R2P
CAPSTONE PROJECT

Team 5

Quantum Neural Networks

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1. PROBLEM STATEMENT

Problem Statement: Quantum Image Classification

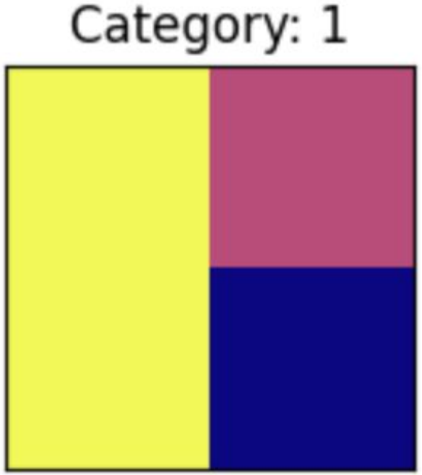
What are we doing?

We train a variational quantum circuit to distinguish three types of 2×2 “images” (lines: horizontal, vertical, diagonal).

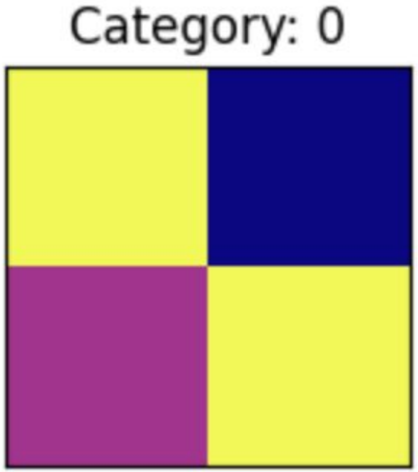
How do we encode the images?

- **Vector representation (length 4):** each of the 4 entries corresponds to one pixel/qubit.
- **Line pixels:** assigned angle value $\pi/2$
- **Background pixels:** uniform random noise in $[0, 1)$

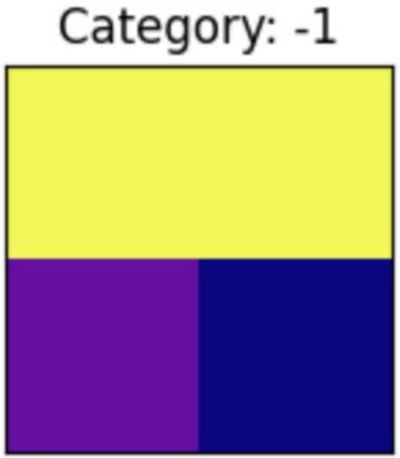
The Dataset



[π/2, 0.15, π/2, 0.54]



[0.44, π/2, π/2, 0.88]



[π/2, π/2, 0.23, 0.67]

2. QUANTUM FEATURE MAP

Quantum Feature Map: From Classical Data to Quantum States

Why a Feature Map?

- **Purpose:** Embed a real-valued vector $\mathbf{x}$ into a quantum state $|\psi(\mathbf{x})\rangle$

Our Chosen Feature Map: ZFeature Map

- **Input:** Vector $\mathbf{x} = [x_0, x_1, x_2, x_3]$
- **Construction:**
  1. Start all qubits in $|0\rangle$
  2. Apply Hadamard H on each qubit to create superposition.
  3. For each qubit i, apply $R_Z(x_i)$
  4. Apply CZ gates between every pair of qubits (full entanglement).

3. PARAMETERIZED QUANTUM CIRCUITS

Parameterized Quantum Circuits: Theory Overview

A Parameterized Quantum Circuit (PQC) is a sequence of quantum gates that depend on continuous parameters $\boldsymbol{\theta}$

It is usually expressed as:

$$U(\boldsymbol{\theta}) = \prod_k U_k(\theta_k)$$

Where each $U_k(\theta_k)$ is a parameterized single-qubit rotation or controlled gate.

Training: the parameters $\boldsymbol{\theta}$ are optimized by minimizing a cost function $C(\boldsymbol{\theta})$.

