

Exploring the Interplay Between Expressivity and Trainability in Quantum Neural Networks for Image and Audio Data

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A thesis submitted to the Department of Computer Science and Engineering
in partial fulfillment of the requirements for the degree of
B.Sc. in Computer Science

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Declaration

It is hereby declared that

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2. The thesis does not contain material previously published or written by a third party, except where this is appropriately cited through full and accurate referencing.
3. The thesis does not contain material which has been accepted, or submitted, for any other degree or diploma at a university or other institution.
4. We have acknowledged all main sources of help.

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Abstract

Quantum Machine Learning architectures consist of ansatzes, a Parameterized Quantum Circuit designed based on educated guesses about the problem to be solved. This design is the most critical aspect of developing a Quantum Neural Network (QNN) structure and has immense implications for its performance. This thesis investigates the expressivity of different ansatzes structures in QNN design through fidelity distribution analysis, which statistically compares the fidelity values between quantum states generated by an ansatz and random states sampled from the Haar measure. The expressivity and trainability of various ansatzes architectures are explored by leveraging different datasets from image and audio domains as test cases. The findings provide valuable insights into designing ansatzes for specific tasks and goals using QNN architectures, advancing the field of quantum machine learning.

Keywords: Ansatz; Quantum Machine Learning Architecture; Parameterized Quantum Circuit; Quantum Neural Network; Expressivity; Fidelity Distribution Analysis; Haar Measure; Trainability; Entangling Capability; Layerwise Expressivity; Layerwise Entangling Capability

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Nomenclature

The next list describes several symbols & abbreviation that will be later used within the body of the document

AI Artificial Intelligence

ANN Artificial Neural Network

CNN Convolutional Neural Network

CNOT Controlled-NOT

CRX Controlled-RX

CRY Controlled-RY

CRZ Controlled-RZ

CZ Controlled-Z

GHZ Greenberger-Horne-Zeilinger

KL Kullback Leibler

MERA MultiScale Entanglement Renormalization Ansatz

ML Machine Learning

MSE Mean Squared Error

NISQ Noise Intermediate Scale Quantum

NLP Natural Language Processing

NN Neural Network

PQC Parameterized Quantum Circuit

QAOA Quantum Approximate Optimization Algorithm

QC Quantum Computing

QC – CNN Quantum-Classical Convolutional Neural Network

QCNN Quantum Convolutional Neural Network

QML Quantum Machine Learning

QNN Quantum Neural Network
QPCA Quantum Principal Component Analysis
QSVM Quantum Support Vector Machine
ResNet Residual Neural Network
RNN Recurrent Neural Network
RY Rotational-Y
VQA Variational Quantum Algorithm
VQE Variational Quantum Eigensolver

Chapter 1

Introduction

Artificial Intelligence (AI) is deployed in a wide array of applications nowadays. Over the past few years, researchers have tried to explore how Artificial Intelligence can be applied to boost human efficiency, automate work, and complete various scientific tasks, especially the deep learning algorithms like Artificial Neural Network (ANN), Convolutional Neural Network (CNN), Recurrent Neural Network (RNN), and Natural Language Processing (NLP). Among them, CNN is widely used for image classification tasks. It has a greater ability to capture spatial correlations and learn important features from data.

Moreover, in the past few years, most organizations and people shifted towards the internet, tools depending on the internet, and many more. Therefore, each application now carries a huge level of data. That shows the necessity of processing this huge data. Especially to know a user's behavior properly, image data classification has become very crucial. Classically, CNN is used to classify these images, but it takes a good amount of computing power and time. If Quantum Computing (QC) is used to process these huge amounts of data, especially data of high dimensions, it can be done in exponentially less time. In Quantum Computing, one of the fields that inherits the classical Machine Learning principles while using Quantum Mechanics principle is called Quantum Machine Learning (QML). One subfield of QML that focuses on applying Neural Network concepts utilizing the quantum mechanical principle is called Quantum Neural Network (QNN). The capabilities of Quantum Convolutional Neural Networks (QCNNs), which operate on classical data, are being investigated in this thesis.

1.1 Research Statement

Despite the future probabilities of QCNNs, several problems are still to be solved before we implement them properly. One of the core components of QCNN is an ansatz. Again, an ansatz's capability can be analyzed through the expressivity and entangling capability.

The term “expressivity” means the ability of an ansatz to access various quantum states in the Hilbert Space whereas the term “entangling capability” measures how effectively an ansatz can create complex, correlated quantum states. Understanding the interplay between expressivity, entangling capability and trainability remains a

big task for the development of efficient and effective QNNs.

Our work explores the interplay between expressivity, entangling capability and trainability in Quantum Neural Networks while applying QCNN to image and audio data. We have also explored Convolution Layer expressivity and entangling capability and their connection with trainability. We start our research by exploring accuracies for image data and audio data classification using various Convolutional Ansatz and Pooling Ansatz. Then we explore the expressivity and entangling capability of our Convolutional Ansatzes as we used the same Pooling Ansatz in our classification test. Finally, we explored the expressivity and entangling capability of Convolutional Ansatzes for the Convolutional Layers (Convolution Layer 1, Convolution Layer 2, Convolution Layer 3). The goal of the research is to choose a better ansatz even before using it for the Quantum Model. This will help quantum researchers reduce cost for model runs and increase trainability.

1.2 Structure of Report

Chapter 1: The introduction chapter discusses our motivation behind the work on Quantum Convolutional Neural Networks and expressivity. We have also started our research objective from the work.

Chapter 2: Literature Review summarized classical and quantum concepts alongside a summary of previous researchers' findings on these topics.

Chapter 3: Work plan showed our detailed plan for the work in a flowchart.

Chapter 4: In Methodology, we described our working procedure to compute expressivity, entangling capability and datasets accuracy on each of the ansatz and convolutional layers.

Chapter 5: In Result Analysis, we analyzed the expressivity, entangling capability and accuracy of our model to find out the correlation between them.

Chapter 6: Conclusion, where we summarized our overall work on this project.

Chapter 2

Literature Review

2.1 Overview of Classical and Quantum Machine Learning

Just like classical Machine Learning, Quantum Machine Learning (QML) inherits the classical Machine Learning Principles. QML is applied in quantum chemistry [4], Artificial Intelligence [16], high energy physics [6], etc. While solving problems in these fields, QML uses Variational Quantum Algorithm (VQA).

Variational Quantum Algorithms (VQA): VQA was first established by researchers who wished to overcome challenges in quantum chemistry. Variational Quantum Eigensolver (VQE) was the first tool they employed [5]. Following that, VQA was combined with Quantum Approximate Optimization Algorithms (QAOAs) [3] to handle combinatorial optimization issues.

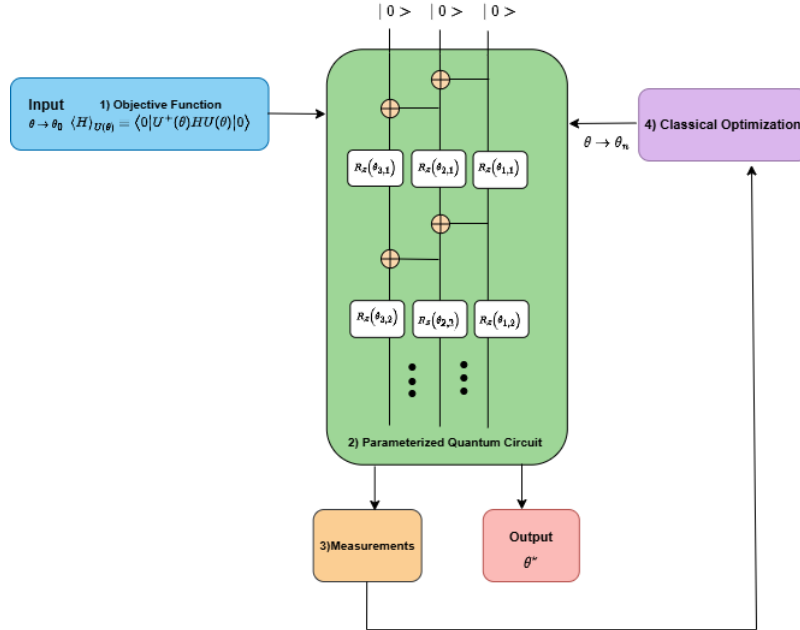


Figure 2.1: VQA with Objective Function, PQC, Measurements, and Classical Optimization [20]

VQA is divided into four parts:

1) **Objective Function:** While using the VQA, firstly we fix a goal. The goal can be said to be an objective function. It is generally a mathematical function that quantifies how close the current quantum state is to our desired goal. It can be presented with this equation:

$$\langle H \rangle_{U(\theta)} \equiv \langle 0 | U^\dagger(\theta) H U(\theta) | 0 \rangle \quad (2.1)$$

2) **Parameterized Quantum Circuit (PQC):** PQCs are quantum circuits built with quantum gates that depend on tunable parameters. It consists of quantum gates and parameterized gates (generally the Rotation gates).

3) **Measurements:** Through measurement, the classical value is extracted from the quantum states. Some of the Noise Intermediate Scale Quantum (NISQ) measurement methods are Measurements of Pauli String, Measurement of overlaps, and Classical Shadows.

4) **Classical Optimizer:** Classical optimizers optimize PQC's parameters to reach the objective function.

One of the fields of QML is Quantum Convolutional Neural Network, which follows the same principle while using gates, encoding techniques, pooling, and convolution through ansatzes and measurement.

2.2 Quantum Convolutional Neural Network Components

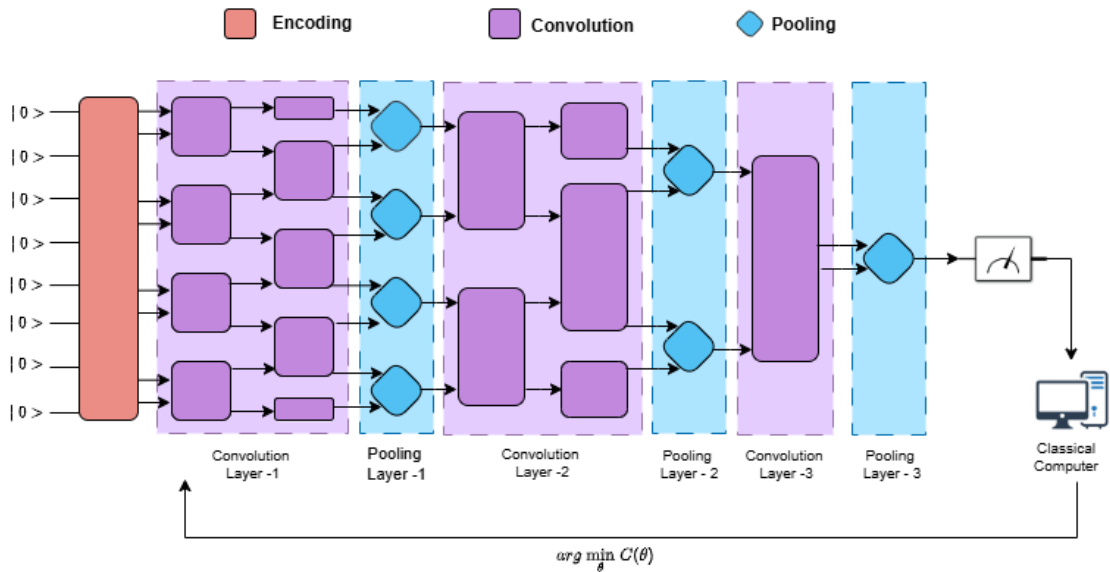


Figure 2.2: Quantum Convolutional Neural Network Architecture [12]

2.2.1 Ansatz

The term Ansatz refers to “educated guess” meaning an assumption that helps solve a problem. It’s a specific form or structure of a PQC that is used to prepare quantum states. Choosing a perfect ansatz is very crucial as it determines expressivity, efficiency of the optimization, and ability to avoid barren plateaus. Generally, there are two types of ansatzes. One is problem-inspired ansatz, and the other one is hardware-inspired ansatz. Problem-inspired ansatzes are designed on knowledge of the problem being solved, often used in physics or chemistry problems where the solution is partially known. Whereas hardware-efficient ansatzes are designed to be compatible with the constraints of the quantum hardware (limited connectivity, gate sets). Ansatzes are used in the Convolutional and Pooling layer of the circuit.

In our work, we use ansatzes in our convolutional circuit and pooling.

Convolutional Layer: Instead of classical filters, QCNN apply Parameterized Unitary Gates. These unitaries act like “Quantum Filters” that extract the features from input.

Once the data is encoded using various ansatzes, the data is passed to the Convolutional Layers.

