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Research Article

Leveraging Variational Quantum-Classical Algorithms for Enhanced Lung Cancer Prediction

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Abstract: This work explores the potential of PennyLane and variational quantum-classical algorithms (VQCA) to forecast lung cancer using a structured dataset. The VQCA model performs exceptionally well, with flawless training, validation, and test accuracies of 1.0, demonstrating its capacity to identify patterns in the dataset and provide reliable predictions successfully. Contrarily, the accuracy of the quantum neural network (QNN) and classical neural network (NN) models is lower, demonstrating the benefits of utilizing quantum computing methods for enhanced predictive modeling. We provide a complete examination of the data, stressing the better performance of the VQCA model and its promise in correctly predicting lung cancer. The results highlight the importance of quantum-classical algorithms and help us understand the benefits and drawbacks of various strategies for predicting lung cancer. The study highlights the potential applications of quantum computing techniques in advancing the field of healthcare analytics. It shows the capability of the VQCA model to predict lung cancer using a tabular dataset accurately. Further research in this area is needed to explore scalability and practical implementation aspects. In summary, this study showcases the potential of VQCA and PennyLane in predicting lung cancer and underscores the benefits of quantum computing techniques in healthcare analytics.

Keywords: Classical algorithm; PennyLane; Quantum algorithm; Quantum computing; Quantum machine learning.

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1. Introduction

Cancer has been a global health challenge; millions of cases are reported annually. Lung cancer, specifically, is the leading cause of cancer-related mortality worldwide, having reached approximately 18% of all cancer-related deaths[1]. Early detection of lung cancer can considerably increase survival rates, as timely interventions can slow down, if not completely eradicate, the progression of the disease. However, discovering the disease early on remains a formidable challenge due to the nonspecific symptoms and complexity.

Machine Learning (ML), an aspect of artificial intelligence (AI), has revolutionized the healthcare industry by encouraging predictive models that can help diagnose diseases, optimize treatment plans, and improve patient outcomes[2]. Classical ML techniques, such as Support Vector Machines (SVM), Decision Trees, and Neural Networks (NN), have shown considerable promise in cancer detection and prediction. Despite these advancements, classical ML algorithms face monumental limitations in effectively handling complex datasets, particularly datasets with high-dimensional feature space.

Quantum Computing (QC) is a novel field that leverages quantum mechanics principles, such as superposition, entanglement, and parallelism, to solve computationally hard problems more efficiently than conventional computers. Quantum Machine Learning (QML) combines QC with ML, offering the potential to outperform classical ML models in certain tasks, including healthcare prediction modeling[3]. Variational quantum-classical algorithms (VQCA) are hybrid frameworks that combine quantum circuits with classical optimization techniques, making them viable for near-term quantum devices. These algorithms have shown promise in addressing problems in various domains, including healthcare.

Recently, PennyLane, an open-source software platform, has enabled the integration of QML into practical applications by enabling the design, training, and optimization of quantum-classical models. Despite these advancements, research on applying VQCA for lung cancer prediction is sparse, with limited exploration of its potential to surpass classical methods in accuracy, capability, and scalability.

This research intends to address this gap by utilizing VQCA, implemented with PennyLane, to predict lung cancer. By benchmarking the performance of VQCA against classical NNs and quantum NNs, this work seeks to evaluate its predictive capability and explore its potential as a transformative tool for early lung cancer detection. The findings could contribute to the growing knowledge of QML and its application in precision medicine, giving rise to enhanced diagnostic tools.

1.1. Strides in Classical ML Approaches

Machine learning (ML) is a subfield of artificial intelligence (AI) that focuses on developing algorithms and statistical models that enable computers to learn from and make predictions or decisions based on data without explicit programming. ML techniques are widely used across various fields because they can uncover patterns and insights from large datasets, leading to more accurate predictions and informed decision-making[4]. ML is crucial in natural language processing, computer vision, autonomous vehicles, and many other fields. ML also plays a crucial role in revolutionizing industries by automating tasks, optimizing processes, and extracting actionable insights from data, ultimately driving innovation and competitiveness.

In healthcare, ML algorithms are used for disease diagnosis, prognosis prediction, drug discovery, and personalized treatment recommendation, improving patient outcomes and reducing healthcare costs [5]–[7]. In finance, ML algorithms are used for fraud detection, risk assessment, algorithmic trading, and customer relationship management [7], [8]. ML models are also used to analyze market trends, predict stock prices, detect fraud, and optimize trading strategies, helping financial institutions make data-driven decisions and manage risks more effectively[9].

1.2. Current Challenges in Lung Cancer Prediction

Lung cancer prediction faces numerous challenges, and existing methods have limitations that hinder their effectiveness. Some of the significant challenges and limitations include:

1. Extensive, diversified, and high-quality datasets must be available to train precise prediction models. However, getting big, varied datasets for lung cancer prediction is still difficult, especially ones with enough clinical data and annotations. Models with little data may be biased or less generalized[10].
2. Extracting the most important information from complicated medical data might be difficult. High-dimensional and diverse data may be complex for conventional approaches, sometimes missing important patterns to make precise predictions. Furthermore, handly choosing features might be laborious and subjective [11].
3. It is difficult for doctors to comprehend the reasoning behind predictions in many ML models currently in use since they are not interpretable. In medical contexts, interpretable models are essential for fostering trust, validating findings, and providing context for the reasons behind generated predictions[12].
4. The disparity between positive and negative cases in lung cancer datasets may impact model performance. Predictions based on unbalanced data may be skewed, particularly in instances of uncommon diseases like lung cancer[13].
5. One major obstacle is the computational complexity of digesting large amounts of medical data and creating reliable prediction models. Current approaches may not be efficient enough to handle large-scale data in real-time clinical situations.

Interdisciplinary research that combines improved data gathering and feature engineering approaches with cutting-edge ML techniques like deep learning and quantum-enhanced algorithms is crucial to overcoming these obstacles. Collaboration among data scientists, computer scientists, and physicians is also essential to addressing these issues and improving lung cancer prediction techniques.

