

Comparative performance analysis of Machine Learning with Quantum Machine Learning for breast cancer prediction.

MSc Research Project
Data Analytics

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Project Submission Sheet
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Student Name:	Sahil Mulani
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Programme:	Data Analytics
Year:	2024
Module:	MSc Research Project
Supervisor:	Paul Stynes
Submission Due Date:	12/09/2024
Project Title:	Comparative performance analysis of Machine Learning with Quantum Machine Learning for breast cancer prediction.
Word Count:	5571
Page Count:	23

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Comparative performance analysis of Machine Learning with Quantum Machine Learning for breast cancer prediction.

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Abstract

In the public health sector, a well-known heterogeneous disease whose incident rate has seen a sharp increase is breast cancer. It is a widely known cause of mortality among women. However, detecting breast cancer in the initial stages can increase survival chances and save lives for many people. The primary focus of this research is to develop a prediction tool using the Wisconsin Breast Cancer (Diagnostic) data set that would help medical practitioners diagnose breast cancer in the early stages. We have selected two prediction models, Classical Machine Learning models (Machine Learning & Deep Learning) and Quantum Machine Learning (QML) models based on the features of the data set. The performance of the models was evaluated on the basis of sensitivity, i.e. true positive rate. The results indicate that the Classical ML models outperformed the QML models, with ANN achieving the highest sensitivity of 98.14% followed by Random Forest with a sensitivity of 94.51%. The QML models gave satisfactory results, achieving the maximum sensitivity of 82.85%; however, its performance was limited due to hardware constraints.

1 Introduction

1.1 Background

Breast cancer is one of the major causes of mortality for women around the world. According to the World Health Organization (WHO) report, 2.3 million women were diagnosed with breast cancer and caused a mortality of 670,000 worldwide in 2022¹. Furthermore, one in 12 women will be diagnosed with breast cancer and would result in a mortality of one in 71 women in countries where the Human Development Index (HDI) is at an extremely high level¹. On the other hand, one in 27 women will be diagnosed with breast cancer and would result in mortality for one in 48 women in countries with a low human development index¹. The disease begins with the unregulated growth of cells within the breast, resulting in the development of a tumor that can be benign or malignant. Benign tumors are non-cancerous and do not spread to other parts of the body, while malignant tumors are cancerous and have a tendency to invade adjacent tissues and migrate to other organs¹. Therefore, detecting a malignant tumor in an early stage increases the likelihood of effective treatment and survival.

¹<https://www.who.int/news-room/fact-sheets/detail/breast-cancer>

1.2 Motivation

Currently, the diagnosis and prediction of malignant tumors are performed manually by medical professionals, based on their experience, knowledge, and physical examination. Traditional diagnostic techniques include mammography, ultrasonography, and biopsy, with mammography and ultrasound aiding in tumor detection, and biopsy that involves microscopic analysis of tissue samples to confirm the presence of cancerous cells. Even though the amount of data collected during diagnosis may be huge, it would be difficult to identify the hidden pattern, resulting in misleading observation and results Gupta et al. (2022a). Traditional methods, while effective, tend to be slow and prone to human error. Consequently, there is an urgent need to improve breast diagnosis, as the conventional approach requires considerable expertise and is often limited by human interpretation errors.

In recent years, the rise of machine learning (ML) and deep learning (DL) has revolutionized medical diagnostics by offering automated, accurate, and efficient methods for disease detection and classification Wankhade et al. (2023). ML and DL techniques, particularly Convolutional Neural Networks (CNNs), have shown considerable promise in the precise analysis of medical images. However, these techniques are computationally inefficient and require a lot of time for training and implementation. Quantum Computing (QC) has gained significant attention due to their potential to solve tasks in feasible time frames that are time-consuming for classical computers Martín-Guerrero and Lamata (2022). A significant recent study claims that it has achieved this milestone by effectively sampling the results of a pseudo-random quantum circuit. Arute et al. (2019), highlighting QC's capabilities. QML has the potential to process large datasets more efficiently and uncover patterns that traditional ML and DL might miss.

1.3 Research Question

"To what extent Classical Machine Learning (Machine Learning & Deep Learning) and Quantum Machine Learning techniques compare in terms of performance for breast cancer prediction using the Wisconsin Diagnostic Breast Cancer dataset ?"

1.4 Research Objectives

1. Evaluate the performance of classical machine learning and deep Learning models.
2. Explore quantum machine learning models for the prediction of breast cancer.
3. Comparative analysis of classical and quantum machine learning techniques.

2 Related Work

In a recent years, a number of research work has been done for early breast cancer prediction. In Section 2.1 the current state of the art in machine learning was reviewed, in Section 2.2 the current state of the art in deep learning was reviewed, and in Section 2.3 review the current state of the art in Quantum Machine Learning in healthcare was reviewed.

2.1 Machine Learning based approach for Breast Cancer Prediction

A review by Kajala and Jain (2020) compared various state-of-the-art machine learning and image analysis methodologies for automated breast cancer detection, demonstrating their ability to improve early diagnosis and reduce unnecessary biopsies. The authors reviewed 22 articles from various journals and conferences from 2014 to 2019. These algorithms were evaluated for their effectiveness in analyzing mammographic images and numerical data to predict breast cancer. The review included several machine learning algorithms, such as Support Vector Machine (SVM), Decision Tree (DT), Artificial Neural Network (ANN), and Convolutional Neural Networks (CNN), with SVM achieving up to 97.7% accuracy. The review suggests that the success of machine learning in breast cancer detection is significantly dependent on the quantity and quality of the training data. The review indicated that SVM consistently exhibits high accuracy in various studies, establishing it as a preferred option among many researchers. Although the performance of ANN was limited by the number of neurons and layers, this highlights the need for more advanced deep learning methods such as CNN to obtain better outcomes. The paper concludes that while machine learning holds significant promise in improving breast cancer diagnosis, challenges such as data availability, computational cost, and integration into clinical workflows need to be addressed.

In another study by Rovshenov and Peker (2022), the authors used the Wisconsin Breast Cancer Dataset (WBCD) and applied various classification algorithms to classify the breast cancer tumor as benign and malignant. The primary objective of the study was to determine the most accurate machine learning technique for early prediction of breast cancer by evaluating algorithms based on precision, recall, and F measure. The findings showed that ANN achieved the highest accuracy at 99%, outperforming SVM and Random Forest, which both had an accuracy of 97%. The authors also used the k-fold cross-validation method, specifically the 10-fold technique, to ensure an accurate evaluation. This method involves dividing the data set into ten subsets, using nine for training and one for testing. The authors carefully selected the Hyper parameter for the algorithms, with the SVM using an RBF kernel and the ANN using ReLU activation functions in hidden layers and a sigmoid function in the output layer. The random forest algorithm was configured with 100 trees and the Gini criterion was split equally. The experimental results showed that ANN not only achieved the highest accuracy, but also performed well on other metrics like precision and recall. The comparative analysis of the literature also suggested that the algorithm performance was similar to previous studies on the same data set.

Similarly, in research work by Ahmed et al. (2020) the performance of six different machine learning classification algorithms including Logistic Regression (LR), K-Nearest Neighbors (kNN), Decision Tree (DT), Support Vector Machine (SVM), Naive Bayes (NB), and Random Forest (RF) was evaluated. The results showed that SVM achieved the highest accuracy at 97.07%, while Naive Bayes had the lowest accuracy at 96%. Other algorithms like RF, kNN, DT and LR also performed well, with accuracies close to 97%. Performance was further evaluated using a receiver operating characteristic (ROC) curve, which indicated that Naive Bayes achieved the highest area under the curve (AUC) for ROC.

