Architecture representations for quantum convolutional neural networks

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The Quantum Convolutional Neural Network (QCNN) is a quantum circuit model inspired by the architecture of Convolutional Neural Networks (CNNs). The success of CNNs is largely due to its ability to learn high level features from raw data rather than requiring manual feature design. Neural Architecture Search (NAS) continues this trend by learning network architecture, alleviating the need for its manual construction and has been able to generate state of the art models automatically. Search space design is a crucial step in NAS and there is currently no formal framework through which it can be achieved for QCNNs. In this work we provide such a framework by utilizing techniques from NAS to create an architectural representation for QCNNs that facilitate search space design and automatic model generation. This is done by specifying primitive operations, such as convolutions and pooling, in such a way that they can be dynamically stacked on top of each other to form different architectures. This way, QCNN search spaces can be created by controlling the sequence and hyperparameters of stacked primitives, allowing the capture of different design motifs. We show this by generating QCNNs that belong to a popular family of parametric quantum circuits, those resembling reverse binary trees. We then benchmark this family of models on a music genre classification dataset, GTZAN. Showing that alternating architecture impact model performance more than other modelling components such as choice of unitary ansatz and data encoding, resulting in a way to improve model performance without increasing its complexity. Finally we provide an open source python package that enable dynamic QCNN creation by system or hand, based off the work presented in this paper, facilitating search space design.

I. INTRODUCTION

Machine learning with a trainable quantum circuit provides promising applications for quantum computing. Among various parameterized quantum circuit (PQC) models, the Quantum Convolutional Neural Network (QCNN) introduced in Ref. [5] stands out due to the shallow circuit depth, absence of barren plateaus [6], and good generalization capabilities [7]. It has been applied in the study of quantum many-body systems and combine techniques from Quantum Error Correction (QEC), Tensor Networks (TNs) and deep learning. Research at this intersection has been fruitful, yielding deep learning solutions for quantum many-body problems [8-11], quantum inspired insights for deep learning [12-14] and equivalences between them [15-17]. On its own, deep learning is ubiquitous in modern society; applications span from content filtering and product recommendations to aided medical diagnosis and scientific research. Its key characteristic is the ability to learn features from raw data rather than requiring manual design from humans [18]. The success of AlexNet [19] demonstrated the power of this which caused a shift of focus from feature design to architecture design [20] and Neural Architecture Search (NAS) aims to take the natural next step in learning network architecture [21]. Already, state of the art deep learning models has been designed automatically [20,22-24], surpassing previous hand crafted ones. As summarized by Elsken et al. [21], there are three main categories within NAS: search space, search strategy and performance estimation strategy. NAS methods can be computationally expensive since evaluating a single architecture requires training a full model. Focusing on the first category, search space, help increase search efficiency and reduce complexity [25] which is achieved by designing a restricted space. Typically, a set of primitive operations are used as building blocks and combined to capture some design motif which constitutes a cell. Different cells are then stacked to form a full architecture. The idea is to make use of repeated motifs which are commonly seen in successfully handcrafted architectures. Interestingly, repeated motifs are also common in quantum circuit design, for example [5] [26-30]. In particular [24] demonstrate that hierarchical architectures based on tensor networks can be used to classify classical and quantum data. Similarly Cong et al. [4] use the multiscale entanglement renormalization ansatz (MERA) as an instance of their proposed QCNN and discuss generalizations for the quantum analogues of convolution and pooling operations. In this work we take inspiration from NAS and QCNNs to formulate these analog operations as directed graphs such that they can be used as primitives for QCNN architectures. Specifically the formalism encodes the architectural and operational information of...
and between primitives in a way that they can be dynamically stacked together to form QCNNs. This facilitates search space design and enable a system to automatically generate QCNN architectures that capture multiple levels of different design motifs.

The QCNN belong to the class of hybrid quantum-classical algorithms, which are parameterized quantum circuits (PQCs) executed on a quantum computer with their parameters optimized classically. In general, there are two key factors to consider when utilizing PQCs for machine learning. That is the way data is encoded (feature map) and choice of quantum circuit. The goal is to find a good quantum circuit for a given feature map of a data set, and the difficulty is finding ones that are both expressive and trainable. The chosen quantum circuit is referred to as ansatz and typically circuit architecture is fixed while continuous parameters such as rotation angles are optimized. However, a defining characteristic of the QCNN is its circuit architecture since one of its main operations, pooling, directly affects it. This is because pooling cause a portion of available qubits to be measured and based on the outcome, unitary operations are applied to the remaining qubits. Thus restricting future convolution and pooling operations since measured qubits aren’t available for consecutive layers, resulting in favourable shallow depth circuits. Furthermore, alternating architecture has been experimentally shown to effect the expressive power and quality of initialization techniques for PQCs. Therefore, circuit architecture is a key component in designing QCNNs and is typically chosen manually along with a gate set that constitute the convolution and pooling operations. The power of both choices rely heavily on the specific classification task and data that is used. With the success of NAS to classical neural networks in mind, we look to explore its possible overlap with QCNNs. There are various techniques in literature focusing on generative architectures for quantum circuits, typically referred to as variable structure ansatz. Of which some explore the intersection and usage of NAS, termed quantum architecture search. In order to be computationally feasible, these are either oriented towards specific tasks such as the variational quantum eigensolver (VQE) and the quantum approximate optimization algorithm (QAOA) or impose additional constraints such as circuit topology or allowable gates. To the best of the authors’ knowledge, no framework yet encapsulates architecture generation for QCNNs.