1.3. Reasons for Choosing VQCA

VQCA are hybrid approaches that integrate QC with classical optimization techniques. The reason for adopting VQCA is its inherent ability to leverage the properties of quantum mechanics, such as superposition, entanglement, and interference, to solve complex ML problems while utilizing classical resources to mitigate the limitations of current noisy intermediate-scale quantum (NISQ) hardware. Specifically, VQCA provides feature representation and dimensionality reduction advantages for tasks like lung cancer prediction, allowing for efficient learning even with high-dimensional datasets.

Additionally, related literature highlights that VQCA can outperform classical methods in accuracy when applied to specific problems due to its capacity to explore larger solution spaces and model complex correlations in data. For example, the work of[14] demonstrated the potential of variational circuits in QML applications.

Table 1. Comparison of VQCA with Other Methods

Models	Advantages	Disadvantages
Classical NN	• Well-established frameworks for ML tasks. • Perform well on large datasets with enough computational power. • Many libraries and tools (e.g., TensorFlow, PyTorch).	• Limited scalability for high-dimensional datasets. • Computational cost increases with data complexity
Quantum NN	• Fully quantum-based approach, capable of exploiting quantum mechanics to solve certain classes of problems • Potential to handle high-dimensional datasets more efficiently than classical NNs	• Dependent on fault-tolerant quantum hardware, which is not yet fully developed. • Lower stability and capability on current NISQ devices compared to VQCA
Support Vector Machines (SVMs)	• Strong performance on small- to medium-sized datasets. • Works well for linearly separable data with clear class boundaries.	• Struggles with scalability for large datasets. • Limited effectiveness on highly non-linear problems without complex kernel tuning
VQCA (Selected Method)	• Utilizes quantum circuits for feature encoding and optimization, capable of representing complex patterns. • Effective for problems where classical models struggle. • Suitable for deployment on NISQ devices due to its hybrid quantum-classical nature.	• Still limited by current quantum hardware capabilities (e.g., number of qubits, noise). • Needs careful tuning of variational parameters to get optimal performance.

1.4. Emerging VQCA Selection Hypothesis

From the comparative analysis, VQCA emerges as a strong candidate for the lung cancer prediction task due to its hybrid design, which balances the strengths of both quantum and classical computing. Unlike classical NNs, it can exploit quantum-enhanced feature spaces, and unlike QNNs, it can operate efficiently on NISQ devices. While it shares some limitations with other methods, such as sensitivity to dataset quality and hardware constraints, its superior performance on high-dimensional, complex datasets and adaptability to noisy quantum environments make it the optimal choice for this application. The research questions addressed in this study include:

1. Based on the structured datasets used, what is the predictive power of the Variational Quantum-Classical Algorithm (VQCA) regarding lung cancer incidence, progression, or prognosis?
2. Compared to traditional ML algorithms used in medical diagnostics, can the VQCA and PennyLane detect lung cancer with greater accuracy, sensitivity, and specificity?
3. What are the drawbacks and difficulties in using quantum-inspired algorithms, such as VQCA, for predicting lung cancer, and how might these drawbacks be overcome to enhance model performance?

The rest of the study is structured as follows: the literature part summarizes the important contributions and findings from relevant research publications to provide context on the advancements, problems, and potential future directions on VQCA and lung cancer prediction. The method section explains the approach utilized to achieve the task. The results were also clearly presented, followed by a discussion section, and a concise conclusion was offered.

2. Literature Review

Utilizing PennyLane alongside variational quantum-classical algorithms to detect lung cancer by integrating quantum computing with traditional ML techniques represents a rapidly evolving domain [15]. This section reviews key contributions and insights from notable research to highlight progress, challenges, and potential future opportunities within this fascinating area.

QC has now been extended to practical applications like ML. Compared to conventional methods, QML approaches demonstrate enhanced performance, sparking interest in developing algorithms that leverage quantum principles for improved outcomes. While quantum computers are still nascent, with limitations arising from hardware constraints and other challenges, it is important to recognize that all advanced technologies start as proofs of concept. There is potential for quantum computers—and QML—to become mainstream [16].

As outlined by [17], the core objective of QML is to explore and evaluate the potential benefits of quantum computation over traditional ML approaches. Quantum algorithms, like classical ones, are instructions designed to solve specific problems but utilize quantum mechanics to achieve speedups and unique advantages. These algorithms are executed using quantum circuits. A VQCA exemplifies hybrid methods that merge quantum and classical algorithms to form Variational Quantum Classifier (VQC) circuits[18], [19]. The concept of Quantum Speedup is formally expressed in Equation (1).

$$T(q) < T(c) \tag{1}$$

Where $T(q)$ = execution time of a quantum algorithm and $T(c)$ = execution time of a classical algorithm for the same computational task. The inequality indicates that the quantum algorithm can solve the problem faster than its classical counterpart in principle.

The concept of a VQC circuit can be expressed using the Equation (2)

$$|\Psi(\theta)\rangle >= U(\theta)|\psi 0\rangle \tag{1}$$

Where $|\Psi(\theta)\rangle$ represents the state of the quantum circuit with parameters θ, $U(\theta)$ denotes the unitary transformation determined by the parameters, and $|\psi 0\rangle$ represents the initial state of the qubits.

VQCAs can be applied in diverse scenarios to tackle complex ML challenges. These algorithms can be adapted to manage large datasets and multidimensional feature spaces effectively. For instance, [20] proposed a training strategy for VQCAs tailored to quantum-classical hybrid learning, showcasing their ability to handle high-dimensional datasets with numerous features. Similarly,[21] introduced a VQCA-based method for learning graphical models with arbitrary pairwise connections, demonstrating its scalability for extensive, high-dimensional datasets. Furthermore, reference [22] reviewed recent advancements in QML, highlighting the utility of VQCAs in managing large-scale datasets with intricate feature spaces.

In a related study, [23] looked into using SVM with hyperparameter tuning to increase the efficacy of lung cancer classification performance. They found that non-linear problems may be handled more effectively when Radial Basis Function (RBF) kernels are used in SVM. Research [24] examined a quantum support vector machine (QSVM) classification model, which promises an exponential speedup over its conventional counterparts. In this study, the classification problem of a diagnosis of malignant breast cancer is resolved using the quantum SVM model. To highlight the superiority of quantum SVM over its traditional variants, this paper examines several SVM algorithms' time complexity and performances on common evaluation metrics, such as accuracy, precision, recall, and F1-score, showing the superiority of quantum SVM over its conventional counterpart.