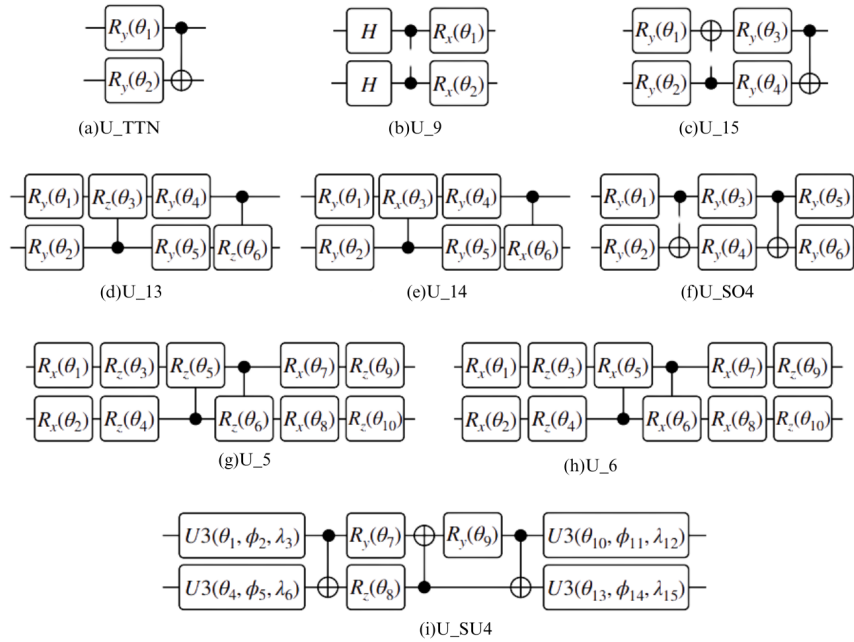


Figure 2.3: Different types of ansatzes that can be used in Convolutional Layers [12]

Pooling Layer: The pooling layer reduces the spatial dimensions. Especially in QCNN, the pooling layer compresses quantum information while preserving important features. In the pooling layer, data is again passed with some pooling layer ansatzes with it. In the Figure 2.4 and 2.5, two pooling layer ansatzes are shown.

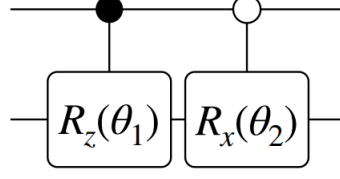


Figure 2.4: Two qubit pooling ansatzes [12]

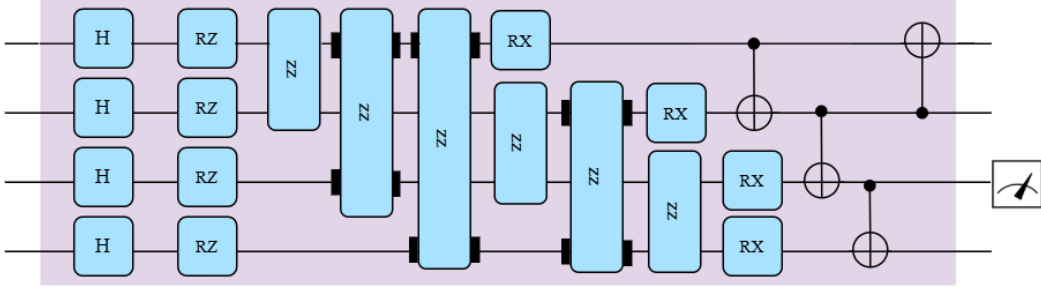


Figure 2.5: Four qubit pooling ansatzes [15]

2.2.2 Quantum Data Encoding

The quantum approach itself is unable to process the classical data. It means that the classical information should be converted to quantum states. There are various encoding methods for data encoding but among them, here are a few:

Encoding Type	Qubit Efficiency	Entanglement	Feature Capacity	User Case
Basis	$\mathcal{O}(2^n)$	No	Binary	Binary Classification, Grover's Search
Amplitude	$\mathcal{O}(\log N)$	No	Continuous	Quantum Neural Networks
Qubit	$\mathcal{O}(N)$	No	Continuous	Simple Embeddings
Angle	$\mathcal{O}(N)$	No	Continuous	Variational Circuits
Angular Hybrid	$\mathcal{O}(\sqrt{N})$	Yes	Continuous	Hybrid Quantum-Classical Models

Table 2.1: Comparison of Quantum Encoding Methods

1) **Basis Encoding:** A quantum system's computational basis states are immediately transferred to the classical binary data throughout this encoding process. Stated differently, it is utilized in the Grover Search Algorithm and quantum walks.

The quantum state $|101\rangle$ can be used to represent the classical number 101.

$$|101\rangle = |1\rangle \otimes |0\rangle \otimes |1\rangle \quad (2.2)$$

Regarding amplitudes:

$$|101\rangle = \alpha|1\rangle \otimes \beta|0\rangle \otimes \gamma|1\rangle \quad (2.3)$$

where the probability amplitudes for each qubit state are denoted by α , β , and γ . Each qubit is taken into consideration independently, as shown by the tensor product sign $\otimes$. [18]

2) **Amplitude Encoding:** In this encoding method, data is stored in the amplitude of a quantum state. Few Quantum Machine Learning Algorithms, such as QSVM and QPCA, have been proposed considering it. Amplitude encoding effectively encodes a huge dataset in a few qubits, and hence Amplitude encoding technique has been followed in this work.

The input data of $x = (x_1, \dots, x_N)^T$ of dimension $N = 2^n$ is represented using the Amplitude encoding. The n qubit quantum state can be expressed as follows:

$$U_\phi(x) : x \in \mathbb{R}^N \rightarrow |\phi(x)\rangle = \frac{1}{\|x\|} \sum_{i=1}^N x_i |i\rangle \quad (2.4)$$

Here $|i\rangle$ presents the i th computational basis state. [12]

3) **Qubit Encoding:** In this encoding, the qubit state can encode the classical data; this is usually considered in many quantum communication protocols.

For instance, data $x = (x_1, \dots, x_N)^T$ is encoded to N qubits using qubit encoding as follows:

$$U_\phi(x) : x \in \mathbb{R}^N \rightarrow |\phi(x)\rangle = \bigotimes_{i=1}^N \left(\cos\left(\frac{x_i}{2}\right) |0\rangle + \sin\left(\frac{x_i}{2}\right) |1\rangle \right) \quad (2.5)$$

Where $x_i \in [0, \pi)$ for all i . The encoding circuit can be expressed thus with a unitary operator, [12]

$$U_\phi(x) = \bigoplus_{j=1}^N U_{x_j} \quad (2.6)$$

Where,

$$U_{x_j} = e^{-i\frac{x_j}{2}\sigma_y} := \begin{bmatrix} \cos\left(\frac{x_j}{2}\right) & -\sin\left(\frac{x_j}{2}\right) \\ \sin\left(\frac{x_j}{2}\right) & \cos\left(\frac{x_j}{2}\right) \end{bmatrix} \quad (2.7)$$

4) **Angle Encoding:** In this encoding, the qubits are considered for the rotational angle which gives them encoding in a classical set. Quantum Neural Network algorithms and Quantum Approximate Optimization Algorithms will be used. We have used Angle Encoding in our work here too.

The first qubit has no rotation ($\theta_0 = 0$), the second qubit has 180-degree rotation ($\theta_1 = \pi$), and the third qubit has no rotation ($\theta_2 = 0$).

So, the rotation acts like: [18]

$$|\psi\rangle = R_{x_2}(0) \cdot R_{x_1}(\pi) \cdot R_{x_0}(0)|0\rangle \quad (2.8)$$

5) **Angular Hybrid Encoding:** It is an encoding technique which combines angle encoding with entanglement. It generally uses Rotational gates to encode classical features as qubits, introduces controlled entangling gates to create connections between features.

2.2.3 Cost function

Cost functions are used to measure how correctly the model is performing. There are various cost functions that can be used, among them these are a few:

Mean Squared Error: The average squared difference between expected and actual values is measured by this popular Machine Learning loss metric. In MSE, $C(\theta)$ is minimized by optimizing θ . The goal is to make $\hat{M}_z(\psi_i(\theta))$ as close as possible to $\tilde{y}_i$ for all inputs. [12]

$$C(\theta) = \frac{1}{N} \sum_{i=1}^N (\hat{M}_z(\psi_i(\theta)) - \tilde{y}_i)^2 \quad (2.9)$$

Cross Entropy Loss: The training of Conventional Neural Networks highly depends on the Cross Entropy loss. It evaluates how well the classification model performs in its output, which is the probability ranging between 0 and 1. Since the odds of witnessing the computational basis states in the single-qubit measurement of a QCNN are in fact provided by the principles of quantum physics, cross entropy loss can be used as a logical choice for this probabilistic description.

Here, the Cross Entropy loss for the i th training data can be shown as: [12]

$$C(\theta) = \sum_{i=1}^N [y_i \log(\Pr[\psi_i(\theta) = 1]) + (1 - y_i) \log(\Pr[\psi_i(\theta) = 0])] \quad (2.10)$$

2.3 Expressivity

Expressivity in Quantum Neural Networks (QNNs) is the capacity of a PQC to produce a broad variety of quantum states in the Hilbert Space [7]. Exploring ansatz structure's expressivity may enable us to design better circuits which might increase the overall performance of a certain QNN. Therefore, informed ansatz design is crucial to achieve an optimal architecture to achieve better accuracy.

There are several ways to quantify the expressivity of a certain ansatz. Our method involves using 'Haar Fidelity Distribution' and comparing them with the fidelity distribution of ansatzes to estimate expressivity.

2.3.1 Haar Fidelity Distribution

Haar Fidelity Distribution represents the statistical distribution between the fidelity values of random quantum states extracted from the Haar measure and quantum states produced by an ansatz. It compares the overlap between these two quantum states within the Hilbert space. The expressivity of various ansatzes are reflected in the degree of similarity between Haar-random quantum states and ansatz-generated quantum states.

Haar Fidelity Distribution can be mathematically expressed as:

$$\text{Fidelity, } F = |\langle \psi_\theta | \psi_\phi \rangle|^2 \quad (2.11)$$

The quantum states ψ_θ and ψ_ϕ are generated by the ansatz with parameter θ and parameter ϕ , respectively. [7]

Here, two random quantum states ψ_θ and ψ_ϕ were generated from uniformly sampled distribution. Using those two random quantum states and [fidelity formula], Haar Fidelity ($P_{\text{haar}}(F)$) is calculated. Now, let us explore the fidelity distribution generated by ansatz. Firstly, two random parameters θ_1 and θ_2 were randomly generated. A specific ansatz has to be selected which will be used to create the two quantum states. The ansatz is then parameterized using θ_1 and θ_2 , two quantum states are generated which are ψ_{θ_1} and ψ_{θ_2} . Finally, $P_{\text{ansatz}}(F)$ is calculated using the quantum states ψ_{θ_1} and ψ_{θ_2} . This entire operation is performed a definite number of times which is equal to the number of samples considered initially. If we generate a graph using the Haar Fidelity distribution and ansatz fidelity distribution, we should observe overlap between these two distributions. Here, the amount of overlap is equal to the amount of expressivity of that certain ansatz possess.

There is another way to quantify Haar Fidelity distribution. At first we have to generate a Haar random unitary matrix. Let us assume, we have a complex matrix U where the variables are sampled from normal distribution. Now, we have to perform QR decomposition on the matrix U and we found an orthonormal matrix at Q . If we normalize the orthonormal matrix where determinant of Q is 1, then we will acquire a Haar random unitary matrix Q . In other words, Q is a quantum gate which is truly random.

Again, we have to quantify the fidelity of $Q^\dagger$ with respect to identity gate using: [2]

$$\begin{aligned} X &= \frac{1}{d} \{Tr(Q^\dagger I)\}^2 \\ \Rightarrow X &= \frac{1}{d} \{Tr(Q)\}^2 \end{aligned} \quad (2.12)$$

Here, $Tr(Q)$ is a random variable which is normally distributed. Now, if $Tr(Q)$ is normally distributed then the $[Tr(Q)]^2$ will be a β distribution. Therefore, the random variable X is β distributed. Again, if X is β distributed then the probability density function will be the same as Haar probability distribution.

$$\text{Haar Probability Distribution, } p_{\text{Haar}}(F) = (N - 1)(1 - F)^{N-2} \quad (2.13)$$

Where,

F = Fidelity value

N = Dimension of the Hilbert space [7]

2.3.2 KL(Kullback Leibler) Divergence

The KL Divergence differentiates between the two probability distributions. Here, the distributions are Haar Fidelity distribution and Ansatz fidelity distribution. It mainly measures how much information is lost while using ansatz fidelity distribution to calculate Haar Fidelity distribution. It can be mathematically expressed as:

$$D_{KL}(P_{\text{ansatz}}(F)||Q_{\text{Haar}}(F)) = \sum_x P_{\text{ansatz}}(F) \log \left(\frac{P_{\text{ansatz}}(F)}{Q_{\text{Haar}}(F)} \right) \quad (2.14)$$

Where:

$P_{\text{ansatz}}(x)$: Ansatz Fidelity Distribution

$Q_{\text{Haar}}(x)$: The Haar Fidelity Distribution [17]

If the value of the KL divergence is low then it implies the Ansatz distribution is closer to Haar randomness which directly implies higher expressivity. On the other hand, if the value is high it signifies poor expressivity of the ansatz.

$$\text{Expr} = D_{KL}(P_{PQC}(F; \theta)||P_{\text{Haar}}(F)) \quad (2.15)$$

Where:

Expr: Expressivity of the ansatz or PQC

DKL: Kullback-Leibler (KL) divergence

$P_{\text{ansatz}}(F; \theta)$: Ansatz probability distribution of fidelities (F) with parameters θ

$P_{\text{Haar}}(F)$: Haar probability distribution of fidelities for Haar-random states, which are uniformly distributed over the state space. [7]

2.4 Entangling Capability

Entangling capability is one of the fundamental features of Quantum Mechanics. Entangling capability refers to the ability of a quantum system to generate entangling states. Entangling states are mostly used in Quantum Teleportation, superdense coding, error correction etc. By measuring entangling capability of a particular circuit, one can define the chances of reaching a desired state.

In our research work, we find the entangling capability using Meyer Wallach's entangling [1].