To achieve this, we formulate the QCNN as a series of directed graphs, each functioning as a primitive operation to represent convolutions, pooling and other architectural operations. These graphs capture the architectural effect of the primitives, controlled by their respective hyperparameters, in such a way that they can be dynamically stacked on top each other. The formalism serve as a language for a system to generate circuit architectures by providing a data structure that encodes QCNNs without needing to specify convolution or pooling unitaries (circuit ansatzes). Making it easy to have a fixed set of ansatzes and enumerating the possible ways of distributing them across a circuit in the form of a QCNN. More importantly, the formalism enables the capture of design motifs on different levels. From overall architecture such as hierarchical motifs resembling reverse binary trees to alternating the distribution of unitaries across the circuit within a single layer. We show this by generating a family of QCNN architectures based on popular motifs seen in literature and benchmark them on a music genre classification dataset, GTZAN. The benchmarks show that alternating circuit architecture impacts model performance more than other components in our experiments. For example, consider the machine learning pipeline we follow in Figure 1 to classify musical genres from audio signals. We start off with a 30-second recording of some song, then transform it in two ways. The first, FIG. 1 (a) represents it in tabular form, by deriving standard digital signal processing statistics from the audio signal. These are then tested across different instances of the architecture family. Out of all these pipeline components, alternating architecture impacted model performance the most. Based on the work presented here, we provide a python package that enable the dynamic creation of QCNNs using these primitives. It serves as a tool to design QCNN search spaces and/or enumerate closely related architectures. Enabling one to experimentally determine good architectures for a specific modelling setup. For example, this can be done to find QCNNs that perform well under a specific noise or hardware configuration, which is favourable in the Noisy Intermediate-Scale Quantum (NISQ) era. Furthermore, as more qubits become available, this formalism allows for a simple and practical way to up scale the same model.

The remainder of this paper is structured as follows: we complete our introduction by summarizing the main contribution of this paper. We then give some background on the related areas of research in Section II by describing quantum machine learning and quantum convolutional neural networks on a high level. Section III is the main content of the paper, containing the architectural representation and its detail. Section IV describes the experimental procedure followed to compare different machine learning components, and section V contain
the result of those comparisons. Finally, we end with a discussion about applications and future steps in section VI.

**Overview of main results**

Figure 2 shows how our work facilitate the architectural design process for QCNNs. We provide a framework, inspired by NAS, that enable automatic QCNN generation and search space design. This is seen in the code block of Figure 2 (e) and (f). These two lines of code is all that is required to generate the circuit in Figure 1 (d), explicitly capturing its motifs. This extends naturally to generating a whole family of related circuits which can be seen in Algorithm 1. The framework enables the creation of intricate and novel architectures which we show to impact model performance more than other modelling components such as circuit ansatz, data encoding, data preprocessing, data format and so on in Section VI. This is achieved through providing an architectural representation for QCNNs and its primitive operations. Consider Figure 2, the primitives such as a convolution or pooling act as level $l = 1$ motifs encoded as directed graphs. They function as building blocks for higher level motifs similar to the hierarchical representation for DNNs by [25]. This allow the capture of modularized design patterns and repeated motifs, often seen in successfully handcrafted PQCs and DNNs. The full QCNN is the highest level motif $l = L$ which when assembled is a sequence of directed graphs. For example, a convolution followed by pooling is a level $l = 2$ motif (a convolution-pooling unit) and repeating that three times a level $l = 3$ motif. Encoding the architectural effect of convolutions, pooling and other primitives allow them to be dynamically stacked together by system or hand to build QCNNs and QCNN search spaces. We further provide a python package that achieves exactly this, compatible with any quantum computing framework. In summary, the contributions are: an architectural representation for QCNNs, a python package facilitating dynamic QCNN creation and experimental results illustrating the impact of alternating circuit architecture on a music genre classification dataset, GTZAN.

**II. BACKGROUND**

**Quantum Machine Learning**

The goal of classification is to utilize some data $X$ alongside a function $f_m$ (model) to accurately represent
Then deciding how to spread these unitaries across the circuit in the form of a QCNN is achieved with the architectural representation of motifs on different levels. On the lowest level $l = 1$ we define primitives which act as building blocks for the architecture. For example: $M^1_1$ is a convolution operation with stride 1, $M^1_3$ a pooling operation with filter $F_{\text{right}}$, combined they form the level two motif (e): a convolution-pooling unit $M^2_1$. Motifs are dynamically stacked to form larger motifs until the final level $l = L$ containing only one motif $M^L_1$, the full QCNN architecture. The code block showcase example usage of the python package, only lines (e) and (f) are required to generate the circuit in Figure 1 (d). The package allow for the dynamic creation of QCNN architectures by system or hand, using the architectural representation provided in this paper.

A discrete categorization $y$, i.e. $f_m(X, \theta) = \hat{y} \approx y$. The data is utilized by iteratively changing the model $f_m$ parameters $\theta$ based on the disparity between the current representation $\hat{y}$ and the actual categorization $y$, measured with a cost function $C(y, \hat{y})$. Minimizing this function or learning is done until some specified critical point is reached, resulting in a set of parameters $\theta^*$ that can be used alongside the model $f_m$ and some new data $X^*$ to estimate their categories. This describes a supervised type of learning, since some actual categorizations $y$ are known beforehand. It is achieved with the aid of computers and forms part of the broader field of machine learning, whose technology is ubiquitous in modern society. One interesting realization of this procedure is with the use of quantum computers, where the function $f_m$ is constructed as a variational quantum circuit that acts on a quantum state $|\psi\rangle$. Learning $\theta$ still makes use of classical (i.e., non-quantum) computation, resulting in a hybrid quantum-classical algorithm [47]. The hope is that the exploration of quantum circuits $f_m$ may lead to new approaches in machine learning that would be difficult to achieve classically [48]. Variational quantum algorithms are also applicable in the NISQ era, making the exploration thereof a step forward in the development of future quantum technologies [46].

The goal is then to find a quantum circuit (often called circuit ansatz) $f_m(X, \theta)$ that estimates $y$ accurately while
keeping the number of required parameters $|\theta|$ as small as possible. A popular candidate for the exploration and construction of different quantum circuits are tensor networks (TNs). This is because they may be used to represent quantum states and have had great theoretical and numerical success in the field of quantum many-body systems [49]. Within this context, tensors can be thought of as multidimensional arrays, where the rank of a tensor indicates the array’s dimension. For example, scalars, vectors and matrices correspond to rank-0, rank-1 and rank-2 tensors respectively. A tensor network is also a tensor but decomposed of other, typically lower rank, tensors through contraction operations. Being able to describe high-rank tensors through low-rank tensors in a network is, in part, what makes TNs powerful (see [49] for a more rigorous explanation). Experiments applying the structure of successful TNs from quantum many-body systems to quantum circuit design for machine learning show promising results. These include structures such as matrix product states (MPS) [50], tensor tree networks (TTN) [26, 51] and the multiscale entanglement renormalization ansatz (MERA) [5, 26]. Specifically, the MERA tensor network overlaps with CNNs in terms of structure of successful TNs from quantum many-body systems to quantum circuit design for machine learning show promising results. These include structures such as matrix product states (MPS) [50], tensor tree networks (TTN) [26, 51] and the multiscale entanglement renormalization ansatz (MERA) [5, 26]. Specifically, the MERA tensor network overlaps with CNNs in terms of architecture [5, 26] and with the combination of QEC give rise to the QCNN presented in [5].