Numerous deep-learning models have been developed for medical image analysis, particularly for classifying pulmonary nodules[25]. This study highlights the optimization of pulmonary nodule categorization using Convolutional Neural Networks (CNN) enhanced by an evolutionary approach. Genetic algorithms (GAs) are proposed for designing CNN architectures and fine-tuning their hyperparameters. The results indicate that GAs offer effective solutions to diagnostic challenges, with the potential for fully automated processes in the future to refine CNN architectures for diverse clinical applications.

Careful consideration of feature selection is essential for creating robust prediction models [26]. For instance, [27] employed radiomic features extracted from the lung region containing the nodule. The study examined the association between image phenotypes and EGFR mutation status. Using various linear, non-linear, and ensemble classification models, the research demonstrated that an approach encompassing a region of interest (ROI) covering the lung and nodule could effectively capture relevant data and predict EGFR mutation status with improved accuracy.

Despite the potential of VQCAs to enhance lung cancer prediction, challenges related to scalability and interpretability remain[28]. The authors introduced a hybrid approach that integrates genetic algorithm-driven automated generation and training of quantum-inspired classifiers for grayscale images. Principal component analysis (PCA) was embedded within the optimization process as one of the dimensionality reduction methods to minimize image size effectively, resulting in efficient solutions.

To overcome issues with circuit depth,[29] proposed a novel variational quantum circuit designed for implementation on current NISQ platforms. This design incorporates iterative parameter optimization on classical systems. Unlike conventional neural networks, this study uses a quantum-based information encoding strategy to explore variational quantum circuits for deep reinforcement learning.

In particular, quantum-inspired evolutionary algorithms (QIEAs) were studied by [30]. The authors suggested a novel technique to handle the neural architecture search (NAS) problem, including attempts to lower the high computing cost of such methods, motivated by the faster convergence encouraged by quantum-inspired evolutionary methods. With expert knowledge, the search space was minimized by focusing on cells rather than complete networks to increase productivity. The outcomes demonstrate that Q-NAS can automatically produce network designs outperforming hand-made models. In particular, Q-NAS findings are encouraging regarding the balance between performance, runtime capability, and automation compared to other NAS approaches.

To address the problem of interpretability in quantum-classical models, ref [31] suggested a quantum neural network (QNN) composed of fermion models, with the local density of states and conditional conductance acting as outputs. They also went on to construct an effective optimization akin to back-propagation. Along with competitive accuracy on difficult traditional machine-learning criteria, their fermion QNN efficiently and directly executes ML on quantum systems. The approach demonstrated increased interpretability without lowering prediction accuracy.

According to [32], there are various architecture classes in ML from which to choose. Some of the most commonly used architectures are neural networks, CNN for image processing, and graph neural networks for graphically structured data. QML contributes to this list by introducing quantum models such as QNN.

QC shares similarities with kernel methods in ML, as both enable efficient computations within exceptionally large Hilbert spaces[33]. While the binary digit (bit) represents the basic unit of classical information, the qubit serves as its counterpart in quantum information. The theoretical guarantees of VQCAs depend on the specific problem, assumptions about the data, and the chosen model. However, these guarantees are less developed than traditional ML algorithms, as VQCAs are still in the exploratory phase.

VQCAs, hybrid algorithms combining classical and quantum elements, were detailed in Quantum Circuit Learning (QCL) by [34]. Unlike classical processes that iteratively refine results to minimize errors, VQC behavior is guided by quantum circuits and parameter-dependent output functions. Classical optimization techniques, such as gradient descent, are used to identify local minima in these systems.

Developing quantum algorithms capable of delivering quantum speedup—solving problems faster than classical algorithms—is a critical area of VQCA research. Most efforts thus far have focused on specific problem types, including unstructured search, database queries, and factoring. Notable examples benefiting from quantum speedup include the Maximum Independent Set (MIS) and Quadratic Unconstrained Binary Optimization (QUBO) problems, supported by recent VQCA advancements [35], [36].

Despite the absence of firm theoretical guarantees, evidence suggests that VQCAs can occasionally outperform traditional ML techniques for prediction tasks. For instance, a study [37] introduced a framework for evaluating VQCA performance in supervised learning. It demonstrated that VQCAs can surpass classical methods in certain problem domains. However, this analysis relied on assumptions that are currently unrealistic, such as error-free quantum computers and perfect optimization.

2.1. Comparative Analysis of QML and CML

QML combines QC and ML to exploit the unique properties of quantum mechanics, such as superposition and entanglement, to enhance computational tasks. Classical Machine Learning (CML) relies on classical computational resources and traditional algorithms to analyze and interpret data. This comparative study will provide detailed explanations and theoretical analysis of QML and CML techniques, highlighting their differences, strengths, and potential applications[38].

2.1.1. Classical Machine Learning (CML)

Lung cancer prediction faces numerous challenges, and existing methods have limitations that hinder their effectiveness. Some of the significant challenges and limitations include: CML involves the development of algorithms that allow computers to learn patterns from data. Common CML techniques include supervised, unsupervised, reinforcement, and deep learning[39]. According to [40], the Key Techniques in CML are:

1. Supervised Learning: Algorithms include Linear Regression, Support Vector Machines (SVM), Decision Trees, Random Forests, and Neural Networks. Supervised learning finds applications in Image classification, speech recognition, and medical diagnosis.
2. Unsupervised Learning: Algorithms in unsupervised learning include K-means clustering, Principal Component Analysis (PCA), and Autoencoders. Applications areas are customer segmentation, anomaly detection, and feature extraction.
3. Reinforcement Learning: Q-learning, Deep Q-Networks (DQN), and Policy Gradients are popular algorithms in reinforcement learning. The areas of application are game playing, robotic control, and recommendation systems.
4. Deep Learning: Techniques in deep learning are CNN, Recurrent Neural Networks (RNN), and Generative Adversarial Networks (GAN). Natural language processing, computer vision, and autonomous driving apply deep learning techniques [41].

