

Enhanced Machine Learning using Quantum Computing

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Abstract—In recent times, increasing amount of the data have enriched the decision making using machine learning. Despite of the growth in the domain of machine learning, the proximity to the physical limits of chip fabrication in classical computing is motivating researchers to explore the properties of quantum computing. A few research efforts have demonstrated that quantum computers which leverages the properties of quantum mechanics, carries the ability to surpass classical computers in machine learning tasks. The study in this paper contributes in enabling researchers to understand how quantum computers can bring a paradigm shift in the field of machine learning. The paper focuses on the concepts of quantum computing that would be used by any machine learning technique to facilitate quantum machine learning. It also studies different quantum algorithms that could be used as core subroutines in machine learning techniques and highlights the famous Grover's algorithm. These subroutines are used to enhance the efficacy of machine learning tasks. The paper towards the end advocates the use of quantum application software and throws light on the existing challenges faced by quantum computers in the current scenario.

Index Terms—Entanglement, Machine Learning, Quantum Computing, Quantum Machine Learning, Quantum Supremacy, Speedup, Superposition, Quantum Algorithms

I. INTRODUCTION

In recent years, owing to increase amount of datasets, success of machine learning has gained momentum in transforming science and technology [1]. The aim of machine learning is to enable computers to act in a manner that barely involves any kind of human intervention and does not require the need of being programmed explicitly [2]. The vast applications of machine learning ranging from predicting protein structure, drug discovery in biology [3] to black hole detection [4], wave analysis in physics [5] to speech recognition, vehicles detection in parking lot [6], data leakage prevention [7], etc. in computers exhibits a remarkable contribution in the existing scenario. However, the ever growing size of dataset, has posed certain challenges in this field. With the Moore's law moving towards its extinction, we might probably attain a peak where current computational methods would not suffice in handling such humongous datasets [8]. This motivated to use the concept of quantum computing which is based on quantum mechanics. The application of quantum mechanics in the discipline of information processing is termed as *Quantum Information Processing* [9].

Quantum information processing offers great advantages over classical information processing, by enabling execution of algorithms in an efficient manner [10] and providing secure communications [11]. The applications developed in the field of machine learning utilizing quantum computing algorithms exceeds the capabilities of any classical computers depicting *quantum supremacy*. A successful demonstration of quantum supremacy would prove that engineered quantum systems can outperform the most advanced classical computers [12].

The *major contribution* of the paper are as follows. The paper presents the concept of machine learning in classical environment and explores the concepts of quantum computing used for enabling machine learning in quantum environment. It further enumerates quantum machine learning and describes the two famous quantum algorithm i.e., Grover's and HHL. The implementation of Grover's algorithm is carried out and its results are analyzed. These algorithms are used as core subroutines in machine learning techniques to enhance their efficiency. The paper also enlists various programming platforms available. These software makes use of actual quantum machines that enables implementation of machine learning techniques in quantum environment. The study also discusses certain challenges faced by quantum computing and how it is still efficient with respect to classical machine learning.

The *motivation* of the paper is to provide technical insights to the community of machine learning researchers and quantum computing scientists about the subject. The *emphobjective* of the paper is to describe how quantum computing can benefit machine learning and what are the challenges faced while implementing machine learning in quantum environment.

The *outline* of the paper is as follows: Section II discusses the related work. Section III describes the concepts and precursors required to study the paper. Section IV analyzes quantum machine learning in detail and provides analysis of speedup for various machine learning techniques which utilizes the concept of quantum computing. Section V discusses various programming platforms for executing quantum machine learning. Section VI discusses the challenges and Section VII concludes the study.

II. LITERATURE SURVEY

Quantum computers are perceived to be exponentially faster for a few tasks that could surpass today's computers computational capabilities. By exploring the properties of quantum computing such as entanglement and superposition, quantum computers could efficiently solve some problems that are perceived as hard problems for classical computers [13]–[15]. The quantum information processing uses qubits as its basic unit analogous to classical bits used for classical information processing.

