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Quantum Machine Learning: Past, Present, and Future

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Abstract: *In recent decades, classical machine learning (CML) has seen rapid development, allowing computers to generate reliable results accurately and quickly. In the last decade, as more powerful computers (both in software and hardware) and significant amounts of data become available, several breakthroughs in CML happened, including but not limited to AlexNet for image classifications, Gated Recurrent Unit for sequential predictions, BERT/transformer for natural language processing. However, there are natural limitations for CML that quantum machine. Thus, computer scientists turned their attention to quantum machine learning (QML), a new field that utilizes quantum properties to produce less time-consuming results while maintaining accuracy.*

Keywords: *classical machine learning (CML); quantum machine learning (QML); Challenges; prospects*

1. Introduction

As shown in Figure 1, CML (blue) generally includes classical data trained with classical models, while QML (orange) consists of any tasks with quantum data or models.

Though the concept of quantum computing was first proposed by Feynman in 1982, breakthroughs in the field were mainly developed after 1990. For instance, Shor's algorithm, introduced in 1994, demonstrated that a quantum computer could factor large numbers exponentially faster than the best classical algorithms known at the time. In 2008, the Harrow-Hassidim-Lloyd (HHL) algorithm allowed linear algebra problems to be solved much quicker on quantum computers [1](Najafi et al., 2022). In recent years, tools like quantum kernel, quantum neural networks (QNN), and quantum support vector machine (QSVM) have allowed quicker calculations and seek to expand quantum advantage to include more applications. However, to understand quantum advantage, one first should understand the fundamental differences that separate QML from CML.

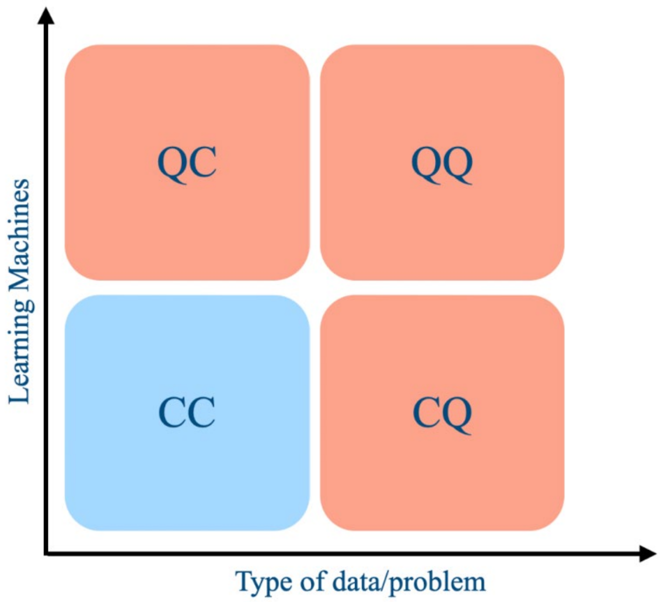

Figure 1: CML (blue) QML (orange)

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2. Quantum Properties

QML differs significantly from CML due to its natural properties. For instance, the fundamental computation units of QML, qubits (quantum bits), possess the superposition property. Where a bit, the basic unit CML, can only possess a state of 0 or 1, a qubit can exist between 0 and 1. This means that under superposition, qubits represent more complicated information than bits. This allows for parallel processing (consider multiple possibilities in parallel) and advanced encoding (multiple pieces of information in one qubit) that can accelerate certain calculations. We can see it in Figure 2.

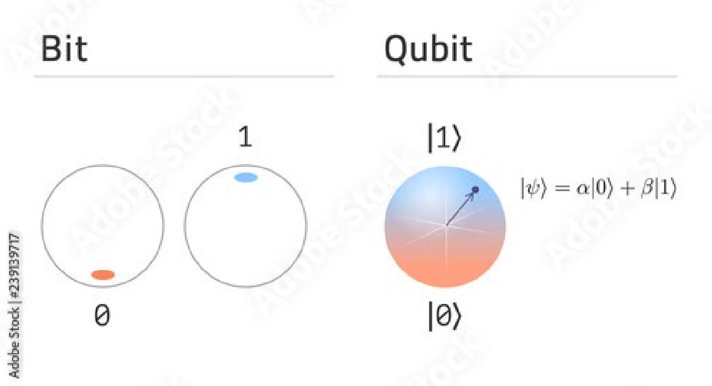

Figure 2: The differences between QML and CML

Specifically, the state of the qubit, $|\Psi >$ can be visualized in a 3D space called the Bloch sphere as shown in Figure 3 and mathematically represented as the following:

