate physical phenomena such as the quantum computer [11]. Moreover, Benioff confirmed that a quantum computer could meet the principles of a Turing machine [7]. It was also shown that a universal quantum computer could perform tasks impossible to solve by a universal Turing machine [10]. Quantum calculations are based on quantum gates, where qubits in the quantum register are initialized in the $|0\rangle$ state due to the z-basis. There are several quantum algorithms such as Shor's algorithm for factoring large integers [21]. Quantum Monte Carlo, quantum phase estimation, and HHL algorithm have potential applications in machine learning [1]. Grover's algorithm searches an unsorted database in time complexity $O(\sqrt{n})$, while the best-known classical algorithm needs $O(n)$ operations [12].

However, constructing a quantum processor is a challenge because of requirements that are in conflict: state preparation, long coherence times, universal gate operations and qubit readout. Processors based on a few qubits have been demonstrated using several technologies such as nuclear magnetic resonance, cold ion trap and optical systems [18]. A calculation operation is required to be completed much more quickly than the decoherence time [4].

The undoubted development of quantum computers goes hand in hand with the intensive development of artificial intelligence. One of the most interesting ideas concerns the implementation of quantum-inspired genetic algorithms [13]. In a quantum-inspired evolutionary algorithm (QEA), a quantum register is defined by a string of qubits [14]. We believe the quantum register ensures a higher population diversity than other known representations. Besides, the evolution quantum operator implemented by the quantum gate replaces the selection and mutation operators [20]. Solutions are represented probabilistically because the quantum register represents the linear superposition of all possible states. The QEA has been developed for the combinatorial optimization problems such as face verification, the knapsack problem and the Travelling Salesman Problem [6, 26]. Besides, the QMEA found solutions close to the Pareto-optimal front for multi-objective 0/1 knapsack problems [16].

Recently, a framework of genetic algorithm-based CNN has been proposed on multi-access edge computing for automated detection of COVID-19 [15]. In this context, we constructed an adaptive multi-objective quantum-based genetic algorithm (MQGA) for supervised training of deep learning models based on Convolutional Neural Networks. The MQGA works with a quantum register that provides a population of chromosomes that represents hyperparameters of CNNs. In this approach, some strategies for adaptive parameters of the algorithm can be developed, too. The MQGA improves proximity to the Pareto-optimal front and preserving diversity by employing advantages of quantum-inspired gates.

Quantum computing can be simulated in computing clouds, too. IBM offers Quantum Computing as a Service, QCaaS [7]. Alibaba and CAS provide public quantum computing services, too [2]. D-Wave launched Leap, the real-time quantum application environment. Rigetti Computing delivers public Quantum Cloud Services, QCS, where quantum processors are integrated with classical computing infrastructure and

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DOI: 10.1007/978-3-031-36030-5_20

made available to user over the cloud [21]. Moreover, Amazon Quantum Solutions Lab allows developers to work with experts in quantum computing, machine learning, and high-performance computing [3]. Azure Quantum enables an access for diverse quantum software, hardware, and solutions from Microsoft and our partners [19].

3 Dataset with X-ray image collection

The COVID-19 pandemic is still having a devastating impact not only on health and the economy, but also on people's sense of security, well-being and satisfaction. The dataset called COVID-19 Image Data Collection is a publicly available dataset for diagnosis using deep learning algorithms. It consists of chest X-ray and CT scan images (https://github.com/ ieee8023/covid-chestxray-dataset). The dataset COVIDx is available at (https://github.com/lindawangg/COVID-Net). The set RSNA COVID-19 Detection Challenge is provided by the Radiological Society of North America (https://www.kaggle.com/c/rsna-pneumonia-detection-challenge/data). Besides, the SIRM COVID-19 CT Dataset consists of CT scan images collected by the Italian Society of Medical and Interventional Radiology available at https://www.sirm.org/ en/category/articles/covid-19/. Also, the dataset COVID-CT can be used to classify COVID-19 patients and patients with other lung diseases by deep learning models. It was created by researchers from the University of San Diego and is available at https://github.com/UCSD-AI4H/COVID-CT.

The COVIDx dataset is was created by researchers from Qatar University, the University of Dhaka, and the University of Malaysia. The dataset contains over 13,000 chest X-ray images, including 5,445 COVID-19 positive images, as well as images of patients with other types of respiratory diseases and healthy individuals. It is available on various online platforms, including Kaggle, GitHub, and the COVID-19 Image Data Collection website [28].

We designed an experimental Covid-19 CXR diagnostic cloud (Covid CXR) to be made available for some clinicians to support the diagnosis of coronavirus 2. In the next stage, the Covid-19 detection application will be available for patients via the Internet. The advantage of this solution is the reduction of costs and a short waiting time for the test result (few seconds), which in turn is of key importance for improving not only the health situation, but also the economic and social situations.

