

PQC Function Evaluation

Weeks 1-3

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Background

- Hayes 2023¹ presents a scheme to prepare a complex vector $\mathbf{h} = \{\tilde{A}_j e^{i\Psi(j)} | 0 \leq j < N\}$ as the quantum state

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

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

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

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

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

¹<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:

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

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

- Currently, \hat{Q}_Ψ is implemented using gate-intensive *linear piecewise functions (LPFs)*

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

²Replacing the conventional QCNN *pooling layers*

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**

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

is applied, at the cost of restricting the search space

- This can be decomposed³ into $3CX$, $3R_z$, and $2R_y$ gates
- A two-parameter real version, $\mathcal{N}_{\mathbb{R}}(\lambda, \mu)$, can be obtained by removing the R_z

³<https://arxiv.org/pdf/quant-ph/0308006>

Convolutional Layers (CLs)

- Two types of convolutional layers are implemented:⁴
 - **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 $\mathcal{O}(m^2)$
- The QCNN uses alternating linear and quadratic CLs

⁴Loosely based on Sim 2019 (<https://arxiv.org/pdf/1905.10876>)

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

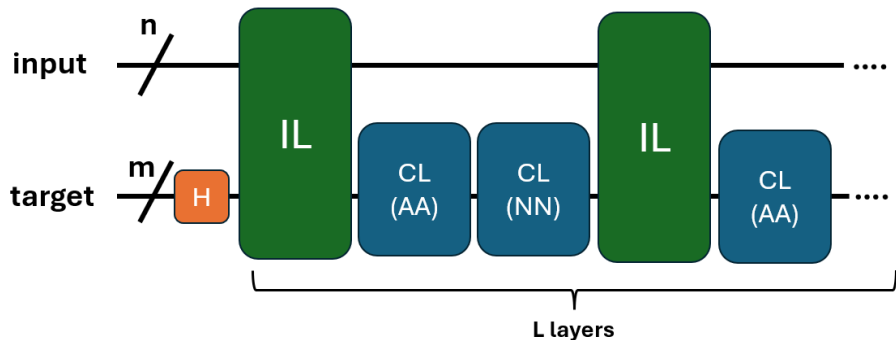


Figure 1: Schematic of QCNN structure

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:

$$M = 1 - | \langle \psi_{\text{target}} | \psi_{\text{out}} \rangle | \quad (6)$$

- There are two ways to train the QCNN on input data:⁵
 - ① Training on **individual states**
 - ② Training in **superposition**

⁵One 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

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

- 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:
 - a Number of layers
 - b Number of epochs
 - c Training mode (individually versus in superposition)
 - d Use of \mathcal{N} and $CU3$ versus $\mathcal{N}_{\mathbb{R}}$ and CR_y
 - e Choice of loss function
 - f Network structure
- This constitutes a **large parameter space** that is difficult to explore systematically
- Overly simple benchmark problems (e.g. $n = m = 2$, $\Psi(x) = x$) do not extrapolate well to more general cases
- Thus, tests are carried out for simplified versions of Ψ in the context of Hayes 2023 ($n = 6$, $m \geq 3$)

Initial Tests

- **Heuristically**: train in superposition with real circuits ($\mathcal{N}_{\mathbb{R}}$ and CR_y) of depth $L = 6$ using 600 epochs and **focus** on optimising the **loss function**
- Best results achieved with *cross entropy* (**CE**) and *sign-adjusted mismatch* (**SAM**):

$$\text{SAM}(x, y) = \left| 1 - \sum_n x_n y_n \right| \quad (8)$$

- SAM is tailored to reduce mismatch and enforce positive amplitudes

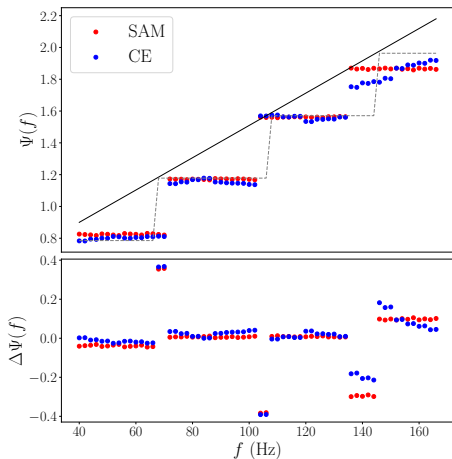


Figure 2: Comparison of loss functions for $\Psi \sim x$ and $m = 4$. Target in black; rounded target dashed in grey.