$$|\Psi\rangle \ = \propto |0\rangle \ + \ \beta\,|1\rangle$$

Where $\propto$ and β are complex numbers that satisfy $|\alpha|^2 + |\beta|^2 = 1$ (Remanan, 2021)[5]. The probability that the state collapse into state |b> (b = 0 or 1) is represented by: $P(b) = |\langle b|\psi\rangle|^2$; $\sum P(b) = 1$

In quantum mechanics, $< \mathrm{b}|$ is known as bra notation and $|\Psi >$ is ket notation, together $< \mathrm{b}|\Psi >$ is bra-ket, measured with the inner product of b and Ψ. It is similar to a dot product that measures the similarity of both by projecting one on the other. <1, 1> and <0, 0> = 1 (normalized, length = 1), where <1, 0> and <0, 1> = 0 (orthogonal, no projection). To simplify the inner product, one can consider P (0) = $|\alpha|^2$ and P (1) = $|\beta|^2$.

Since $\mathrm{a} + \mathrm{bi} = \cos\theta + \mathrm{i}\sin\theta$, the equation can be written as:

$$|\psi\rangle = \ e^{i\gamma}\left(\cos\frac{\theta}{2}|0\rangle + \ e^{i\phi}\sin\frac{\theta}{2}|1\rangle\right)$$

After omitting the common factor $e^{i\gamma}$ (which does not affect the location of a point on the Bloch sphere), we obtain the state of qubit that lies anywhere on the sphere (Meyer et al., 2022)[3].

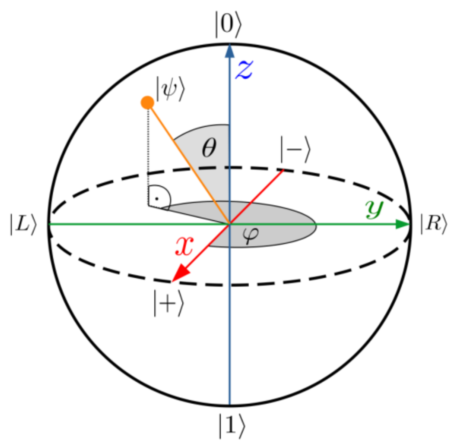

Figure 3: The Bloch sphere

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In this representation, the points on positive x axis (+) and positive y (R or +i) axis are

$$|+\rangle = \frac{|0\rangle + |1\rangle}{\sqrt{2}}$$

And

$$|R\rangle = \frac{|0\rangle + i|1\rangle}{\sqrt{2}}$$

Multiple qubits (n-qubit system) create a Hilbert space of multiple (n^2) dimensions, where the state is defined as:

$$|\psi\rangle = c_0|00\cdots00\rangle + c_1|00\cdots01\rangle + \cdots + c_{2^n-1}|11\cdots11\rangle$$

where

$$\sum_{i=0}^{2^n-1} |c_i|^2 = 1$$

This means that a system of n qubits can encode information scaling in O(2^n) compared to O(n) in bits in CML (Zeguendry et al, 2023)[8].

To perform matrix operations on qubits, each qubit has a unique 2*1 matrix representation. For instance, states |0> and |1> are:

$$|0\rangle = \begin{pmatrix}1\\0\end{pmatrix} \ ; \ |1\rangle = \begin{pmatrix}0\\1\end{pmatrix}$$

To compute, qubits may go through quantum gates (single and/or multi-qubit operations) that manipulate their states. Examples of single-qubit gates include Pauli X, Y, and Z gates as represented in Figure 4 (Zeguendry et al, 2023)[8].