Quantum Convolutional Neural Networks

In the classical CNN setting, a convolution refers to an operation that produces some feature map by cross correlating a kernel with a given input. The input is the previous layer, and by having the same kernel applied to all of its values result in weights being shared to the following layer. Sharing of weights is an important characteristic of a CNN, since it shapes feature maps to be translational equivariant representations of the previous layer [51]. After the convolution operation, non-linearity is introduced through an activation function. This is typically followed by a pooling operation, which down-samples the feature map to introduce local translational invariance and to reduce model complexity.

While there have been various proposals for the quantum analogue of convolutional neural networks [5, 26, 30, 52, 55], our work focuses on the framework proposed by Cong et al. [5] and the findings of Grant et al. [26]. As with many of these proposals, the key components are weight sharing, sequential reduction of system size via pooling and translational invariance of convolutions. This way the QCNN (Figure [1]) implements analogous convolution and pooling operations in a quantum circuit setting. These operations are applied on a circuit architectural level, where a convolution consist of unitary operations $U_i$ being applied to all available qubits in a given layer. It’s applied to all available qubits in order to achieve a type of translational invariance and being identical unitaries allows the sharing of their weights. This relates to a CNN applying a single kernel to all input neurons in a given layer. Weight sharing is an important characteristic of the QCNN, as it causes the magnitude of its cost function gradients to increase, which is desirable in the face of barren plateau’s since it counteracts vanishing gradients [6]. Pooling consist of measuring a portion of the available qubits within a layer and then applying unitary rotations $V_i$ to the remaining ones based on the measurement outcomes. This leads to a reduction in parameters to optimize, which introduces non-linearity to the model while also reducing its computational overhead [5]. Convolution and pooling operations are repeated until the system size is sufficiently small. For binary classification, one of the qubits are measured, and the expectation value defined as the probability for binary class membership.

Considering the MERA structure in reverse satisfies the above description, giving rise to a valid QCNN architecture. The QCNN circuit architecture has been successfully applied to problems surrounding quantum phase recognition (QPR) and quantum error correction (QEC). The partial measurement performed during pooling relates to syndrome measurements in QEC, giving the intuition that a QCNN is viewed as some combination of MERA and QEC [5].

III. ARCHITECTURE REPRESENTATIONS

The chosen architecture of quantum circuits [26, 27, 43] and deep neural networks [21] is an important component for their success. This is emphasized for DNNs by NAS which seek to automate that choice. To this end, a search space is required that determine which architectures are reachable by an algorithm. Effective search spaces will greatly reduce the computational complexity of the algorithm, making NAS methods feasible. Creating them requires a method of architectural representation that is able to capture design motifs on multiple levels of abstraction. DNNs have well defined primitive operations, for instance $n \times n$ depthwise convolutions, $n \times n$ maxpooling and many more, that can be combined dynamically to form a full model. Repeated motifs are often seen in handcrafted designs where a specific combination of primitive operations is reused throughout the model. Recent proposals in NAS [21] attempt to learn such motifs by combining primitive operations to form cells and then stack the cells in some predefined manner resulting in a full architecture. Liu et al. [26] presented a hierarchical representation where the macro architecture is also learnt by using lower level motifs as building blocks for higher level ones. Directed graphs are used to capture motifs, where edges correspond to operations and nodes to feature maps. On the lowest level primitive operations are used as edges and going up the hierarchy use previous graphs (motifs) as edges for the new graph. The highest level consists of one motif which constitutes a full architecture. This is a powerful technique that capture
modularized design patterns often seen in handcrafted architectures. Similar design patterns occur in quantum circuits and is emphasized by QCNNs. Consider Figure 2 from a gate set, unitaries are built according to some ansatz. They are then placed on the circuit according to design motifs on different levels. Lower level motifs, Figure 2 (a)-(d), such as convolutions (identical unitaries, translational invariance) and pooling (system reduction) to higher level ones such as overall architecture being hierarchical or based on tensor network structures [5] [29]. These motifs are implemented implicitly in QCNN designs and we aim to capture them explicitly so that a system can learn them. Therefore a method of architectural representation is required that can capture design motifs for QCNNs. To this end, we also use directed graphs and define primitives for QCNNs to be used as building blocks for their architecture.

Digraph Formalism

Consider the motif levels \( l \) in Figure 2 we encode the QCNN as a sequence of directed graphs, each acting as a primitive operation that capture level \( l = 1 \) motifs such as a convolution (Qconv) or pooling (Qpool). The effect of a primitive is based of its hyperparameters and the effect of its predecessor. This way their individual and combined architectural effect is captured, enabling them to be dynamically stacked one after another to form second level \( l = 2 \) motifs. Stacking these stacks in different ways constitute higher level motifs until a final level \( l = L \) where there is only one motif constituting the full QCNN architecture. We also define a special primitive Qfree that free up pooled qubits to be used again for future operations. For a primitive \( G = (Q,E) \), its nodes \( Q \) represent available qubits, and oriented edges \( E \) the corresponding unitary applied between a pair of them. The direction of an edge indicates the order of interaction for the unitary. For example a CNOT gate with qubit \( i \) as control and \( j \) as target is represented by the edge from qubit \( i \) to qubit \( j \). In the case of pooling, controlled unitaries are used in place of measurement due to the deferred measurement principle [50]. We define the full QCNN architecture as follow:

**Definition 1.** The \( k^{th} \) motif \( 1,2, \ldots, K_l \) on level \( l \) \( L = 1,2, \ldots, L \) is the tuple \( M_k^l = (M_{k-1}^{l-1}|j \in \{1,2, \ldots, K_{l-1}\}) \). At the lowest level \( M_1^l \) corresponds to a primitive operation which is part of the set \( M^{(l)} = \{M_1^1, M_2^1, \ldots, M_{K_1}^1\} \), for instance \( M_1^1 = \{Q\text{conv}, M_2^1 = \text{Qpool(right)}, \ldots \). At the highest level \( l = L \) there is only one motif \( M_1^{L-1} \) which is a hierarchy of tuples. \( M_1^1 \) is flattened through an assemble operation: \( M = \text{assemble}(M_1^1) \) which encodes each primitive into a directed graph \( G_m = (Q_m,E_m) \) where \( m \) is the index such that the full QCNN architecture is represented by \( M = (G_1, G_2, \ldots, G_{|M|}) \).