Initial Tests

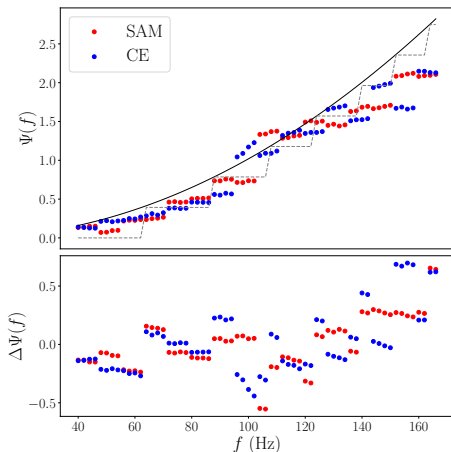


Figure 3: Comparison of loss functions for $\Psi \sim x^2$ and $m = 4$. Target in black; rounded target dashed in grey.

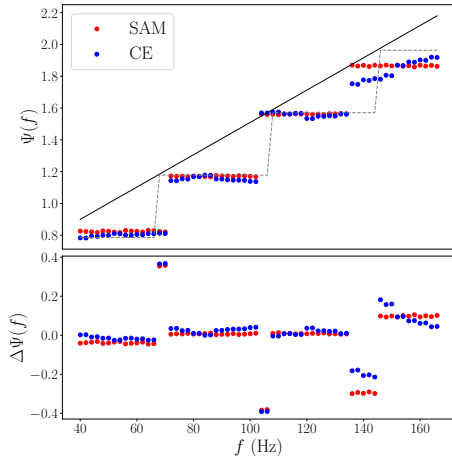


Figure 4: Comparison of loss functions for $\Psi \sim \sin x$ and $m = 4$. Target in black; rounded target dashed in grey.

Initial Tests

look into effects of increasing L and or epochs...

SAM significantly outperforms CE when taking into account state amplitudes

USE GRADIENT-BASED WEIGHTING, tailored to function shape (MEG: mismatch entailing gradients)

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

$$\tilde{A}(f) = f^{-7/6}, \quad (9)$$

$$\Psi(f) = c_0 + c_1 f + c_2 f^{-1/3} + c_3 f^{-2/3} + c_4 f^{-1} + c_5 f^{-5/3}, \quad (10)$$

with $40 \text{ Hz} \leq f \leq 168 \text{ Hz}$

- 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

Encoding the Amplitude

- The **QCNN** outperforms the **QGAN** and **nearly reaches GR** w.r.t. mismatch
- The QCNN ($L = 3, n = 6$) was trained in 600 epochs with SAM

| Method | CX | Mismatch |
|-----------------|--------|----------------------|
| QGAN | 100 | 8.6×10^{-3} |
| GR ⁶ | 23,796 | 5.7×10^{-4} |
| QCNN | 72 | 7.1×10^{-4} |

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

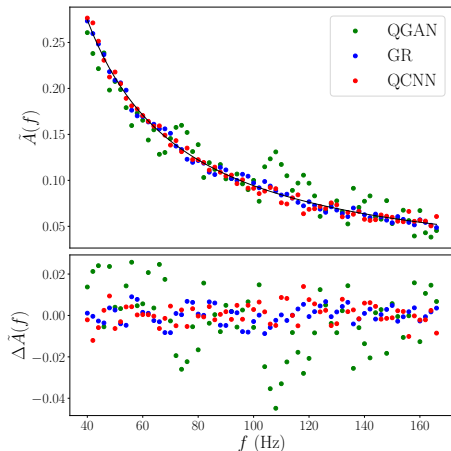


Figure 5: Reconstruction of $\tilde{A}(f)$ from different methods. Target in black.

⁶Hayes 2023 reports a mismatch of 4.1×10^{-4}

Encoding the Amplitude

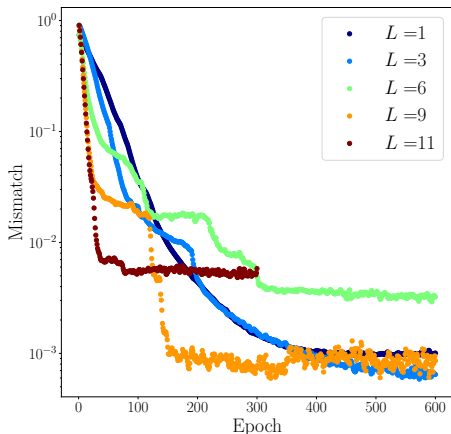


Figure 6: QGAN training for different circuit depths.

