QOC: Quantum On-Chip Training with Parameter Shift and Gradient Pruning

1Hanrui Wang*, 2Zirui Li*, 3Jiaqi Gu, 4Yongshan Ding, 3David Z. Pan, 1Song Han
1Massachusetts Institute of Technology, 2Shanghai Jiao Tong University, 3University of Taxes at Austin, 4Yale University

https://qmlays.mit.edu

ABSTRACT

Parameterized Quantum Circuits (PQC) are drawing increasing research interest thanks to its potential to achieve quantum advantages on near-term Noisy Intermediate Scale Quantum (NISQ) hardware. In order to achieve scalable PQC learning, the training process needs to be offloaded to real quantum machines instead of using exponential-cost classical simulators. One common approach to obtain PQC gradients is parameter shift whose cost scales linearly with the number of qubits. We present QOC, the first experimental demonstration of practical on-chip PQC training with parameter shift. Nevertheless, we find that due to the significant quantum errors (noises) on real machines, gradients obtained from naive parameter shift have low fidelity and thus degrading the training accuracy. To this end, we further propose probabilistic gradient pruning to firstly identify gradients with potential large errors and then remove them. Specifically, small gradients have larger relative errors than large ones, thus having a higher probability to be pruned. We perform extensive experiments with the Quantum Neural Network (QNN) benchmarks on 5 classification tasks using 5 real quantum machines. The results demonstrate that our on-chip training achieves over 90% and 60% accuracy for 2-class and 4-class image classification tasks. The probabilistic gradient pruning brings up to 7% PQC accuracy improvements over no pruning. Overall, we successfully obtain similar on-chip training accuracy compared with noise-free simulation but have much better training scalability. The QOC code is available in the TorchQuantum library.

1 INTRODUCTION

Quantum Computing (QC) has great potential to achieve exponential acceleration over classical computers, which represents a computational paradigm shift in various domains. Parameterized Quantum Circuits (PQC) are circuits containing trainable weights and are promising to achieve quantum advantages in current devices. Among them, Quantum Neural Network (QNN) is one of the popular algorithms for machine learning tasks.

In order to achieve PQC quantum advantage, the number of qubit needs to be large enough, which casts great difficulty in the parameter training process. In existing PQC work [4, 11], the primary focus has been building quantum models that can outperform classical model accuracy. Thus they typically perform training on classical computers through software simulations and then perform inference with simulators as well (Figure 1 top). Although classical simulation is useful in understanding the capabilities of small-size PQC, it is not scalable due to the exponentially increased time and memory costs (O(2^n), n is the qubit number). As shown in Figure 2(a), the space (#Regs) and time (#Ops) complexity of classical simulation grow exponentially as the number of qubits increases. To the authors’ knowledge, this is the first experimental demonstration of efficient and scalable PQC on-chip training protocol. The optimization of parameterized quantum gates is offloaded to the quantum chips with in-situ gradient computation using parameter shift [14]. We also perform PQC evaluation on real quantum machines, making the results more practical as in Figure 1 bottom.

One of the major challenges to enable scalable and efficient PQC on-chip learning is the robustness against quantum noise. In the current Noisy Intermediate Scale Quantum (NISQ) [16] era, the gate error rates on real quantum devices are non-negligible (10^{-3} to 10^{-2}). In the context of PQC, such errors will lead to noisy gradients which can slow down convergence or even make training unstable. As shown in Figure 2(b), large gaps exist between the quantum on-chip training results and the classical noise-free simulation results.

By carefully investigating the on-chip training process, we observe that small gradients tend to have large relative variations or even wrong directions under quantum noises, as shown in Figure 2(c). Among them, we find that due to the significant quantum errors (noises) on real machines, gradients obtained from naive parameter shift have low fidelity and thus degrading the training accuracy. To this end, we further propose probabilistic gradient pruning to firstly identify gradients with potential large errors and then remove them. Specifically, small gradients have larger relative errors than large ones, thus having a higher probability to be pruned. We perform extensive experiments with the Quantum Neural Network (QNN) benchmarks on 5 classification tasks using 5 real quantum machines. The results demonstrate that our on-chip training achieves over 90% and 60% accuracy for 2-class and 4-class image classification tasks. The probabilistic gradient pruning brings up to 7% PQC accuracy improvements over no pruning. Overall, we successfully obtain similar on-chip training accuracy compared with noise-free simulation but have much better training scalability. The QOC code is available in the TorchQuantum library.

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We are the first work to demonstrate the practicality of parameter shift on NISQ machines, achieving high PQC learning accuracy.