2.4.1 Meyer Wallach's Entangling

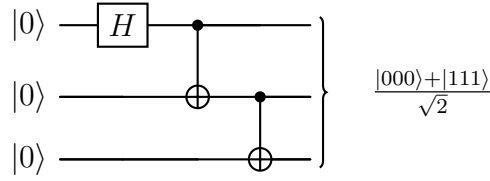
In the Meyer Wallach entangling rule, the function on pure states of n qubits are defines as $Q(|\psi\rangle)$. This function only depends on the pure states because pure states provide a direct representation of quantum correlations, making the detection more efficient without any requirement of full state reconstruction.

Here, for each qubit in the multi-qubit system, the purity can be detected using the reduced density matrix, $\text{Tr}[\rho_k^2]$. Highly entangling systems have low purity whereas product states have high purity.

$$Q(|\psi\rangle) = 2 \left(1 - \frac{1}{n} \sum_{k=0}^{n-1} \text{Tr}[\rho_k^2] \right) \quad (2.16)$$

The closer the Meyer Wallach value is near 1, the more entangling the ansatz is.

For example, the GHZ (Greenberger-Horne-Zeilinger) state is an entangled quantum state for 3 states.



$$|\text{GHZ}_3\rangle = \frac{1}{\sqrt{2}} (|000\rangle + |111\rangle) \quad (2.17)$$

Theoretically, the GHZ state has maximum entanglement and therefore, the Q value should be 1. While using the Meyer Wallach Entangling law, the full density matrix ρ of GHZ State,

$$|\rho\rangle = \frac{1}{2} (|000\rangle\langle 000| + |000\rangle\langle 111| + |111\rangle\langle 000| + |111\rangle\langle 111|) \quad (2.18)$$

Therefore,

$$\rho_k = \frac{1}{2} \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$$

The purity is thus,

$$\text{Tr}[\rho_k^2] = \text{Tr} \left(\frac{1}{2} I_2 \times \frac{1}{2} I_2 \right) = \frac{1}{2}$$

Using the Meyer Wallach, we got the entangling capability of, $Q = 1$ as a result.

$$Q(|\psi\rangle) = 2 \left(1 - \frac{1}{n} \sum_{k=0}^{n-1} \text{Tr}[\rho_k^2] \right)$$

For 3 qubits:

$$Q(|GHZ_3\rangle) = 2 \left(1 - \frac{1}{3} \sum_{k=0}^2 \frac{1}{2} \right)$$

Solving:

$$= 2 \left(1 - \frac{3}{6} \right)$$

$$= 2(1 - 0.5)$$

$$= 2 \times 0.5 = 1.0$$

As the Meyer Wallach value is 1, it shows highest entangling capability just the like theoretical concept.

2.5 Correlation

The correlation coefficient signifies how two variables are related to each other. Here, we will use Pearson Correlation Coefficient to find the relationship between Image and Audio data accuracy with KL Divergence and entangling capability.

The Pearson Correlation Coefficient mathematically expressed as:

$$\rho_{X,Y} = \frac{S_{xy}}{\sqrt{S_{xx}S_{yy}}} \quad (2.20)$$

Where,

$$S_{xx} = \sum (X_i - \bar{X})^2 \quad (2.21)$$

$$S_{yy} = \sum (Y_i - \bar{Y})^2 \quad (2.22)$$

$$S_{xy} = \sum (X_i - \bar{X})(Y_i - \bar{Y}) \quad (2.23)$$

Here,

X = KL Divergence or Entangling Capability

Y = Image Accuracy or Audio Accuracy

2.6 Related Work

Some of the work focused on fidelity and expressivity. Du and colleagues (2022) [11], in their paper, sought to offer a meaningful measure of the expressivity of variational quantum algorithms (VQAs). This states that a simple VQA will simply not be able to achieve the desired target states, while more expressive architectures may on the other hand be impeded by barren plateaus and flattened loss landscapes on which parameterized quantum circuits become hard to train. Therefore, it appears to be expressivity that prescribes the performance and limitations of VQAs for arriving at an optimum solution. Here, regarding their Q-learning framework for measuring expressivity, covering number is a measure of representativity covered what counts against an upper expressivity bound given the gate action and measurement observable. Secondly, they considered quantifying expressivity for near-term quantum chips, investigating the subsequent parameterized circuit expressivity through VQA system noise. According to these implications, the maximum number of qudits has a sublinear dependence on the number of quantum gates and an exponential reliance on the generalization bound. Is it necessary to increase the quantity of training examples? Improvement in the generalization bound would then ensue. Secondly, from the analysis of VQAs on near-term quantum chips, the expressivity of VQAs showed an exponential decay as the circuit depth increased. The result in the simulation of VQE showed that a moderate-sized ansatz with balanced expressivity is the most suitable for good performance since a restricted ansatz with little expressivity could not reach the target solution and an overly flexible ansatz with large expressivity may hinder its trainability. Therefore, expressivity can be quantified against other ansatzes to improve the performance of VQAs.

Sim et al. (2019) [7] focus on addressing the challenge of selecting an effective ansatz or Parameterized Quantum Circuits (PQCs) for better performance in variational quantum algorithms. In this paper the objective was to identify certain ansatzes that retains minimal circuit depth and parameter count while balancing expressivity and entangling capability. The authors highlighted the importance of employing practical descriptors for assessing Parameterized Quantum Circuits (PQCs) in the NISQ era, where limitations in circuit depth and qubit connectivity present significant challenges. As hybrid quantum classical algorithms depends on ansatz or PQC, it is important to effectively describe the solution space. The authors defined two prime descriptors - expressivity and entangling capability to study the capabilities of PQCs. To identify the expressivity of certain ansatzes they have used Haar fidelity distribution which compares the overlap between Haar-random states and quantum states generated by the ansatzes. Then, KL divergence has been used between the Haar fidelity distribution and ansatz fidelity distribution, which provides an operational meaning for the Haar fidelity distribution. The Welch bounds were cited to define the theoretical limits on the expressivity of parametrized quantum circuits. After performing simulations among different ansatzes, it was observed that circuit-6 showed the highest expressivity by achieving a low KL divergence value at $L=1$. The authors also identified ‘expressivity saturation’, where the expressivity value does not necessarily exhibit continuous improvement as additional layers were added. Again, it was observed that different ansatzes saturate at different expressivity values and to different number of layers. The saturation behavior may offer valuable information

in determining the appropriate number of layers in each circuit fragment. Therefore, the expressivity value can serve as an indicator of a PQC’s representational capacity, which provide insights into the number of circuit layers required for a given application. On the other hand, to estimate the entangling capability Meyer Wallach entanglement measure was used. The MW measure was selected due to its effectiveness as an entanglement probe across diverse quantum information applications. Generating entangling states was necessary as it allowed the ability to effectively describe the solution space for particular tasks. It was observed that circuit 9 was able to generate highly entangled states with Q values near to 1. Controlled X-rotation gates demonstrated superior performance over controlled Z- rotation (CRZ) gates in terms of both expressivity and entangling capability. On the other hand, three circuit configuration of two-qubits gates – nearest neighbor, ring topology and all-to-all connectivity were compared to identify the most effective circuit structures which will balance expressivity and entangling capability well. Both ring and all-to-all connectivity topologies significantly outperformed linear configurations in the field of expressivity. The ring architecture yielding KL divergence values up to 2-3 times lower than those observed in linear arrangements which clearly shows high expressivity. It was evident that ring and all-to-all configuration were able to produce high entangling states. Again, in case of circuit 5 and 6, the performance of ansatzes may vary in terms of specific gate choice. The authors tried to present a theoretical to compare the performance of the PQCs applying several approaches. They described that rate of saturation can also be an important indicator for the performances of ansatzes. The salient note is that the importance of expressivity, entangling capability and circuit configurations can significantly affect the overall performance of hybrid quantum classical algorithm. This work introduced a theoretical for characterizing and comparing parameterized quantum circuits, independent of any specific problem or application. This approach makes the framework broadly applicable for circuit design and benchmarking. Although a direct and universal correlation between these descriptors and algorithm performance has not yet been established, the study lays a foundational framework for the systematic evaluation and selection of parameterized quantum circuits, particularly for hybrid quantum-classical algorithms. Finally, this paper advocates for a more informed approach to PQC design which will become increasingly vital as quantum hardware progresses and the range of hybrid quantum-classical applications broadens.

Brennen (2003) [1] proposed an operational framework for quantifying multi-qubit entanglement in pure quantum state which offers a practical approach to assess entanglement in quantum systems. Although entanglement is fundamental to quantum information processing, many existing measures for multi qubit systems are computationally intensive or rely on full quantum state tomography, which poses significant experimental challenges. The author emphasize the need for an entanglement measure that is both physically meaningful and experimentally feasible, which ideally requires only a number of measurements that scales linearly with the system size. The approach focuses on Meyer Wallach entanglement measure (Q), defined for pure states of n qubits. The measure quantifies the amount of entanglement in a multi qubit quantum states. This equation provides a way to quantify the entanglement in a quantum state by averaging the generalized distance over all qubits in the system. The author demonstrate that Q can be efficiently estimated

by measuring the purity of each qubit, which can be achieved using entanglement witnesses and controlled- SWAP (c-SWAP) gates. The method requires only two copies of the quantum state along with a set of ancillary qubits. The paper presents the formal mathematical definition of the Meyer Wallach measure Q , highlighting its invariance under local unitary operations and its bounded range between 0 and 1. The structure of the quantum states plays a crucial role, as the measure effectively distinguishes between globally entangled states, sub-globally entangled states and fully separable or product states. The paper presents explicit calculations of the Meyer Wallach measure (Q) for various important quantum states, demonstrating its effectiveness in distinguishing between different classes of entanglement. The paper calculate the Q for several important classes of multi-qubit pure states such as GHZ state (Maximum entangled, $Q=1$), Cluster states, W states, Product states ($Q=0$), Eigenstates of the Heisenberg interaction. The analysis also addresses the limitations of the Meyer Wallach measure Q , which is its inability to differentiate between certain forms of sub-global entanglement - for example, two bell pairs and four-qubit GHZ state both yield $Q=1$. The author suggested that this limitation can partially mitigated by examining the purity of specific subsets of qubits. The protocol for measuring Q , is compatible with current quantum technologies, including trapped atoms in optical lattices. This measure can be implemented using only nearest-neighbor interactions and standard quantum gate operations. This method effectively bridges the gap between abstract theoretical entanglement measures and experimentally measurable quantities, providing a valuable tool for characterizing entanglement in quantum information experiments.

The paper by Kinha et al. (2023) [14] addresses the problem of classifying heart sounds to detect different kinds of heart diseases with accurate classification. This represents a crucial way to provide early diagnosis and appropriate treatment of cardiovascular conditions. The authors proposed a CNN-based model based on ResNet18 and a Neural Network extending the ResNetXt50 model. Both architectures also feature a new component, the shuffle attention layer, to enhance the representation of features. Data for this paper come from the PhysioNet/CinC 20216 Challenge Dataset, containing 3240 heart sound recordings. These recordings fall further into two categories: 2575 normal heart sounds and 665 abnormal heart sounds. The audio data is pre-processed by converting it into spectrogram images. Further, ResNet18 achieved a performance rate of 91.27% accuracy, while ResNeXt0 had an accuracy of 88.72% accuracy. The ResNet18 model also showed better precision of 90.38%, recall of 94.75% accuracy, and F1 Scores of 92.51% accuracy compared to ResNetXt50. These results further show that the ResNet18 model is more efficient in classifying heart sounds. It hereby affirms that neural network models, in particular ResNet18, with shuffle attention layers, classify heart sounds efficiently for disease detection.

In the quantum computing aspect, Chen et al. (2022) [13] address the problem of accurately classifying binary images using QCNNs. The goal is to enhance the image classification performance by leveraging quantum computing techniques. Moreover, the author proposed MultiScale Entanglement Renormalization Ansatz (MERA) which is a local feature extraction method and box-counting fractal features. Just Like classical CNN, the data is downsampled using this before feeding it into QCNN.

In this study, we compare the performance of a QCNN and two hybrid quantum-classical QCNN models with that of a classical CNN. The researchers employed a dataset of breast cancer photos that included 50 pictures of normal tissue, 67 pictures of benign fibrous tumors, and 205 pictures of malignant breast cancer. However, when it comes to recognition accuracy, the QCNN and hybrid QCNN models perform better than the traditional CNN. The QCNN achieved accuracies of about 78-93% in the first group and 83-88% in the second group. Finally, the study shows that QCNNs combined with scale-inspired feature extraction methods can effectively classify binary images and outperform classical CNNs. Finally, it can be said that these findings show the prospective of using quantum computing for image classification.

V. Rajesh et al.(2021) in their work [9], address enhancing image recognition and object detection performance by the use of QCNNs to leverage quantum computing-based advantages in their application to computer vision tasks. The researchers have proposed an innovative model, which integrates some principles of quantum computing into conventional CNNs; the QCNN retains the convolution and pooling layers of classical CNN architecture but replaces its neurons with qubits. The model extracts features and performs classification using the quantum circuit, which has the capabilities of superposition and entanglement. With regard to the structure of the dataset, the paper does not specify anything but generally talks about the domains in which QCNN can find its application: image recognition, signal processing, or pharmaceuticals. This shows how powerful QCNNs are in handling large-scale, higher-dimension data with much more efficiency than the classical methods. This work established the fact that QCNNs can offer great improvements in computational speeds and performance metrics compared to their classical CNNs. Authors have discussed various experiments and applications where QCNNs outperformed traditional models, demonstrating their potential in real-world scenarios. Hence, this work postulates that QCNN is a promising approach to solving complex problems in computer vision and other fields.