In 1994, Peter Shor manifested integer factorization in polynomial time with the help of quantum algorithm. This proved a major breakthrough in breaking public-key crypto systems based on integer factorization method [16], [17]. Quantum algorithms envisaged that speedup could be seen when the quantum environment is used as against the classical environment. Quantum simulation enables modeling of atomic scale interactions that helps to approximate behavior in drugs, material science and organics. It also enables simulation of quantum field theories [18]–[20]. Swap Test is used to estimate distance between any two input vectors of the dataset and is exponentially faster as compared to the classical method [21]. Quantum Fourier transform, which is analogous to classical discrete fourier transform experiences exponential speedup as against the classical version of calculating Fourier transforms [22]–[24]. Grover's search algorithm facilitates quadratically faster search operation in an unstructured database [25]. HHL algorithm provides exponential speedup for solving system of linear equations [26]. This paper discusses Grover's and HHL algorithms along with its use cases.

Quantum computing also provides security to the algorithms due to its exceptional properties. Quantum communication is inherently secure. It ensures confidentiality and integrity of data respectively. A lot of research has taken place with regards to authentication of participation entities in quantum channel which provides considerable advantages over the conventional channel especially against Man In The Middle attacks [27]–[30].

TABLE I
COMPLEXITIES FOR VARIOUS SUBROUTINES IN CLASSICAL AND QUANTUM ENVIRONMENT

Subroutines	Classical	Quantum
Distance Calculation	$\mathcal{O}(\log n)$	$\mathcal{O}(\log n)$
Searching	$\mathcal{O}(2^n)$	$\mathcal{O}(\sqrt{2^n})$
Solving systems of Linear Equations	$\mathcal{O}(n \log n)$	$\mathcal{O}((\log n)^2)$
Fourier Transform	$\mathcal{O}(n 2^n)$	$\mathcal{O}(n \log n)$

III. PRELIMINARIES

This section describes machine learning in classical environment. It also enumerates the concepts of quantum computing.

A. Classical Machine Learning

Machine learning, is a sub-discipline of artificial intelligence where learning from data is involved. Arthur Samuel, in 1959, described machine learning as “a field of study that gives computers the ability to learn without being explicitly programmed” [31]. Machine learning is used to find hidden structures and interesting patterns from the given dataset. The intrinsic value of data can be augmented with machine learning. This value can be fetched in different manner depending upon the nature of the dataset available. Broadly, the term *learning* in machine learning can be divided into three types: *Supervised Learning*, *Unsupervised Learning* and *Reinforcement Learning*. In *Supervised Learning* a computer is fed with input-output data pairs that helps to infer an algorithm and predict the output. It is generally used for classification of data based on the labels. Examples of supervised learning classifier includes K Nearest Neighbors, Decision Tree, Naive Bayes and Random Forest models. In *Unsupervised Learning* input-output data pairs are not given to the machine, rather the system is fed with unlabeled data and hence it builds an algorithm to find the patterns. It is basically used for clustering of data. Some of the examples are Apriori, K-means and Principal Component Analysis. *Reinforcement Learning* uses software agents to earn cumulative rewards and thus proceed to train the algorithm in a certain manner. In all these learning methods, the indispensable role is of training phase. Training phase is often considered as most costly phase of any machine learning process. When dealing with extremely large datasets efficient training methods plays a vital role.

Irrespective of what learning method is adopted, an optimal machine learning algorithm is the one which produces a minimum error rate by consuming minimum resources. Due to ever increasing rate of data, current machine learning systems are nudging the limit of classical computational resources. Challenges lies in the problem of finding an optimal solution to any problem, that helps to minimize the complexity class of the problem [32]. This is where the need arises to shift to quantum computing.

B. Quantum Computing

Quantum computing enable researchers to deal with *quantum information*. The quantum information involves processing, storing and transferring of information which is encoded in quantum mechanical systems. Quantum information is processed by acting upon quantum systems. Basic quantum computing concepts that influence any algorithm to perform in an efficient manner [33].