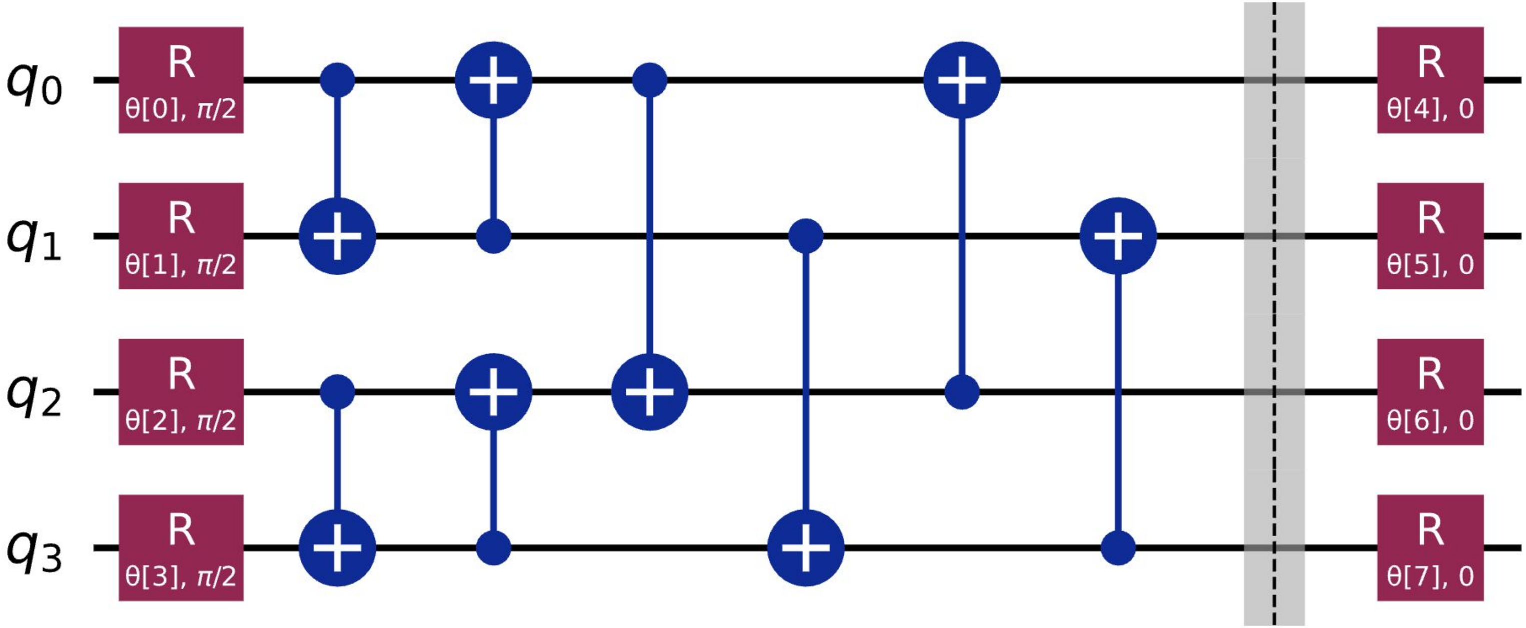
Our Chosen Ansatz Architecture

- **Parameter vector:**

  $\boldsymbol{\theta} = [\theta_0, \ldots, \theta_7]$ (two angles per qubit, here 2 x 4 = 8).

