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Contents

Chapter 1

Introduction

1.1 Relevant work

1.1.1 Cerezo et al. (2021)

Variation quantum algorithms (VQAs) are envisioned as the most likely candidate for quantum advantage to be achieved. By optimising a set of parameters that describe the quantum circuit, classical optimisation techniques are applicable, and only using the quantum hardware for what can be interpreted as function calls, limits the circuit depths needed. Running the same circuit many times with slightly different parameters and inputs in a classical-quantum-hybrid fashion, rather than a complete quantum implementation, means that the quantum operations can be simple enough for the noise and decoherence to be manageable.

Generally, VQAs start with defining a cost function, depending on some input data (states) and the parametrised circuit, to be minimised with respect to the parameters of the quantum circuit. For example, the cost function for the variational quantum eigensolver (VQE) is the expectation value of some Hamiltonian, which is the energy of a system. The cost function should be meaningful in the sense that the minimum coincides with the optimal solution to the problem, and that lower values generally implies better solutions. Additionally, the cost function should be complicated enough to warrant quantum computation by not being easily calculated on classical hardware, while still having few enough parameters to be efficiently optimised.

The optimisation of the cost function is often done with gradient descent methods. To evaluate the gradient of the quantum circuit w.r.t. the parameters, the very convenient parameter shift rule is often used. Though appearing almost as a finite difference scheme, relying on evaluating the circuit with slightly shifted parameters, it is indeed and exact formula. Furthermore, it may be used recursively to evaluate higher order derivatives, which is useful for optimisation methods that require the Hessian.

VQA's applications are numerous. The archetypical example is finding the ground state of a Hamiltonian for a molecule. Such problems are exponential in the particle count, and thus intractable on classical hardware for larger molecules, while the problem of evaluating the Hamiltonian on quantum hardware is typically polynomial. VQAs are also well suited for general mathematical problems and optimisation, even machine learning, another common example being QAOA for the max-cut problem.

Still, there are many difficulties when applying VQAs. Barren plateaus are a common occurrence, making the optimisation futile. The choosing of the ansatz determines the performance and feasibility of the algorithms, and there are many strategies and options. Some rely on exploiting the specific quantum hardware's properties, while some use the specifics of the problem at hand. Finally, the inherent noise and errors on near-term hardware will still be a problem and limit circuit depths.

1.1.2 Moll et al. (2018)

The computational performance of quantum computers is decided by five main factors. Naturally, the total qubit count is important, but also their connectivity (if they are not connected, intermediate operations like swapping is needed). How many gates/operations can be used before decoherence, noise and errors ruins the result also determines what programmes are feasible. Furthermore, which physical gates are available also matters, as transpiling to native gates will increase the circuit depth. Lastly, the degree of gate parallelisation can allow for shallower circuits and increased performance.

With all these factors in mind, the metric of quantum volume is defined, giving a single number describing the performance. It is effectively defined as the largest rectangular circuit of two-qubits a quantum computer may execute.

1.1.3 Torlai et al. (2020)

Due to the probabilistic nature of quantum computers and their exponentially great number of states, measuring complex observables accurately requires many samples. By post-processing the measurements using an artificial neural network, the variance of the samples are significantly reduced, though at the cost of some increased bias.

1.1.4 Schuld et al. (2019)

In optimising the parameters of variational circuits, having access to the gradient of the cost function (with respect to the parameters) is beneficial. The individual measurements are probabilistic, but the expectation is a deterministic value whose gradient can be calculated. Often, this is possible exactly using the parameter shift rule, allowing for evaluating the gradient using the same circuit with changed parameters. For circuits containing gates whose derivatives are not as nice, a method of linear combination of unities can be used. This method requires an extended circuit including an ancillary qubit.

1.1.5 Pesah et al. (2021)

The problem of barren plateaus plagues the optimisation of variational circuits and quantum neural network; for randomly initialised ansätze, the gradient of the cost function may exhibit exponentially small gradients, prohibiting gradient based optimisation. Under certain assumptions, it is shown that for quantum convolutional neural networks, the gradient of the cost function is no worse than polynomially small, such that the networks can be trainable.

1.1.6 Farhi et al. (2018)

Quantum neural networks (QNNs) are simply an abstraction of parametrised quantum circuits with some sort of data encoding. As with classical neural networks or supervised learning in general, the parameters are optimised by minimising a cost function. For QNNs, the output can be a single designated read-out qubit, where the states are interpreted as classes in a binary classification problem. This was shown to indeed be feasible for handwritten digit recognition, using downsampled MNIST data. With the qubit count on current quantum devices and the

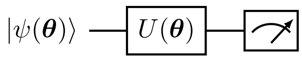

Figure 1.1: Test figure.

amount that can be easily simulated, the dimensionality of the data can not be much more than a dozen.

1.1.7 Abbas et al. (2021)

Whether quantum neural networks have inherent advantages is still an open question. Using the Fisher information of models, the authors calculate the effective dimension as a measure of expressibility. For models comparable in their input, output and parameter count, the effective dimension of particular quantum neural networks can be significantly higher. This advantage is empirically shown to be useful with a particular model on real quantum hardware, showing convergence in fewer steps than a similarly specced classical network.

The importance of feature maps is remarked upon, affecting both the expressibility of the model and the risk of barren plateaus, which in turn determines trainability.

1.2 Quantikz

Admire fig. 1.1. It is a quantum circuit. It is drawn using the package `quantikz`.