2.2 Deep Learning based approach for Breast cancer Prediction

2.2.1 Breast Cancer Prediction using Image Classification

In a review conducted by Ramalakshmi et al. (2023), the authors investigated how deep learning algorithms can be used to analyze breast histopathological images for the early diagnosis of breast cancer. The authors reviewed several deep-learning based image analysis techniques such as AlexNet, Inception V3, and ResNet-50, with a primary focus on their effectiveness in detecting and classifying breast cancer from histopathology images. The study examines key data sets used to train and evaluate the deep learning model. This includes Spanhol et al. (2016) BreKHis dataset 7,900 images of breast biopsy specimens from 82 patients, with four different magnification levels : 40, 100, 200, and 400. These images were specifically captured for the classification of breast cancer histopathology images. The MITOS dataset, provided by the MITOS ATYPIA 14 contest, which contains 1,80,000 nonmitotic images and 748 mitotic histopathological images stained with mitotic hematoxylin and eosin. Another important dataset that was discussed was the Camelyon data set Bejnordi et al. (2017), which contains 400 images on the whole side. The authors explored various performance metrics used to evaluate the effectiveness of deep learning models in the detection of breast cancer. Metrics such as sensitivity, specificity, and accuracy are important to determine the ability of the models to correctly identify cancerous tissues. For example, the paper highlights a study in which the AlexNet model achieved a 89% accuracy rate on the BreakHis dataset, while another CNN-based model achieved an accuracy of 97.25%.

In the research by Chandra et al. (2024), the authors evaluated the performance of various deep learning models primarily using two distinct types of dataset: histology images and thermal images. The authors used the Gleason Case website ² to obtain breast histological images and thermal images. The histology dataset comprises 1,282 patches of 50x50 pixel images for training and 240 test images, with a distribution of 15.8% cancer-positive and 84.2% cancer-negative patches. The deep learning models, such as CNN, ResNet50, and a combined architecture of CNN and ResNet50, were trained using a stochastic gradient descent optimizer with a learning rate of 0.001 and a batch size of 32. For histology images, the CNN model showed highest accuracy at 88%, with balanced precision and recall rates. However, the ResNet50 model showed inconsistent performance metrics. The Concatenated Model achieved a notable accuracy of 87%, with balanced precision, recall, and a F1 score of 77%. For thermal images, the ResNet50 model demonstrated a balance between precision and recall, resulting in moderate performance. On the other hand, the CNN model achieved greater accuracy along with a balanced precision and recall rate. The findings suggest that although deep learning models are proficient in detecting breast cancer, their performance is greatly influenced by the type of imaging data used.

2.2.2 Breast Cancer Prediction using Wisconsin Breast Cancer data

In a research work by Khuriwal and Mishra (2018), the authors compared deep learning techniques to diagnose breast cancer, primarily using the Wisconsin Breast Cancer Database (WBCD) which contains 569 rows and 30 features. The authors identified 11 important features of the data set using recursive feature elimination with cross-validation

²<https://glean.co/>

(RFECV). Further, Principal Component Analysis (PCA) was used to reduce the dimensionality and convert the dataset into a 2-dimensional feature subspace. The main aim of the research is to implement a Convolutional Neural Network (CNN) for diagnosing breast cancer. The architecture consists of 12 neurons in the input layer, 8 neurons in the hidden layer, and a single neuron in the output layer. The CNN model achieved a highest accuracy of 99.67% as compared to other machine learning algorithms including Neural Network, Nearest Neighbour, Random Forest, and Support Vector Machine. The findings revealed that CNN performed the best among these algorithms in terms of precision, recall, and F-measure, establishing it as the most accurate model.

2.3 Quantum Machine Learning in Health Care

The review conducted by Ullah and Garcia-Zapirain (2024) provides an in-dept analysis of the potential and challenges of integrating the quantum computing(qc) with Machine Learning in healthcare domain. The authors focused on how Quantum Computing through Quantum Machine Learning can handle complex health care data, better than the traditional machine learning model in terms of speed and accuracy. The review identifies key areas where QML has be applied such as : Medical Imaging: QML has shown significant potential in enhancing various image analysis tasks critical for early disease diagnosis such as segmentation, classification and anomaly detection. For example, a hybrid model combining classical AlexNet and Variational Quantum Classifier (VQC) achieved an accuracy of 97% and 96% on MRI datasets from PPMI and ADNI, respectively. Drug Discovery: Quantum algorithms excel at efficiently modeling intricate molecular interactions, thus hastening the drug discovery process. In contrast to conventional techniques, QML methodologies have significantly enhanced the prediction of pharmacological properties, such as toxicity and efficacy, resulting in quicker identification of potential drug candidates and the optimization of medication formulations. Electronic Health Records (EHRs) QML techniques have been applied to analyze large and diverse EHR datasets, extracting valuable insights for improved disease prediction and patient management. For instance, using quantum-enhanced support vector machines (QSVM) and Quantum Random Forests (QRF), researchers achieved a 10%-15% improvement in accuracy for diabetes classification by correctly observing patterns in the dataset. The paper concludes that QML has the potential to revolutionize healthcare by providing more accurate, efficient, and scalable diagnostic tools. However, challenges such as qubit stability, error correction, scalability, and data encoding need to be addressed.

In another research by Gupta et al. (2022b), the authors proposed two predictive models, on with Deep learning and other with Quantum Machine Learning. The primary objective was to create a robust prognosis tool utilizing the PIMA Indian Diabetes dataset, which could help medical practitioners in reducing diabetes-related complications. The findings of the research reveal that the Deep Learning model out-performs the QML model and state-of-the-art techniques in terms of accuracy, precision, recall, F1 score, and other performance metrics. Specifically, the DL model achieved an accuracy of 95%, while the QML model attained an accuracy of 86%. The study concludes that, although the DL model demonstrates superior performance, the QML model shows promising results and potential for future integration with deep learning frameworks to further enhance its predictive capabilities.