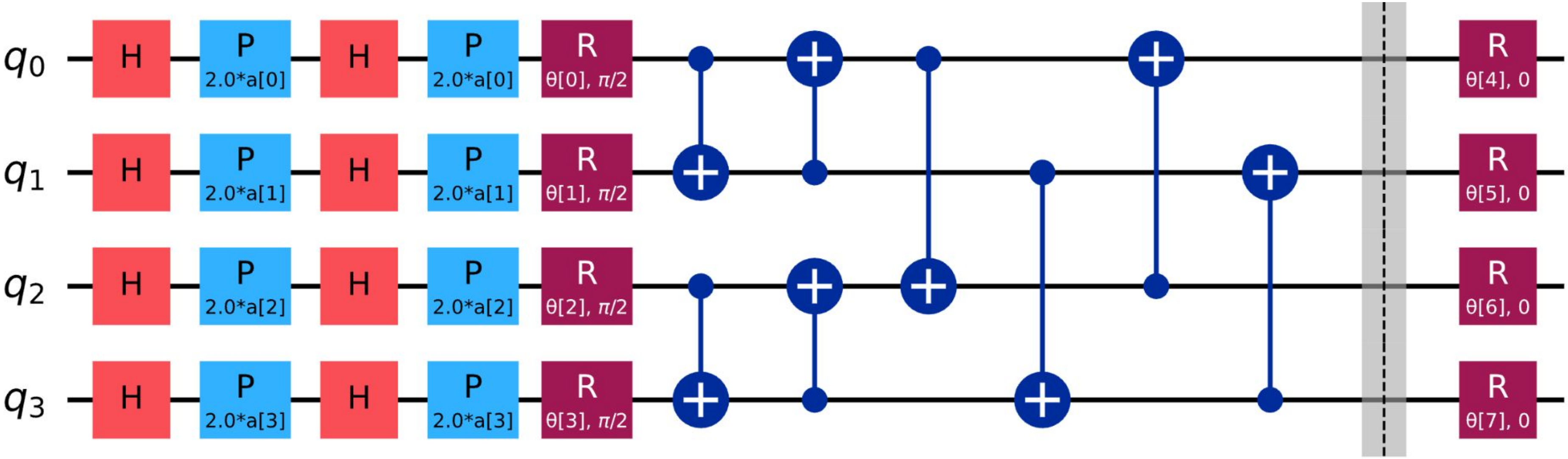
- **Layer 1:**
  - Single-qubit rotations $R_Y(\theta_i)$ on each qubit i
- **Entanglement:**
  - **CNOTs connecting neighboring qubits horizontally and vertically** (in the 2×2 grid).
- **Layer 2:**
  - Single-qubit rotations $R_X(\theta_{4+i})$ on each qubit.

Our Chosen Ansatz Architecture



Merging both ansatz and feature map

We compose the feature map and ansatz into a single circuit, then define the measurement operator $O = Z^{\otimes n}$ (using SparsePauliOp.from_list([("Z"*n,1)])) whose expectation value $\langle O \rangle$ serves as the classifier output.



4. TRAINING

Quantum Forward Pass

What is the Forward Pass?

- **Definition:** The computation that maps input data and circuit parameters to measurement outcomes.
- **Purpose:** Produces predictions $\hat{\boldsymbol{y}}$ by executing the quantum circuit and measuring the chosen observable.

$$(\mathbf{x}, \boldsymbol{\theta}) \to \langle Z^{\otimes n} \rangle$$

- **Analogy:** Like the “forward propagation” in a classical neural net, but replacing matrix multiplications with quantum operations.

Loss functions

The **loss function** $C(\boldsymbol{\theta})$ quantifies the discrepancy between the measured expectation values and the true labels.

$$C(\boldsymbol{\theta}) = \frac{1}{N}\sum_{i=1}^{N}\left(\langle Z^{\otimes n}\rangle_i - y_i\right)^2$$

where:

$$\langle Z^{\otimes n}\rangle_i = \langle \psi(\mathbf{x}_i;\boldsymbol{\theta}) \,|\, Z^{\otimes n} \,|\, \psi(\mathbf{x}_i;\boldsymbol{\theta})\rangle$$

$$y_i \in \{-1, 0, +1\}$$

.

It drives the classical optimizer to update $\boldsymbol{\theta}$ so that the quantum circuit's outputs match the target labels.

Training Process: Mini-Batch Optimization

1. **Initialization**

$$\boldsymbol{\theta}^{(0)} \sim \mathcal{U}(0, 2\pi)^{2n}$$

   Random two-angle-per-qubit vector for the ansatz.