Chapter 2

Machine learning

2.1 Introduction

2.2 Neural networks

2.2.1 Universal approximation theorem

Chapter 3

Quantum computing

3.1 The qubit

3.2 Quantum circuits

3.3 Limitations of NISQ hardware

3.4 Variational quantum algorithms

Chapter 4

Quantum machine learning

4.1 Data encoding

4.2 Quantum neural networks

4.2.1 QNN versus NN

Using the same data, model structure and optimiser as in [1], measuring instead performance using 10-fold cross validation, the quantum neural networks clearly outperform the classical. The mean accuracy during training is shown in fig. 4.1. For simulation of noise, the 27-qubit IBM Montreal architecture was chosen, as it was the actual hardware used in [1] The model with noise was only trained for ten epochs, due to the significant time required for the noisy simulation, but the results show that noise did not have a significant impact on the performance. While the QNNs always reached perfect accuracy, the classical NN occasionally got stuck in local minima, always predicting one of the classes.

4.2.2 Quantum convolutional neural networks

Testing a QCNN on synthetic data shown in fig. 4.2; classify pictures as either horizontal or vertical lines. The model without errors achieve 100% accuracy on both training and test data, while the noisy model only managed around 90% accuracy on the training data and 80% on test data. The loss function of the noisy and exact model during training is shown in fig. 4.3.

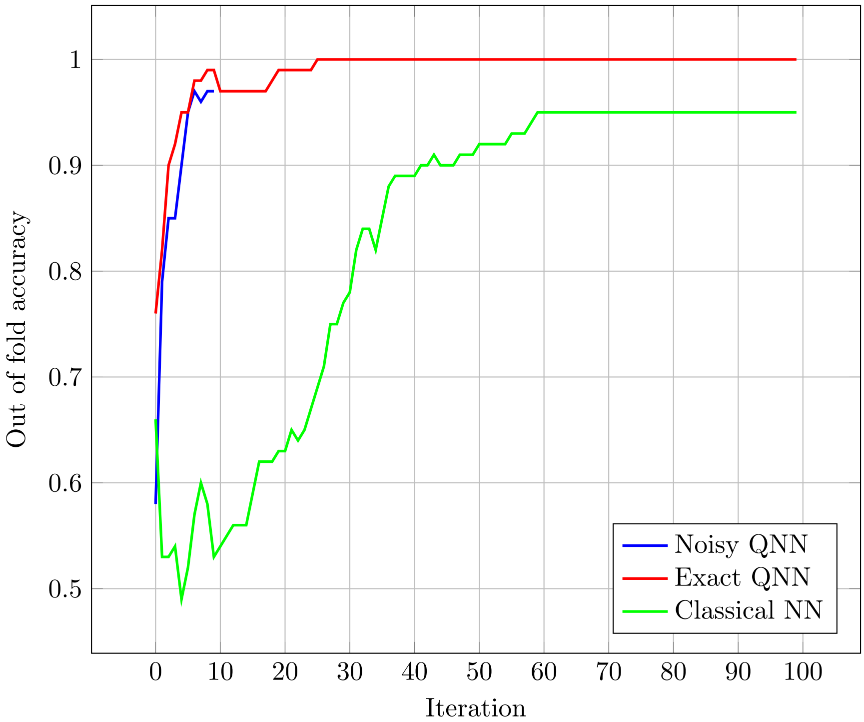

Figure 4.1: Mean accuracy during training for the Iris dataset using 10-fold cross validation.

Figure 4.2: Synthetic data for the QCNN.

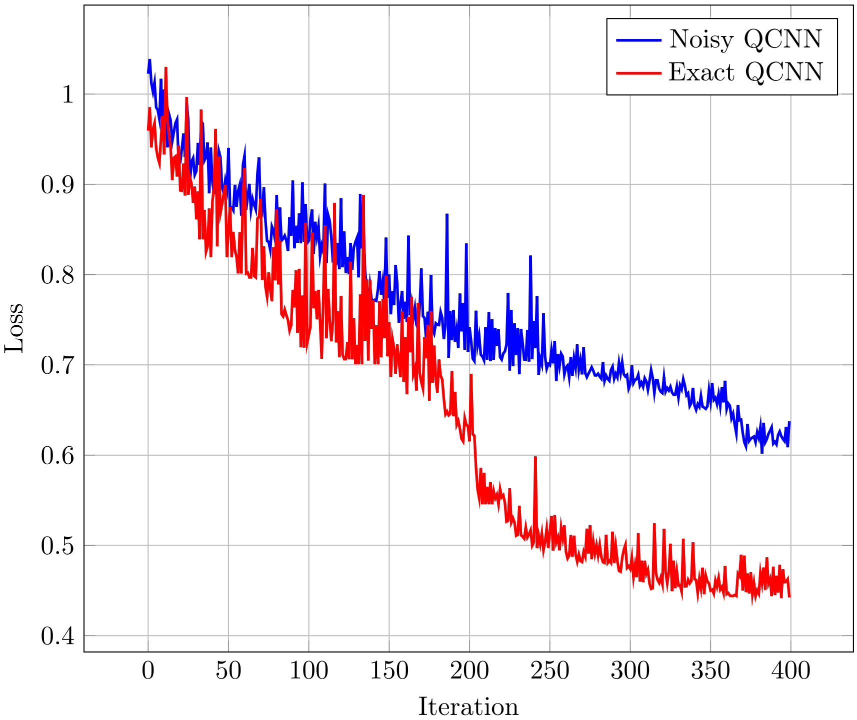

Figure 4.3: Loss function of QCNN model during training with both exact simulations and noisy.

Chapter 5

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