1) *Qubit*: Quantum bits or qubit is the basic unit of processing information in quantum systems analogous to a bit in classical systems. A qubit can exist in one or more than one state simultaneously. However, the information content stored in a qubit that is equivalent to a single bit in classical medium. It is defined as linear superposition of states.

$$|\psi\rangle = \alpha|0\rangle + \beta|1\rangle \quad \alpha, \beta \in \mathbb{C}$$

where, $|\alpha|^2 + |\beta|^2 = 1$. The complex numbers α and β are probabilities of the basic states of $|0\rangle$ and $|1\rangle$, and $|0\rangle$ and $|1\rangle$

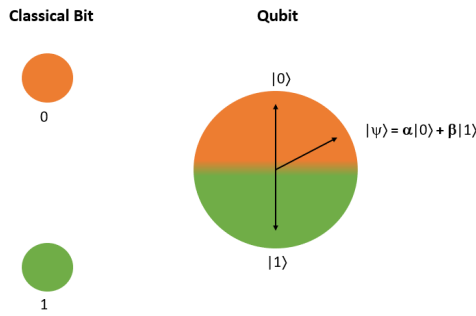


Fig. 1. Difference between Classical bit and Qubit

represent the orthogonal states. Fig. 1 depicts the difference between classical bit and qubit.

2) *Superposition*: A qubit can be in a state of $|0\rangle$ and $|1\rangle$ at the same time. This implies that to store two bit worth of value only one qubit is required. On similar lines for 4 bits, 2 qubits will be required and hence, $2^N \text{Classical Bits}$ can be stored on $N \text{Qubits}$. This means that a particle has an ability to exist in multiple quantum states and when the measurement is performed, it undergoes certain changes resulting in a probabilistic value, thereby losing its individuality. Fig. 1 states that as qubit can exist in multiple states at the same time hence it could provide a reduction in storage space and handle complex computations by inducing *parallelism*.

3) *Entanglement*: In a multi qubit system, qubits exist in a manner that they lose their individuality. It means the property of one qubit is connected to the property of another qubit. Thus, this property helps the qubits to be correlated with each other despite of being separated by large physical distances.

4) *No cloning theorem*: This theorem states that it is not possible to create an identical copy of an arbitrary unknown quantum state. It helps to infer that once a measurement is performed, it is not sure to get the same information after another measurement being performed on an already measured state.

5) *Wave Function Collapse*: Quantum measurement depends on the wave function collapse. Due to interaction with the external world, the wave function which is initially in a superposition of several states gets reduced to a single state. This leads to measurement of a quantum state which is probabilistic in nature.

6) *Quantum Gates*: Quantum gates are the quantum operations used to transform qubit from input state to desired output state. Once a quantum gate is applied it is expected that the norm of the state vectors maintain its unity i.e., the sum of the squares of probability of amplitudes should be equal to one. These gates are reversible in nature. These quantum gates are used as a basic building block in machine learning to perform computations.

Few basic quantum gates that may be used in machine learning are listed in Table II.

TABLE II
BASIC QUANTUM GATES

Quantum Gate	Matrix Representation
Hadamard	$\frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}$
Not	$\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$
Pauli-X	$\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$
Pauli-Y	$\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$
Pauli-Z	$\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$
CX (Controlled Not)	$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix}$
SWAP	$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$
Fredkin(CSWAP)	$\begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix}$
$R_x(\Theta)$ (Rotation X)	$\begin{pmatrix} \cos(\Theta/2) & i\sin(\Theta/2) \\ i\sin(\Theta/2) & \cos(\Theta/2) \end{pmatrix}$
$R_y(\Theta)$ (Rotation Y)	$\begin{pmatrix} \cos(\Theta/2) & \sin(\Theta/2) \\ \sin(\Theta/2) & \cos(\Theta/2) \end{pmatrix}$
$R_z(\Theta)$ (Rotation Z)	$\begin{pmatrix} e^{-i(\alpha/2)} & 0 \\ 0 & e^{i(\alpha/2)} \end{pmatrix}$
$U3(\Theta, \phi, \lambda)$	$\begin{pmatrix} \cos(\Theta/2) & e^{i\phi}\sin(\Theta/2) \\ e^{i\lambda}\sin(\Theta/2) & \cos(\Theta/2) \end{pmatrix}$

These paramount features offered by quantum computers are required for high speed computing which paves way to delve deeper and integrate machine learning with quantum computing.