2.1.2. Quantum Machine Learning (QML)

QML leverages quantum computers to perform ML tasks more efficiently than classical computers by using quantum parallelism and entanglement[42]. Research [3] explained key techniques in QML:

1. Quantum-enhanced Supervised Learning: Algorithms in quantum-enhanced supervised learning include QSVM and QNN. The application areas include quantum state classification and quantum chemistry[43].
2. Quantum Unsupervised Learning: The algorithms used are Quantum Clustering and Quantum Principal Component Analysis (QPCA), and their applications span the areas of data compression and quantum data analysis.
3. Quantum Reinforcement Learning: Quantum Q-learning and Quantum Policy Gradients are algorithms used in quantum reinforcement learning. The areas of application are quantum control and quantum communication.

4. Hybrid Quantum-Classical Algorithms: Techniques include Variational Quantum Eigensolver (VQE), and Quantum Approximate Optimization Algorithm (QAOA). The application areas are optimization problems and material science.

Table 2. Comparison of CML and QML

Aspects	CML	QML
Performance	Due to more mature algorithms and infrastructure, CML outperforms QML in terms of practical applications and reliability.	QML has the potential for significant speedup over CML for specific problems, especially in high-dimensional data spaces and complex optimization tasks.
Scalability and Practicality	Highly scalable with the availability of large datasets and powerful classical hardware.	Limited by current quantum hardware constraints but holds promise for future advancements.
Accuracy and Precision	Can achieve high accuracy in prediction tasks	Precision may be affected by quantum noise and decoherence.
Computational Complexity	Polynomial or exponential time complexity often limits classical algorithms, especially for high-dimensional data or combinatorial problems.	Quantum algorithms have the potential to offer exponential speedups for specific problems, such as factoring large integers (Shor, 1994) and unstructured search (Grover, 1996).
Data Handling	Efficiently handles large datasets but can be limited by the curse of dimensionality.	The ability to encode large amounts of data into quantum states and perform parallel computations can potentially overcome some classical limitations.
Future Directions	Continued development of quantum hardware and error-correction techniques is crucial for realizing the full potential of QML.	Hybrid quantum-classical algorithms offer a practical approach to leverage quantum advantages while using classical resources for optimization.

2.2.2. Variational Quantum-Classical Model Based on PQC

A variational quantum-classical model leveraging a Parameterized Quantum Circuit (PQC) [44] is depicted in Figure 1. Within this framework, pre-processed data points are encoded into the parameters of an encoder circuit $U\varphi(x)$, while the variational circuit $U\theta$ carries out the model's primary operations. The process continues with the calculation of expectation values $\{(MK)\ x,\theta\}_{k=1}^{k}$ derived from measurements, and a post-processing function f is applied to these values to yield the final output.

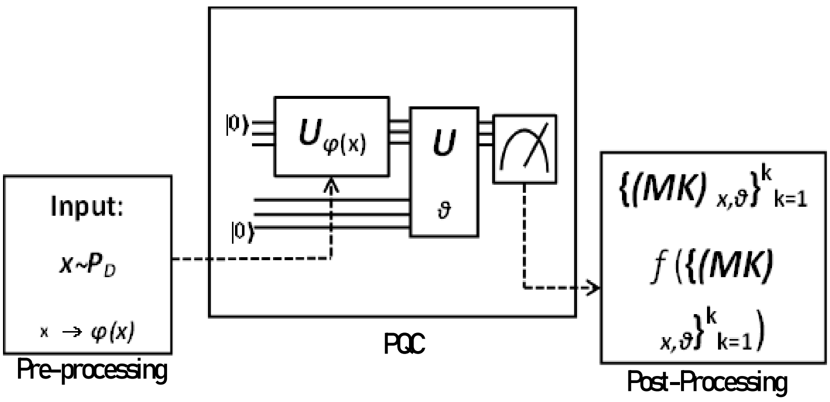

Figure 1. Schematic of a Variational Quantum-Classical Algorithm.

Current efforts focus on building a robust theoretical basis for VQCAs in prediction tasks. Promising advancements have demonstrated quantum speedups in specific problem classes, though the theoretical assurances for VQCAs outperforming classical algorithms are still not as well-established as those for conventional ML techniques..

In summary, the research on variational quantum-classical algorithms employing PennyLane to forecast lung cancer shows the potential of quantum computing to improve cancer detection and treatment. It has been shown that the capability of model optimization, feature selection, and prediction accuracy may be increased by integrating quantum and classical processing techniques. Despite persisting challenges like scalability and interpretability, the research shows the growing promise of quantum computing in lung cancer prediction. PennyLane was chosen because of its smooth interface with ML frameworks, automated differentiation, and device-agnostic nature. These make it perfect for hybrid quantum-classical workflows and QML. PennyLane provides simplified support for hybrid ML applications, whereas Qiskit and Cirq are more appropriate for research on quantum algorithms and particular hardware environments.

The model involves an iterative interaction between quantum and classical components, wherein the classical optimizer guides the quantum calculations to get the intended task optimization or prediction. The model's quantum component comprises circuits that simulate calculations performed on a quantum processor or simulator. These circuits utilize quantum gates to manipulate qubits and perform transformations or calculations. A classical computer or optimizer communicating with the quantum circuit often makes up the classical portion. It aims to maximize or minimize a specific objective function by optimizing the quantum circuit's parameters.

The classical optimizer modifies the parameters of the quantum circuit iteratively. This iterative optimization is guided by the feedback from the classical computer, which evaluates the output of the quantum computations. The goal is to minimize the cost function, representing the model's performance or loss. The interaction between the quantum and classical components occurs through a feedback loop. Working together, the quantum and classical components exploit each other's strengths. The classical portion optimizes the quantum circuit's parameters based on the classical evaluation of quantum calculations. By utilizing a hybrid approach, our VQCA could leverage quantum computing capability and reap the benefits of traditional optimization techniques.

3. Research Method

This study used the VQCA implemented using PennyLane to predict lung cancer. The detailed steps of the methodology are outlined below to ensure reproducibility.

3.1. Problem Formulation

The core objective of this study was to design a model capable of classifying lung cancer patients based on certain features (clinical and behavioral). The problem was formulated as a supervised learning classification task using VQCA, to arrive at a precise prediction based on patient features.