2. **Batch Loop** (for epoch $e = 0, \ldots, E - 1$)
   - Partition $\{(\mathbf{x}_i, y_i)\}_{i=1}^{N}$ into batches of size b.
   - For each batch $\mathcal{B}$:
     - **Define cost** $C_{\mathcal{B}}(\boldsymbol{\theta}) = \dfrac{1}{b} \sum_{i \in \mathcal{B}} \left(\langle Z^{\otimes n} \rangle_i(\boldsymbol{\theta}) - y_i \right)^2$
     - **Update** $\boldsymbol{\theta} = \underset{\theta}{\operatorname{argmin}}\ C_{\mathcal{B}}(\boldsymbol{\theta})$

       using the derivative-free COBYLA optimizer (maxiter = 100)

Training Process: Mini-Batch Optimization

3. **Output:**
    - Trained parameters $\boldsymbol{\theta}^*$
    - Recorded loss history $\{C_{\mathcal{B}}(\boldsymbol{\theta})\}$

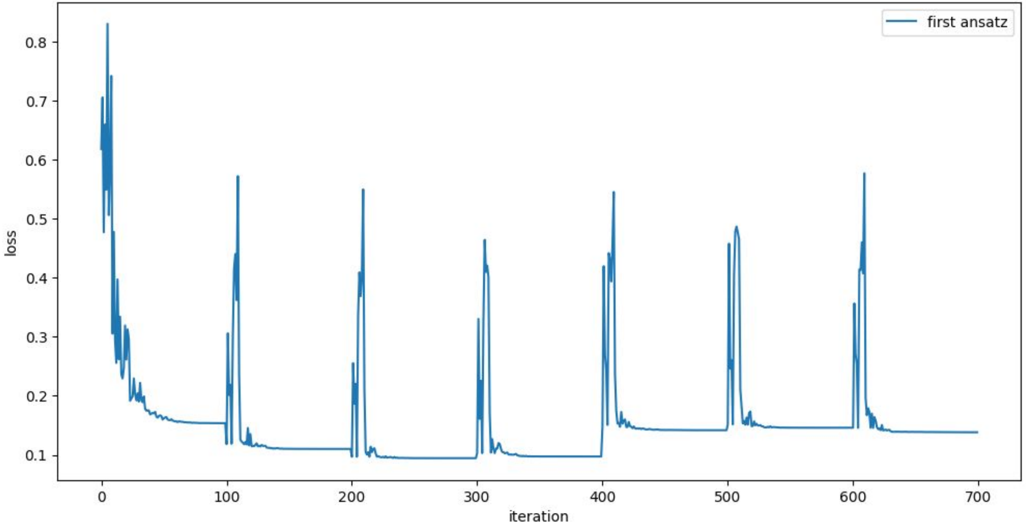
5. RESULTS

Results & Performance

Train accuracy: 84.14%

Test accuracy: 82.67%

Modest train–test gap (~1.5 pp) indicates good generalization.

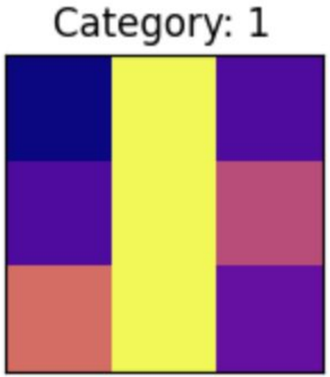


- **Spikes at ~0, 100, 200, …:** the very first evaluation in each new mini-batch—random weights on fresh data → high initial loss.
- **Rapid decay after each spike:** COBYLA quickly lowers the MSE within that batch.

