PQC Function Evaluation

Weeks 1-3

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01/07/2024 - 19/07/2024

1/18

Table of Contents

- Background
- 2 Approach: a QCNN

Convolutional Layers Input Layers Summary: QCNN Structure

- Training the QCNN
- 4 Initial Tests
- 6 Results

Encoding the Amplitude Encoding the Phase

2/18

Background

• Hayes 2023¹ presents a scheme to encode a complex vector ${m h}=\{\tilde A_j e^{i\Psi(j)}|0\leq j< N\}$ as the state

$$|h\rangle = \frac{1}{|\tilde{A}|} \sum_{j=0}^{2^{n}-1} \tilde{A}(j)e^{i\Psi(j)} |j\rangle, \qquad (1)$$

using $n = \lceil \log_2 N \rceil$ qubits

ullet This requires operators \hat{U}_A and \hat{U}_Ψ such that

$$\hat{U}_A |0\rangle^{\otimes n} = \frac{1}{|\tilde{A}|} \sum_{j=0}^{2^{n-1}} \tilde{A}(j) |j\rangle, \qquad (2)$$

$$\hat{U}_{\Psi} |j\rangle = e^{i\Psi(j)} |j\rangle \tag{3}$$

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https://arxiv.org/pdf/2306.11073

Background

• \hat{U}_{Ψ} is constructed via an operator \hat{Q}_{Ψ} that performs function evaluation in an ancilla register:

$$\hat{Q}_{\Psi} |j\rangle |0\rangle_{a}^{\otimes m} = |j\rangle |\Psi'(j)\rangle_{a}, \qquad (4)$$

with $\Psi'(j) \equiv \Psi(j)/2\pi$

• Currently, \hat{Q}_{Ψ} is implemented using gate-intensive linear piecewise functions (LPFs)



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Background

Aim

Implement \hat{Q}_{Ψ} in a gate-efficient way using a parametrised quantum circuit (PQC)

Remark

The n-qubit register containing the $|j\rangle$ and the m-qubit register containing the $|\Psi'(j)\rangle$ will be referred to as the input register and target register, respectively.

Approach: a QCNN

- A quantum convolutional neural network (QCNN) is used to tackle the problem
- A QCNN is a parametrised quantum circuit involving multiple layers
- Two types of network layers are implemented:
 - Convolutional layers (CL) involve multi-qubit entanglement gates
 - Input layers (IL)² involve controlled single-qubit operations on target qubits
- Input qubits only appear as controls throughout the QCNN

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6/18

Convolutional Layers (CLs)

- Each CL involves the cascaded application of a two-qubit operator on the target register
- A general two-qubit operator involves 15 parameters
- To reduce the parameter space, the canonical three-parameter operator

$$\mathcal{N}(\alpha, \beta, \gamma) = \exp\left(i\left[\alpha X \otimes X + \beta Y \otimes Y + \gamma Z \otimes Z\right]\right) \tag{5}$$

7 / 18

is applied, at the cost of restricting the search space

- This can be decomposed into 3 CX, 3 R_z , and 2 R_y gates
- A two-parameter real version, $\mathcal{N}_{\mathbb{R}}(\lambda,\mu)$, can be obtained by removing the R_z

³https://arxiv.org/pdf/quant-ph/0308006 ←□ → ←② → ←② → ←② →

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Convolutional Layers (CLs)

- Two types of convolutional layers are implemented:
 - Neighbour-to-neighbour / linear CLs: the \mathcal{N} (or $\mathcal{N}_{\mathbb{R}}$) gate is applied to neighbouring target qubits
 - All-to-all /quadratic CLs: the \mathcal{N} (or $\mathcal{N}_{\mathbb{R}}$) gate is applied to all combinations of target qubits
- The \mathcal{N} -gate cost of neighbour-to-neighbour (NN) layers is $\mathcal{O}(m)$ while that of all-to-all (AA) layers is $\mathcal{O}(m^2)$
- Currently, the QCNN uses alternating linear and quadratic CLs

David Amorim PQC Function Evaluation 22/07/2024 8 / 18

Input Layers (ILs)

- ILs, replacing pooling layers, feed information about the input register into the target register
- An IL involves a sequence of controlled generic single-qubit rotations (CU3 gates) on the target qubits, with input qubits as controls
- For an IL producing states with real amplitudes, the CU3 gates are replaced with CR_y gates
- Each input qubit controls precisely one CU3 (or CR_y operation), resulting in an $\mathcal{O}(n)$ gate cost (no CX gates!)
- ILs are inserted after every second convolutional layer, alternating between control states 0 and 1

Summary: QCNN Structure

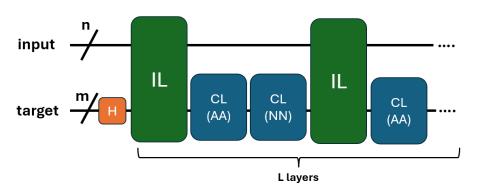


Figure 1: Schematic of QCNN structure

David Amorim PQC Function Evaluation 22/07/2024 10 / 18

Training the QCNN

- For training, the QCNN is wrapped as a SamplerQNN object and connected to PyTorch's Adam optimiser via TorchConnector
- The optimiser determines improved parameter values for each training run (epoch) based on the loss between output and target state
- Beyond loss, mismatch is an important metric:

$$M = 1 - |\langle \psi_{\mathsf{target}} | \psi_{\mathsf{out}} \rangle| \tag{6}$$