IV. QUANTUM MACHINE LEARNING

Quantum Machine Learning (QML) is the intersection of machine learning process with the concepts of quantum computing. In QML, quantum algorithms are devised to solve intricate problems of machine learning by utilizing the potency of quantum computing. This is achieved by enabling expensive subroutines of classical algorithms to be executed on a quantum computer. The properties of quantum computing such as superposition induces *parallelism* in quantum computers which allows to evaluate function on many inputs in machine learning algorithms simultaneously. Entanglement provides a mechanism for improving the storage capacity as well as retrieving corrupted or incomplete information [34], [35]. These properties thus provide significant speedup of any computation evaluated on the basis of complexity [36]. By speedup it means the advantages obtained in run time by any quantum algorithm as compared to the classical methods used for the same task [37].

A. Core Subroutines

The paper studies two major quantum algorithms used as a subroutine by various machine learning techniques to gain speedup.

1) *Grovers Algorithm*: Grover's algorithm is used as a core-routine in many machine learning algorithms. Most of the NP-complete algorithms like K-Means, Traveling Salesman Problem etc. require searching of a key element or entity from the dataset as their subroutine and lack of an efficient searching algorithm may degrade the performance of the entire machine learning algorithm. NP-Complete is a set of decision problems which can be solved by non deterministic Turing Machines in polynomial time. Hence, the time required to solve the problem using any currently known technique increases expeditiously as the size of the data grows. Grover's algorithm helps to find an element in an unordered set quadratically faster compared to the theoretical limit for any classical algorithm. While classical algorithms can take $\mathcal{O}(n)$ to detect the matching element in a dataset having n input values, Grover's algorithm can carry out the same task on a quantum computer in $\mathcal{O}(\sqrt{n})$ steps. In machine learning, it is applied on optimization problem, where minima is to be computed. Grover's algorithm applies quantum oracle which is a unitary operator and is used to checks if the searched result is correct. It does this by stating which items are smaller than the threshold value and executes it several times to find out the correct solution. The effect of Grover algorithm results in speedup and therefore, majority of the machine learning algorithms uses it as a sub-routine.

The experimental analysis of the algorithm is depicted. Qiskit software offered by IBM is selected for performing the experiment. Qiskit provides access to various quantum machines and simulators with varied qubit configurations. For more information on Qiskit refer Table IV. This paper uses *ibmq_qasm_simulator* for the execution of code and analysis of the result.

The algorithm finds the required number from a given set of values. Here, total 16 values are given as input and the algorithm will notify the required number by indicating the highest probability for that value. For our analysis, we have given value as 0 or (in binary "0000") to be searched by the algorithm. The different instances from Fig. 2, Fig. 3 and Fig. 4 depicts that the highest probability is noted for "0000". But in all the three figures the probability value is different though it is the highest amongst all. This is because the quantum measurements are probabilistic in nature and does not produce the exact same results every time. Similarly, if the value as 3 (in binary "0011") is to be realized from the given set of possible numbers, then it has the highest probability in all the three cases as depicted in Fig. 5, Fig. 6 and Fig. 7. But again due to the uncertainties in quantum measurements due to its probabilistic nature, it follows the same line where the probabilities of the searched element are not constant, but the highest amongst all the possible values. This denotes that even though quantum measurements have uncertainties due