Figure 2 contain examples of motifs on different levels for a QCNN. Higher level motifs are tuples and the lowest level ones directed graphs. The dependence between successive motifs is specified in the following definition:

**Definition 2.** Let \( x \in \{c,p,f\} \) indicate the primitive type for \( \{\text{Qconv, Qpool, Qfree}\} \) and \( M_1^L \) be the highest level motif for a QCNN. Then assemble\((M_1^L)\) flattens depth-wise into \( M = (G_1, G_2, \ldots, G_{|M|}) \) where \( G_m = (Q_m,E_m) \). \( G_1 \) is always a Qfree\((N_f)\) primitive specifying the number of available qubits with \( N_q \). For \( m > 1 \), \( G_m \) is defined as:

If \( G_m \) is a Qfree\((N_f)\) primitive then:

\[
Q_m^f = \{1,2, \ldots, N_f\} \\
E_m^f = \{\}
\]

If \( G_m \) is a convolution primitive:

\[
Q_m^c = \begin{cases} Q_{m-1}^c & \text{if } x \in \{c,f\} \\ Q_{m-1}^c \setminus \{|i,j) \in \{i,j) \in Q_m^c \times Q_m^c\} \text{ if } x = p \\
E_m^c = \{(i,j)|j \in Q_m^c \times Q_m^c\}
\end{cases}
\]

If \( G_m \) is a pooling primitive:

\[
Q_m^p = \begin{cases} Q_{m-1}^p & \text{if } x \in \{c,f\} \\ Q_{m-1}^p \setminus \{|i,j) \in |i,j) \in Q_m^p \times Q_m^i, i \neq j, d^{-}(i) = 0, d^{+}(i) = 1, d^{-}(j) \geq 1, d^{+}(j) = 0) \}
\end{cases}
\]

with \( d^{-}(i) \) and \( d^{+}(i) \) referring to the indegree and out-degree of node \( i \), respectively and \( \setminus \) to set difference.

Figure 3 show a three level motif implementation using both definitions. It’s the same circuit from Figure 1 (d) represented through the digraph perspective. If the \( m^{th} \) graph in \( M \) is a convolution, we denote its two qubit unitary acting on qubit \( i \) and \( j \) as \( U_{ij}^m(\theta) \). Similarly, for pooling, we note the unitary as \( V_{ij}^m(\theta) \). The action of \( V_{ij}^m(\theta) \) is measuring qubit \( i \) (the control) which causes a unitary rotation \( V \) on qubit \( j \) (the target). With this figure and notational scheme in mind, definition 2 read as follows:

\( Q_m^f \) is the set of available qubits for the \( m^{th} \) primitive in \( M \), where \( x \in \{c,p,f\} \) for convolution, pooling or Qfree respectively. The first primitive \( G_1 \) is Qfree\((N_q)\) which specifies the number of available qubits \( N_q \) for future operations. Any proceeding \( m > 1 \) primitive \( G_m \) only has access to qubits not measured up to that point. This is the previous primitive’s available qubits \( Q_{m-1}^f \) if its type \( x \in \{x,f\} \) is a convolution or Qfree. Otherwise, for pooling, it’s the set difference: \( Q_{m-1}^f \setminus \{|i,j) \in E_m^f\} \) when \( x = p \) since the \( i \) indices during pooling \( |i,j) \in E_m^f \) indicates measured qubits. This is visualized as small red circles in Figure 3. The only way to make those qubits available again is through Qfree\((N_f)\), which can be used to free up \( N_f \).
FIG. 3: Graph view for the circuit architecture in Figure 1 (d). The same two qubit unitary is used in all layers for the convolution operation, i.e. $U_{ij}^m = U_m$. Similarly in this example we use the same two qubit pooling unitaries $V_{ij}^m = V_m$. Consider layer $l = 1$, the top left graph is $C_1$ with all eight qubits $Q_{c1}$ available for the convolution operations $U_{ij}^1$, $(i,j) \in E_{c1}$. Below $C_1$ is $P_1$ with half the qubits of $Q_{p1}$ measured, indicated by the $i^{th}$ indices of $V_{ij}^m$, $(i,j) \in E_{p1}$. For example, qubit 8 $\in Q_{p1}$ is measured and $V_1$ applied to qubit 1 $\in Q_{p1}$ as indicated by $V_{81}^1$, $(8,1) \in E_{p1}$. This pattern repeats until one qubit remain in $P_3$, which is measured and used to classify the music genre.

qubits. For the convolution primitive, $E_{c_m}$ is the set of all pairs of qubits that have $U_{ij}^m(\theta)$ applied to them. Finally for the pooling primitive, $E_{p_m}$ is the set of pairs of qubits that have pooling unitaries $V_{ij}^m(\theta)$ applied to them. The restriction being that if qubit $i$ is measured, it cannot have any other rotational unitary $V$ applied to it within the same primitive $G_m$. This means the indegree $d^-$ of node $i$ is zero. Similarly, if qubit $i$ is measured it may only have one corresponding target, meaning that the outdegree $d^+$ of node $i$ is one. In the same vein, no target qubit $j$ can be the control for another, $d^+(j) = 0$. Every target qubit $j$ have at least one corresponding control qubit $i$, $d^-(j) \geq 1$. It is possible for multiple measured qubits to have the same target qubit, giving $E_{p_m}$ a surjective property.