3 Methodology

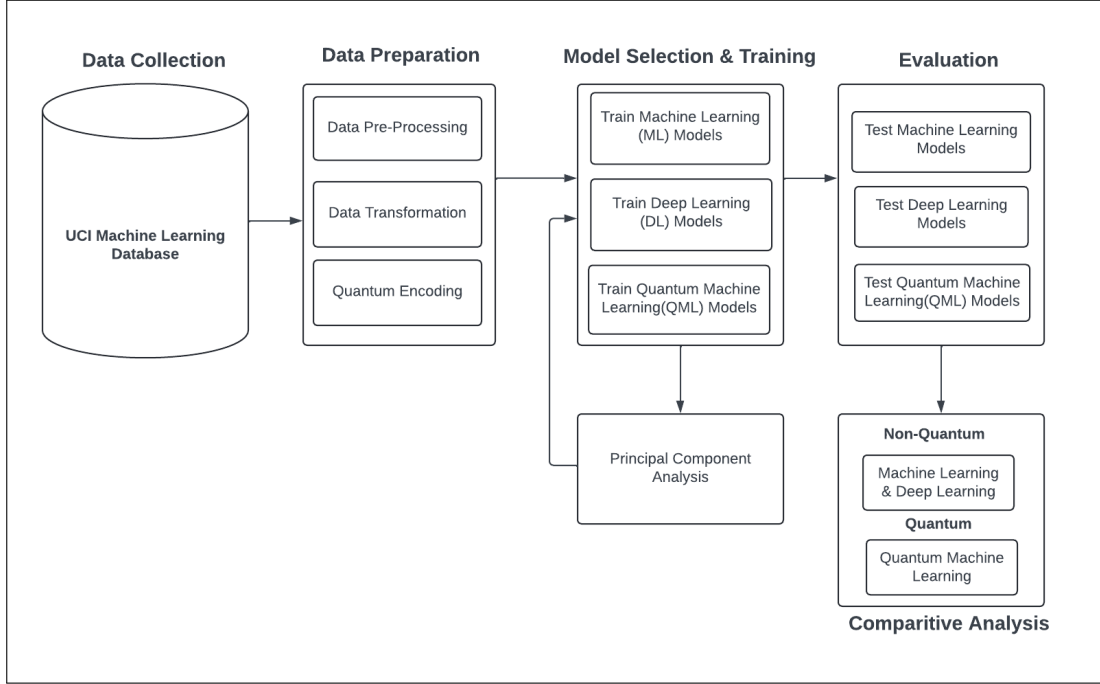


Figure 1: Project Methodology

In this research, a public dataset was used. The data set was sourced from the UCI Machine Learning repository, which contains breast cancer information from the University of Wisconsin hospital, provided by Dr. William H. Walberg. The data set contains 569 rows and 32 attributes. Table 3 provides a detailed description of all attributes of the data set.

3.1 Data Pre-Processing

In this step, the data is cleaned as some datasets may contain noise that can impact the outcome and overall performance of the models. After thorough analysis, it was found that the data set does not contain missing values or noise that can potentially impact the performance of the models.

3.2 Data Transformation

Data Transformation consists of steps to transform the data into a form that is ideal for analysis and modeling according to the requirement. Therefore, according to our requirement, the target variable of the Wisconsin dataset consists of categorical values, i.e. B: Benign Tumor & M: Malignant tumor which needs to be transformed into binary numerical values 0 & 1. The numerical values "0" represent benign tumors and "1" represent malignant tumors, respectively.

Table 1: Dataset Description

Attributes	Description	Domain (values)
diagnosis	Type of tumour	Benign(B) and Malignant(M)
radius	Mean distance from centre	decimal
texture	Standard deviation of values on grey scale	decimal
smoothness	Radius length variations (local)	decimal
concavity	Strength of concave curves on the boundary	decimal
concave points	Count of concave curving segments on the boundary	decimal
fractal dimension	Structure of an object and its relational characteristics	decimal
perimeter	Total length of the boundary	decimal
area	Area inside the boundary	decimal
compactness	$(\text{Perimeter}^2 / \text{Area} - 1)$	decimal
symmetry	Equal distribution between two parts	decimal

3.3 Exploratory Data Analysis

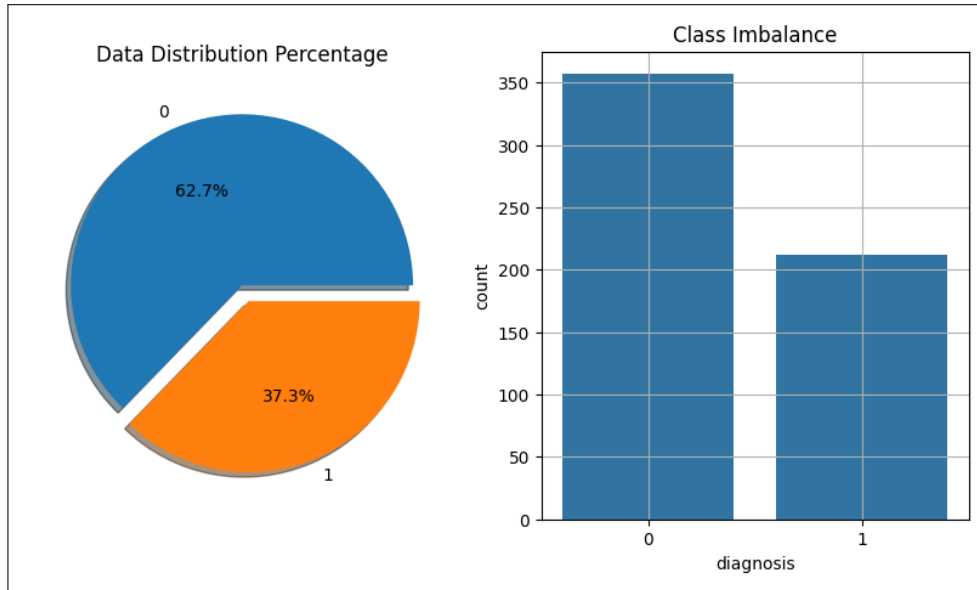


Figure 2: Data Imbalance

Figure 3.3 shows the distribution of diagnosis data in the Wisconsin Breast Cancer dataset. The bar chart indicates the imbalance in the dataset, with approximately 350 benign cases compared to approximately 200 malignant cases. It is important to address this imbalance during the training of the models, as the benign cases are more prevalent, the predictions might be skewed in favor of benign class.