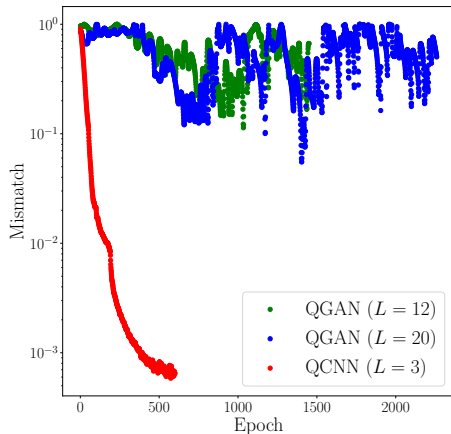


Figure 7: Comparison of QGAN and QCNN training. Note: QGAN results do not match Hayes 2023!

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 $m \gtrsim 6$
- The LPF approach in Hayes 2023 uses $m = 8$

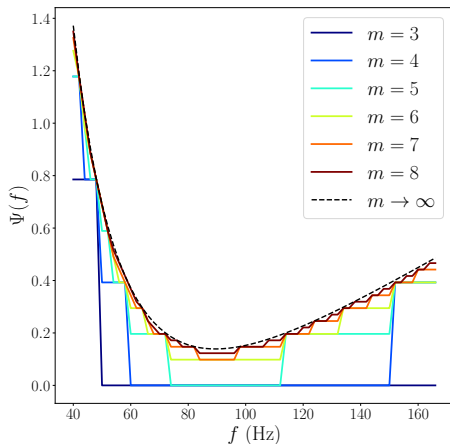


Figure 8: Attainable precision due to rounding for different target register sizes

Encoding the Phase

- right now: using -l MM -TS -r -L 3 -e 600 for different m values ... not learning even for m=3 ...
- at least MM quickly stagnates ...
- take-aways so far:
 - a -TS is far superior to individual training
 - b CE worse than MM ; L1 worse than MM but better than CE

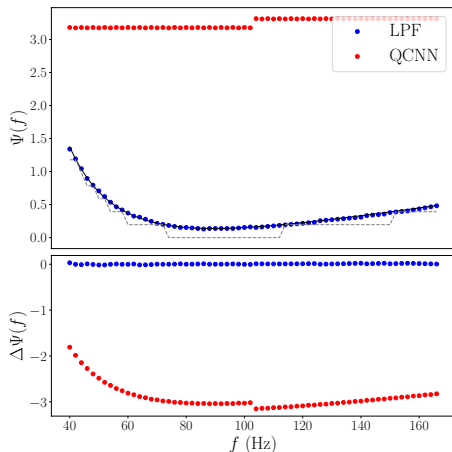


Figure 9: Encoding of $\Psi(f)$ using LPFs versus a QCNN. Target in black; rounded target dashed in grey.

Full Waveform

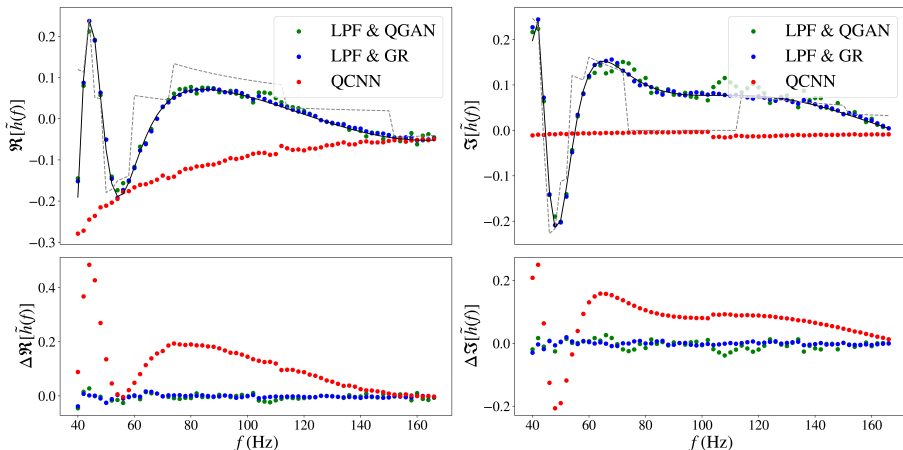


Figure 10: Encoding of $h(f)$ as waveform $\tilde{h}(f)$ using different methods. Target in black; rounded target dashed in grey.

Next Steps

- more fully explore PQC parameter space ...
- look into barren plateau mitigation (layer-by-layer training....)