Following this definition, we can express a convolution or pooling operation for the $m^{th}$ graph in $M$ as:

$$\tilde{U}_m = \prod_{(i,j) \in E_{c_m}} U_{ij}^m(\theta)$$  \hfill (1)

$$\tilde{V}_m = \prod_{(i,j) \in E_{p_m}} V_{ij}^m(\theta)$$  \hfill (2)

Let $\tilde{W}_m = \tilde{U}_m$ or $\tilde{V}_m$ be the $m^{th}$ primitive in $M$ based on whether it’s a convolution or pooling and the identity $I$ if it’s a Qfree primitive. Then the state of the QCNN after one training run is:

$$|\psi\rangle = \tilde{W}|\psi_{[M]}\rangle \cdots \tilde{W}_4 \tilde{W}_3 \tilde{W}_2 \tilde{W}_1 U_{\text{encoding}} |0\rangle$$  \hfill (3)

We note that the choice of $V$ is unrestricted, which means that within one layer each $V$ can be a different rotation. Figure 1(d) shows a special case where the same $V$ is used per layer, which is computationally favourable compared to using different ones. To enable weight sharing, the QCNN require convolution unitaries to be the
same i.e. $U^{ij}_{nm} = U^{kh}_{nm}$ where $(i, j) \in (k, h) \in E^c_m$. This formulation only regards one and two qubit unitaries for convolutions, one qubit unitaries being described with $E^c_m = (i, i), i \in Q^c_m$. It is possible to use $n$-qubit unitaries where $n > 2$ since multiple two qubit unitaries may be used to construct any arbitrary $n$-qubit unitary. Although in practice mostly two qubit unitaries are used, and the focus of this paper.

After training, $|\psi\rangle$ in eq. 3 is measured based on the type of classification task, in this work we focus on binary classification allowing us estimate $\hat{y}$ by measuring the remaining or specified qubit in the computational basis:

$$\hat{y} = P(y = 1) = |\langle 1|\psi\rangle|^2$$

(4)

We note that multi-class classification is also possible by measuring the other qubits and associating each with a different class outcome. Following this, we calculate the cost of a training run with $C$ and $\hat{y}$, then using numerical optimization the cost is reduced by updating the parameters from Equations 1 - 2 and repeating the whole process until some local minimum is reached. Resulting in a model alongside a set of parameters to be used for classifying unseen data.

Equation 8 captures the case where there are only two qubits available for a convolution and equation 9 when there is only one which implies the convolution unitaries only consist of single qubit gates. A stride of $s_{c} = 1$ is a typical design motif for PQCs and the graph formalism allow for a simple way to capture and generalize it. To achieve translational invariance for all strides the two constraints: $|E^c_m| = |Q^c_m|$ and $(i, j) \neq (k, h)$ where $(i, j) \in (k, h) \in E^c_m$ are added. Another option for translational invariance is a Qdense primitive, which only differs from Qconv in that $E^c_m$ generates all possible pairwise combinations of $Q^c_m$. This primitive is available in the python package but left out from the definition (because of its similarity). Figure 4 show different ways in which $s_c$ generate $E^c_m$ for $|Q^c_m| = 8$.

The pooling primitive has two hyperparameters, a stride $s_p$ and filter $E^p_m$. The filter indicates which qubits to measure and the stride how to pair them with the qubits remaining. We define the filter as a binary string:

$$F^p_m = w_1w_2 \cdots w_{|Q^p_m|}$$

where $w_i = 1$ if qubit $i$ is measured and $w_i = 0$ otherwise

(10)

For $N = 8$ qubits, the binary string $F^p_m = 00001111$ translates to measuring the rightmost qubits, i.e. $\{i | i \in Q^p_m, i \geq 5\}$. Figure 3 is an example where the pattern $F^p_m = 00001111 \rightarrow F^p_4 = 0011 \rightarrow F^p_6 = 01$ is used, visually the qubits are removed from top to bottom. Encoding filters as binary strings is useful since generating them becomes generating languages, enabling the use of computer scientific tools such as context free grammars and regular expressions to describe families of filters. Pooling primitives enable hierarchical architectures for QCNNs and in section (search space design) we illustrate how they can be implemented to create a family resembling reverse binary trees. The action of the filter is expressed as: $F^p_m \ast Q^p_m = Q^p_{m+1}$ where * slices $Q^p_m$ corresponding to the 0 indices of $F^p_m$, i.e. $w_i = 0$ (not measured). For example $010 \ast \{4, 7, 2\} = \{4, 2\}$. This example illustrates the case where an ordering was given to the set of available qubits to represent some specific topology of the circuit. Let $Q^p_{m+1} = F^p_m \ast Q^p_m$ then the pooling primitive stride $s_p = \{1, 2, \ldots\}$ is defined as:

$$E^p_m = \{(i, (j + s_p) \mod |Q^p_{m+1}|) | i \in Q^p_m \}$$

(11)

### Search Space Design

We show how the digraph formalism facilitates QCNN generation and search space design. Grant et al. exhibit the success of hierarchical designs that resemble reverse binary trees. To create a space of these architectures we only need three levels of motifs. The idea is to

**Controlling the primitives**

We define basic hyperparameters that control the individual architectural effect of a primitive. There are two broad classes of primitives, special and operational. A special primitive has no operational effect on the circuit, such as Qfree. Its purpose is to make qubits available for future operational primitives and therefore has one hyperparameter $N_f$ for this specification. $N_f$ is typically an integer or set of integers corresponding to qubit numbers:

$$Q^f_m = \{1, 2, \ldots, N_f\} \quad \text{if } N_f \text{ is an integer}$$

$$Q^f_m = N_f \quad \text{if } N_f \text{ is a set of integers}$$

(5)

Each operational primitive has its own stride parameter analogous to classical CNNs. For a given stride $s$, each qubit gets paired with the one $s$ qubits away modulo the number of available qubits. For example a stride of 1 pairs each qubit with its neighbour. This depends on the qubit numbering used which is based on the circuit topology. For illustration purposes, we use a circular topological ordering, but any layout is possible as long as some ordering is provided for $Q^f_1$. For the convolution primitive we define its stride $s_c \in \{1, 2, 3, \ldots\}$ as:

$$E^c_m = \{(i, (i + s_c) \mod |Q^c_m|) | i \in Q^c_m \} \quad \text{if } |Q^c_m| > 2$$

$$E^c_m = \{(i,j) | i, j \in Q^c_m, i \neq j \} \quad \text{if } |Q^c_m| = 2$$

$$E^c_m = \{(i,i) | i \in Q^c_m \} \quad \text{if } |Q^c_m| = 1$$

(7)

(8)

(9)
reduce the system size in half until one qubit remain while
alternating between convolution and pooling operations.
Given \( N \) qubits, a convolution stride \( s_c \), pooling stride
\( s_p \) and a pooling filter \( F^* \) that reduce system size in half,
a reverse binary tree QCNN is generated in algorithm [1].