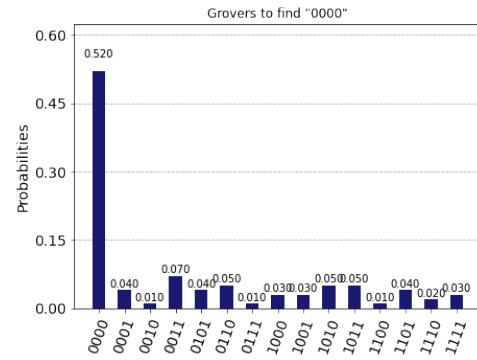


Fig. 2. Grovers Search to find "0000"; Instance: 1

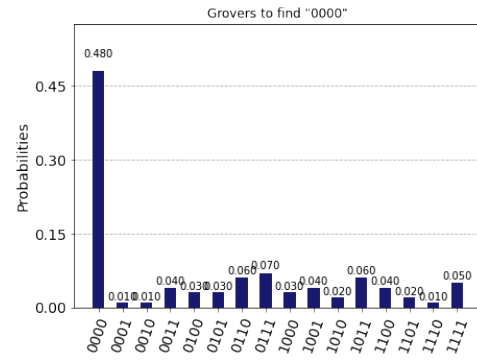


Fig. 3. Grovers Search to find "0000"; Instance: 2

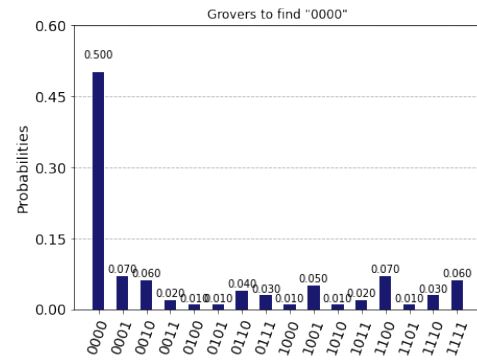


Fig. 4. Grovers Search to find "0000"; Instance: 3

to the nature of quantum particles, the expected result is still obtained. Hence such algorithms play a vital role in enhancing machine learning techniques.

2) *Harrow-Hassidim-Lloyd (HHL) Algorithm*: HHL algorithm is another famous quantum algorithm which is used as a core subroutine in various machine learning techniques to offer speedup. This technique is used to solve system of linear equations. In the field of science and engineering, linear systems plays a major role. As HHL algorithm attains exponential speedup over classical algorithm, it can be widely used in data processing, numerical calculation, quantum machine learning models including the support vector machines, linear

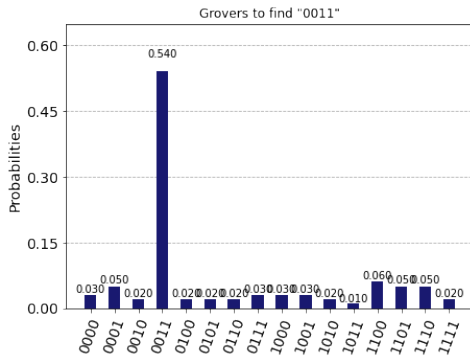


Fig. 5. Grover's Search to find "0011"; Instance: 1

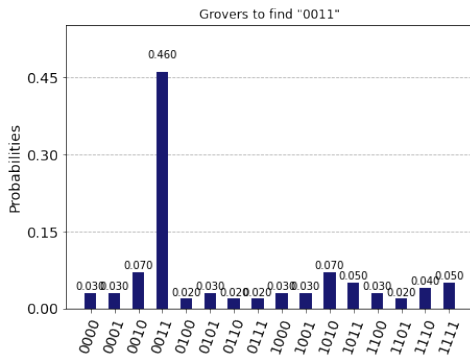


Fig. 6. Grover's Search to find "0011"; Instance: 2

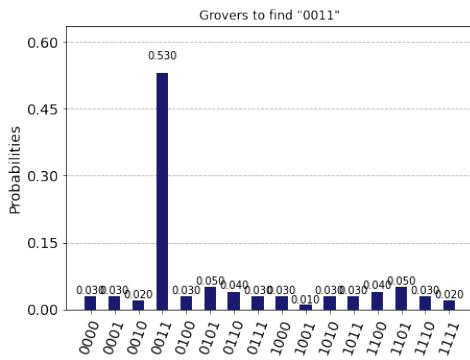


Fig. 7. Grover's Search to find "0011"; Instance: 3

regression and recommendation systems etc.

B. Performance Enhancement using Core Subroutines

This section describes performance enhancements in various machine learning techniques. It uses the core sub routines that rely on quantum computing and enriches the performance of any machine learning technique if used. The part of algorithm which requires complex calculations can be integrated with quantum resources and the data can be trained, analyzed and evaluated in an efficient and rigorous manner. That part can be integrated with the above mentioned subroutines to produce efficacy. Table III gives a general overview of the different machine learning algorithms and their speedups when executed

on quantum computers. It also states if the Grover and HHL subroutine is used in the algorithms. These core subroutines are used by these machine learning algorithms which uses the properties of quantum computing as discussed to enhance their efficiency. It will thus help to understand how quantum computers can revolutionize machine learning.