When infected patients are effectively screened, they can receive immediate treatment and care, and be isolated to reduce the spread of the virus. It is worth mentioning that reverse transcriptase-polymerase chain reaction (RT-PCR) testing is currently being used to detect COVID-19 cases. However, RT-PCR tests are very time-consuming, complicated, and also require the involvement of diagnosticians, who are few in relation to the needs. The sensitivity of RT-PCR tests varies depending on the manufacturer and the batch, and the studies show relatively low precision. Some studies even suggest that radiographic data analysis could be used as a primary screening tool for COVID-19. In particular, most positive cases show bilateral abnormalities in the CXR images, including lack of transparency and interstitial abnormalities. An initial diagnosis can also be made using the mobile application [28].

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4 Multi-objective quantum deep learning

A multi-objective quantum-inspired genetic algorithm MQGA operates on the quantum register that represents hyperparameters of CNNs. It is made up of several layers that perform different operations on the input chest X-ray images. The basic structure consists of three types of layers. A convolutional layer applies a set of learnable filters to extract relevant features from the input image. The filters are small, square-shaped matrices that slide over the image in a specific pattern, performing a convolution operation at each position. The convolutional layer provides a set of feature maps that highlight the most important features of the input image. The pooling layer reduces the spatial dimensions of the entered feature maps. The most common type of pooling is *max pooling*, which takes the maximum value of each non-overlapping subregion of the feature map.

The fully connected layer classifies the chest X-ray image based on the pooling layer. It takes the flattened output of the previous layers and applies a set of weights to produce a final output vector. A sequence of these three layers are repeated L times. The final output layer is *softmax* layer that produces a set of probabilities of the chest X-ray image belonging to two of the possible classes. The class with the highest predicted probability is then assigned as the final output.

Training adjusts the filter weights so that the CNN can learn to recognize important features. This is done using a form of gradient descent optimization algorithm, such as stochastic gradient descent (SGD) or ADAM with the learning rate to control the updates of weights during training. We need to know the number L of weave layers with parameters related to the number of neurons in three dimensions. The size of the input image determines the size of the feature maps and there are both L filters and feature maps generated in the convolutional layers. Besides, the given size of the filters determines the size of the receptive field and the features that are extracted. We tune the stride level S (in %) that determines the amount of shift of the filter.

The padding value PV (in %) determines extra rows and columns of pixels to the input image to preserve the spatial dimensions of the output feature maps. We consider the most widely used activation function ReLU Besides, a sigmoid activation function and a tanh activation function (Hyperbolic Tangent) are used. Their limitations for gradient based algorithms, such as vanishing gradients, can be easily omitted by MQGA. Moreover, softmax is used to produce a probability distribution over two classes, with the sum of all probabilities equal to 1. Another hyperparameter of the CNN is the number of hidden layers in the network that affects the complexity of the learned features. The batch size BS determines the number of samples used in each iteration.

A qubit can exist in more than one state (a superposition) at the same moment in time and can be represented by the Bloch sphere. The qubit can be modeled as a two-layer quantum bit from the Hilbert space H_2 with the base $B = \{|0\rangle, |1\rangle\}$. The qubit may be in the "1" binary state, in the "0" state, or in any superposition of them [17]. The state x_m of the mth qubit in the Q-chromosome can be written, as follows [5]:

$$Q_m = \alpha_m|0\rangle \oplus \beta_m|1\rangle, \tag{1}$$

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DOI: 10.1007/978-3-031-36030-5_20

where
α_m and β_m – the complex numbers that specify the amplitudes of the states 0 and 1, respectively;
$\oplus$ – a superposition operation;
m – the index of the gene in the chromosome, $m = \overline{1, M}$.

The value $|\alpha_m|^2$ is the probability that we observe the state "0". Similarly, $|\beta_m|^2$ is the probability that state "1" is measured. The qubit is characterized by the pair (α_m, β_m) with the constraint, as below [21]:

$$|\alpha_m|^2 + |\beta_m|^2 = 1. \quad (2)$$

Dirac notation is often used to select a basis. The basis for a qubit (two dimensions) is $|0\rangle = (1,0)$ and $|1\rangle = (0,1)$. The most commonly used representation of a chromosome in a genetic algorithm is the matrix, as follows [22]:

$$Q = \begin{bmatrix} |\alpha_1| & \dots & |\alpha_m| & \dots & |\alpha_M| \\ |\beta_1| & \dots & |\beta_m| & \dots & |\beta_M| \end{bmatrix} \quad (3)$$

However, the state $Q_m = \alpha_m|0\rangle \oplus \beta_m|1\rangle$ of the mth qubit can be represented as the point on the 3D Bloch sphere (Fig. 1), as follows [23]:

$$\left|Q_m\right\rangle = \cos\frac{\theta_m}{2}\left|0\right\rangle + e^{i\phi_m}\sin\frac{\theta_m}{2}\ |1\rangle, \quad m = \overline{1, M} \quad (4)$$

where $0 \le \theta_m \le \pi$ and $0 \le \phi_m \le 2\pi$.