- Pauli X Gate: “not” operator

$$X := \begin{pmatrix}0 & 1\\1 & 0\end{pmatrix}$$

- For instance, applying this gate to |0> will produce |1>

$$\begin{pmatrix}0 & 1\\1 & 0\end{pmatrix}\begin{pmatrix}1\\0\end{pmatrix} = \begin{pmatrix}0\\1\end{pmatrix}$$

- Pauli Y Gate: similar to X gate but also change phase (|0> to i|1>)

$$Y := \begin{pmatrix}0 & -i\\i & 0\end{pmatrix}$$

- Pauli Z Gate: 180 degrees rotation around the z-axis (axis of |0> and |1>)

$$Z := \begin{pmatrix}1 & 0\\0 & -1\end{pmatrix}$$

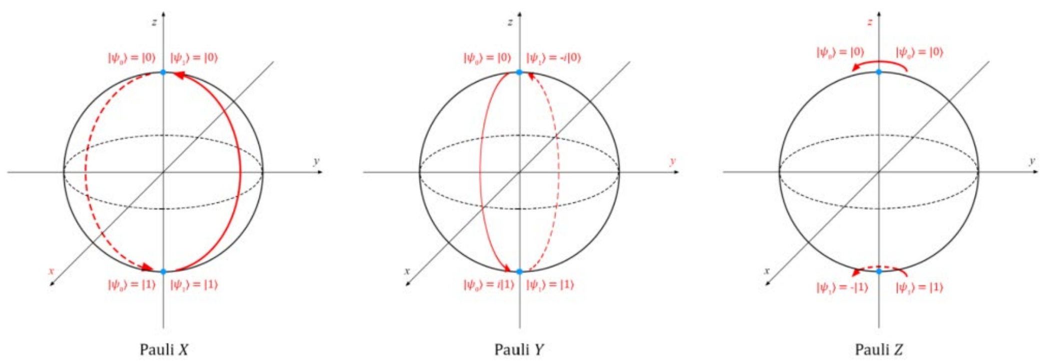

Figure 4: Pauli X, Y, and Z gates

Another important property of QML is quantum entanglement (performed with CNOT multi-qubit gate), where two or more qubits are connected in a way where the states of each qubit are dependent on

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the others. This allows QML to establish hidden connections between features that are impossible to achieve with CML. Entanglement allows for quantum systems to excel in factoring (Shor's algorithm, essential to cryptography and cybersecurity), optimization (for more effective complex/high dimensional solution space), database search (Grover's algorithm), etc.

3. Quantum Advantages

With the special properties of quantum computing, QML algorithms have the potential to outperform any CML algorithms in specific problems. This is known as quantum speedup. In the following section, we will discuss problems that quantum advantage may likely occur.

3.1. Linear Algebra Problems and Complex Matrix

Many linear algebra problems, like solving a system of linear algebra equations, finding eigenvectors and eigenvalues, and completing Fourier transformation, can be done exponentially faster with QML (e.g., HHL algorithm) than CML (Biamonte et al., 2018)[2].

3.2. Optimization

Minimizing the loss function and reaching the absolute minimum of the cost function is crucial to the success of any ML model. Compared to CML, which requires many iterations and is often costly, QML could explore multiple solutions at the present state thanks to the superposition property, making it potentially more reliable and less time-consuming than CML. For instance, the Quantum Approximate Optimization Algorithm (QAOA) utilizes quantum gates to adjust the states of the qubits. Then, it adjusts the status of gates using classical optimization techniques. This combinatory optimization tackles many real-world problems like navigation, finance, and healthcare.

3.3. Quantum Principle Component Analysis

Principle Component Analysis reduces the dimension of large data sets with large feature sizes. In this case, CML largely fails to compute the weight of each feature as the program becomes too complicated. Without simplification, training and testing of models will be extremely difficult and cost-inefficient. However, QML can utilize Quantum Random Access Memory (qRAM, still in the theoretical stage) to decompose any quantum data into its fundamental units, achieving this goal.

3.4. Kernel methods

Kernel methods are algorithms with linear classifiers that solve non-linear problems.(The most notable method, the Support Vector Machine (SVM), performs regression and classification. SVM increases the dimension of data (with a maximum threshold) until it becomes linearly separable as shown in Figure 5 (Tychola et al., 2023)[7]. QSVM, the quantum counterpart of this method, could perform matrix inversions and exponentials much more efficiently. This means that QSVM can map data into higher dimensions than SVM's threshold to achieve classification.