### Algorithm 1 QCNN, reverse binary tree architecture

**Input:** \( N, s_c, s_p, F^* \)

**Output:** QCNN \( \rightarrow M = \{G_1, G_2, \ldots, G_M\} \)

\[
\begin{align*}
\triangleright & \text{ Primitives:} \\
M_1^l & \leftarrow \text{Qconv}(\text{stride} = s_c) \\
M_2^l & \leftarrow \text{Qpool}(\text{stride} = s_p, \text{filter} = F^*) \\
\triangleright & \text{ Motif: alternate convolution and pooling} \\
M_1^2 & \leftarrow M_1^1 + M_2^1 \\
\triangleright & \text{ Motif: repeat until one qubit remain} \\
M_1^1 & \leftarrow \text{Qfree}(N) + M_1^2 \times \log_2 N \\
M & \leftarrow \text{assemble}(M_1^1)
\end{align*}
\]

It shows how instances of this architecture family can be
created. Two primitives are defined on level one, con-
volution and pooling, which are sequentially combined
on level two as \( M_2^1 \) to form a convolution-pooling unit.
This second level motif is repeated until the system size
is one which is \( \log_2(N) \) times for \( N \) qubits, since \( F^* \)
is chosen to reduce system size in half. The addition
and multiplication operations act as append and extend
for tuples. For example \( M_1^1 + M_2^1 = (M_1^1, M_2^1) \) and
\( M_1^2 \times 3 = (M_1^2, M_1^2, M_1^2) \), which allow for an intuitive
way to build motifs. It’s easy to expand the algorithm
for more intricate architectures, for instance increasing
the number of motifs per level and the number of level-
s. A valid level four motif for algorithm [1] would be
\( M_1^4 = (M_1^2 + M_2^2) \times 3 \), where \( M_1^4 = \text{Qfree}(4) + M_2^4 \) and
\( M_2^4 = M_1^2 \times 2 \) which is the reverse binary tree archi-
tecture \( M_1^4 \) then two convolutions and one convolu-
tion-pooling unit on four qubits, all repeated three times.
Motifs can also be randomly selected on each level to gen-
erate novel architectures. The python package we provide
act as a tool to facilitate architecture generation exactly
this way.

We now analyze the family of architectures generated by
algorithm [1] in more detail. First we consider the possible
pooling filters \( F^* \) that reduce system size in half. It’s
equivalent to generating strings for the language \( A = \{w|w\}
has an equal number of 0s and 1s , |w| = \lfloor Q_{n-1}^m \rfloor \). Let \( N_{m-1} = |Q_{n-1}^m| \) indicate the number of available
qubits for the filter \( F^*_n \). Then based on the \( \binom{N}{1} \) = 6 possible
equal binary strings [57] of length 4 we construct the follow-
ing pooling filters:

\[
\begin{align*}
F_{\text{right}}^*_m & = \{0^m 1^m 1^m | n = N_{m-1}\} \\
F_{\text{left}}^*_m & = \{1^m 0^m 0^m | n = N_{m-1}\} \\
F_{\text{odd}}^*_m & = \{(01)^m | n = N_{m-1}\} \\
F_{\text{even}}^*_m & = \{(10)^m | n = N_{m-1}\} \\
F_{\text{inside}}^*_m & = \{0^m 1^m 0^m 0^m | n = N_{m-1}\} \quad \text{if } N_{m-1} > 2 \\
& \quad \{01\} \quad \text{if } N_{m-1} = 2 \quad \text{(16)} \\
F_{\text{outside}}^*_m & = \{1^m 0^m 1^m 0^m | n = N_{m-1}\} \quad \text{if } N_{m-1} > 2 \\
& \quad \{10\} \quad \text{if } N_{m-1} = 2 \quad \text{(17)}
\end{align*}
\]

where the exponent \( a^b \equiv \{a\} \cap \{a\} \cap \{a\} = aaa \) refers to
the regular operation concatenation: \( A \circ B = \{xy | x \in
A, y \in B\} \). The pooling filter \( F_{\text{inside}} \) yields 0110, visually
this pattern pools qubits from the inside (the middle of the circuit),
see Figure 5 (c). Figure 5 (a) shows the repeated usage of \( F^* \)
for pooling. This particular pattern is useful for data preprocessing
techniques such as principal component analysis (PCA) since PCA intro-
duces an order of importance to the features used in the model.
Typically, the first principal component (which explains the most variance)
encoded on the first qubit, the second principal component on the second qubit
and so on. Therefore, it makes sense to pool the last qubits
and leave the first qubits in the model for as long as possible.
If \( N = 8, s_c = 1, s_p = 0 \) and \( F^* = F_{\text{right}}^* \) then
Algorithm [1] generates the circuit in Figure 3 (d), Figure
2, Figure 5 (f) and Figure 3 (a). Specifically Figure
5 show how different values for \( s_c, s_p, F^* \) represent
the size of the search space / family. Since \( F^* \) reduces system
size in half, it’s required that the number of available

\begin{figure}[h]
\centering
\begin{tabular}{cccc}
\textbf{s}_c = 1 & \textbf{s}_c = 3 & \textbf{s}_c = 5 & \textbf{s}_c = 7 \\
\end{tabular}
\caption{Diagram showing how changing the convolution stride \( s_c \) generates different configurations for \( E_m^* \).}
\end{figure}
FIG. 5: An example of how the hyperparameters of the primitives effect the circuit architecture of the family generated by Algorithm 1. Three are shown, the convolution stride $s_c$, pooling stride $s_p$ and pooling filter $F^*$. These are specified in Section III. Controlled-$R^z$ gates are used for convolutions and CNOTs for pooling as an example. The convolution stride $s_c$ determine how convolution unitaries are distributed across the circuit. Each convolution primitive typically consist of multiple unitaries and the QCNN requires them to be identical for weight sharing. The pooling stride $s_p$ determine how pooling unitaries are distributed, for a given pooling primitive, a portion of available qubits gets pooled via controlled unitary operations and $s_p$ dictates which controls match to which targets. The pooling filter $F^*$ dictates which qubits to pool according to some recursive pattern/mask. For example, circuit d) always pools the outside qubits during pooling primitives, resulting in the middle qubit making it to the end of the circuit.

qubits $N$ be a power of two. Using integer strides cause the $|E_{m_0}| = |Q_{c_m}|$ constraint (see section III controlling primitives) which enable translational invariance. The complexity of the model(in terms of number of unitaries used) then scale linearly with the number of qubits $N$ available. Specifically, $N$ qubits result in $3N - 2$ number of unitaries [58].