Two angles θ_m and ϕ_m determines the localization of mth qubit on the Bloch sphere. In addition to the representation of (3), we can therefore distinguish the following other models of the chromosome [27]:

$$Q^{sign} = \begin{bmatrix} |\alpha_1| & \dots & |\alpha_m| & \dots & |\alpha_M| \\ sign(r_1) & \dots & sign(r_m) & \dots & sign(r_M) \end{bmatrix} \quad (5)$$

where r_m – the random number from the interval [-1; 1], and also it is, as below [29]:

$$Q^{vector} = [|\alpha_1|, \dots, |\alpha_m|, \dots, |\alpha_M|] \quad (6)$$

$$Q^{angle} = \begin{bmatrix} \theta_1 & \dots & \theta_m & \dots & \theta_M \\ \phi_1 & \dots & \phi_m & \dots & \phi_M \end{bmatrix} \quad (7)$$

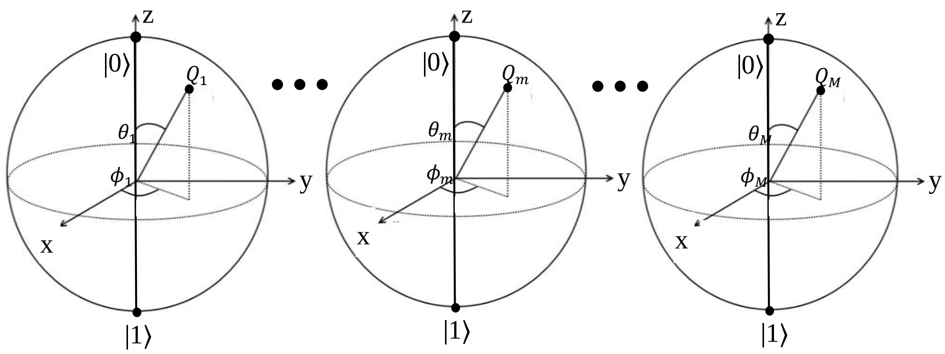

Fig. 1. The set of Bloch spheres for the quantum register Q.

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DOI: 10.1007/978-3-031-36030-5_20

There are two important criteria for deep learning. The first one is an accuracy and the second criterion is F_1-score. We determine non-dominated solutions from the current population and copy them to the archive after verification. Figure 2 shows the initialization *Q(t)* by Hadamard gates and rotation gates. Then, digital population *P(t)* is created by observation the states of *Q(t)*.

Fig. 2. A diagram of the quantum evolution circuit at Quantum Inspire platform.

Figure 3 shows a histogram after updating the register *Q*(*t*) using the rotation gates *Rx*, *Ry*, *Rz* refer to best group. Digital algorithms for calculation this probability distribution is exponentially more difficult as the number of qubits (width) and number of gate cycles (depth) raise [24].

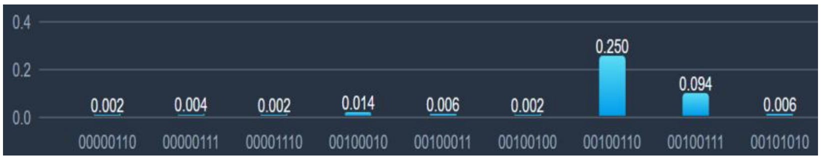

Fig. 3. Histogram after updating the population *Q*(*t*).

5. Numerical experiments

We consider an instance of the multi-objective seep learning instance for the dataset COVIDx with 13,975 CXR images across 13,870 patient cases. Table 1 shows characteristics for three CNNs. By comparison three models, we can recommend QCNN regarding its dominance regarding accuracy and F1-score.

Table 1. Comparison of Convolutional Neural Networks.

	QCNN		RESNET		SENET	
	Value	#	Value	#	Value	#
Accuracy	0.982	1	0.952	3	0.951	2
F1-score	0.984	1	0.949	2	0.948	3

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Concluding remarks

We presented QCNN trained by a quantum-inspired multi-objective evolutionary algorithm in an attempt to gain deeper insights into critical factors associated with COVID-19 cases, which can aid clinicians in improved screening. Development of Pareto-optimal deep learning solutions for detecting COVID-19 cases from CXR images can predict hospitalization duration which would be useful for triaging, patient population management, and individualized care planning.

We also introduces a new machine learning paradigm based on quantum computers. Our futures work will be focused on developing this approach to the other Covid datasets. Besides, the other artificial neural networks will be tested.

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DOI: 10.1007/978-3-031-36030-5_20