In their work from 2022, Xinmiao Chen et al. talked about [10] using QCNN to efficiently classify images on a quantum computer. It uses quantum computers to improve these image categorization methods more effectively. The authors proposed a QCNN model with an encoding circuit. It proposes expressing high-dimensional classical data as quantum states via quantum amplitude encoding. Additionally, the QCNN model will be built and tuned for image recognition applications. The MNIST dataset was used in the work. It demonstrates that, in terms of accuracy, the QCNN model outperforms the traditional CNN models. On a quantum computer, the QCNN model seems capable of handling image classification tasks effectively. Finally, it can be said that this QCNN model may work well for classifying images utilizing quantum computing techniques. The work illustrates how quantum computers could improve the efficacy and efficiency of picture classification techniques. Therefore, additional research on QCNN model optimization should be carried out in other domains.

Thakar et al. (2024) [19] address the problem of efficiently classifying high-dimensional and complex audio signals using hybrid Quantum-Classical Convolutional Neural

Networks (QC-CNNs). The authors proposed a QC-CNN model that uses quantum effects like superposition and entanglement for audio classification. The model uses mel spectrograms obtained from audio data and evaluates the performance on both small-sized and large-sized datasets. Here, two different datasets (GTZAN) with 100 audio files for each of the 10 genres. A large-sized birdsong classification dataset was collected from the Zeno-canto public API with 1000 audio files for each bird species. The QC-CNN model achieved comparable training accuracy with classical CNN on the smaller dataset but outperformed the classical CNN on test accuracy (95.04% vs. 92.88%) for the larger birdsong dataset. The QC-CNN model also exhibited reduced overfitting and higher cross-entropy loss on the small-sized dataset, which actually reduced when evaluated on the large-sized dataset. Finally, it can be said that the work showed the potential advantages of QC-CNNs for handling high-dimensional and complex audio data.

Tak Hur et al. (2022) [12] address the problem of accurately classifying classical data using QCNNs. The authors proposed a fully parameterized QCNN model inspired by classical CNN. The model used two qubit circuits and in total 8 qubit architecture. The work achieved 94% accuracy on the Fashion MNIST data and 99% accuracy on the MNIST data while utilizing a variety of data encoding techniques, pre-processing, cost functions, and optimizers. Therefore, the work shows that QCNNs can effectively classify data and outperform classical CNNs in terms of accuracy.

Hubregtsen et al. (2021) [8] investigate the power of PQC to span over the Hilbert space uniformly. This is known as expressivity. It also explores the entangling capability to evaluate the correlation with accuracy. The paper uses 9 datasets to build a strong ground to showcase their correlation. The correlation between accuracy and expressivity, as well as between accuracy and entangling capability, has been established. It is motivated by the idea that quantum circuits can outperform classical Neural Networks. A supervised learning approach has been used here. The key differences between classical and Quantum Neural Networks show that the input layer of CNN and QNN are referred to as the input layer and embedding layer, respectively. Additionally, the weights in NNs are termed as parameters or variational angles in QNNs. Most importantly, the QNN needs to be run several times to show the output. The paper suggests that there is a strong negative correlation between expressivity and accuracy. In addition, there is a weak positive correlation between entangling capability and accuracy. These in turn support that expressivity has greater power of suggesting the property of the ansatz, compared to entangling capability.

Chapter 3

Work Plan

In Pre-Thesis 1, we formed a team and explored basic Quantum Computing under the supervision of our supervisor and co-supervisor. We initially decided to proceed with the Barren Plateau problem in Quantum Computing. Then we were given some papers on related topics. We summarized the papers. We were in touch with our supervisor every week and reported our paper-reading activity.

In Pre-thesis 2, we narrowed down more and chose this topic. We did explore Takhur's QCNN code with the audio dataset. Alongside that, we explored expressivity and custom pooling ansatz in our code. Finally, we successfully to run the QCNN with our audio dataset and custom pooling ansatz.

In the final thesis, we proceeded with a detailed result and analysis phase, where we explored entangling capability on each of the ansatzes alongside expressivity. We performed a convolutional layerwise analysis on both expressivity and entangling capability. Also, we trained the QCNN architecture across multiple datasets and extracted the results. We then conducted correlation analysis of both expressivity and entangling capability with the datasets accuracy values. Finally, we evaluated our results and proceeded to write the final thesis paper and prepared for the final defense.

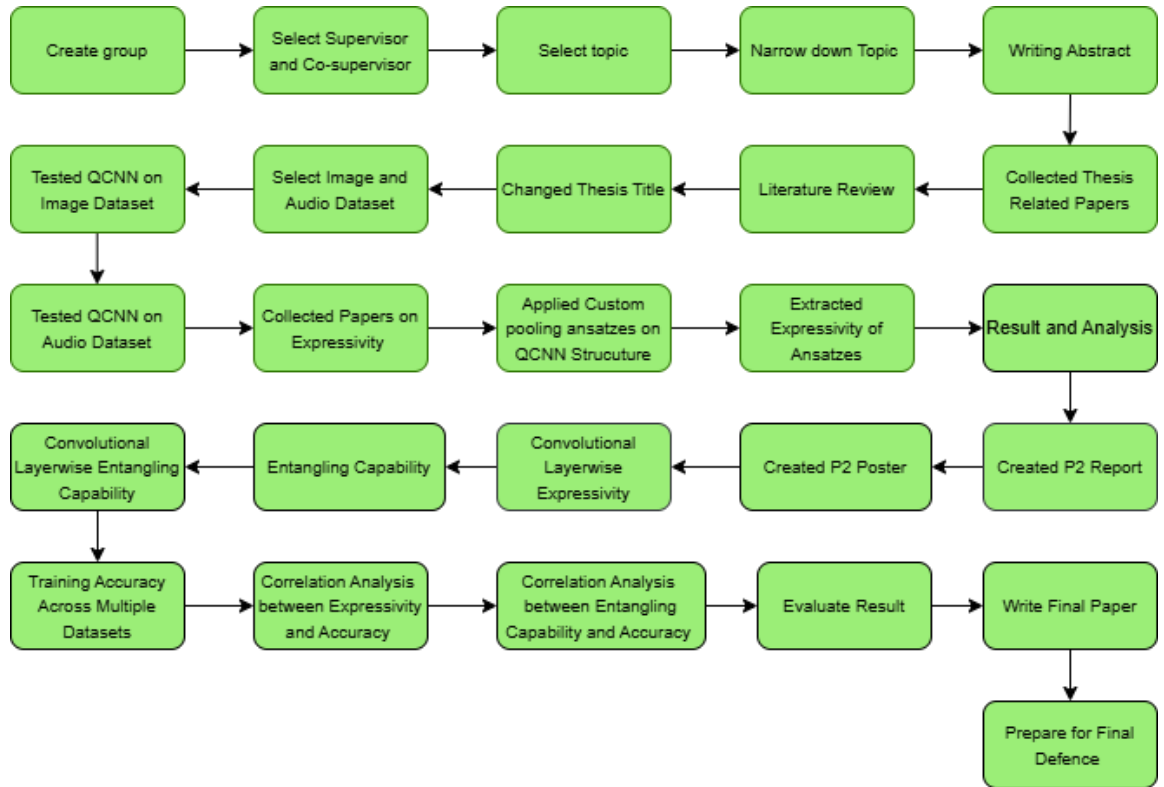


Figure 3.1: Work Plan

Chapter 4

Methodology

As the classical Machine Learning field is expanding and getting implemented in every field of human life, researchers are very hopeful of implementing Quantum Machine Learning as successfully as classical Machine Learning. While training Quantum Machine Learning models, we need to run ansatzes, which are applied in multiple layers of the model. But running these models is not that easy, as generation of qubits is a very complex and expensive task. Organizations like Google, IBM, and Amazon Braket use superconducting qubits, which are very expensive. The superconducting circuits are cooler near absolute zero temperature. Whereas organizations like IonQ and Honeywell Quantum use trapped ion qubits. Xanadu, PsiQuantum, Alibaba Quantum Lab, etc. use photonic qubits. Different types of quantum computers have different challenges and expenses. So, if we can analyze an ansatz's capability prior to the training, it may reduce the cost for model runs and pick a better ansatz for better research. Therefore, we have tried to find a correlation between expressivity, entangling capability, and trainability (accuracy).

4.1 Dataset

We have used various image classification datasets like MNIST dataset, Fashion MNIST dataset and QMNIST dataset for the image classification.

Image Dataset:

Dataset Name	Image Size	Labels	Train Size	Test Size
MNIST	28×28 pixels	10 (digits)	60,000	10,000
Fashion MNIST	28×28 pixels	10 (clothes)	60,000	10,000
QMNIST	28×28 pixels	10 (digits)	120,000	60,000

Table 4.1: Image Datasets used in our image classification

4.1.1 MNIST Dataset

It consists of gray scaled images of handwritten digits from 0 to 9. Each image is of 28*28 pixels. For training, it has 60,000 gray scaled images and for testing it has gray scaled 10,000 images. It has 10 labels indicating 10 digits from 0 to 9.

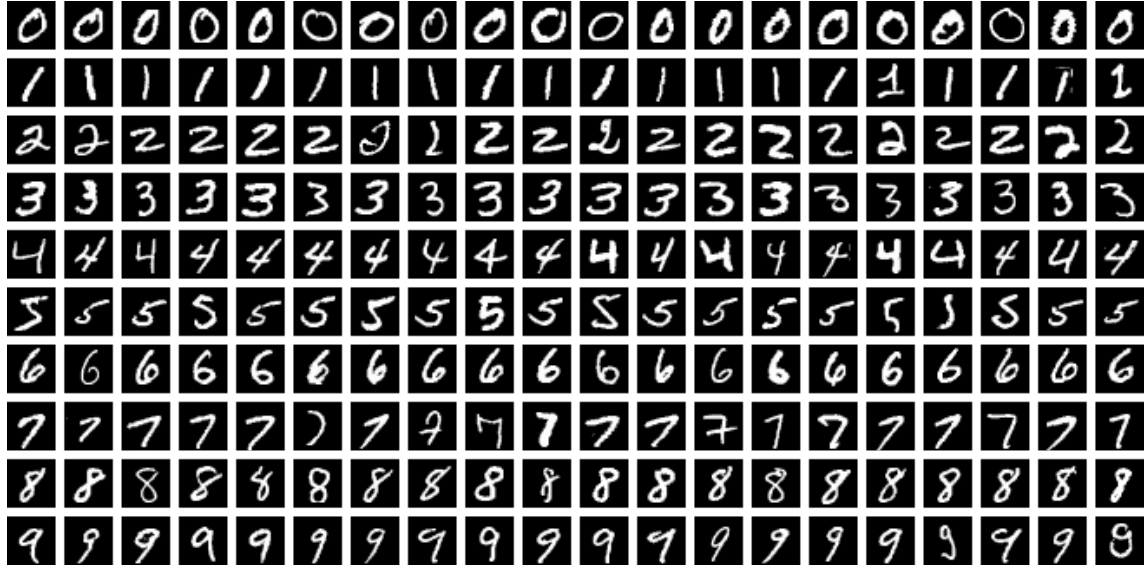


Figure 4.1: MNIST Dataset

4.1.2 Fashion MNIST Dataset

The Fashion MNIST dataset is an alternative dataset of MNIST mostly used in image classification. It consists of gray scale images of clothing items just like MNIST. There are 60,000 training images and 10,000 testing images. The image sizes are 28*28 pixels. It has 10 labels which indicate T-shirt, trouser, pullover, dress, coat, sandal, shirt, sneaker, bag, ankle boot.

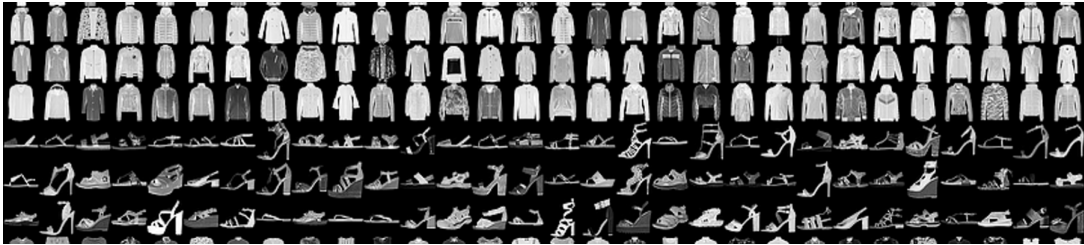


Figure 4.2: Fashion MNIST Dataset

4.1.3 QMNIST Dataset

It is an extended version of MNIST dataset where additional hand written samples and labels are added. It has 120,000 training images and 60,000 testing images. This dataset provides more detailed metadata than the MNIST dataset with an image size of 28*28 pixels.



Figure 4.3: QMNIST Dataset

Moreover, we have used Capuchin bird Audio from Kaggle for audio classification.

4.1.4 Audio Dataset

The audio samples include voices of Capuchin bird as well as different other birds making it a perfect dataset for audio classification. The dataset has 80 training samples and 20 testing samples. The dataset has 2 labels.

For our QCNN model, we have generated Mel-spectrograms from the audio sample to apply in our QCNN model. Each mel-spectrogram consists of 370*969 pixels.