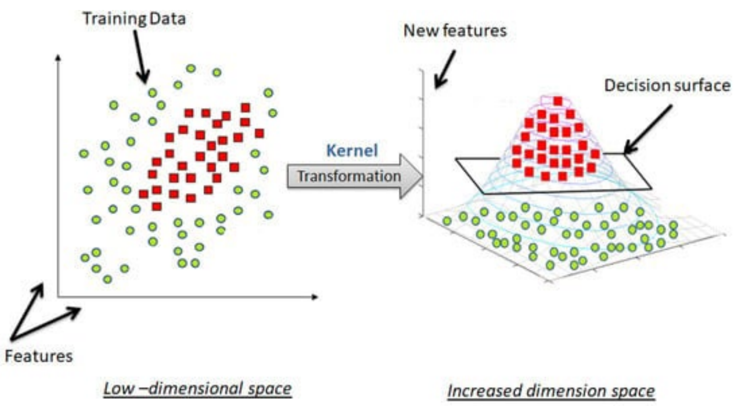

Figure 5: Kernel transformation

Figure 6 is an example completed by researchers that demonstrate quantum advantages (Huang et

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al., 2021)[4].

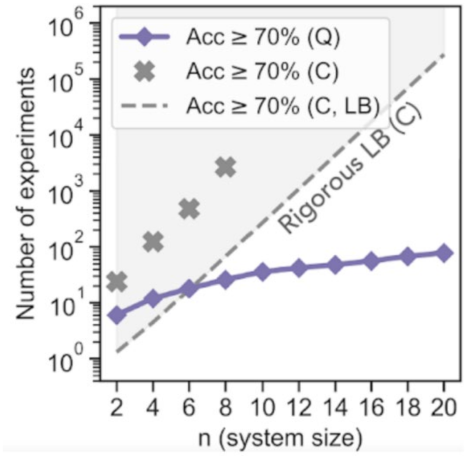

Figure 6: Number of experiments relative to system size using QML and CML

Experimental comparison of OML vs. CML algorithms for predicting a quantum state's observables.While the number of experiments needed to achieve 70% accuracy with a CML algorithm ("C" above) grows exponentially with the size of the quantum state n, the number of experiments the QML algorithm ("O") needs is only linear in n. The dashed line labeled "RigorousLB (C)" represents the theoretical lower bound (LB) - the best possible performance - of a classical machine learning algorithm.

4. Challenges

While QML is theoretically superior to CML in certain tasks, the QML field is still largely experimental. Due to the limitations in hardware and algorithms, many practical tasks are still completed with CML.

Due to a property called quantum decoherence, QML has a limited length of computation time. Quantum decoherence is the collapse of superposition. Since superpositions only exist when the atoms are not observed or acted on, they are very sensitive to outside disruption. As a result, when researchers activate a quantum environment, unwanted outside noises (temperature change, sound, etc.) can cause quantum decoherence, meaning that atoms collapse into state 0 or 1 completely when computing, leading to erroneous results (Collapse of one entangled atom will immediately collapse other entangled atoms as well). And the longer the quantum environment operates, the higher the chance of inaccurate results.

5. Current Works (examples)

5.1. Geometry G-test

One of the challenges in ML is identifying which approach researchers should take to solve a particular problem. A group of researchers demonstrated that with a newly developed Geometry Test, they can evaluate the potential for QML for any problem. This prevents researchers from taking the wrong approach and wasting time. In addition, the researchers demonstrated a new path toward ML problems – the projected quantum kernel (PQK)– that performs well above any existing approach, as shown in Figure 7 (Huang et al., 2021)[6].

