Quantum Neural Network Design via Quantum Deep Reinforcement Learning

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The workshop is organized by the Machine Learning research group (www.cs.ubbcluj.ro/ml) and the Romanian Meteorological Administration (https://www.meteoromania.ro/)

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Outline

Quantum Neural Network Architecture Search

Quantum Neural Networks

- Networks which combine classical layers and parametrized quantum circuits (PQCs).

Challenges of Designing QNNs

- Designing PQCs is very hard and labor-intensive, requiring deep knowledge of quantum mechanics.
- Automation is essential to simplify this complex process and make QNNs more accessible and efficient.

Quantum Neural Network Search

- Automating the process of designing optimal parametrized quantum circuits which are integrated into QNNs along with classical layers for data encoding and decoding.

Quantum Neural Network Architecture Search

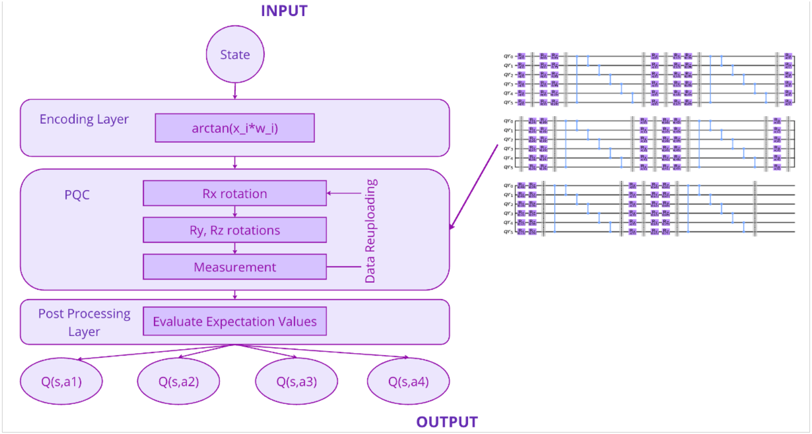

Figure: Instance of a Quantum Neural Network

Quantum Neural Network Architecture Search

Impact on:

- **Optimization of Neural Network Architectures**
  - Efficient Hyperparameter Tuning
  - Advanced Architecture Selection
- **Enhancing Training Efficiency**
  - Minimizing Training Parameters
  - Simplifying Architectural Complexity
- **Accelerating Scientific Research in Various Domains**
  - Chemistry and Material Science
  - Financial Modeling and Prediction
  - Medical Diagnosis and Healthcare

Research Motivation

The research is motivated by addressing the following questions:

- **Research Question 1:**
  - How do quantum gate selection and entanglement strategies affect the performance and expressivity of QNNs?
- **Research Question 2:**
  - Under what conditions can QNNs be optimized to outperform classical ANNs?

Original Contributions

Theoretical Perspective

- Novel Approach to Modelling the Reinforcement Task
- First Implementation of RL which integrates the generated circuits in a QNN that is trained on real data

Practical Implementation

- One of the first publicly accessible frameworks designed explicitly for optimizing PQCs

Current State of the Art

Key Points

- Research in Quantum Neural Network Architecture Search (QNNAS) is still in its infancy and is very limited.
- It is based on Neural Architecture Search (NAS), which has over thousands of research papers.
- Most existing work consists of quantum implementations of classical neural network search algorithms.
- Proposed algorithms for generating quantum circuit architectures have often been tested only on regular, non-parameterizable circuits, not being fully integrated within Quantum Neural Networks (QNNs).

Neural Architecture Search Literature

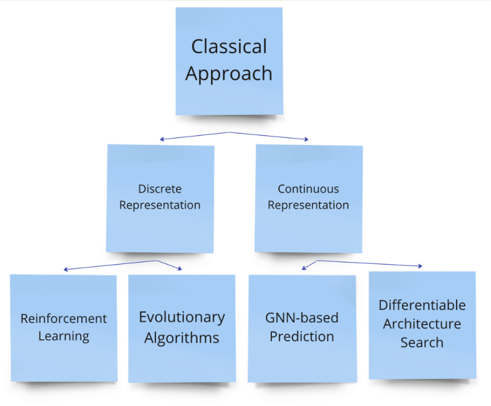

Figure: Overview of Neural Architecture Search Literature

Quantum Neural Architecture Search Literature

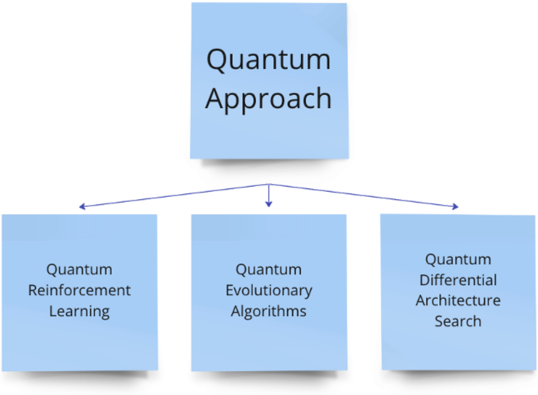

Figure: Overview of Quantum Neural Architecture Search Literature

Employed Dataset

- **Benchmark QNNs Architectures** used in:
  - Reinforcement Learning
    - CartPole Environment
    - Frozen Lake
  - Supervised Learning - Classification Problems
    - Iris Dataset
    - Breast Cancer Wisconsin Dataset

The Reinforcement Task I

Description:

- The agent must choose a layer action in order to build a PQC architecture which has the best performance on its specific task and respects the constraints of a PQC architecture.