IV. EXPERIMENTAL SETUP

Figure 1 gives a broad view of the machine learning pipeline we implement for the benchmarks. There are various factors influencing model performance during such a pipeline. Each step from raw audio signal to classified musical genre contains a wide range of possible configurations, the influence of which propagates throughout the pipeline. For this reason, it is difficult to isolate any one configuration and evaluate its effect on the model. With our goal being to analyse QCNN
architectures (Figure 1(d) on the audio data, we perform random search in the family created by algorithm 1 with different choices of circuit ansatz and quantum data encoding. These are evaluated on two different datasets: Mel spectrogram data (Figure 1(b)) and 2D statistical data (Figure 1(c)) both being derived from the same audio signal (Figure 1(a)). We preprocess the data based on requirements imposed by the model implementation before encoding it into a quantum state. These configurations are expanded on below:

Data

For the data component, we aimed to use a practical and widely applicable dataset, and chose the well known music genre dataset, GTZAN. It consists of 1000 audio tracks, each being a 30-second recording of some song. These recordings were obtained from radio, compact disks and compressed MP3 audio files. Each is given a label of one of the following ten musical genres: blues, classical, country, disco, hip-hop, jazz, metal, pop, reggae, rock. Binary classification is used for the analysis of model performance across different architectures. Meaning, there are 10 possible genre pairs to build models from. Each pair being equally balanced since there are 100 songs for each genre. The dataset therefore enables the comparison of 45 models per configuration within the audio domain.

Model Implementation

For all experiments, we evaluate instances of Algorithm 1 with $N = 8$ qubits, resulting in $3(8) - 2 = 22$ two qubit unitaries. We test each model based on different combinations of model architecture, two qubit unitary ansatz and quantum data encoding. The specific unitaries for $U_m$ are chosen from a set of eight ansatzes that were used by 28. They are based on previous studies that explore the expressibility and entangling capability of parameterized circuits 61, hierarchical quantum classifiers 26 and extensions to the VQE 62. These are shown figure A.1, the ansatz for pooling also comes from 28 and is shown in figure 6. For quantum data encoding, we compare qubit encoding 48 with IQP encoding 63 on the tabular dataset. Amplitude encoding 64 is used for the image data.

Each model configuration considers all 45 genre pairs for classification, for example, rock vs reggae. Cross entropy is used as the cost function $C(y, \hat{y})$ during training, for rock vs reggae this would be:

$$C(y, \hat{y}) = -(y \log(\hat{y}) + (1 - y) \log(1 - \hat{y}))$$

(18)

where

$$y_i = \begin{cases} 1 & \text{if song } i \text{ is labelled rock}, \\ 0 & \text{if song } i \text{ is labelled reggae} \end{cases}$$

(19)

$\hat{y}_i$ is obtained from equation 4. $i$ represents one observation and both $y$, $\hat{y}$ are all the observations in vector form.

Data Creation

We benchmark the model against two different forms of data, namely tabular and image. To construct the dataset in tabular form, specific features are extracted from each audio signal using librosa 65 as shown in Figure 1(b). Each row represents a single audio track with its features as columns. The specific features extracted are those typically used by music information retrieval applications. For these features, we encode each feature into a quantum state, where $N$ is the number of available qubits. Using $N = 8$ qubits, we scale the image down to $8 \times 32 = 256 = 2^8$ pixels, normalizing each pixel between 0 and 1. The down scaling is done by binning the mel frequencies into eight groups and taking the first three seconds of each audio signal.

Data Preprocessing

Two main forms of preprocessing are applied to the data: min-max scaling and feature selection. The features are scaled using min-max scaling, where the range is based on the type of quantum data encoding used. With amplitude encoding, the data is scaled to the range $[0, 1]$, qubit encoding to $[0, \pi/2]$ and IQP encoding to $[0, \pi]$. Feature selection is only applied to the tabular data. Using qubit encoding
with \( N = 8 \) qubits result in selecting eight features. Principal Component Analysis (PCA) and decision trees are used to perform the selection. The tree based selection is used to compare against the PCA, to verify whether the results of the model is not heavily biased by PCA.

Model Evaluation

The model is trained with 70% of the data while 30% is held out as a test set to evaluate performance. During training five-fold cross validation is used on each model. The average classification accuracy and standard deviation of 30 separate trained instances are calculated on the test set as performance metrics.

V. RESULTS

To illustrate the impact of architecture on model performance, we compare the fixed architecture from the experiments of Hur et al. \cite{28} to related architectures in the same family, while keeping all other components the same. Meaning the only difference in each comparison is architecture (how the unitaries are spread across the circuit). Within our framework, the architecture in \cite{28} is represented as: \((s_e, F^*, s_p) = (1,\text{even},0) \leftrightarrow Q\text{free}(8) + (Q\text{conv}(1) + Q\text{pool}(0,F^{\text{even}})) \times 3\), see algorithm \ref{alg}. The comparison is performed on the country vs rock genre pair, since it proved to be one of the most difficult classification tasks from the 45 possibilities. We compare eight unitary ansatzes with different levels of complexity, shown in figure \ref{fig:a.1}.

### Table I: Country vs Rock average accuracy and standard deviation on a held out test set after 30 separate trained instances on the same family vs rock genre pair. The overall accuracy of the whole space is 63.11% indicating that the reference architecture from table II was close to the mean performance. The alteration is part of the best performing architectures \((s_e, F^*, s_p) = (6,\text{left},2)\) with an average accuracy of 75.93. It seems that the combination of \(F^{\text{left}}\) and \(s_e=6\) perform particularly well for this task, with an average accuracy of 72.52%. In general it seems that the convolution stride \(s_e\) and pooling filter \(F^*\) effect performance the most. It’s also worth noting that convolution strides of \(s_e = 3, 4, 5\) performed badly compared to the others. The range of performance goes from a minimum of 43.75% to a maximum of 75.93%, showing the potential impact of the architectural choice.