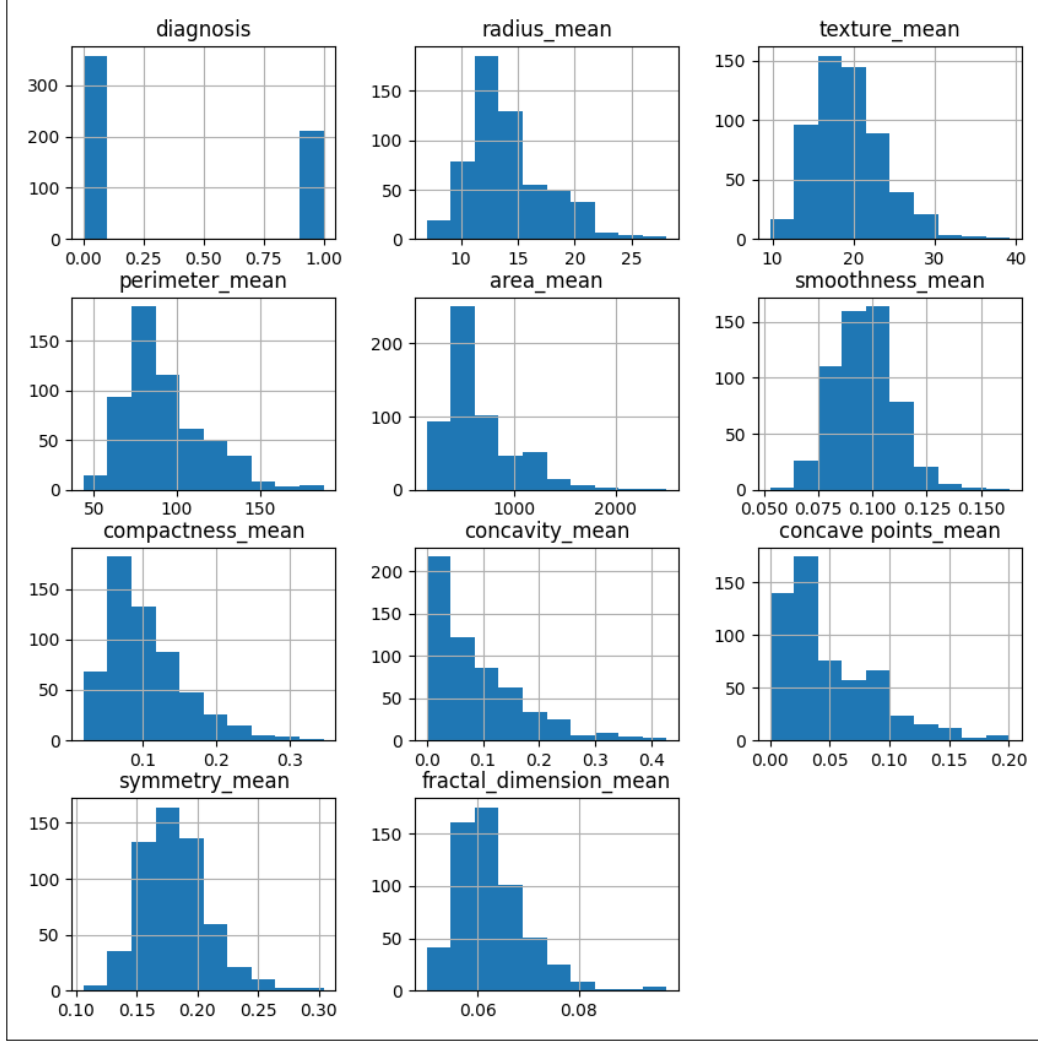


Figure 3: Distribution of Key Features in the Dataset.

3.4 Feature Selection

The Wisconsin Breast Cancer dataset has 32 features, all of which may not be pertinent to the prediction of the target variable, that is, the diagnosis. Therefore, it is crucial to determine and eliminate non-significant attributes of the dataset to get a higher prediction accuracy. To perform feature selection, we normalize the data using the StandardScaler³ method to ensure that all features were on a comparable scale. Furthermore, to determine the statistically significant features, we performed a T-test comparing the means of benign and malignant cases for each feature. The significance of the features was determined using a p-value threshold of 0.05, the features that exhibited p-values below this threshold were selected for further analysis.

3.4.1 Principal Component Analysis

Principal Component Analysis is a widely used dimensionality reduction approach Song et al. (2010). In classical principal component analysis, the dimensionality is reduced by

³<https://scikit-learn.org/stable/modules/generated/sklearn.preprocessing.StandardScaler.html>

transposing the covariance matrix of the data on to its diagonal Zeguendry et al. (2023). Quantum Principal Component Analysis uses QRAM to encode a quantum state in a randomly chosen data vector, resulting in the formation of a density matrix $\frac{1}{N} \sum_j |u_j\rangle\langle u_j|$, where N is the number of input vectors Zeguendry et al. (2023). By applying density matrix exponentiation, continuous data sampling, and quantum phase estimation, this method extracts the principal components of the input vectors Zeguendry et al. (2023).

3.5 Model Application & Comparative Analysis

Model Application is an important step in methodology as it consists in selecting appropriate algorithms according to the data set and research objectives. Based on the data in Wisconsin dataset we have selected various classification algorithms for Machine Learning such as Logistic Regression, Decision Tree Classifier, Random Forest, Support Vector Machine, KNN and Naive Bayes. For Deep Learning we have selected Artificial Neural Network, Convolutional Neural Network and Recurrent Neural Network. Finally, for Quantum Machine Learning, we have selected Variational Quantum Classifier and Quantum Support Vector Classifier. The performance of Machine Learning & Deep Learning (Non-Quantum) models is compared with Quantum Machine Learning Models on the basis of parameters such as accuracy, sensitivity and specificity.

4 Design Specification

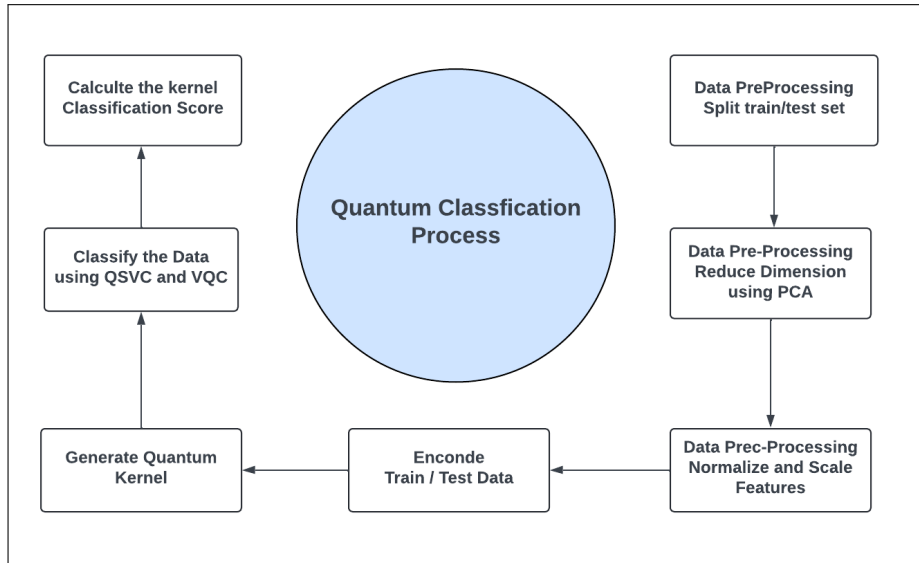


Figure 4: Quantum Classification Process

Quantum data refers to the information which adheres to the principles of quantum mechanics and can be stored and processed using the quantum bits or qubits Rath et al. (2023). Although classical data can exist in two states and are represented in binary form of 0 & 1, the quantum data can exist in multiple states at the same time because of superposition which aids in efficient encoding and information processing.

- Quantum Feature Maps : Kernel techniques use data mapping into high-dimensional spaces for pattern analysis and data recognition. This can be further extended into

an infinite-dimensional space. The "kernel trick" facilitates this by substituting the inner products of vectors with a kernel function within the algorithm, enabling efficient computation without explicitly performing the transformation Zeguendry et al. (2023). Quantum Kernel techniques use this concept into the realm of quantum computing. They identify hyperplanes through nonlinear transformations of data, referred to as "feature maps." These quantum feature maps, including the ZZ feature map, Z feature map, or Pauli feature maps (using Pauli X, Y, Z gates), can be implemented using frameworks like Qiskit, developed by IBM Zeguendry et al. (2023). The construction of quantum feature maps often involves the use of Hadamard gates and entangling unitary gates, which allow the encoding of classical data into quantum states that can then be processed by quantum algorithms Zeguendry et al. (2023).

Based on the type of data in the Wisconsin dataset, the following encoding methods were selected:

1. ZZ Feature Map: The ZZ Feature Map encodes classical information into quantum states by using single-qubit rotations and two-bit entangling interactions.
 2. Z Feature Map: The Z feature map is directly a form of angle encoding, where the classical information is encoded into quantum states using only single-qubit Z rotations.
 3. Pauli Feature Map: Pauli feature Maps are one of the most commonly used maps used in classification experiments due to their optimal depth and complexity Alexander and Widdows (2022). Pauli Feature Map uses combination of rotation around the Pauli-X, Pauli-Y and Pauli-Z axes.
- Quantum States - Quantum data generally refers to the condition of a quantum system, characterized by quantum states. The feature maps encode the data into quantum states, which is then further used as input for quantum computing.
 - Quantum Gates - Quantum Gates are used to construct the feature map itself and other parts of quantum circuit. They are the operations applied to the qubits. The quantum gates include elementary gates like Pauli gates & X gate, Hadamard gates, Phase gates, CNOT gate and Toffoli gates.
 - Quantum Circuits - The feature map is part of large quantum circuit that is designed for a particular algorithm. The circuit includes series of quantum gates that process the quantum data.