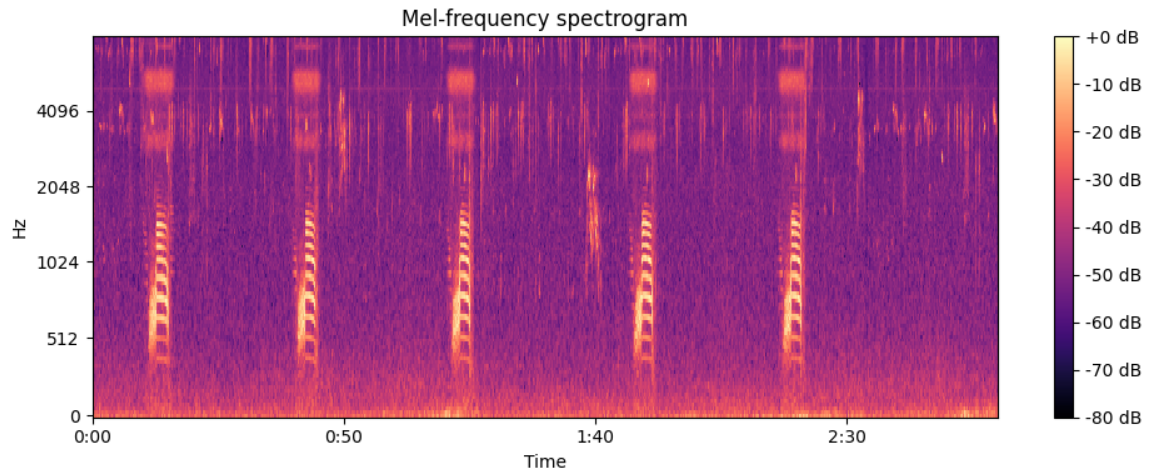


Figure 4.4: Mel-spectrogram for an audio sample

4.2 Data Pre-Processing

After loading the MNIST, Fashion MNIST, and QMNIST datasets, we need to normalize the pixel values. Firstly, we have normalized our pixel values from $[0, 255]$ to $[0, 1]$. Then we have created class pairs $[0, 1]$ and $[1, -1]$ for classification, as all

of our image datasets have 10 labels. After that, we have resized our 28*28 pixel images to (256,1) to cover it with 8 qubits.

For the Capuchin bird audio dataset, we initially generated Mel-spectrogram images from the audio dataset. Then we gray-scaled the image of size 370*969 pixels. After that, we have normalized the pixel values to [0,1] and labelled the dataset to [0,1] and [1,-1]. Finally, we have resized the 370*969 images to (256,1) to cover it with 8 qubits.

4.2.1 Feature Reduction

After data loading, we have to reduce the dimensions to process through our QCNN model.

Principal Component Analysis (PCA): PCA is a technique that minimizes the complexity of data and transforms the original variables into a new set of variables. It is mostly used in data compression, noise reduction, visualization, and feature extraction. In our research, we have reduced the dimensions to 30 dimensions using PCA for all of the image datasets. For the audio dataset, we have reduced the dimensions to 32 dimensions using PCA as well.

4.2.2 Encoding

After feature reduction, the classical data need to be encoded into quantum data.

In our work we have used Angular Hybrid Encoding (Angular_Hybrid_4-1). It is a quantum circuit based technique to map high dimensional data into a quantum state using Rotational Gates (RY) and Controlled Gates (CNOT,CRY).This is a hybrid encoding system which can process 15 input features into 4 qubits.

$$|\psi\rangle = \sum_{i=0}^{15} c_i |i\rangle$$

where the amplitudes c_i nonlinearly depend on all 15 input features.

While encoding, the classical data is converted to highly entangled quantum state suitable for Quantum Machine Learning models. Once the data is encoded, we then passed it to our QCNN model.

4.2.3 Quantum Convolutional Neural Network (QCNN) Architecture

In the QCNN structure, various types of ansatzes are passed through various convolutional and pooling layers.

For our QCNN model, we have used 9 different ansatzes in the convolutional layer 1, convolutional layer 2 and convolutional layer 3.

Convolutional Layer 1 takes 8 inputs and returns 8 outputs while using multiple ansatzes structure. After that the qubits go through Pooling Layer 1. It then down-scales the qubit to 4 qubits. We then pass the qubits through Convolutional Layer 2 and Pooling Layer 2 to downscale the qubits to 2 qubits. Later, the convolutional layer 3 and pooling layer 3 are used to downscale it to 1 qubit. Finally, we measure the qubit.

4.2.4 Training Process

We have then used Cross Entropy loss function for training. We have trained in batches with 200 iterations. Finally, we have tracked the loss history and computed the accuracy.

4.3 Expressivity

4.3.1 Expressivity for ansatz

We conducted an expressivity analysis to quantify each ansatz’s capability to approximate the Haar-random unitary distribution. The output states generated by each ansatz was compared against the Haar-random distribution to measure how effectively the ansatz can produce quantum states that can approximate truly random quantum states. The Kullback-Leibler (KL) divergence was computed between the Haar-random fidelity distribution and the ansatz-generated fidelity distribution to serve as a quantitative metric of expressivity. A lower KL divergence indicates the higher expressivity of the ansatz, which reflects the ansatz’s ability to traverse a broader portion of Hilbert space.

4.3.2 Expressivity for Convolutional layers

Following the individual ansatz’s expressivity analysis, we conducted layerwise expressivity analysis to understand how expressivity evolves through the convolutional layers of the QCNN architecture. There are three convolution layers within the QCNN architecture which we had followed. For each of the ansatz, specific convolutional layers within the QCNN architecture were selected for evaluation. Quantum states were generated by applying the specific ansatz to the selected layer. These output states were then compared against the Haar-random distribution to determine how effectively they can emulate the characteristics of truly random quantum states.

To quantify this comparison, we calculated the KL divergence between those fidelity distributions in order to provide a layerwise expressivity metric for each ansatz. The procedure was systematically repeated for Convolutional Layer (layer-1, layer-2, and layer-3) to observe how the expressivity of the layer evolves as the layer changes.

4.4 Entangling Capability

4.4.1 Entangling Capability for Ansatz

As the entangling capability of an ansatz refers to the ability of an ansatz to form complex and correlated quantum states, the metric can define the chances of an ansatz to generate a quantum state and find our desired result.

Therefore, in our work we have found the entangling capability for all of the nine ansatzes used in convolutional layers to find their relationship with accuracy. To find the entangling capability, we firstly detected the purity of the ansatz using reduced density matrix. Then we computed the Meyer Wallach Entangling using the equation 2.16.

The entangling capability of the nine convolutional layer ansatzes are shared in Table 5.5.

4.4.2 Entangling Capability for Convolutional layers

After we have analyzed the entangling capability of ansatzes, we used the same methods to find the entangling capability of the convolutional layers.

The goal was to give a comprehensive idea of the entangling capability after passing through the Convolutional Layer 1, Convolutional Layer 2 and Convolutional Layer 3. As the data passes through Convolutional layers, it is important to check it is relationship with accuracy. This can give us an idea of how ansatzes are performing in certain Convolutional layers.

4.5 Correlation Procedure

The final stage of our analysis involved examining the relationship between expressivity, entangling capability with trainability by calculating the correlation between the KL divergence values, entangling capability values and the corresponding accuracy of both image datasets and the audio data. We computed Pearson Correlation Coefficient between the classification accuracy, the expressivity and entangling capability of each ansatz across all the datasets. Similarly, we conducted the correlation analysis on a convolution layerwise basis to assess how individual convolutional layers expressivity correlated with the trainability (accuracy).

By comparing these correlation values, we aimed to identify consistent patterns which will link the expressive and entangling power of quantum circuits to the effectiveness in classification tasks. It could provide information on the relationship between practical learning performance and quantum characteristics.