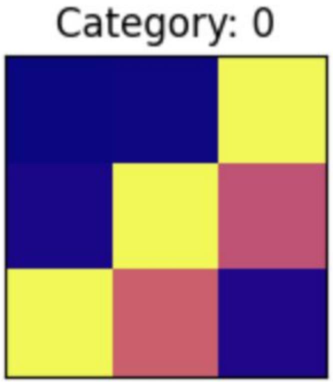
6. Increasing the data size: 3x3 images

The Dataset

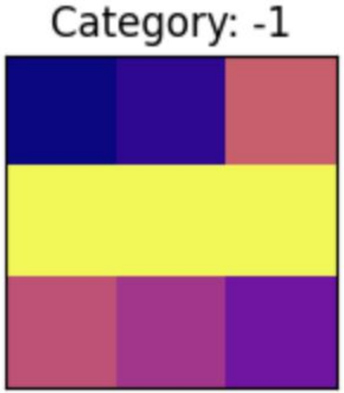
- **Input dimension:** n = 9 qubits (3×3 image)
- **Line length:** 3 pixels



$$\begin{bmatrix} n_{00} & \frac{\pi}{2} & n_{02} \\ n_{10} & \frac{\pi}{2} & n_{12} \\ n_{20} & \frac{\pi}{2} & n_{22} \end{bmatrix}$$

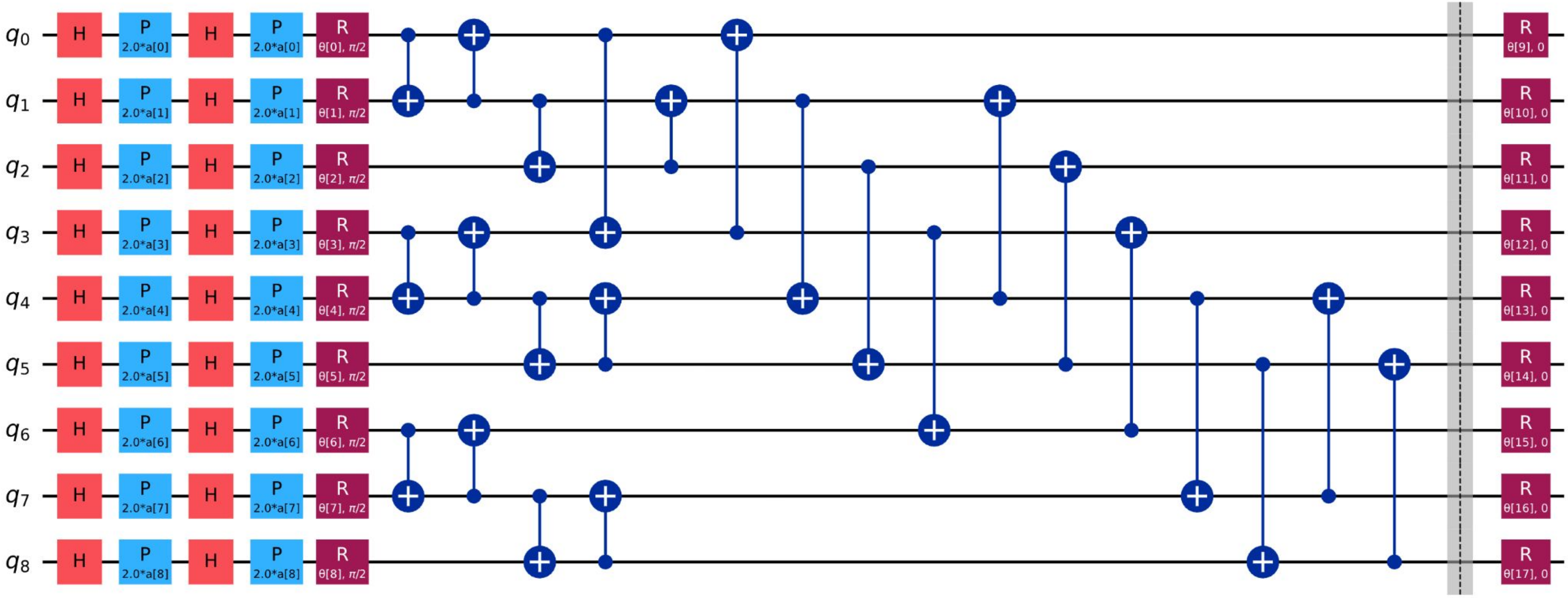


$$\begin{bmatrix} n_{00} & n_{01} & \frac{\pi}{2} \\ n_{10} & \frac{\pi}{2} & n_{12} \\ \frac{\pi}{2} & n_{21} & n_{22} \end{bmatrix}$$



$$\begin{bmatrix} n_{00} & n_{01} & n_{02} \\ \frac{\pi}{2} & \frac{\pi}{2} & \frac{\pi}{2} \\ n_{20} & n_{21} & n_{22} \end{bmatrix}$$