Finally, we compared the performance of two different architectures on the image data across all genres. This time using ansatz Figure \ref{fig:a.1g} to compare the \(F^{\text{right}}\) and \(F^{\text{even}}\) pooling filters, shown in Figures \ref{fig:a.5} and \ref{fig:a.6}. As mentioned in Section IV the image data is a low-resolution \((8 \times 32 = 256 = 2^8\) pixels) spectrogram of the audio signal. We therefore did not expect high accuracy, but were interested in the variation of performance for different architectures. Figures \ref{fig:a.5} and \ref{fig:a.6} indicate the

\[\text{Meaning the number of parameters to optimize is mostly}\]

\[\text{represents average model accuracy } \pm \text{its standard deviation}\]

\[\text{from 30 separate trained instances on the the same held out test set. Ansatz refers to the unitary used for}\]

\[\text{for the convolution operations of a model, for example the}\]

\[\text{A.1A}\]

\[\text{A.1B}\]

\[\text{A.1C}\]

\[\text{A.1D}\]

\[\text{A.1E}\]

\[\text{A.1F}\]

\[\text{A.1G}\]

\[\text{A.1H}\]

\[\text{Algorithm }\text{1}\]

\[\text{The model is trained with } N = 8 \text{ qubits and have the same number of unitaries}\]

\[\text{Meaning the number of parameters to optimize is mostly}\]

\[\text{represents average model accuracy } \pm \text{its standard deviation}\]

\[\text{from 30 separate trained instances on the the same held out test set. Ansatz refers to the unitary used for}\]

\[\text{for the convolution operations of a model, for example the}\]

\[\text{A.1A}\]

\[\text{A.1B}\]

\[\text{A.1C}\]

\[\text{A.1D}\]

\[\text{A.1E}\]

\[\text{A.1F}\]

\[\text{A.1G}\]

\[\text{A.1H}\]

\[\text{Algorithm }\text{1}\]

\[\text{The model is trained with } N = 8 \text{ qubits and have the same number of unitaries}\]

\[\text{Meaning the number of parameters to optimize is mostly}\]

\[\text{represents average model accuracy } \pm \text{its standard deviation}\]

\[\text{from 30 separate trained instances on the the same held out test set. Ansatz refers to the unitary used for}\]

\[\text{for the convolution operations of a model, for example the}\]

\[\text{A.1A}\]

\[\text{A.1B}\]

\[\text{A.1C}\]

\[\text{A.1D}\]

\[\text{A.1E}\]

\[\text{A.1F}\]

\[\text{A.1G}\]

\[\text{A.1H}\]

\[\text{Algorithm }\text{1}\]
TABLE II: Country vs Rock average accuracy within the reverse binary tree search space, all with $\text{A, In} \text{as ansatz.}$ The convolution stride $s_c$ is shown on the horizontal axis and the combinations of pooling filter $F^*$ and stride $s_p$ on the vertical. The best pooling filter and convolution stride combinations are presented in bold along with the overall best architecture $(s_c, F^*, s_p) = (6, \text{left}, 2).$

difficulty some genre pairs. Interestingly, the $F_{m}^{\text{right}}$ pooling filter outperformed the $F_{m}^{\text{even}}$ filter on almost all genres. If we focus on the genre pairs that the models were able to classify, we see that $F_{m}^{\text{right}}$ had 14 models that achieved an accuracy above 75% compared to the 5 of $F_{m}^{\text{even}}.$ We also note that the image data had no PCA or tree based feature selection applied on it, and the $F_{m}^{\text{right}}$ filter was still favored. A similar result was obtained with the ansatz $\text{A, In}\text{.}$

VI. OUTLOOK

The main contribution of this paper is a framework enabling the dynamic generation of QCNNs and the creation of QCNN search spaces. It’s provided theoretically in this paper and practically as a python package ready for use. Our experimental results justify the importance of alternating architecture for PQCs, illustrating a means to increase model performance without increasing its complexity. Our next step is to explore search strategies using this architectural representation to automatically find good performing QCNNs for different classification tasks. The method of representation is particularly useful for evolutionary algorithms as shown by [25]. Reinforcement learning and random search algorithms are also applicable. Another interesting consideration is the theoretical analysis of QCNN architectures generalizing well across multiple data sets. The framework also allow for different qubit orderings that can correspond to physical hardware setups, therefore benchmarking the effect of noise of different architectures on NISQ devices would be a useful exploration.
FIG. 8: QCNN with the $F_{m}^{even}$ pooling filter using low resolution image data. The accuracies for all genre pairs are provided.

DATA AVAILABILITY

The dataset analysed during the current study is available on TensorFlow Datasets, https://www.tensorflow.org/datasets/catalog/gtzan. The source code used to generate QCNNs is available on github as a package, https://github.com/matt-lourens/dynamic-qcnn.

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**Appendix A: Circuit ansatz**

![Circuit diagrams](image)

**FIG. A.1:** The different unitary ansatzes used for the convolution operation $U_m$ across all experiments. The same ansatzes were used in the benchmarks of [28]. They are based on previous studies that explore the expressibility and entangling capability of parameterized circuits [61], hierarchical quantum classifiers [26] and extensions to the VQE [62].

**Appendix B: Feature Summary**

| Feature                          | Description                                                                                                                                 |
|----------------------------------|---------------------------------------------------------------------------------------------------------------------------------------------|
| Chroma frequencies               | Bins the different pitches of a song into the equal tempered 12-tone scale commonly used in western music.                                    |
| Harmonic and percussive elements | The harmonic and percussive components present in the signal separated via median filtering.                                                   |
| Mel-frequency cepstral coefficients | Coefficients that make up the mel frequency cepstrum, where mel frequency is the transformation of a signal to the mel scale which characterizes human audio perception. It’s commonly used for speech recognition, mobile phone identification and genre classification. |
| Root-mean-square                 | The square root of the average of the square of the signal, $\sqrt{\frac{1}{T_2-T_1}\int_{T_1}^{T_2} x(t)^2 \, dt}$ where $x(t)$ is the amplitude of the signal at time $t$. |
| Spectral centroid                | The expected value of the frequency spectrum in a time interval. A type of centre of mass which can be used as an indication of tone brightness.     |
| Spectral bandwidth               | The standard deviation of the frequency spectrum around its centroid in a time interval.                                                    |
| Spectral rolloff                 | The frequency bin where the cumulative spectral energy is a specified percentage.                                                             |
| Tempo                            | The speed of the music, estimated in beats per minute.                                                                                      |
| Zero crossing rate               | The rate at which the amplitude of the signal crosses zero or changes sign.                                                                 |

**TABLE III:** The information gathered from audio signals to produce the tabular form data set for genre classification benchmarks.
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