5 Implementation

5.1 Machine Learning Models

5.1.1 Logistic Regression

Logistic Regression is commonly used to classify data where the target variable is binary or categorical in nature. It is particularly useful in situations that involve categorical

outcome variables, with a special emphasis on binary cases where 1 represents a positive outcome and 0 represents a negative outcome. To classify breast cancer data, logistic regression model was implemented using the 'LogisticRegression' class from 'sklearn.linear_model' ⁴. The model was initialized with a fixed 'random_state' for reproducibility and trained it using the `fit` method with selected features ($X_{\text{train_selected}}$) and target labels (Y_{train}) from the training data set.

5.1.2 Random Forest

Random forest is a supervised machine learning algorithm that uses multiple decision trees to classify data. The random forest performance is good during binary classification. For classifying breast cancer data, Random Forest Model was implemented using `RandomForestClassifier` from the `sklearn.ensemble` module ⁵. The classifier was configured with 10 decision trees (`n_estimators=10`), using the `entropy` criterion for evaluating the quality of splits, and a fixed `random_state` of 42 to ensure reproducibility. The model was trained on the selected features ($X_{\text{train_selected}}$) and corresponding labels (Y_{train}) using the `fit` method.

5.1.3 Support Vector Machine

Support vector Machine: SVM is a supervised machine learning algorithm that can be used for classification. Ghantasala et al. (2023). SVM is used to classify data into two linear classes, such as benign and malignant, using the hyperplane to separate the data into distinct classes Ghantasala et al. (2023). To classify breast cancer data, Support Vector Machine (SVM) classifiers was implemented using the `SVC` class from `sklearn.svm`. The SVM model was initialized using linear kernel using `SVC` class with the parameter `kernel='linear'` ⁶ and a fixed `random_state` for reproducibility. The model was trained on the selected features ($X_{\text{train_selected}}$) and corresponding labels (Y_{train}) using the `fit` method.

5.1.4 K-Nearest Neighbours

KNN is one of the easy-to-use supervised machine learning algorithms that uses the distance between the data points to classify the data Bansal et al. (2022). To classify breast cancer data, K-Nearest Neighbors (KNN) classifier was implemented using the `KNeighborsClassifier` class from `sklearn.neighbors` ⁷. The classifier was configured with 5 neighbors (`n_neighbors=5`), using the Minkowski distance metric with a parameter $p = 2$ (which corresponds to the Euclidean distance). The KNN model was trained on the selected features ($X_{\text{train_selected}}$) and the corresponding labels (Y_{train}) using the `fit` method.

⁴https://scikit-learn.org/stable/modules/generated/sklearn.linear_model.LogisticRegression.html

⁵<https://scikit-learn.org/stable/modules/generated/sklearn.ensemble.RandomForestClassifier.html>

⁶<https://scikit-learn.org/stable/modules/generated/sklearn.svm.LinearSVC.html>

⁷<https://scikit-learn.org/stable/modules/generated/sklearn.neighbors.KNeighborsClassifier.html>

5.2 Deep Learning Models

5.2.1 Artificial Neural Network

The artificial neural network is a deep learning model based on the characteristics and working of biological neural networks Singhal and Pareek (2018). ANN is considered as one of the most effective algorithms when it comes to binary classification tasks Mridha (2021) such as classifying between benign and malignant cancer.

To classify breast cancer data, a neural network model was implemented using the Sequential API from `tf.keras` ⁸. The architecture of the model consists of multiple dense (fully connected) layers with ReLU activations and a final output layer with a sigmoid activation function for binary classification.

Layer (Type)	Output Shape	Parameters
Dense (ReLU)	(None, 24)	$input_dim \times 24 + 24$
Dense (ReLU)	(None, 8)	$24 \times 8 + 8$
Dense (ReLU)	(None, 16)	$8 \times 16 + 16$
Dense (ReLU)	(None, 64)	$16 \times 64 + 64$
Dense (ReLU)	(None, 16)	$64 \times 16 + 16$
Dense (ReLU)	(None, 8)	$16 \times 8 + 8$
Dense (Sigmoid)	(None, 1)	$8 \times 1 + 1$

Table 2: Architecture of the Neural Network Model

The compilation of model done using `binary_crossentropy` ⁹ and the Adam optimizer at a learning rate of 0.0005. Accuracy was used as an evaluation metric. To prevent overfitting, early stopping was used with a 20 epoch patience and monitoring the validation loss. The model was trained on the training data ($X_{\text{train}}, Y_{\text{train}}$) for up to 100 epochs, with validation on the test data ($X_{\text{test}}, Y_{\text{test}}$).

5.2.2 Convolutional Neural Network

Convolutional Neural Network is a deep learning algorithm that can be trained on data sets with a large number of records and hundreds of parameters Chauhan et al. (2018). It is commonly used in classification tasks. To classify breast cancer data, the convolutional neural network (CNN) was implemented using the `keras` library ¹⁰. The network architecture and compilation were designed as follows.

The model was compiled using the Adam optimizer ¹¹ with a learning rate of 0.00005. The loss function was set to binary cross-entropy, appropriate for binary classification tasks, and the model was evaluated using the accuracy metric. The model was then trained for 100 epochs to learn and classify the breast cancer data effectively.

5.2.3 Recurrent Neural Network

A Recurrent Neural Network (RNN) represents a deep learning model with the characteristics of supervised learning models Kaur and Mohta (2019). To classify breast cancer

⁸https://www.tensorflow.org/api_docs/python/tf/keras/activations

⁹https://www.tensorflow.org/api_docs/python/tf/keras/losses/BinaryCrossentropy

¹⁰<https://www.tensorflow.org/tutorials/images/cnn>

¹¹https://www.tensorflow.org/api_docs/python/tf/keras/optimizers/Adam

Layer (type)	Output Shape	Param #
conv1d (Conv1D)	(None, 29, 32)	96
batch_normalization (BatchNormalization)	(None, 29, 32)	128
dropout (Dropout)	(None, 29, 32)	0
conv1d_1 (Conv1D)	(None, 28, 64)	4,160
batch_normalization_1 (BatchNormalization)	(None, 28, 64)	256
dropout_1 (Dropout)	(None, 28, 64)	0
flatten (Flatten)	(None, 1792)	0
dense (Dense)	(None, 64)	114,752
dropout_2 (Dropout)	(None, 64)	0
dense_1 (Dense)	(None, 1)	65

Table 3: Architecture of CNN Model

data, we implemented a Recurrent Neural Network (RNN) using the `keras` library ¹². The network architecture and compilation were designed as follows.

Layer (Type)	Output Shape	Parameters
SimpleRNN (ReLU)	(None, 64)	$64 \times (\text{time_steps} + 1) + 64$
Dense (Sigmoid)	(None, 1)	$64 \times 1 + 1$

Table 4: Architecture of the RNN Model

The compilation was performed using the Adam optimizer ¹³. The loss function was set to binary cross-entropy and appropriate for binary classification tasks.