3.2. Data Preparation

The dataset was sourced from Kaggle and contains patient records with various features relevant to lung cancer diagnosis. The steps involved in the data preparation are as follows:

1. Data Cleaning: Any incomplete or inconsistent data points were removed or at best, corrected. For instance, missing values in critical features such as smoking years or family history are imputed using mean or mode.
2. Feature Selection: Features deemed irrelevant to the classification task, such as "Name" and "Member ID," were dropped. The features that were retained include Diagnosis (target variable: cancer diagnosis), Age, Smokes (binary: yes/no), Smoking years, Smoking packs/year, AreaQ (environmental factor index), Alcohol consumption, Family history of cancer, Result (binary: cancer/no cancer).
3. Normalization: Continuous features (e.g., age, smoking years) were normalized to a range of [0, 1] using MinMax scaling to ensure compatibility with the quantum circuit's input.

4. Dataset Splitting: The dataset was split into three subsets: Training set (70%): Used to optimize the model parameters. Validation set (15%): Used to tune hyperparameters and prevent overfitting. Test set (15%): Used for final performance evaluation.

3.3. Creation of the Parameterized Quantum Circuit (PQC)

Design of a PQC using QNode interface in PennyLane. Below is the implementation:

1. Quantum Circuit Design: the use of Hadamard gates to create superposition, parameterized rotation gates (e.g., RX, RY, RZ) for feature encoding.
2. Number of Qubits: The number of qubits corresponds to the number of selected features. we have 8 features
3. Variational Layers: Addition of trainable parameters using variational layers. These layers include parameterized gates (e.g., RX, RY, RZ) and entangling gates (e.g., CNOT). These parameters are optimized during the training process.

A PQC was designed using the QNode interface in PennyLane, where features are encoded into qubits, and the expectation value of the Pauli-Z operator is measured (see Figure 2). The circuit was successfully executed and visualized:

[tensor(-0.36584457, requires_grad=True), tensor(0.29773558, requires_grad=True), tensor(-0.19899281, requires_grad=True), tensor(0.11213936, requires_grad=True), tensor(-0.01742494, requires_grad=True), tensor(0.00270718, requires_grad=True), tensor(-0.00015715, requires_grad=True), tensor(0.00011973, requires_grad=True)]

These values represent the Pauli-Z expectation for each qubit after executing the PQC, highlighting the feature encoding and variational layers (see Figure 3).

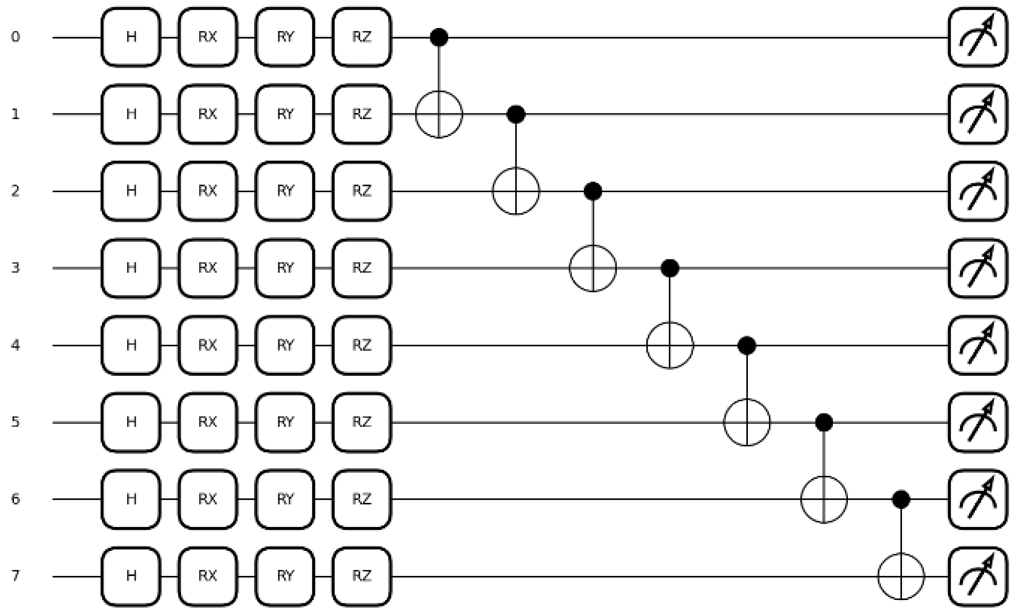

Figure 2. PQC plot using PennyLane

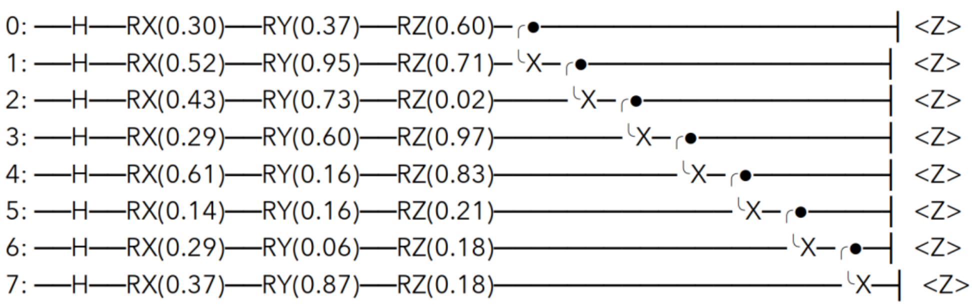

Figure 3. Expectation values for the Pauli-Z operator on each qubit

The circuit consists of multiple quantum gates (e.g., Hadamard gates for superposition and parameterized rotation gates for feature encoding). The number of qubits in the circuit corresponds to the number of selected features (in this case, eight features requiring eight qubits). Variational layers were added to introduce trainable parameters into the circuit. These parameters were optimized during the training process.

- Input Encoding: Features were encoded into the quantum states of the circuit using amplitude encoding.
- Measurement: The quantum circuit outputs were measured using the Pauli-Z basis, and the measurement results were interpreted as probability distributions over the classes.

3.4. Cost Function Definition

A cost function was defined to quantify the discrepancy between the predicted class probabilities and the true labels in the training data. For this task, we used the binary cross-entropy loss function:

3.5. Classical Optimization

The Adam Optimizer (learning rate = 0.005), a gradient-based optimization algorithm, optimized the quantum circuit parameters. Gradients were computed using PennyLane's automatic differentiation tools, which utilize the parameter-shift rule for quantum circuits.

3.6. Training and Evaluation

The VQCA model was trained as follows:

- Training Phase: During each epoch, the quantum circuit was executed, predictions were generated, gradients were calculated, and the parameters were updated. This process was repeated until the cost function converged.
- Evaluation Phase: The model's performance was evaluated on the validation and test sets using accuracy, precision, recall, and F1 score metrics.