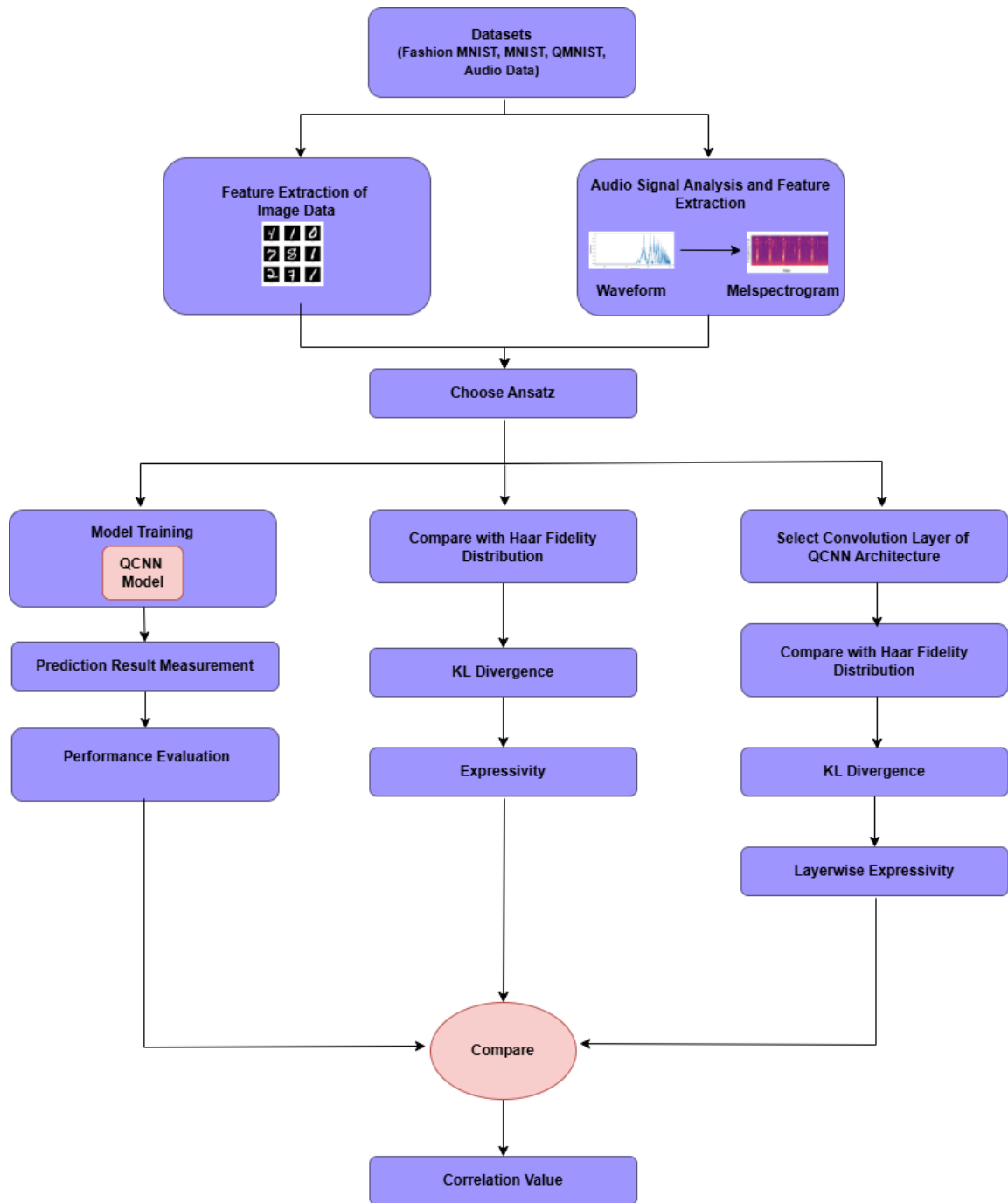


Figure 4.5: Expressivity Workflow

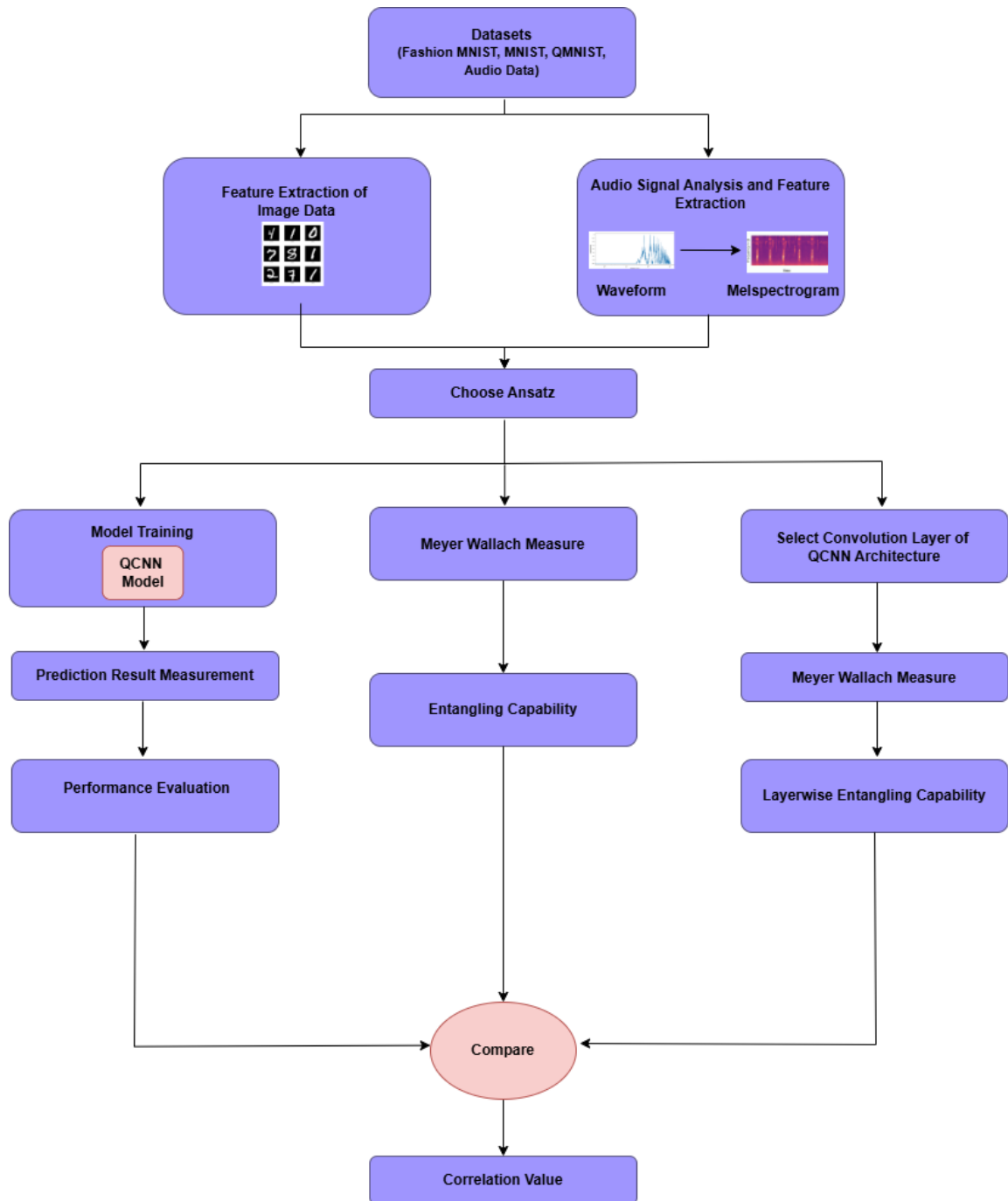


Figure 4.6: Entangling Capability Workflow

Chapter 5

Result Analysis

5.1 Expressivity Analysis

5.1.1 Ansatz Expressivity Analysis

To evaluate the expressivity of our convolutional circuit ansatzes, we conducted a series of experiments using nine convolutional ansatzes. The primary goal was to determine which ansatz architectures demonstrated the highest and lowest levels of expressivity. Among the nine convolutional circuit ansatzes evaluated, U_{SU4} exhibited the highest expressivity, whereas U_9 demonstrated the least expressivity. The understanding of our results are described below.

For example, using the Haar Probability Distribution for Convolutional circuit 2 (U_9) ansatz, we get the Fidelity graph:

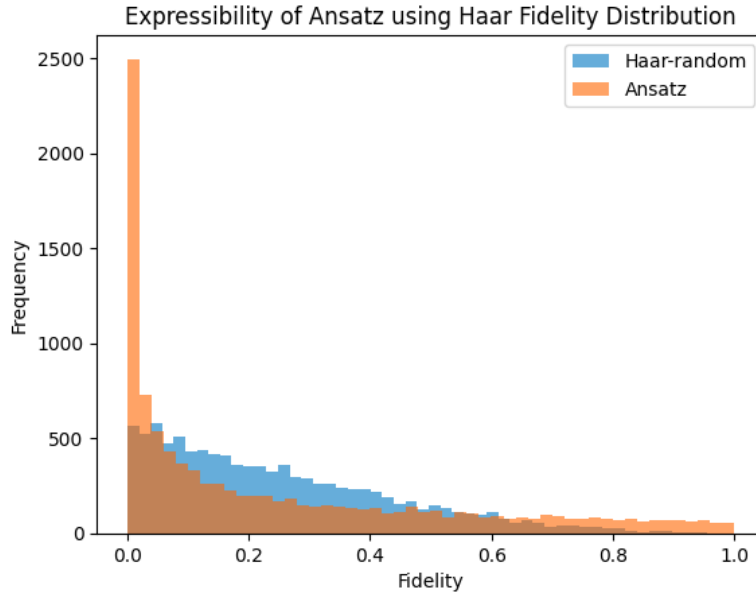


Figure 5.1: Fidelity graph for Convolutional U_9 ansatz

The fidelity graph for the USU4 ansatz:

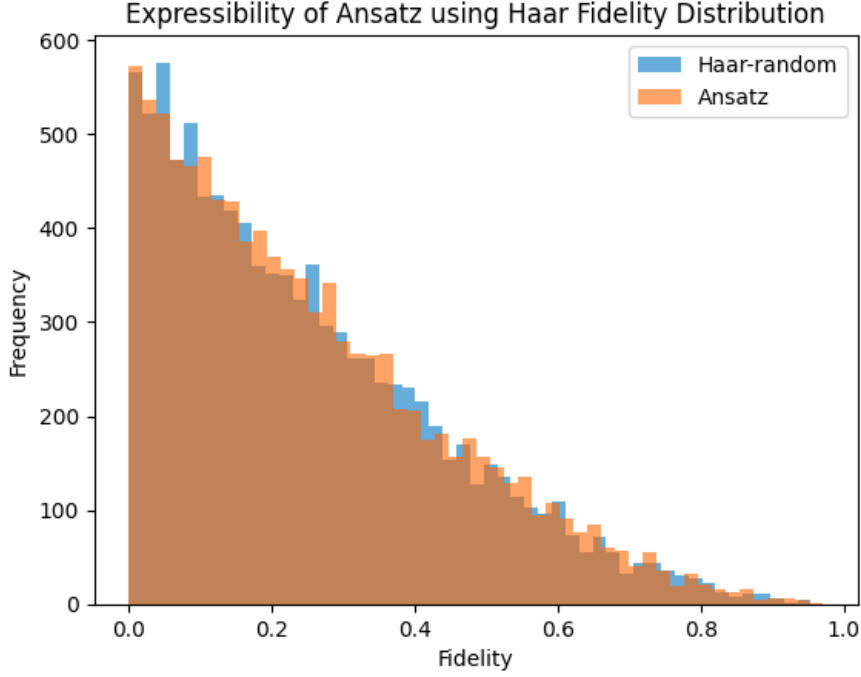


Figure 5.2: Fidelity graph for U_{SU4} ansatz

Here, the blue bars indicate the fidelity distribution between two random quantum states from the Haar measure, and the orange bars indicate the fidelity distribution values generated by the ansatz using random parameters θ . There are 1000 samples in each circuit. The Y-axis displays the frequency of a certain fidelity value, while the X-axis indicates the range of fidelity values.

In Figure 5.1, the U_9 ansatz (orange curve) is unable to generate states to span the quantum state space compared to Haar-random states (blue curve). We can say that the ansatz fidelity distribution does not sufficiently overlap with the Haar Fidelity distribution. As a result, it is observed that the amount of overlap between states generated by ansatz and Haar-random states is lower. It indicates that the ansatz is less expressive.

Moreover, in Figure 5.2, it is observed that the U_{SU4} ansatz can generate diverse quantum states to explore a wide scale of quantum states like the Haar random states. The ansatz (orange curve) closely overlaps the Haar-random states (blue curve), which implies the higher expressivity of the ansatz.

The analysis of the KL divergence value of U_9 and U_{SU4} ansatzes:

a) The KL Divergence of the circuit ' U_9 ' is $= 0.5682$. It indicates a higher value, which states that the fidelity distribution of the ansatz significantly differs from the Haar Probability distribution. Therefore, the ansatz is unable to closely approximate the Haar-random states, which leads to poor expressivity of the ansatz.

b) The KL Divergence of the circuit ‘ U_{SU4} ’ is 0.0054. It indicates a lower value, which implies that the fidelity distribution of the ansatz closely matches the Haar-random states. Therefore, the ansatz can explore the Hilbert space effectively, which is a clear indicator of a highly expressive ansatz.

Therefore, U_9 is less expressive than U_{SU4} .

5.1.2 Layerwise Expressivity Analysis

We conducted a layerwise expressivity analysis across the three convolutional layers of the QCNN using nine different convolutional circuit ansatzes.

A layerwise reduction in KL divergence was observed across all ansatzes, indicating that deeper layers progressively enhance expressivity by producing quantum states that more closely resemble Haar-random distributions.

Among the evaluated architectures, the U_{SU4} ansatz consistently exhibited the highest expressivity across all three layers. The KL divergence value gradually decreased from 1.1824 at Layer 1 to 0.0055 at Layer 3. The analysis clearly depicts that the U_{SU4} ansatz consistently showed high expressivity at each convolutional layer of the QCNN architecture.

On the other hand, U_{TTN} ansatz was recorded the highest KL divergence values at each of the three convolutional layers and it was 4.0712, 1.7850 and 0.5682 respectively. This performance of U_{TTN} indicates that it was the least expressive across each of the layers. The U_9 ansatz exhibited one of the highest KL divergence values at Layer 3, which indicates the lowest expressivity alongside U_{TTN} . Similar to U_{TTN} , U_9 consistently demonstrated higher KL Divergence across convolutional layers, establishing it as the second least expressive ansatz within the set of ansatzes analyzed.

5.1.3 Correlation of Ansatz Expressivity with Accuracy

The ansatzes exhibited consistently high classification performance across the majority of the datasets. Notably, U_{SU4} was able to achieve the best MNIST accuracy (0.9833) and demonstrated high performance on most of the datasets. It indicates that expressivity may contribute positively to model performance as it demonstrated the least KL divergence, reflecting the highest expressivity among the nine ansatzes assessed.

In contrast, U_9 consistently yielded lower accuracies across multiple datasets, including MNIST, Fashion MNIST and QMNIST. This consistent underperformance underscores the limitations of ansatzes which directly correlates to its highest KL divergence, depicting the least expressivity of the ansatz. The summary of the ansatz trainability across multiple datasets and expressivity are shown below.

Ansatz	MNIST Accuracy (%)	Fashion MNIST Accuracy (%)	QMNIST Accuracy (%)	Audio Data Accuracy (%)	KL Divergence
U _{TTN}	98.18	87.81	93.61	60	0.5682
U ₅	98.19	89.93	96.10	65	0.0154
U ₆	98.30	89.36	97.26	60	0.0411
U ₉	98.04	83.64	94.14	60	0.5682
U ₁₃	98.24	88.23	94.51	65	0.0388
U ₁₄	98.19	87.84	96.91	75	0.0292
U ₁₅	98.24	88.91	95.45	60	0.2301
U _{SO4}	98.11	88.85	97.02	80	0.2117
U _{SU4}	98.33	90.08	95.40	70	0.0054

Table 5.1: Performance and Expressivity Comparison of Quantum Ansatzes on Multiple Datasets

Datasets	Pearson Correlation Coefficient (r)
MNIST	-0.6660
Fashion MNIST	-0.7310
QMNIST	-0.6650
Audio Data	-0.1166

Table 5.2: Pearson Correlation Coefficients for Various Datasets

From the above Pearson Correlation Coefficient table, we can observe overall strong negative correlations (-0.6660 , -0.7310 , and -0.6650), which indicates that ansatzes with lower KL divergence (higher expressivity) tend to show better performance. This pattern highlights expressivity as a valuable descriptor for predicting model accuracy in QCNN.

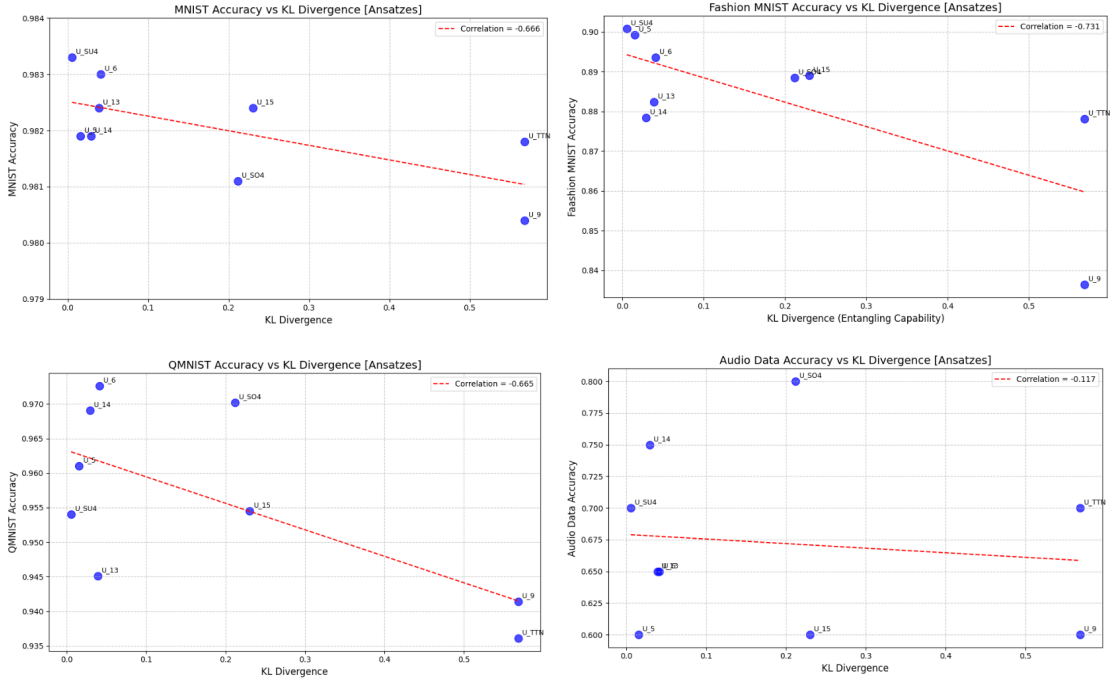


Figure 5.3: Image and Audio Accuracy vs KL Divergence

From the above correlation plot, we can observe that image data accuracy has a

strongly negative correlation with KL Divergence. The plot indicates that ansatzes exhibiting high expressivity tend to achieve correspondingly high accuracy values.