5.2.4 Multi-layer Perceptron

Multi-Layer Perceptron, as the name suggests, consists of multiple layers such as input, hidden, and output layers with each layer containing a set of neurons¹⁴. To classify breast cancer data, we implemented a multilayer perceptron (MLP) using the `keras` library ¹⁵. The network architecture and compilation were designed as follows:

Layer (Type)	Output Shape	Number of Parameters	Activation Function
Dense	(None, 8)	72	SELU
Dense	(None, 16)	144	SELU
Dense	(None, 32)	544	SELU
Dense	(None, 8)	264	ReLU
Dense	(None, 2)	18	ReLU
Dense	(None, 1)	3	Sigmoid

Table 5: Architecture of MLP Model

¹²https://www.tensorflow.org/guide/keras/working_with_rnns

¹³https://www.tensorflow.org/api_docs/python/tf/keras/optimizers/Adam

¹⁴<https://www.sciencedirect.com/topics/computer-science/multilayer-perceptron>

¹⁵https://www.tensorflow.org/guide/keras/working_with_rnns

5.3 Quantum Machine Learning Models

5.3.1 Variational Quantum Classifier

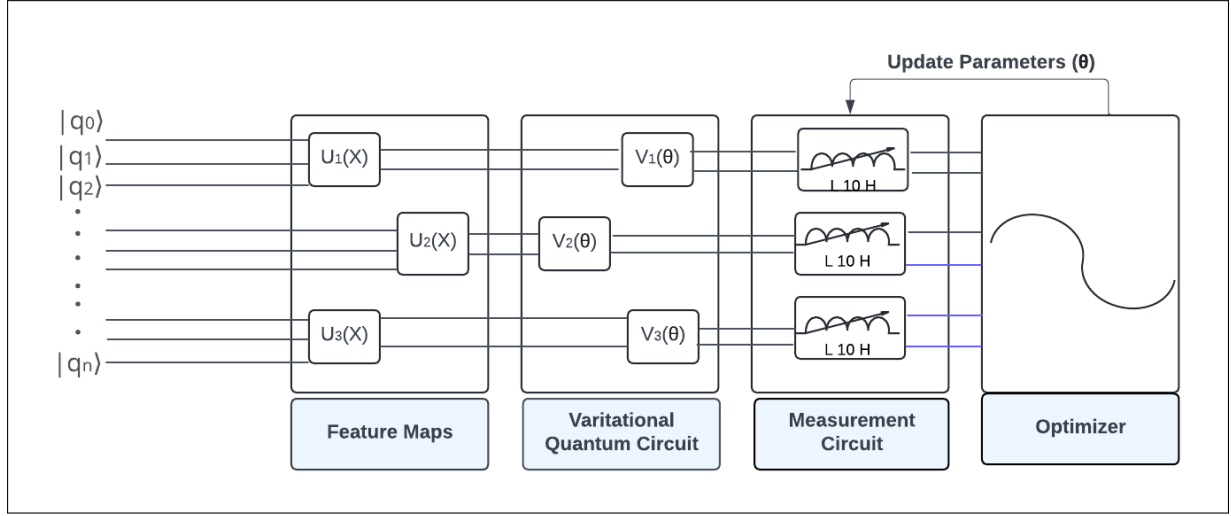


Figure 5: Architecture of Variational Quantum Classifier

The variable quantum classifier is a supervised Quantum Machine Learning algorithm that is widely used in classification problems Havlíček et al. (2019). To classify breast cancer data, Variational Quantum Classifier (VQC) was implemented using the `qiskit` library. The implementation involved the following steps:

1. The feature maps were prepared using the different classes from `qiskit.aqua.components.feature_maps`¹⁶. The feature map was initialized with the number of features (`num_features`) in the dataset and one repetition (`reps=1`).
2. The ansatz was prepared using distinct classes from `qiskit.circuit.library`¹⁷ and was initialized with the number of qubits equal to the number of features and three repetitions (`reps=3`).
3. The optimizer were implemented from `qiskit_algorithms.optimizers`¹⁸, setting a maximum number of iterations to 100.
4. The `Sampler()` function was used from `qiskit.primitives`¹⁹ to sample the quantum circuits.
5. The VQC model was then created using the `VQC` class from `qiskit_machine_learning.algorithms`²⁰. The model was initialized with the sampler, feature map, ansatz, optimizer, and a callback function for graph visualization.

¹⁶https://docs.quantum.ibm.com/api/qiskit/0.28/qiskit.aqua.components.feature_maps

¹⁷https://docs.quantum.ibm.com/api/qiskit/circuit_library

¹⁸<https://docs.quantum.ibm.com/api/qiskit/0.28/qiskit.algorithms.optimizers>

¹⁹<https://docs.quantum.ibm.com/api/qiskit/qiskit.primitives.Sampler>

²⁰<https://github.com/qiskit-community/qiskit-machine-learning>

5.3.2 Quantum Support Vector Classifier

Quantum Support Vector Classifier works in the same manner as the supervised machine learning algorithm, i.e., Support Vector Machine, by separating the data groups with a boundary that separates the data Maheshwari et al. (2022). To classify breast cancer data, we implemented a Quantum Support Vector Classifier (QSVC) using the Pegasos algorithm with the `qiskit` library ²¹. The implementation involved the following steps:

1. The feature maps were prepared using the different classes from `qiskit.aqua.components.feature_maps` ²². The feature map was initialized with the number of features (`num_features`) in the dataset and one repetition (`reps=1`). The random seed was set for reproducibility using the `algorithm_globals` ²³ module.
2. The quantum kernel was created using the `FidelityQuantumKernel` class from `qiskit_machine_learning.kernels` ²⁴ and was initialized with the previously defined feature map.
3. The QSVC model was implemented using the `PegasosQSVC` class from `qiskit_machine_learning`. The model was initialized with the quantum kernel, a regularization parameter (`C`) and the number of steps (`tau`).
4. The QSVC model was trained using the `fit` method on the training features (`train_features`) and labels (`train_labels`). The training accuracy was evaluated using the `score` method.
5. The testing accuracy of the model was evaluated using the `score` method on the testing features (`test_features`) and labels (`test_labels`).

6 Evaluation

In this section, we evaluate the performance of the model after implementing different techniques. Performance is calculated using various methods and criteria. The primary objective of this evaluation is to determine the results achieved, by analyzing the outcomes, based on following metrics:

1. Accuracy: Accuracy is the number of total correct predictions made by the model on the total number of overall predictions. The formula for calculating accuracy is given by the following equation :

$$Accuracy = \frac{True\ Positive + True\ Negative}{Total} \quad (1)$$

2. Sensitivity: Sensitivity is know as the True Positive rate and is calculated using following equation:

$$Sensitivity = \frac{True\ Positive}{True\ Positive + False\ Negative} \quad (2)$$

²¹https://qiskit-community.github.io/qiskit-machine-learning/tutorials/07_pegasos_qsvc.html

²²https://docs.quantum.ibm.com/api/qiskit/0.28/qiskit.aqua.components.feature_maps

²³https://docs.quantum.ibm.com/api/qiskit/0.28/qiskit.utils.algorithm_globals

²⁴https://qiskit-community.github.io/qiskit-machine-learning/stubs/qiskit_machine_learning.kernels.FidelityQuantumKernel.html

3. Specificity: Specificity is known as the False Positive rate and is calculated using following equation:

$$Specificity = \frac{True\ Negative}{True\ Negative + False\ Positive} \quad (3)$$

In this research, even though the metrics including accuracy, sensitivity, and specificity were considered when evaluating the performance of a model, the model with best performance was determined on the basis of Sensitivity or True positive rate. In the prognosis of breast cancer, it is crucial to accurately identify patients with breast cancer from general patients, as it would affect the chances of survival. Therefore, sensitivity was selected as a metric to judge the models.