Merging both ansatz and feature map



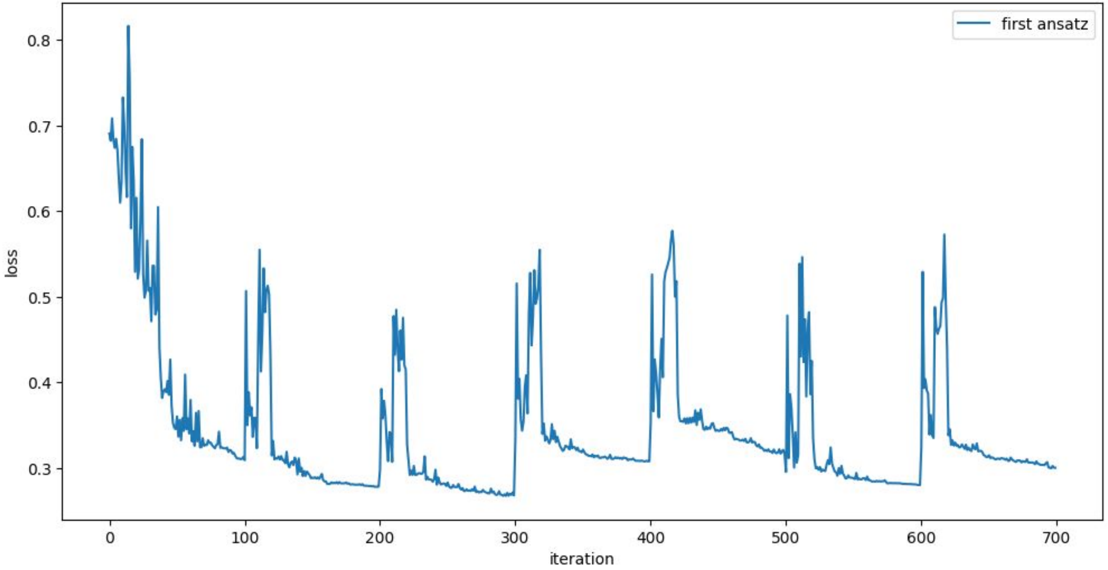
Results & Performance

Train accuracy: 72.57 %

Test accuracy: 73.33%

Train–test gap (~ -0.76 pp) indicates no overfitting.

Lower overall accuracy than the 2×2 case (~82.7% test)