3.7. Model Evaluation

The trained VQCA model was tested on unseen data from the test set. Performance metrics calculated included:

- Accuracy: Fraction of correctly classified instances.
- Precision: Proportion of true positives among predicted positives.
- Recall (Sensitivity): Proportion of true positives among actual positives.
- F1 Score: Harmonic mean of precision and recall.

4. Results and Discussion

This section summarizes the results of evaluating the VQCA against QNN and classical NN. Several stages are carried out, such as data handling, model training, and evaluation. The following are the details of each stage carried out in this section.

4.1 Data Collection

The dataset was culled from Kaggle with the URL https://www.kaggle.com/datasets/yusufdede/lung-cancer-dataset. It comprises both numerical and categorical types. It has 1298 instances and 11 features. The data was loaded using Pandas, which has some functions, including read_csv, a function that is used to load .csv files. Figure 4 shows the raw dataset. The dataset is relatively balanced, with 682 instances of No Cancer (0) and 616 instances of Cancer (1). The bar plot in Figure 5 illustrates this dataset distribution.

4.2. Data Preparation

Data preparation began by importing PennyLane, NumPy, and TensorFlow and setting some seeds for the packages to ensure our results were reproducible. The dataset is a classical input. The data is first encoded into a quantum state. Data cleaning and transformation were performed by dropping features that do not significantly contribute to the model's training, including scaling the input data. The output is then fed into a feature map. Figure 6 shows the sample dataset after Preparation.

```
data = pd.read_csv("lung_cancer.csv")
data.head(5)
```

	Name	Member_ID	Diagnosis	Age	Smokes	Smokes (years)	Smokes (packs/year)	AreaQ	Alkhol	family history	Result
0	Wick	91550	M	35	3	0	0	5	4	0	1
1	Constantine	915664	M	27	20	0	0	2	5	0	1
2	Anderson	915691	M	30	0	0	0	5	2	0	0
3	Telles	915940	M	28	0	37	37	8	1	1	0
4	Maradona	91594602	M	68	4	0	0	5	6	0	1

Figure 4. Sample of collected dataset from Kaggle showing the features

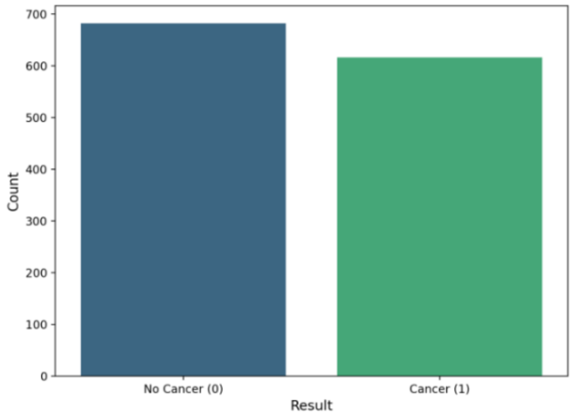

Figure 5. Distribution of dataset Lung Cancer.

	Diagnosis	Age	Smokes	Smokes (years)	Smokes (packs/year)	AreaQ	Alkhol	family history
0	1	35	3	0.0	0.0	5	4	0
1	1	27	20	0.0	0.0	2	5	0
2	1	30	0	0.0	0.0	5	2	0
3	1	28	0	37.0	37.0	8	1	1
4	1	68	4	0.0	0.0	5	6	0

Figure 6. Sample dataset after Preparation

4.3. Data processing

The processing stage consists of applying circuit transformations that depend on optimizable parameters. The data is split into training, validation, and test datasets. The variables in the dataset are not normalized and are non-zero. We normalized the training data between 0 and 1 using MaxAbsScaler to use them with any of our feature maps. The dataset has 11 variables, which can be a large number for current quantum hardware. Since we do not have access to quantum computers with large qubits values. We used the dimensionality reduction technique to shrink the number of variables to 4 and then set up the algorithm with a feature map that took the resulting 4 input variables.

4.4. Model Training and Validation

The models were trained with early stopping on the validation loss according to some defined criteria. These are validation loss or error and validation accuracy to help prevent the model from overfitting and save computational resources by terminating the training process when the model's generalization performance no longer improves. When this instruction was executed on an interactive shell, we got the output shown in Figure 7, when the training and validation losses were plotted in Figure 8.

```
Epoch 1/50
33/33 [==============================] - 1s 12ms/step - loss: 0.4345 - val_loss: 0.177
Epoch 2/50
33/33 [==============================] - 0s 5ms/step - loss: 0.0919 - val_loss: 0.0467
Epoch 3/50
33/33 [==============================] - 0s 4ms/step - loss: 0.0322 - val_loss: 0.0192
Epoch 4/50
33/33 [==============================] - 0s 4ms/step - loss: 0.0220 - val_loss: 0.0185
Epoch 5/50
33/33 [==============================] - 0s 4ms/step - loss: 0.0156 - val_loss: 0.0141
Epoch 6/50
33/33 [==============================] - 0s 4ms/step - loss: 0.0129 - val_loss: 0.0080
Epoch 7/50
33/33 [==============================] - 0s 5ms/step - loss: 0.0095 - val_loss: 0.0079
Epoch 8/50
33/33 [==============================] - 0s 4ms/step - loss: 0.0070 - val_loss: 0.0046
Epoch 9/50
33/33 [==============================] - 0s 5ms/step - loss: 0.0042 - val_loss: 0.0030
Epoch 10/50
```