3.1 Parameter Shift Rule for Quantum Gradients

Parameter shift rule states that we can calculate the gradient of each parameter in some quantum circuits by simply shifting the parameter twice and calculating the difference between two outputs, without changing the structure of circuits or using any ancilla qubits. Prior works elaborate it based on quantum circuit function [2], however, in the next subsection we will show how parameter shift rules combined with backpropagation can be used in a real PQC task. Suppose an $m$-qubit quantum circuit is parametrized by $n$ parameters $\theta = (\theta_1, \ldots, \theta_n)$, the expectation value of measurements of this circuit can be represented by a circuit function,

$$f(\theta) = \langle \psi(\mathcal{U}(\theta_1) \cdots \mathcal{U}(\theta_n) | \psi) \rangle$$

where $\mathcal{U}(\theta_i)$ is the gate where $\theta_i$ is the parameter whose gradient is to be calculated, and $\mathcal{U}$ is the gate that $\theta_i$ lies in. Here, for notation simplicity, we have already absorbed the unitaries before $\mathcal{U}(\theta_i)$ into $\hat{Q}$. Usually, the

Quantum noise. In real quantum computer systems, errors (noises) would occur due to unwanted interactions between qubits, imperfect control signals, or interference from the environment [6]. For example, quantum gates introduce operation errors (e.g., coherent errors and stochastic errors) into the system, and qubits also suffer from decoherence error (spontaneous loss of its stored information) over time. These noisy systems need to be characterized [13] and calibrated [7] frequently to mitigate the noise impact.

Quantum neural networks. Quantum Machine Learning (QML) [1, 9, 17, 18, 21] aims to leverage QC techniques to solve machine learning tasks and achieve much higher efficiency. The path to quantum advantage on QML is typically provided by the quantum circuit’s ability to generate and estimate highly complex kernels [5], which would otherwise be intractable to compute with conventional computers. They have been shown to have potential speed-up over classical counterparts in various tasks, including metric learning [12], data analysis [10]. As shown in Figure 3, the quantum neural network is one type of QML model using variational quantum circuits with trainable parameters to accomplish feature encoding of input data and perform complex-valued linear transformations thereafter. Most of QNN trainings are exploratory and rely on classical simulation of small quantum systems. In our work, on the contrary, we explore the practical setting: the QNN training and inference are both performed on real quantum devices.

Pruning. Pruning techniques are widely used in the field of DNN [3, 19, 20, 23], performing an important role of the trade-off between accuracy and memory or time cost [15]. Recently, pruning techniques have been used in quantum tasks. Pruning the ansatz can bring time-efficient circuit and even higher performance on real QC [17]. In our work, we apply pruning techniques to prune unreliable gradients in order to mitigate the noise during training.
Negative shift

Then the gradient of the loss function with respect to \( \theta \) is the Hermitian generator of matrix with only 2 unique eigenvalues +1 and -1.

Firstly, the RX gate is,

\[
R_X(\alpha) = e^{-\frac{i}{2} \alpha X} = \sum_{k=0}^{\infty} (-i\alpha/2)^k X^k/k!
\]

and

\[
R_X(\alpha) = e^{-\frac{i}{2} \alpha X} = \sum_{k=0}^{\infty} (-i\alpha/2)^k X^k/k! = \sum_{k=0}^{\infty} (-1)^k (\alpha/2)^k X^k/(2k+1)!
\]

where \( \alpha \) is the Pauli-X matrix.

As \( f(\theta) = \langle \psi | R_X(\alpha) | \psi \rangle \), we have

\[
\frac{\partial f(\theta)}{\partial \theta} = \langle \psi | R_X(\alpha) | \psi \rangle \gamma X R_X(\alpha) = \frac{i}{2} X R_X(\alpha)
\]

and

\[
\frac{\partial f(\theta)}{\partial \theta} = \left( \langle \psi | R_X(\alpha) | \psi \rangle - \frac{i}{2} X R_X(\alpha) \right) \gamma X R_X(\alpha)
\]

where \( \gamma = \frac{\alpha}{2} \).

In the second part, we run the circuit without shift and get the measurement result \( f(\theta) \). Then we apply Eq. 2 to obtain the Jacobian via parameter shift.

\[
J = \{ \frac{\partial f(\theta)}{\partial \theta} \}
\]

Finally, we obtain the Jacobian matrix \( \frac{\partial f(\theta)}{\partial \theta} \).

**Down-stream gradient backpropagation.** In the third part, we calculate the dot-product between down-stream gradients and the Jacobian and get the final gradients

\[
\frac{\partial f(\theta)}{\partial \theta} = \left( \frac{\partial f(\theta)}{\partial \theta} \right) \gamma X R_X(\alpha)
\]

Without loss of generality, the derivation holds for all units of the form \( e^{-\frac{i}{2} \theta H} \), e.g., RX, RY, RZ, XX, YY, ZZ, where \( H \) is a Hermitian matrix with only 2 unique eigenvalues +1 and -1.

In our circuit functions, we assume each parameter lies in exactly one gate. However, there are cases that one parameter lies in multiple gates. In that case, we only need to calculate the gradient of the parameter in those gates separately and sum the gradients up to get the gradient of that parameter.