Reinforcement Key Points:

- **State:** A Parameterized Quantum Circuit
- **Action:** Placement of a Quantum Gate in the Architecture
- **Reward:** Accuracy of the Generated QNN measured on its specific task

The Reinforcement Task II

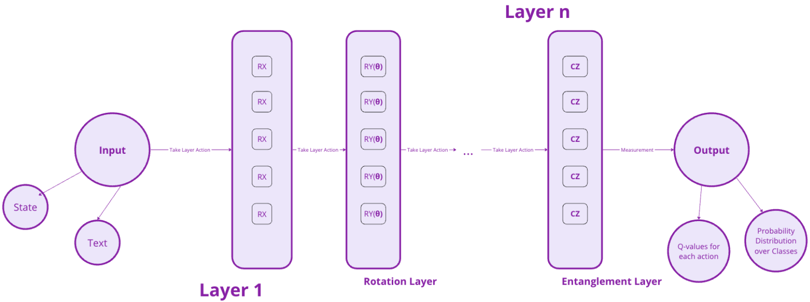

Figure: Overview of the Generated Circuit from the Environment State

The Reinforcement Task III

Layer Action

- Rotation Parameterizable Gates: RX(θ), RY(θ), RZ(θ)
- Entaglement Gates: CX, CY, CZ
- Standard Gates: RX, RY, RZ
- Measurements

Our Methodology Overview

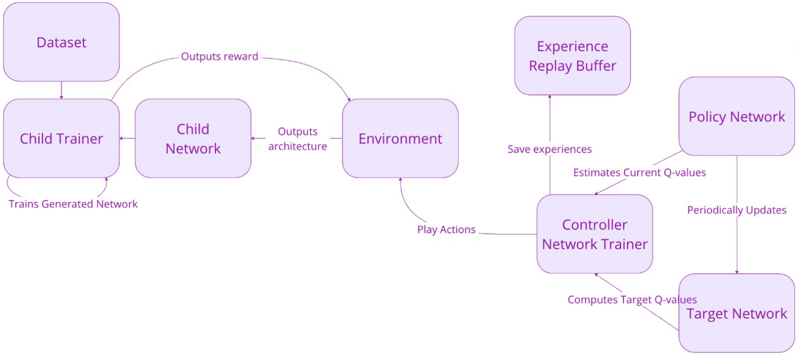

Figure: Overview of the QNNAS Methodology

Agent Training Process

- The agent places quantum gates in the **Environment**, creating the **Child Network** by integrating the generated circuit into a QNN, which is later trained on its problem with its specific dataset.
- The performance of the Child Network is evaluated, and the reward (accuracy obtained) is collected by the agent.
- The agent's experiences, including actions taken and rewards received, are stored in the **Experience Replay Buffer**.
- The **Controller Network Trainer** uses the stored experiences to compute optimal action values.
- The **Policy Network** is updated based on these computed values to improve the agent's decision-making process, with periodic updates from the **Target Network** to ensure consistent and stable training.

Experimental Results I

The initial experiments were conducted using the following settings:

- **Reinforcement Hyperparameters:**
  - **Architecture Max Length (State Max Length):** 4
  - **Possible Gates:** RX(θ), RY(θ), RZ(θ), CX, CY, CZ
  - **Discount Rate:** 0.99
  - **Learning Rate:** 1×10^{-4}
- **Architecture of Controller Network:**
  - **Layers:** Linear ($4 \rightarrow 16$), ReLU, Quantum Layer with RX(θ), RY(θ), RZ(θ) rotations operating on a 16-qubit register and outputting one observation value, then Linear ($1 \rightarrow 7$) actions

Experimental Results II

- **Problem:** Classification of Iris flowers in 3 categories
- **Dataset:** Iris dataset consisting of 150 samples.
- **Input Features**: the length and the width of the sepals and petals, in centimeters

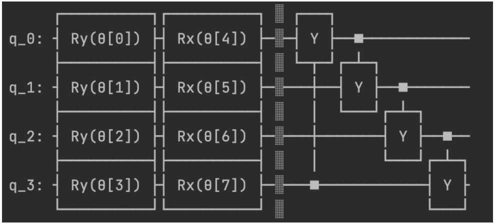

Figure: Generated Architecture

Best Accuracy Attained: 70%

Limitations and Challenges

- **Computationally Intensive:**
  - Training the generated quantum architectures at each step.
  - Controller network training required after a few episodes.
- **Quantum Hardware:**
  - Limited number of qubits available.
  - Long waiting time for circuit compilation and execution.
  - Currently feasible to use only simulators.
- **Quantum Noise:**
  - Quantum noise can induce errors in QNN computations.
  - Reduces accuracy of predictions.
  - Simulated to some extent on simulators.

Thank You!

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