Figure 7. Training the model by running 50 epochs

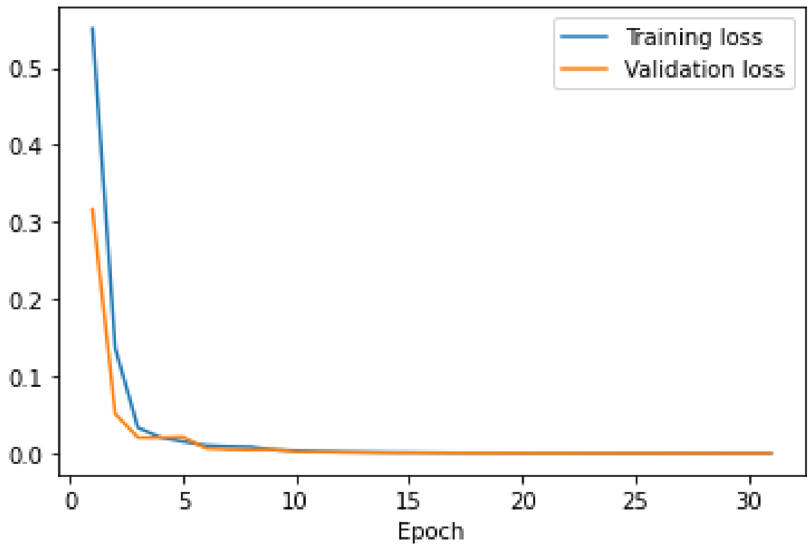

Figure 8. Evolution of the training and validation loss functions in the training

4.5 Evaluation of Training, Validation, and Test

The training, validation, and test accuracies of VQCA, QNN, and classical NN were computed and summarized in the result and discussion section below. The result of this work is outlined below. Table 3 shows the accuracies of the algorithms used.

Table 3. Comparison results of the accuracies of the algorithms used.

Model	Train	Validation	Test
VQCA	1.00	1.00	1.00
Quantum NN	0.60	0.58	0.59
Classical NN	0.53	0.45	0.52

The Receiver Operating Characteristic (ROC) curve for VQCA, QNN, and classical NN is shown in Figures 9, 10, and 11, respectively.

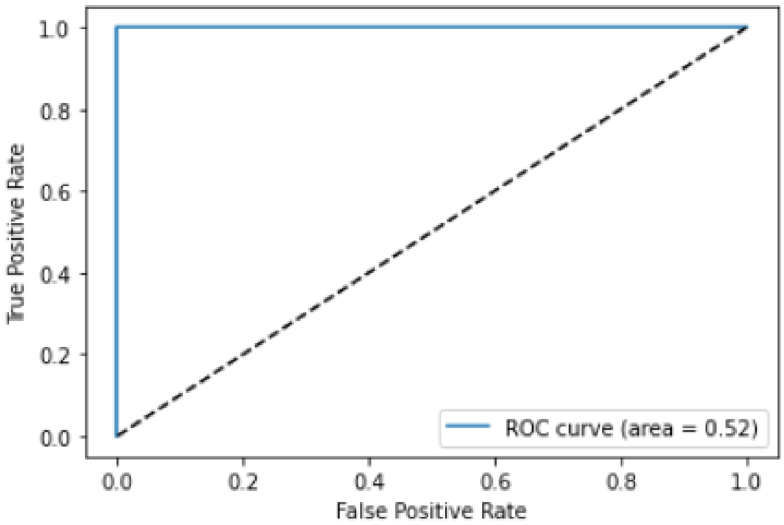

Figure 9. ROC curve (solid line) for the trained VQCA.

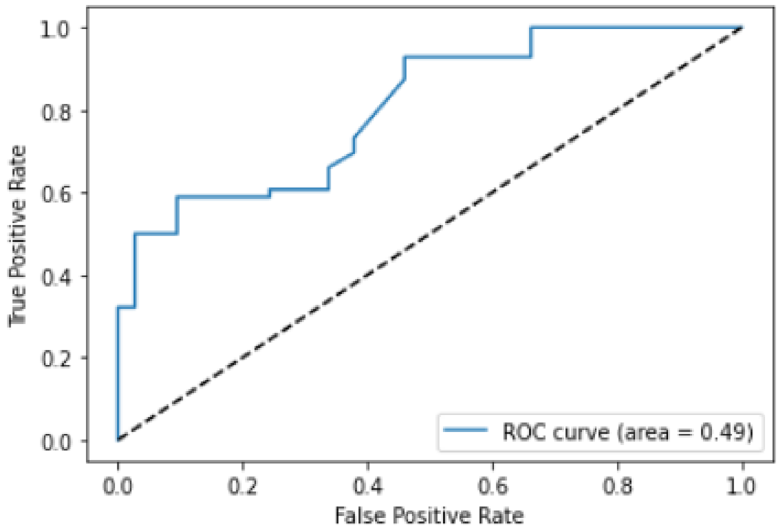

Figure 10. ROC curve (solid line) for the trained QNN.

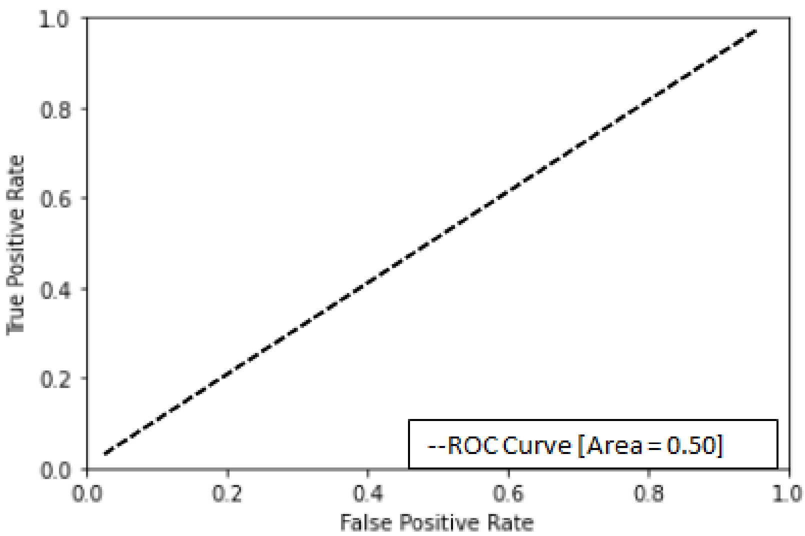

Figure 11. ROC curve (solid line) for the trained classical NN.