11 / 18

- There are two ways to train the QCNN on input data:⁴
 - Training on individual states
 - 2 Training in superposition

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⁴One can also train the QCNN to produce a target distribution independent of the input register, which is equivalent to constructing \hat{U}_A

Training the QCNN

1. Training on Individual States

- One of the 2^n input states, $|j\rangle$, is randomly chosen each epoch
- The network is taught to transform $|j\rangle\,|0\rangle\mapsto|j\rangle\,|\Psi'(j)\rangle$ for each of the states individually

2. Training in Superposition

- The same input state is chosen each epoch
- The network is taught to transform

$$\left(\frac{1}{\sqrt{2^n}}\sum_{j=0}^{2^n-1}|j\rangle\right)|0\rangle\mapsto\frac{1}{\sqrt{2^n}}\sum_{j=0}^{2^n-1}|j\rangle\,|\Psi'(j)\rangle\tag{7}$$

• By linearity, this teaches the network to transform $|j\rangle\,|0\rangle\mapsto|j\rangle\,|\Psi'(j)\rangle$ for each $|j\rangle$

Initial Tests

- Initial tests need to be carried out to inform QCNN design choices regarding:
 - Number of layers
 - 6 Number of epochs
 - **6** Training mode (individually versus in superposition)
 - f d Use of ${\mathcal N}$ and CU3 versus ${\mathcal N}_{\mathbb R}$ and R_y
 - Choice of loss function
 - Metwork structure
- The case n=m=2, $\Psi(x)=x$ (the simplest non-trivial configuration) is an ideal benchmark problem
- Unclear, however, how well these findings extrapolate to more general cases

David Amorim PQC Function Evaluation 22/07/2024 13 / 18

Results

• In the following, a QCNN is applied to implement both \hat{U}_A and \hat{U}_Ψ for the problem studied in Hayes 2023:

$$\tilde{A}(f) = f^{-7/6},\tag{8}$$

$$\Psi(f) = c_0 + c_1 f + c_2 f^{-1/3} + c_3 f^{-2/3} + c_4 f^{-1} + c_5 f^{-5/3},$$
 (9)

with 40 Hz $\leq f \leq$ 168 Hz

- In the paper, \hat{U}_A is implemented via a quantum generative adversarial network (QGAN) as well as the Grover-Rudolph (GR) algorithm while LPFs are used for \hat{U}_Ψ
- Hayes 2023 uses n=6 as well as 22 ancilla qubits



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Encoding the Amplitude

- The QCNN outperforms the QGAN and nearly reaches GR w.r.t. mismatch
- L = 3 with mismatch as loss function and 600 epochs of training was used

Method	CX	Mismatch
QGAN	100	8.6×10^{-3}
GR^5	23,796	5.7×10^{-4}
QCNN	72	6.5×10^{-4}

Table 1: Comparison of \hat{U}_A implementations

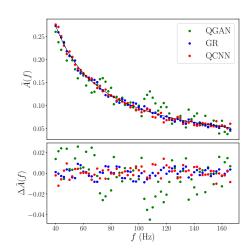


Figure 2: Reconstruction of $\tilde{A}(f)$ from different methods. Target in black.

15 / 18

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⁵Hayes 2023 reports a mismatch of 4.1×10^{-4}

Encoding the Amplitude

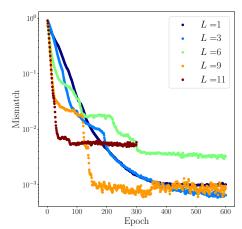


Figure 3: QCNN training for different circuit depths.

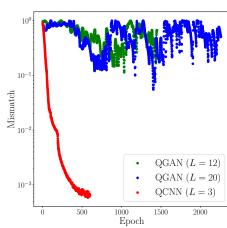


Figure 4: Comparison of QGAN and QCNN training. Note: QGAN results do not match Hayes 2023!

Encoding the Phase

- The implementation of \hat{U}_{Ψ} is not the only factor affecting the encoding of $\Psi(f)$
- The size, m, of the target register limits the available precision due to rounding to $\sim 2^{-m}$
- A meaningful representation of $\Psi(f)$ requires $m\gtrsim 6$
- In combination with n=6 this gives a state-space of size $\gtrsim 2^{12}=4,096$ resulting in long training times

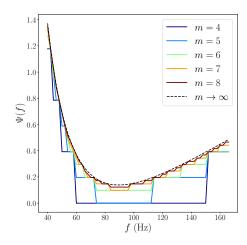


Figure 5: Attainable precision due to rounding for different target register sizes

Encoding the Phase

• ... USE L1 TS r L3 ???

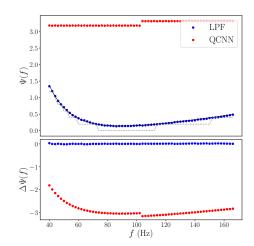


Figure 6: Encoding of $\Psi(f)$ using LPFs versus a QCNN