TABLE III
SPEED UP OF MACHINE LEARNING ALGORITHMS IN QUANTUM ENVIRONMENT

Algorithm	Speedup	Grover	HHL
Associative Memory [38]	Exponential improvement in capacity	✓	
Divisive Clustering [39]	Quadratic	✓	
K-Means [36], [40]	Exponential	✓	
K-Medians [39]	Quadratic	✓	
K Nearest Neighbors [41]	Quadratic	✓	
Pattern Recognition [42]	Exponential improvement in capacity	✓	
Principal Components Analysis [43]	Exponential		✓
Recommendation Systems [44]	Exponential	✓	✓
Support Vector Machines [45]	Exponential		✓

V. QUANTUM APPLICATION SOFTWARE

The gap between the computational models and its actual implementation has been narrowed down to a great extent with the development of open-source quantum software platforms around the globe. Some leading-edge quantum platforms like *QISKIT* [46], *D-Wave* [47], *ProjectQ* [48], *Forest* [49], *Strawberry Fields* [50], *Quantum Development Kit* [51] and *Cirq* [52]. allow these algorithms to be implemented on real quantum computers which can be accessed through cloud based services or quantum simulators which runs on classical machines [53]. Thus these software makes it possible to implement machine learning in quantum environment and experience the enhanced outcomes.

Table IV lists the software that provides platform for execution of machine learning techniques using the built in modules and libraries. It also states which software offers the maximum number of qubits when the real quantum device is accessed or while accessing quantum simulators. According to the need of number of qubits and flexibility of environment, a programmer may chose the software best suited to cater to the demands.

VI. CHALLENGES

QML poses a great challenge in the field of Quantum Information Processing as quantum computing is still in its infancy stage of development. Qubits are affected by various disturbances such as vibrations, electromagnetic waves, temperature fluctuations, cosmic rays, etc. that are induced by the effects of quantum mechanics which are extremely sensitive to external conditions. This fragile nature of qubits makes them prone to high errors. Due to this, any kind of vibration impacts the atoms and causes de-coherence which leads to inaccuracy in the desired results of quantum algorithms [54]. The researchers

are working in the field of mitigating errors induced due to noise and fragile nature of quantum computers [55]. A major challenge is the architecture and design of quantum machines that have a significant effect on measurement values. The deviation in probability measurement and impact of noise due to various factors enables better appreciation of obtained results and provides an estimation of degree of erroneous measurements that may arise depending on the configuration chosen to execute a quantum circuit [56]. A rigorous study is required to decide upon how many logical qubits are required by quantum computers to exceed the capabilities of classical computers, that are extremely powerful [57].

TABLE IV
COMPARATIVE STUDY OF VARIOUS QUANTUM SOFTWARE

Quantum Software	Institution	Quantum Hardware Max. no. of qubits	Quantum Simulator Max. no. of qubits
Qiskit	IBM	65 [58]	32 [58]
Quantum Development Kit	Microsoft	IonQ [59]: 79 and Honeywell (H1) [60]: 10	40
Ocean	D-Wave Systems	2000	
Cirq	Google	72	40
Strawberry Fields	Xanadu	8 [61]	
Forest	Rigetti	31 [62]	26

VII. CONCLUSION

The study in this paper reveals that with the existence of quantum supremacy a drastic change will be seen in the field of machine learning. The immense challenges require different approaches of quantum computing to be devised and investigated to enhance machine learning methods. Table II depicts that the properties leveraged by quantum computers helps to achieve considerable speedups in the field of machine learning. Table IV conveys different types of software platform to implement machine learning along with its processing capabilities. The paper also states certain challenges faced by QML in the existing situations. Although QML has gained a lot of awareness amongst quantum scientists and machine learning researchers, yet in order to gain maximum benefits areas which remain unfolded may be explored and delved deeper.

Future Scope. The various quantum machine learning algorithms as discussed incorporates core quantum subroutines which may be realized on different quantum machines.

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