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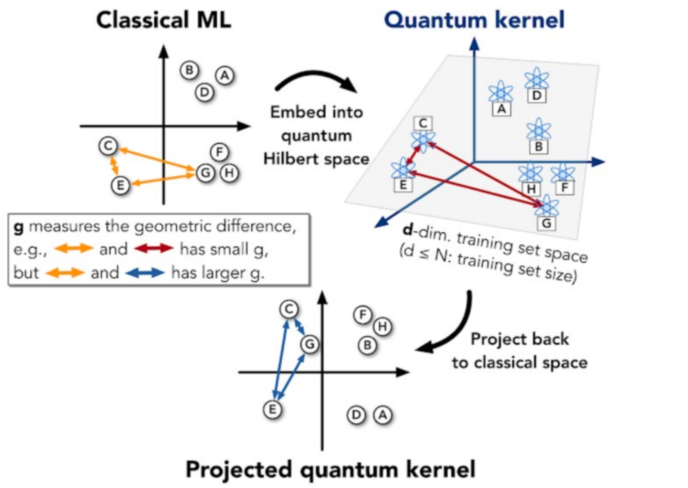
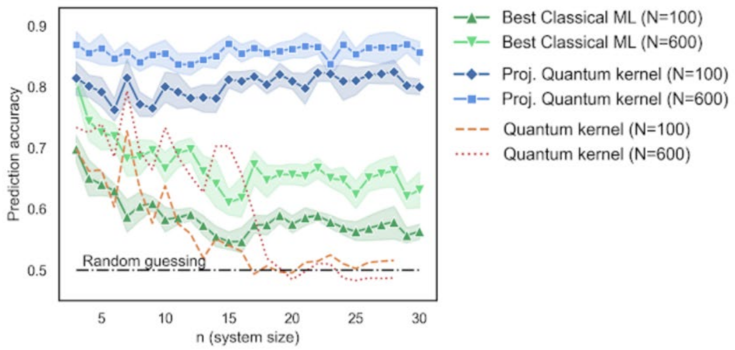


Geometric quantity g, which quantifies the potential for quantum advantage, depicted for several embeddings, including the projected quantum kernel introduced here.

Figure 7: Projected quantum kernel

As the classical representation of quantum kernel, PQK has access to well-developed non-linear kernels and can produce accurate results in less time, recorded by Figure 8. Interestingly, when comparing PQK, quantum kernel, and classical kernel, researchers found that between 20-30 qubits (real-world problem size), CML can perform better than QML if enough data are provided, even for inherently QML intuitive problems.



Prediction accuracy as a function of the number of qubits (n) for a problem engineered to maximize the potential for learning advantage in a quantum model. The data is shown for two different sizes of training data (N).

Figure 8: Prediction accuracy of CML, PQK, and quantum kernel in relation to system size

5.2. Drug design on quantum computers

Researchers examined the QML potential in the drug design field. They concluded that QML computing could offer an advantage over CML in computational chemistry (CC), which predicts a compound's pharmacokinetic properties (how it interacts with the body) and binding affinity (required local concentration). This is crucial to developing new drugs as it shortens the time needed for development. However, several obstacles prevent this potential from being realized.

- Quantum Error Correction: To maintain the accuracy of computations, thousands of physical qubits are required for each logical unit.

- Initial state: Like CML, the initial state of optimization needs to approach the final state. Otherwise, optimization will be cost-inefficient and time-consuming.

5.3. QSVM vs. SVM

In this experiment, researchers tested quantum advantage over three sets of problems (Tychola et al.,

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2023). All tests were run 10 times to obtain the average to evaluate the performance of QSVM and SVM.

• Breast cancer data set: 10 features, 699 data points, simplest out of all three. SVM outperforms QSVM by 2% on average. (roc score, accuracy, f1-score)

• Ionosphere data set: 34 features, 351 data points, medium difficulty. QSVM outperforms SVM by a small amount on average

• Spam data set: 57 features, 4601 data points, hardest of the three. QSVM outperforms SVM by 1-2% on average.

Researchers demonstrate that the quantum SVM is superior when the feature number increases. It's important to note that the quantum environment is simulated on a classical computer, so results may differ if it is produced with a quantum computer.

6. Prospects and conclusion

Though still in its early development phase, QML has the potential to revolutionize ML. Instead of replacing CML, QML can work with CML to produce faster, more accurate results by combining the strength of CML and QML (such as QAOA). A new development loop may occur as CML is already producing QML processors, which provide quantum resources for themselves. In the future, we will likely see practical implementation of QML on real-world problems. Of course, further research into the field to optimize or create algorithms and hardware is necessary to make this happen. Nonetheless, technological advancement often comes with downsides. For instance, QML's ability to decrypt passwords with the optimized number factoring (Shor's algorithm) could damage privacy and data security, so the future security system may require fundamental changes. Despite this, QML offers a promising future to efficiently process the increasing amount of data. Together with CML, they could make our lives more convenient and enjoyable.

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