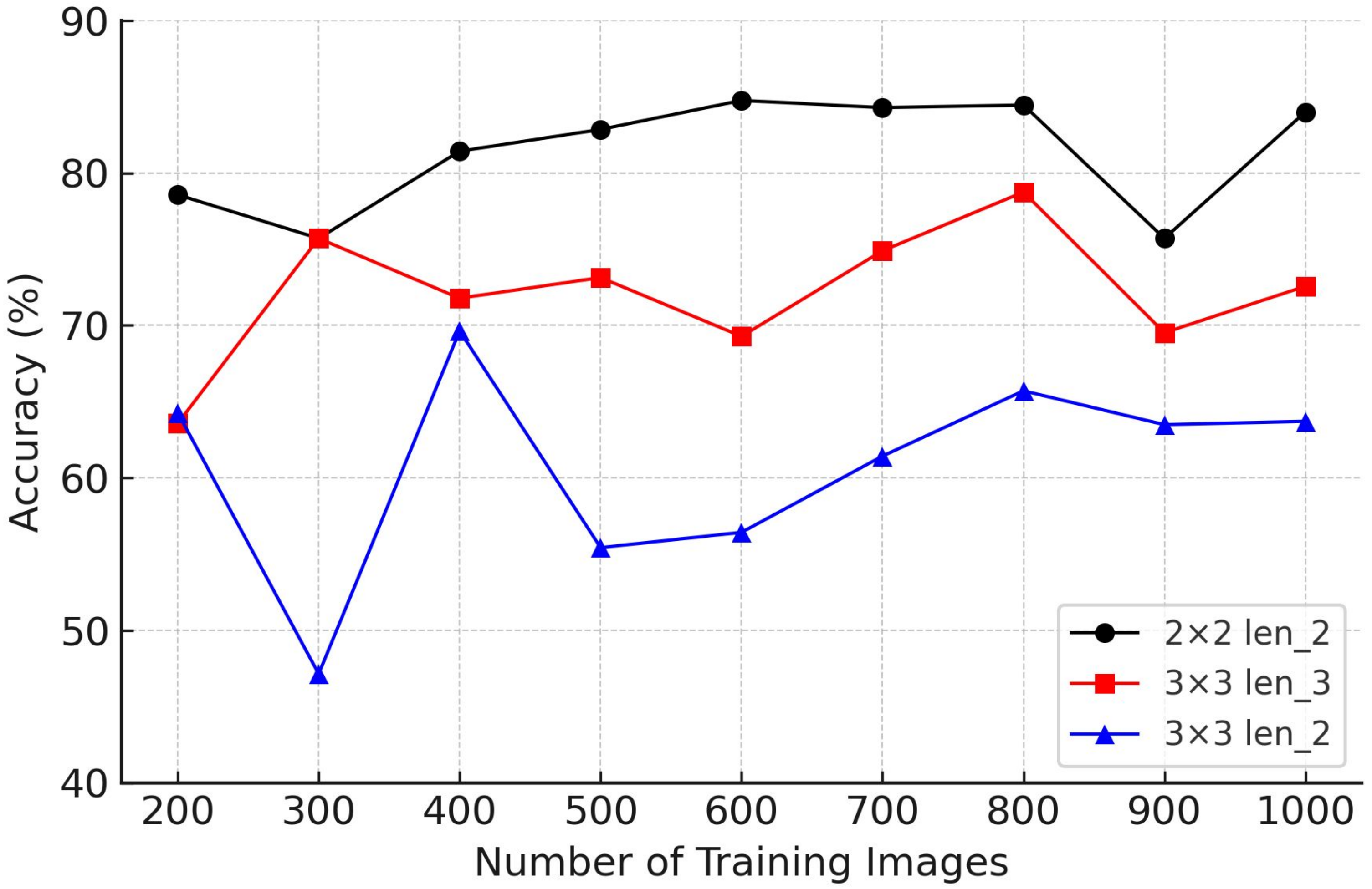


- **Spikes at ~0, 100, 200, …:** the very first evaluation in each new mini-batch—random weights on fresh data → high initial loss.
- **3×3 variant plateau** around **0.30 – 0.32**
- **2×2 baseline plateau** was around **0.14**

7. Testing the program

Prediction Accuracy

Training Images	2x2 images (len 2)	3x3 images (len 3)	3x3 images (len 2)
200	78%	64%	63%
300	75%	47%	75%
400	81%	69%	71%
500	82%	55%	73%
600	84%	56%	69%
700	84%	61%	74%
800	84%	65%	78%
900	75%	63%	69%
1000	84%	63%	72%



90
80
70
60
50
40
Accuracy (%)
200
300
400
500
600
700
800
900
1000
Number of Training Images
2×2 len_2
3×3 len_3
3×3 len_2

8. BIBLIOGRAPHY

Bibliography

- A review of Quantum Neural Networks: Methods, Models, Dilemma
  arXiv:2109.01840v1
- Training Quantum Embedding Kernels on Near-Term Quantum Computers
  arXiv:2105.02276
- Variational Quantum Classifier, Elies M. Gil Fuster & J.I. Latorre
- Quantum neural networks and variational circuits course (link)

[GitHub Repository]