5.1.4 Correlation of Layerwise Expressivity with Accuracy

Among the nine evaluated ansatzes, U_{SU4} repeatedly achieved higher classification accuracy across all datasets, including MNIST (98.33%), Fashion MNIST (90.08%), QMNIST (95.40%), and the audio dataset (70%). This strong performance is closely aligned with its expressivity characteristics, as evidenced by the lowest KL divergence values recorded across the three convolutional layers (Layer 1 - 1.1824, Layer 2 - 0.1845, Layer 3 - 0.0055). These results indicate U_{SU4} 's exceptional ability to approximate Haar-random quantum states which suggests a greater capacity for state space exploration.

Ansatz	MNIST Accuracy (%)	Fashion MNIST Accuracy (%)	QMNIST Accuracy (%)	Audio Data Accuracy (%)	KL Divergence [Layer 1]	KL Divergence [Layer 2]	KL Divergence [Layer 3]
U_{TTN}	98.18	87.81	93.61	60	4.0712	1.7850	0.5682
U_5	98.19	89.93	96.10	65	2.1365	0.2487	0.0154
U_6	98.30	89.36	97.26	60	2.9681	0.4172	0.0411
U_9	98.04	83.64	94.14	59	3.7903	1.2536	0.5682
U_{13}	98.24	88.23	94.51	65	2.2237	0.3147	0.0388
U_{14}	98.19	87.84	96.91	75	1.8290	0.2836	0.0292
U_{15}	98.24	88.91	95.45	60	2.0630	0.4281	0.2300
U_{SO4}	98.11	88.85	97.02	80	1.8908	0.4036	0.2117
U_{SU4}	98.33	90.08	95.40	70	1.1824	0.1845	0.0055

Table 5.3: Performance and Layerwise Expressivity Comparison of Quantum Ansatzes on Multiple Datasets

On the other hand, U_9 exhibited the weakest performance across most datasets, achieving accuracies of 0.9804 on MNIST, 0.8364 on Fashion MNIST, 0.9414 on QMNIST, and 0.60 on the audio dataset. This comparatively weaker performance is strongly associated with its high KL divergence values (Layer 1 - 3.7903, Layer 2 - 1.2536, Layer 3 - 0.5682), reflecting limited expressivity. The elevated KL divergence implies that U_9 's circuit struggles to approximate Haar-random quantum states, thereby restricting its ability to capture complex data patterns.

Datasets	Pearson, r (Layer 1)	Pearson, r (Layer 2)	Pearson, r (Layer 3)
MNIST	-0.474	-0.493	-0.666
Fashion MNIST	-0.644	-0.611	-0.731
QMNIST	-0.546	-0.698	-0.665
Audio Data	-0.299	-0.0875	-0.1167

Table 5.4: Pearson Correlation Coefficients (r) for Different Datasets Across Layers 1, 2, and 3

According to the correlation values in the above table, deeper convolution layers reveals significantly higher correlation values. This trend demonstrates that expressivity's impact on model performance increases at greater circuit depths. Fashion MNIST was able to represent this pattern with an increasing negative correlation value of -0.731 at Layer 3 compared to -0.644 at Layer 1. These outcomes collectively establishes that layerwise expressivity may serve as an important factor for optimizing ansatz selection.

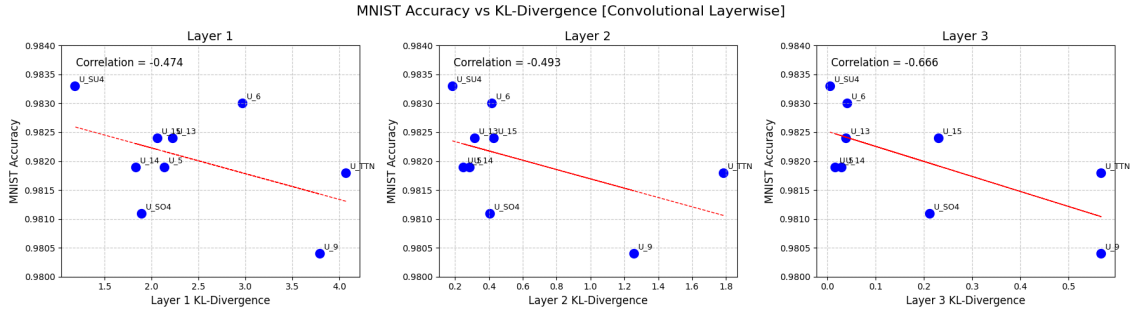


Figure 5.4: Plotting MNIST Accuracy against Layer 1, Layer 2 and Layer 3 KL Divergence

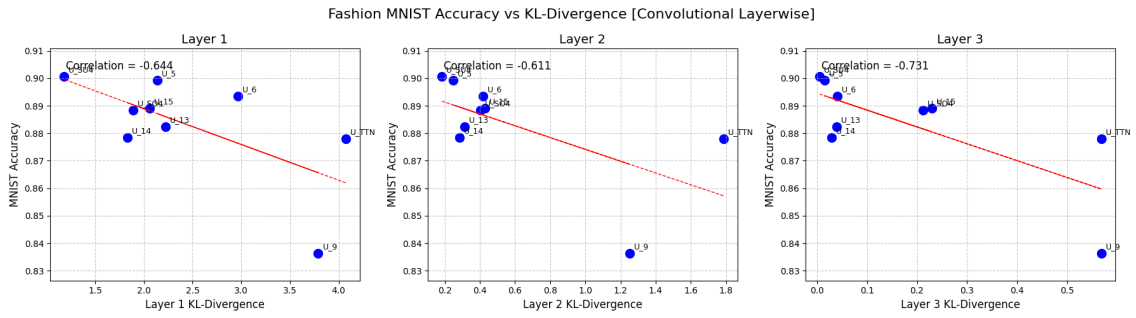


Figure 5.5: Plotting Fashion MNIST Accuracy against Layer 1, Layer 2 and Layer 3 KL Divergence

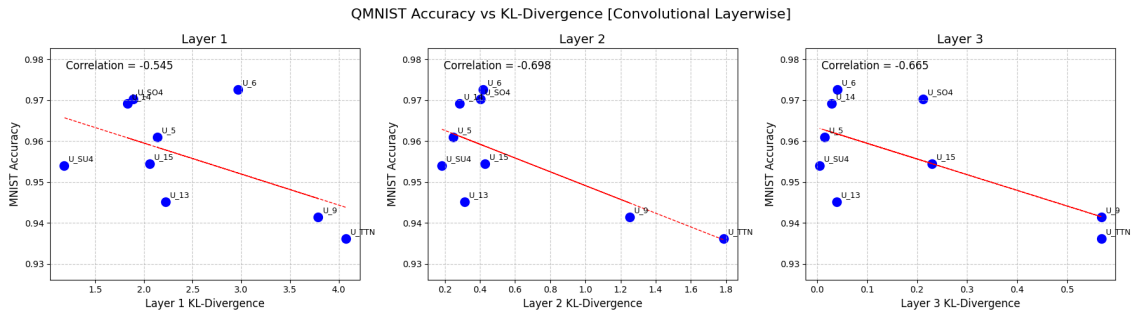


Figure 5.6: Plotting QMNIST Accuracy against Layer 1, Layer 2 and Layer 3 KL Divergence

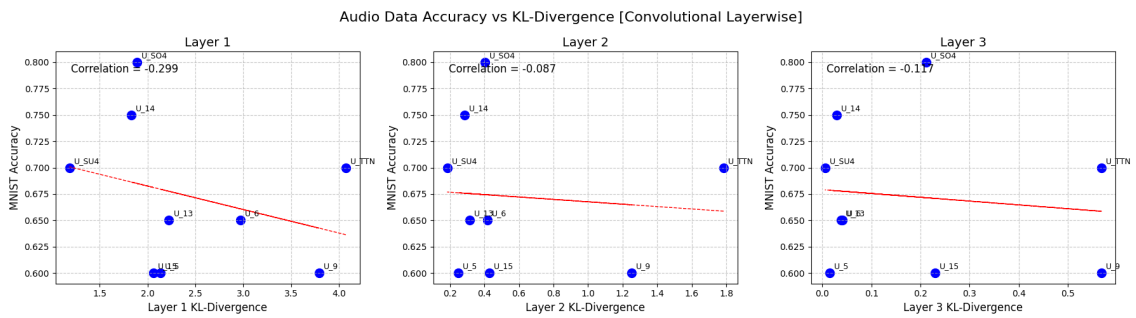


Figure 5.7: Plotting Audio dataset Accuracy against Layer 1, Layer 2 and Layer 3 KL Divergence

Referring to the above correlation plot, we can observe that the correlation between expressivity and model accuracy (MNIST) increases progressively with the deepening of convolutional layers within the QCNN architecture. Therefore, it is observed there is strong negative correlation which demonstrates that the model performance increase as the number of convolution layer increases.

5.2 Entangling Capability Analysis

5.2.1 Ansatz Entangling Capability Analysis

To evaluate the entangling capability of our convolutional circuit ansatzes, we conducted a series of experiments on our convolutional layer ansatzes. The primary goal was to determine which ansatz architectures demonstrated the highest and lowest levels of entangling capability. Among the nine convolutional circuit ansatzes evaluated, U_9 exhibited the highest expressivity, whereas U_5 demonstrated the least entangling capability. The understanding of our results are shown in the table below.

Ansatz	MNIST Accuracy (%)	Fashion MNIST Accuracy (%)	QMIST Accuracy (%)	Audio Data Accuracy (%)	Entangling Capability
U_{TTN}	98.18	87.81	93.61	60	0.2702
U_5	98.19	89.93	96.10	65	0.1342
U_6	98.30	89.36	97.26	60	0.3160
U_9	98.04	83.64	94.14	60	1.0000
U_{13}	98.24	88.23	94.51	65	0.2068
U_{14}	98.19	87.84	96.91	75	0.2237
U_{15}	98.24	88.91	95.45	60	0.3119
U_{SO4}	98.11	88.85	97.02	80	0.3405
U_{SU4}	98.33	90.08	95.40	70	0.3346

Table 5.5: The entangling capability of 9 ansatzes and their accuracy across different datasets

From Table 5.5, we can see that U_9 ansatz shows strongest entangling capability as it has Controlled Gates (CZ) applied on the first two qubits. Whereas, U_6 and U_{SU4} continuously maintain high entangling capability between 0.39 to 0.42. Moreover, ansatzes like U_5 , U_{13} , U_{14} which show low entangling capability. The table also shows CRX gate (U_6 , U_{14}) outperforms CRZ gate (U_5 , U_{13}).

5.2.2 Layerwise Entangling Capability Analysis

Once we found the entangling capability of ansatzes, we have conducted a layerwise entangling capability analysis across the three convolutional layers of the QCNN using nine different convolutional circuit ansatzes. Table 5.6 summarizes the entangling capability across the three convolutional layers of the nine ansatzes.

Ansatz	MNIST Accuracy (%)	Fashion MNIST Accuracy (%)	QMNST Accuracy (%)	Audio Data Accuracy (%)	Entanglement [Layer 1]	Entanglement [Layer 2]	Entanglement [Layer 3]
U _{TTN}	98.18	87.81	93.61	60	0.3451	0.3381	0.1668
U ₅	98.19	89.93	96.10	65	0.3354	0.3468	0.1177
U ₆	98.30	89.36	97.26	60	0.6449	0.5424	0.2796
U ₉	98.04	83.64	94.14	60	1.0000	0.7500	1.0000
U ₁₃	98.24	88.23	94.51	65	0.4100	0.4417	0.1705
U ₁₄	98.19	87.84	96.91	75	0.4431	0.4985	0.1605
U ₁₅	98.24	88.91	95.45	60	0.5907	0.5719	0.3351
U _{SO4}	98.11	88.85	97.02	80	0.5896	0.4496	0.2723
U _{SU4}	98.33	90.08	95.40	70	0.5835	0.5303	0.3003

Table 5.6: The entangling capability of 9 ansatzes in Convolutional Layer 1, Convolutional Layer 2, and Convolutional Layer 3

From Table 5.6, it can be seen that U₉ has high entangling capability in all of the layers whereas U₆ maintains strong entanglement in Convolutional Layer 1 and decreases when the Layer increases. Moreover, U_{TTN} consistently has low entangling capability.

5.2.3 Correlation of Ansatz Entangling Capability with Accuracy

When we plot the accuracy and entangling capability to understand the relationship between ansatzes' entangling capability and accuracy, we can see that entangling capability has a weak positive correlation with accuracy. For MNIST dataset the correlation value is 0.225, for Fashion MNIST it is 0.100, for QMNIST it is 0.153 and for the audio dataset it is 0.422.