Model	Accuracy %	Sensitivity %	Specificity %
Logistic Regression	95.10	88.89	98.87
Random Forest	93.00	94.51	92.13
SVM	95.10	89.89	98.85
KNN	92.31	90.74	93.25

Table 6: Comparison of Machine Learning Models

Table 6 shows the performance of all the Machine Learning models in terms of accuracy, sensitivity, and specificity. The model with best performance, i.e. highest sensitivity or true positive rate, is Random Forest with 94. 51% sensitivity and KNN with 90. 74% sensitivity.

Deep Learning	Accuracy %	Sensitivity %	Specificity %
ANN	97.20	98.14	96.66
CNN	97.20	94.33	98.88
RNN	96.50	94.44	97.77
MLP	97.20	94.44	98.87

Table 7: Comparison of Deep Learning Models

Table 7 shows the performance of all the Deep Learning models in terms of accuracy, sensitivity and specificity. The model with the best performance, that is, the highest sensitivity or the true positive rate is ANN with 98.14% Sensitivity and MLP & RNN with 94.44% Sensitivity.

Model	Accuracy %	Sensitivity %	Specificity %
Variational Quantum Classifier	86.84	63.41	1.00
Quantum Support Vector	93.00	82.85	96.29

Table 8: Comparison of Quantum Models

Table 8 shows the performance of all the Deep Learning models in terms of accuracy, sensitivity, and specificity. The model with best performance, i.e. highest sensitivity or true positive rate, is the quantum support vector with 82. 85% sensitivity

6.1 Experiment 1 : Choosing different feature maps and ansatz for Variational Quantum Classifier

In Variation Quantum Classifier, it is important to choose appropriate feature map as it can impact the performance of the model and the characteristics of the data encoded. Therefore, the performance Variation Quantum Classifier was evaluated for different feature maps including ZZFeatureMap, ZFeatureMap and PauliFeatureMap, in order to determine the best suitable one for VQC implementation. Additionally, another important step that directly impacts the performance of the model is ansatz. Thus, the performance of VQC was evaluated for two ansatz, including EfficientSU2 and the Real Amplitudes Ansatz.

6.1.1 Variational Quantum Classifier with EfficientSU2

Results before Principal Component Analysis			
Model	Accuracy %	Sensitivity %	Specificity %
ZZFeatureMap	71.05	34.15	91.78
ZFeatureMap	65.79	4.88	1.00
PauliFeatureMap	67.54	51.22	76.71

Table 9: Comparison of VQC Models with Efficient Su2 before PCA

Table 9 shows the performance of Variation Quantum Classifier for all the feature maps in terms of accuracy, sensitivity and specificity using EfficientSU2 ansatz. The feature map using which the variational quantum classifier gives best performance i.e. highest sensitivity or true positive rate is PauliFeatureMap with 51. 22% sensitivity before the principal component analysis.

Results after Principal Component Analysis			
Model	Accuracy %	Sensitivity %	Specificity %
ZZFeatureMap	79.82	81.25	78.79
ZFeatureMap	72.81	20.51	1.00
PauliFeatureMap	68.42	27.91	92.96

Table 10: Comparison of VQC Models with Efficient Su2 after PCA

Table 10 shows the performance of Variation Quantum Classifier for all the feature maps in terms of accuracy, sensitivity and specificity using EfficientSU2 ansatz. The feature map using which the variational quantum classifier gives best performance i.e. highest sensitivity or true positive rate is ZZFeatureMap with 81.25% sensitivity before the principal component analysis.

6.1.2 Variational Quantum Classifier with Real Amplitude

Table 11 shows the performance of Variation Quantum Classifier for all the feature maps in terms of accuracy, sensitivity, and specificity using Real Amplitude ansatz. The feature map using which the variational quantum classifier gives best performance i.e. highest sensitivity or true positive rate is PauliFeatureMap with 63.41% sensitivity before the principal component analysis.

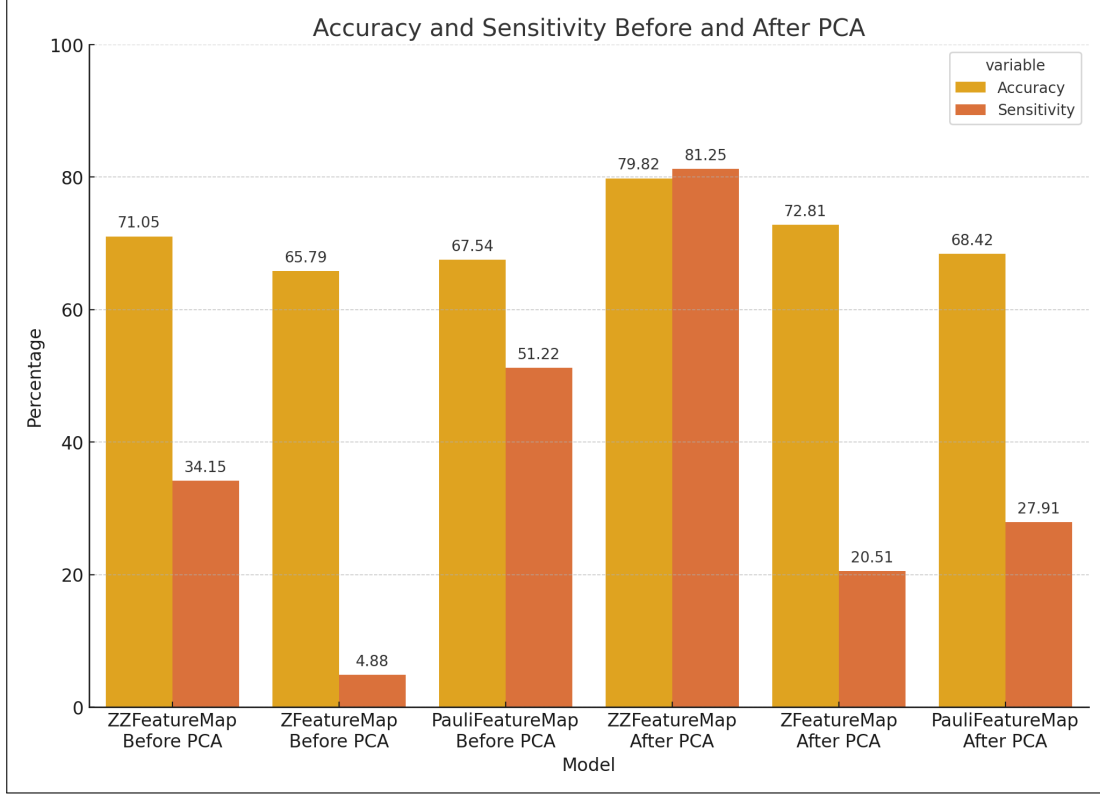


Figure 6: VQC accuracy and sensitivity with different feature maps & EfficientSU2

Results before Principal Component Analysis			
Model	Accuracy %	Sensitivity %	Specificity %
ZZFeatureMap	68.42	24.39	93.15
ZFeatureMap	70.18	17.07	1.00
PauliFeatureMap	86.84	63.41	1.00

Table 11: Comparison of VQC Models with RealAmplitude before PCA

Table 12 shows the performance of the Variation Quantum Classifier for all feature maps in terms of accuracy, sensitivity, and specificity using the Real Amplitude ansatz.