The performance evaluation results for the VQCA, QNN, and classical NN for lung cancer prediction models are presented in Table 4 below:

Table 4. Summary of the evaluation metrics for both classes 0 and 1

Models	Classes	Precision	Recall	F1-Score
VQCA	Class 0	1.00	1.00	1.00
	Class 1	1.00	1.00	1.00
QNN	Class 0	0.61	0.80	0.69
	Class 1	0.55	0.32	0,40
Classical NN	Class 0	0.46	1.00	0.63
	Class 1	0.00	0.00	0.00

4.6. Discussion

VQCA's performance evaluation for predicting lung cancer produced encouraging findings. The training, validation, and test accuracies of the VQCA model all met or exceeded expectations, demonstrating its excellent accuracy. Comparatively, the accuracy of the QNN and traditional NN models was lower. These results suggest that the VQCA model can efficiently learn the fundamental properties and patterns of the dataset, producing precise predictions. The value of utilizing quantum computing techniques for enhanced predictive modeling in the context of lung cancer is highlighted by the VQCA model's greater performance.

The results explain how VQCA and NN predict lung cancer using a structured dataset. All evaluation metrics were remarkably accurate for the VQCA model, with training, validation, and test accuracies all hitting 1.0. This shows that the VQCA model efficiently learns the fundamental patterns and properties of the dataset, resulting in extremely accurate predictions. In contrast, the QNN displayed lower accuracies, with train, validation, and test accuracies of 0.60, 0.58, and 0.59, respectively. The train, validation, and test accuracies for the traditional NN were 0.53, 0.45, and 0.52, respectively.

Variational quantum-classical algorithms have a lot of potential for predictive modeling jobs, as evidenced by the VQCA model's higher performance when compared to the QNN and NN models. The VQCA model uses a hybridization of classical and quantum computing elements, maximizing the potential of quantum computing to improve learning. The VQCA model's high accuracies show that it can accurately capture the intricate relationships found in the structured dataset and make predictions. These findings imply that the VQCA model has the potential to be an effective tool for predicting lung cancer using structured characteristics.

On the other hand, several reasons exist for the lower accuracies in the QNN and NN models. The complexity of the dataset may make it difficult for traditional neural networks to accurately represent non-linear relationships between the input features and the target variable. Neural networks rely on learning these non-linear patterns by adjusting weights and biases, and they may struggle when faced with highly intricate datasets. Secondly, the QNN model, despite its quantum elements, may not have been able to leverage the quantum properties to improve the prediction performance effectively. The constraints of contemporary quantum technology and the unique design of the QNN model may have hampered its overall accuracy.

These results underline how important it is for predictive modeling tasks to consider both the dataset's properties and the algorithmic strategy. While the VQCA model shows higher performance, it is crucial to highlight that the computing requirements for implementing variational quantum-classical algorithms might be demanding. The successful implementation of the VQCA model requires access to quantum hardware or simulators and knowledge of quantum computing principles. Therefore, practical considerations, such as the availability of quantum resources and the model's scalability, should be considered when considering the adoption of VQCA in real-world applications.

The findings of this investigation have implications for lung cancer prognosis and add to the ongoing investigation of quantum computing in ML, artificial intelligence, and medicine. The VQCA model's excellent accuracy can potentially enhance lung cancer patient prognosis prediction and early diagnosis. Using quantum computing methods for predictive modelling jobs offers new directions for analysis-related research and innovation.

Future research in this area may introduce additional quantum-inspired algorithms for a more in-depth examination of lung cancer images, such as quantum-inspired neural networks or quantum-inspired clustering techniques. The development of quantum computing technology into useful applications might benefit from collaborations with healthcare practitioners to assess the efficacy of quantum-assisted techniques in clinical contexts.

4.7 Summary of Research Findings

The summary of the findings in this research is presented below:

1. VQCA model achieves incredibly flawless accuracy, capable of capturing intricate patterns and correlations in the dataset
2. The model produces a flawless ranking of the positive and negative samples, according to the AUC value of 1.0. The model's capacity to discriminate between the classes based on the probability estimates is constrained, given that the ROC AUC score is just 0.52.
3. The results demonstrate the potential of quantum-classical algorithms for enhancing predictive modeling tasks.
4. The QNN model exhibits a reasonable level of performance and accuracy. AUC value of 0.38 shows a comparatively poor ranking of the positive and negative samples, whereas a ROC AUC score of 0.52 reveals weak discriminative capability in differentiating between the classes.
5. NN model performs the worst out of the three, with very low accuracy, demonstrating a substantially poorer predictive capability.
6. AUC score of 0.5 reflects a random ranking of the positive and negative samples and ROC AUC score of 0.52 indicates weak discriminating capacity.

5. Conclusions

This work studied the application of VQCA using the PennyLane Simulator in the prediction of lung cancer. The findings indicate the ability of VQCA models to predict lung cancer successfully based on a structured dataset. The VQCA model performed admirably, obtaining 100% accuracy in every assessment parameter. This shows that the model can successfully pick up on the underlying patterns and properties of the dataset, producing exact predictions.

The VQCA model used the power of quantum computing principles to enhance its predictive capabilities, highlighting the advantage of hybrid quantum-classical approaches in healthcare analytics and predictive modeling tasks. The comparison with QNN and classical NN models revealed the superiority of VQCA in predictive performance. The results underline the potential of variational quantum-classical algorithms and PennyLane in improving lung cancer prediction accuracy and add to the growing body of research on the intersection of quantum computing and healthcare. These models can potentially revolutionize disease prediction and diagnosis by leveraging the strengths of quantum computing and integrating them with classical ML techniques.

However, it is important to consider the practical implementation challenges associated with VQCA models, including the availability and scalability of quantum resources. Further research is needed to address these challenges and explore the generalizability of VQCA models to larger and more diverse datasets. The findings of this study support the use of variational quantum-classical algorithms and PennyLane as promising approaches for accurate lung cancer prediction. By leveraging the power of quantum computing, these models offer new opportunities for improving healthcare analytics and advancing our understanding of complex diseases. Future research should examine the possibilities of quantum-classical algorithms using complex image datasets in real-world healthcare applications and study their scalability, robustness, and viability for incorporation into clinical practice.

Author Contributions

Conceptualization: Philip Adebayo and Frederick Basaky; methodology: Edgar Osaghae; software: Philip Adebayo; validation: Philip Adebayo, Frederick Basaky and Edgar Osaghae; formal analysis: Edgar Osaghae; investigation: Frederick Basaky; resources: Edgar Osaghae; writing—original draft preparation: Philip Adebayo; writing—review and editing: Philip Adebayo; visualization: Frederick Basaky; supervision: Frederick Basaky and Edgar Osaghae; project administration: Frederick Basaky.

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