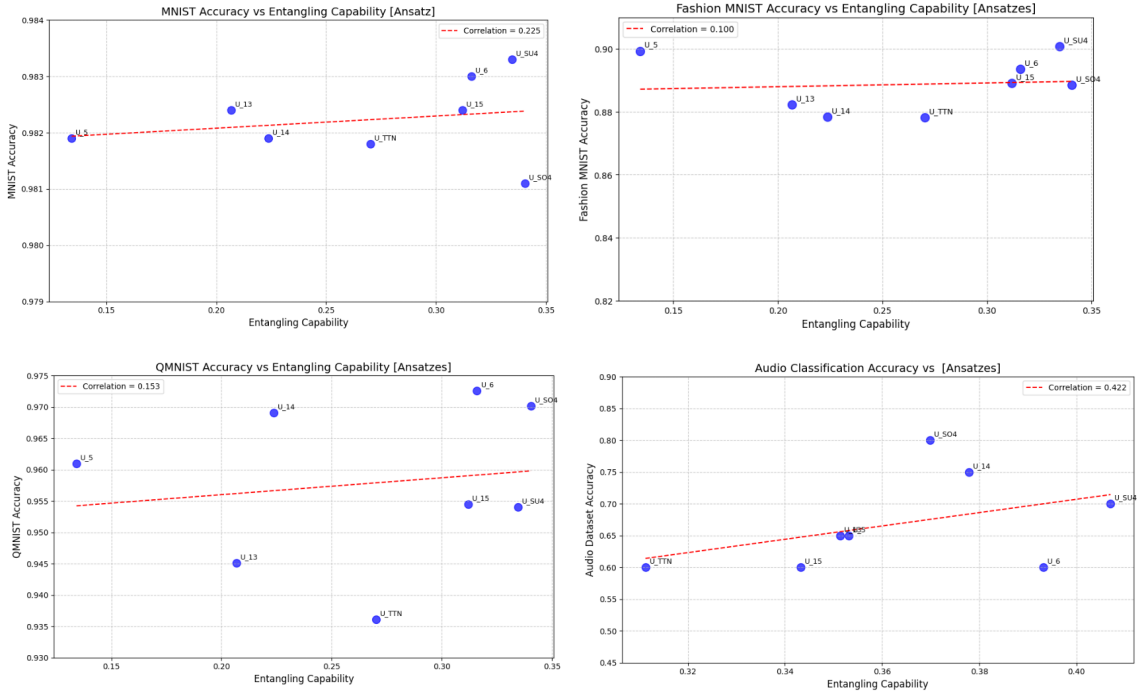


Figure 5.8: Image and Audio Accuracy vs Entangling Capability

Dataset	Pearson Correlation Coefficient (r)
MNIST	0.225
Fashion MNIST	0.100
QMNIST	0.153
Audio Dataset	0.422

Table 5.7: Pearson Correlation Coefficients for Various Datasets

This implies that high accuracy is not always guaranteed by an ansatz with high entangling capability. However, an ansatz with a moderate capacity for entanglement has demonstrated a moderate level of accuracy. For instance, U_9 consistently displayed poor accuracy despite having a high entangling capability ($Q = 1$). In contrast to other ansatzes, however, we can observe a moderate entanglement for ansatz, such as U_{SU4} . Additionally, it has continuously demonstrated high accuracy across the datasets. Ansatzes such as U_{14} and U_6 demonstrated a moderate level of accuracy and entanglement across all datasets.

5.2.4 Correlation of Layerwise Entangling Capability with Accuracy

Once we plot the MNIST dataset accuracy with Convolutional Layer 1, Convolutional Layer 2 and Convolutional Layer 3 entangling capability, we found a weak positive correlation.

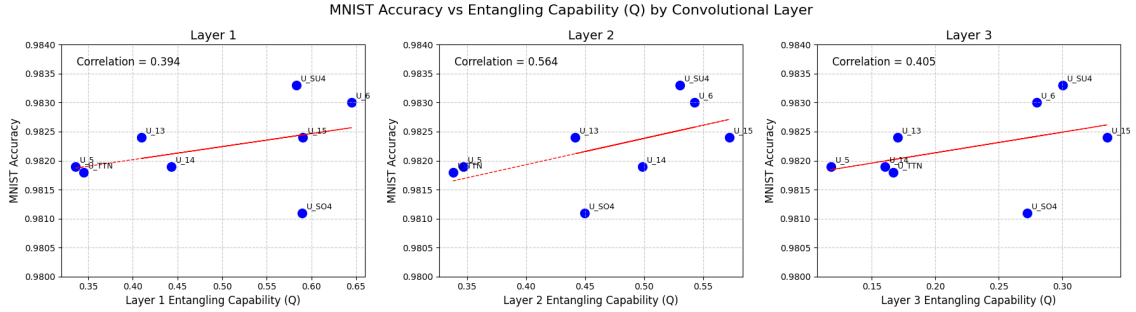


Figure 5.9: Plotting MNIST Accuracy against Layer 1, Layer 2 and Layer 3 Entangling Capability

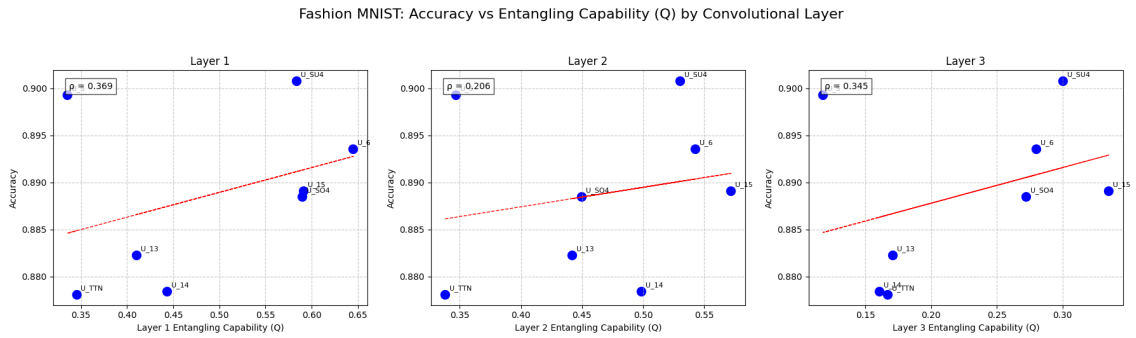


Figure 5.10: Plotting Fashion MNIST Accuracy against Layer 1, Layer 2 and Layer 3 Entangling Capability

QMNST: Accuracy vs Entangling Capability (Q) by Convolutional Layer

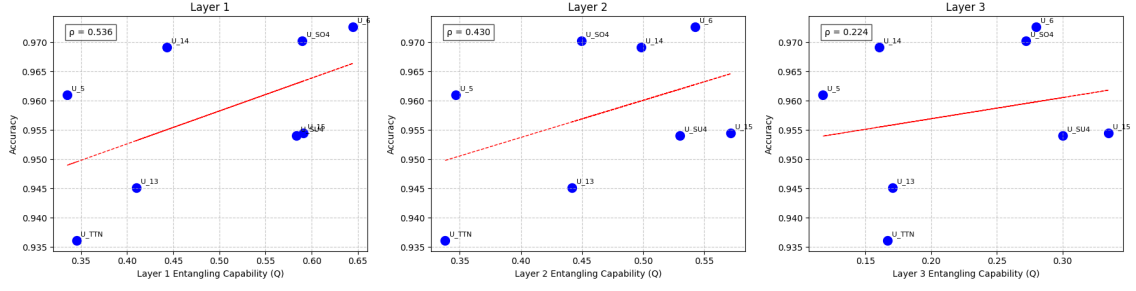


Figure 5.11: Plotting QMNST Accuracy against Layer 1, Layer 2 and Layer 3 Entangling Capability

Audio: Accuracy vs Entangling Capability (Q) by Convolutional Layer

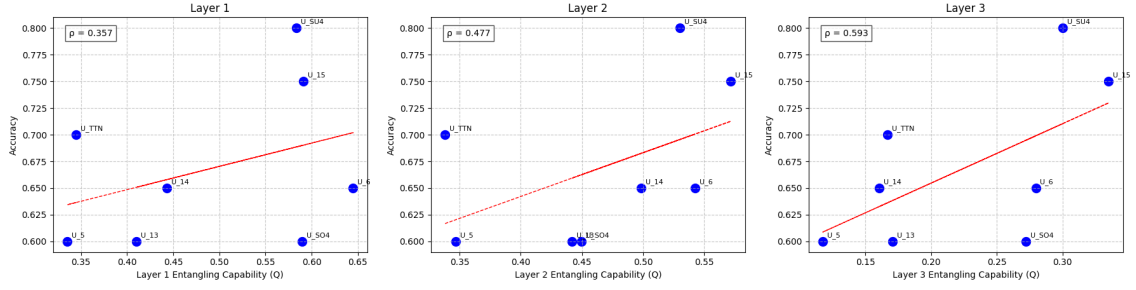


Figure 5.12: Plotting Audio dataset Accuracy against Layer 1, Layer 2 and Layer 3 Entangling Capability

Datasets	Pearson, r (Layer 1)	Pearson, r (Layer 2)	Pearson, r (Layer 3)
MNIST	0.394	0.564	0.405
Fashion MNIST	0.369	0.206	0.345
QMNST	0.536	0.430	0.224
Audio Data	0.357	0.477	0.593

Table 5.8: Pearson Correlation Coefficient for Convolutional Layer Entangling Capability and Accuracy

This correlation again indicates that when the entangling capability increases, the accuracy is better, but there is no guarantee of getting the highest accuracy with the highest entangling capability. For example, U_9 had the highest entangling capability over all the Convolutional Layers had low accuracy after the whole model run. Whereas U_{SU4} had a moderate entangling capability over all the convolutional layer and showed consistently high accuracy over various datasets. Ansatzes like U_6 , U_{15} also showed the same characteristics as U_{SU4} .

5.3 Relation of Expressivity, Entangling Capability and Accuracy

From our earlier work in Section 5.1 and 5.2, it is clear that there is a relationship between expressivity and accuracy as well as entangling capability and accuracy.

In our research, we found that U_9 has low expressivity and high entangling capability. Despite having high entangling capability, it consistently had low accuracy. Therefore, the high entangling capability could not contribute much to the accuracy of the ansatz, as it had low expressivity.

Ansatz	KL Divergence	Entangling Capability	MNIST Accuracy (%)	Fashion MNIST Accuracy (%)	QMIST Accuracy (%)	Audio Data Accuracy (%)
U_{TTN}	0.5682	0.2702	98.18	87.81	93.61 (Lowest)	60 (Lowest)
U_5	0.0154	0.1342 (Lowest)	98.19	89.93	96.10	65
U_6	0.0411	0.3160	98.30	89.56	97.26 (Highest)	60 (Lowest)
U_9	0.5682 (Highest)	1.0000 (Highest)	98.04 (Lowest)	83.64 (Lowest)	94.14	60 (Lowest)
U_{13}	0.2068	0.2237	98.24	88.23	94.51	65
U_{14}	0.0292	0.2237	98.19	87.84	96.91	75
U_{15}	0.2301	0.3119	98.24	88.91	95.45	60 (Lowest)
U_{SO4}	0.2117	0.3405	98.11	88.85	97.02	80 (Highest)
U_{SU4}	0.0054 (Lowest)	0.3346	98.33 (Highest)	90.08 (Highest)	95.40	70

Table 5.9: Comparison of KL Divergence and Entangling Capability for Various Ansatzes

Whereas U_{SU4} has the highest expressivity and a moderate entangling capability, the ansatz has also shown consistently high accuracy over all datasets. This indicates that an ansatz’s expressivity contributes more to finding the desired goal state. Because entangling capability is just the ability to generate complex quantum states, but expressivity gives one ansatz the ability to explore the Hilbert state to find the desired state.

These results indicate that if an ansatz has a greater entangling capability, it creates excessive quantum relations and lead to overfitting to training data and barren plateaus in the optimization process. Whereas, when ansatzes have high expressivity, they continuously explore more states in Hilbert space and finally end up having high accuracy.

Therefore, while choosing an ansatz for Quantum Models, expressivity is an important factor to be considered. Entangling capability surely helps create quantum relations but does not contribute more towards the accuracy.

Chapter 6

Conclusion

This thesis aimed to investigate the potential of expressivity and entangling capability as key metrics for guiding the selection of ansatzes structures in Quantum Neural Network design. The motivation initiates from the high computational demands involved in training and validating various ansatzes' configurations, especially within Quantum Convolutional Neural Network (QCNN). The primary objective was to identify alternative metrics that could predict ansatzes' effectiveness prior to full-scale training which will enhance the efficiency in both computational resource allocation and model development timelines. Through comprehensive experimentation on diverse image and audio datasets, we established a strong negative correlation between expressivity and model accuracy, indicating that ansatzes exhibiting lower KL divergence consistently yielded superior model performance. This outcome validates the application of expressivity as a principal criterion for ansatz assessment. In contrast, the analysis demonstrated only a weak and inconsistent relationship between entanglement capability and trainability. Although entanglement remains a fundamental quantum resource, our findings indicate that it does not serve as a reliable standalone predictor of ansatzes' performance. However, entangling capability may serve as a secondary metric, providing additional insight into the efficiency with which a circuit explores its accessible state space. We observed that ansatzes exhibiting moderate entangling capability in conjunction with high expressivity frequently achieved robust performance. This observation supports the interpretation that, although entangling capability indicates a circuit's efficiency in state space traversal and expressivity determines the extent of this traversal and exerts a more critical influence on trainability. Our study was constrained by limitations in runtime and hardware capabilities, which restricted the range of ansatzes' architectures examined. As a result, we analyzed only a limited number of ansatzes. Including more number of ansatzes could have made the results more complete and reliable. We recognize this as a limitation of our work. In conclusion, our findings support a descriptor-driven approach to ansatzes' selection strategy, emphasizing expressivity as the primary criterion and entangling capability as a complimentary factor. The strategy has the potential to substantially amplify the efficiency of quantum model design during the NISQ era and beyond.

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