Results after Principal Component Analysis			
Model	Accuracy %	Sensitivity %	Specificity %
ZZFeatureMap	52.63	16.67	78.79
ZFeatureMap	68.42	7.69	1.00
PauliFeatureMap	67.54	25.58	92.96

Table 12: Comparison of VQC Models with RealAmplitude after PCA

The feature map using which the variational quantum classifier gives best performance i.e. highest sensitivity or true positive rate is PauliFeatureMap with 25.71% sensitivity after the principal component analysis.

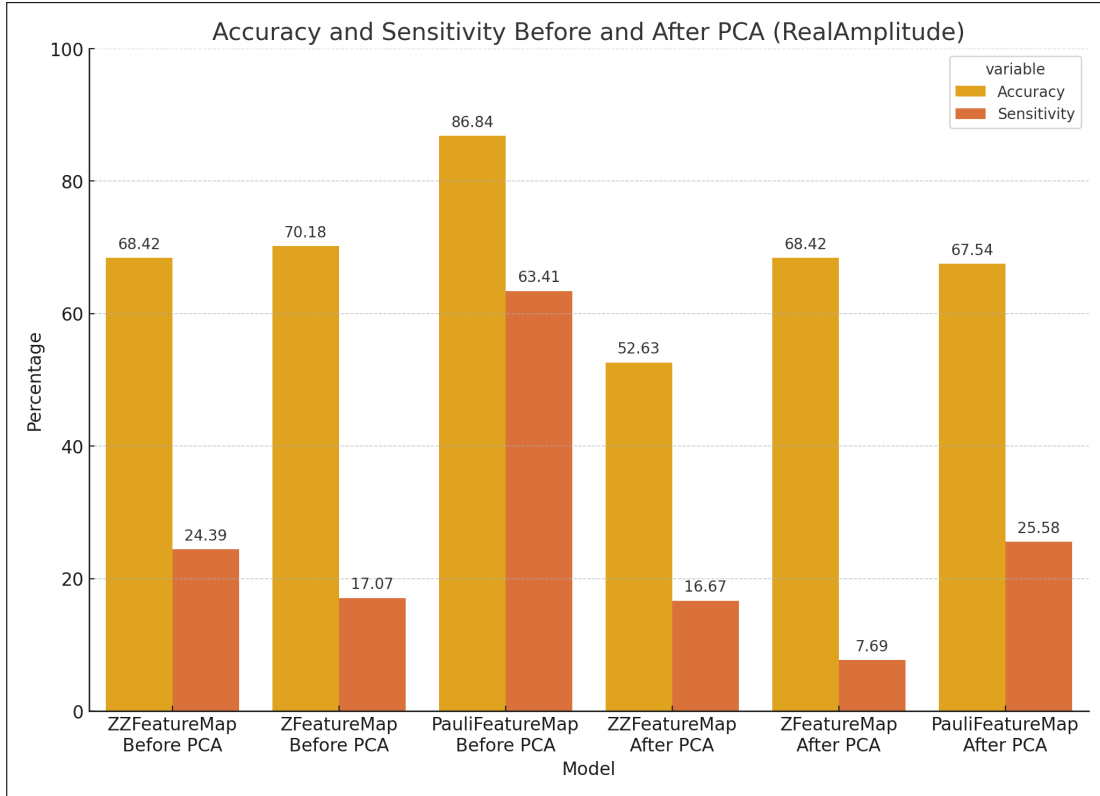


Figure 7: VQC model accuracy and sensitivity across different feature maps

Model	Accuracy %	Sensitivity %	Specificity %
ZZFeatureMap	27.28	1.00	3.70
ZFeatureMap	93.00	82.85	96.29
PauliFeatureMap	81.82	25.71	1.00

Table 13: Comparison of Quantum Support Vector Models

6.2 Experiment 2: Choosing different feature Maps for QSVC

Table 13 shows the performance of the Quantum Support Vector for all feature maps in terms of accuracy, sensitivity, and specificity. The feature map using which the QSVC gives best performance i.e highest Sensitivity or true positive rate is ZFeatureMap with 83.85% Sensitivity.

6.3 Discussion

Model	Accuracy	Sensitivity	Specificity
Quantum Support Vector	93.00	82.85	96.29
ANN	97.20	98.14	96.66
Random Forest	93.00	94.51	92.13

Table 14: Comparative Analysis of Classical and Quantum Machine Learning Models with highest sensitivity

The results show that machine learning models such as **Random Forest** and **SVM**

as well as deep learning models such as **ANN** and **MLP**, consistently perform well on the Wisconsin dataset. The Quantum models give satisfactory performance but are highly dependent on the feature map and preprocessing steps such as Principal Component Analysis(PCA). The **Quantum Support Vector** with **ZFeatureMap** in particular showed performance comparable to that of classical models. However, the performance variability in terms of sensitivity and specificity suggests that more work is needed to optimize these quantum models. Preprocessing techniques such as Principal Component Analysis appear to improve the performance of certain models, particularly the **Variational Quantum Classifier** with **Efficient Su2** configuration.

While Sensitivity was the main criterion for evaluating the models, another performance metric, specifically Time Complexity, must also be taken into account. The time complexity for training Machine Learning models can be as high as $O(n^2 \times d)$, where n is the number of samples and d is the dimensionality of the data Groning et al. (2022). Furthermore, training a deep neural network can have a time complexity ranging from $O(n \times d \times m)$ to $O(n^2 \times d \times m)$, where m is the number of layers or parameters in the network Groning et al. (2022). The Quantum Machine Learning algorithm specifically the Quantum Support Vector Classifier can reduce the time complexity to approximately $O(\log(n) \times \text{poly}(d))$, Gentinetta et al. (2022), demonstrating exponentially faster performance compared to the machine learning algorithms. However, in this research, due to Hardware limitations and lack of access to quantum computing resources, the performance of quantum models couldn't be fully illustrated.

7 Conclusion and Future Work

The primary focus of this study was to determine a model that will accurately identify the type of breast cancer tumors in the patient. The analysis of various machine learning, deep learning, and quantum machine learning models on the Wisconsin data set provides several important insights. Machine learning models, particularly Random Forest with a sensitivity of 94.51% and deep learning models such as ANN with a sensitivity of 98.14%, demonstrate strong and consistent performance. Thus, these models can help medical practitioners detect benign and malignant cancer tumors in the early stages. Quantum Machine Learning models, particularly the Quantum Support Vector, gave satisfactory performance achieving sensitivity of 82.85%. Despite the ability of quantum machine learning models to deliver comparatively faster performance, the research was restricted by hardware limitation and the lack of advanced quantum computing resources, preventing a full illustration of the potential speed advantage of quantum models.

For future research, it is recommended to focus on optimizing the quantum feature maps, exploring advanced preprocessing techniques and developing hybrid models that combine classical and quantum approaches to enhance breast cancer prediction. The time complexity of quantum models must be evaluated using real-world quantum hardware and extend the application of these models to other medical datasets.

Acknowledgement

I am profoundly thankful to my supervisors, Dr. Paul Stynes, Dr. Musfira Jilani, and Professor Mark Cudden for their constant support and guidance throughout the research process.

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