3.3 In-situ Gradient Computation on Real QC

To realize PQC on-chip learning, we implement a TrainingEngine, described in Alg. 1. This TrainingEngine contains three parts.

**Jacobian calculation via parameter shift.** In the first part, we sample a mini-batch of training data \( I \) in Line 6. For each example of the mini-batch, we set up the quantum encoder gates and then iteratively evaluate gradients for all parameters. In each iteration, we shift the parameter \( \theta \) twice by \( +\pi/2 \) and \(-\pi/2 \) respectively. After each shift, we execute the shifted circuit on quantum hardware. The circuit will be created, validated, queued, and finally run on real quantum machines. As soon as we get the returned results of the two shifted circuits, i.e., \( f(\theta) \) and \( f(\theta, \ldots) \), we apply Eq. 2 to obtain the Jacobian matrix \( \frac{\partial f(\theta)}{\partial \theta} \). In the left part of Figure 4.

Finally, we get the training loss \( L(\theta) \). Then we run backpropagation only from the loss to the logits to get the down-stream gradients \( \frac{\partial f(\theta)}{\partial \theta} \) shown in the right part of Figure 4.

**Gradient calculation.** In the third part, we calculate the dot-product between down-stream gradients and the Jacobian and get the final gradients

\[
\frac{\partial f(\theta)}{\partial \theta} = \left( \frac{\partial f(\theta)}{\partial \theta} \right) \gamma X R_X(\alpha)
\]

3.3 Probabilistic Quantum Gradient Pruning

On quantum chips, there exist various noises and errors that could potentially diminish the fidelity of the computation results. When the gradient magnitude is small, noises could easily overwhelm the signals, such that the gradients calculated on real quantum circuit become unreliable when they have small magnitude. Those unreliable gradients have harmful effects on training convergence. Skipping the evaluation on those unreliable gradients can benefit both training convergence and efficiency. Besides, we observe that for most parameters, if the gradient magnitudes are far from zero for several
steps, it will likely keep far from zero in the next several steps. Similarly, if the gradient magnitude remains small for some steps, it will likely keep small in the next several steps. This means the gradient reliability is predictable to some extent. Therefore, we propose the gradient pruning method to sample the parameters whose gradients are more reliable. This method helps training converge faster while also saving time by skipping the evaluation of unreliable gradients.

Alg. 1 describes the PQC on-chip training flow with probabilistic gradient pruning. We divide all the training steps into 5 stages and perform the pruning method periodically on each stage. For every stage, we split it into two phases, shown in Figure 5. The first phase is called magnitude accumulation with an accumulation window width $w_a$, and the second is called probabilistic gradient pruning (PGP) with a pruning window width $w_p$. We only apply pruning in the second phase, while the parameter subset is sampled from a probability distribution $\tilde{\theta} = \{\theta_i \sim P_M(\theta)\}_{1 \leq i \leq (1-r)n}$ based on the gradient information collected within the accumulation window.

In Lines 4-9, within the accumulation window, we record the magnitude of gradients of each parameter in each step and accumulate them until the window is over. At the end of the first phase, we can get an accumulator $M$ that records the accumulated gradient magnitude for each parameter. Thus, when the pruning phase starts, we normalize the accumulated gradient magnitude and pass it to our sampler as the sampling distribution. In each pruning step, the sampler samples a subset of parameters $\tilde{\theta}$ with a pruning ratio of $r$, and we only evaluate gradients for them while the rest $\theta / \tilde{\theta}$ is temporarily frozen.

There are three important hyper-parameters in our gradient pruning method: 1) accumulation window width $w_a$, 2) pruning ratio $r$, and 3) pruning window width $w_p$. The accumulation window width and pruning window width decide the reliability of the gradient trend evaluation and our confidence in it, respectively. The pruning ratio can be tuned to balance the gradient variances caused by noise perturbation and pruning. Thus, the percentage of the time saved by our probabilistic gradient pruning method is $r \frac{w_p}{w_a+w_p} \times 100\%$. In our experiments, we find that the setting ($w_a=1, w_p=2-3, r=0.3-0.5$) usually works well in all cases.

4 EXPERIMENTS

In this section, we deploy our PQC on-chip learning framework on real QC and evaluate it on 5 QNN tasks for image and voice recognition. Compared with classical QNN training protocols, we can achieve 2-4% real QC test accuracy improvement with 2× convergence speedup. We also conduct extensive ablation studies to validate our scalability and the effectiveness of the proposed probabilistic gradient pruning method.

4.1 Experiment Setups

Benchmarks. We conduct our experiments on 5 QML tasks. QML are all classification tasks including MNIST [8] 4-class (0, 1, 2, 3), 2-class (3 and 6); Fashion [22] 4-class (t-shirt/top, trouser, pullover, dress), 2-class (dress and shirt); Vowel 4-class(hid, hld, had, hOd). MNIST and Fashion 2-class use the front 500 images as the training set and randomly sampled 300 images as the validation set. MNIST, Fashion 4-class uses the front 100 images as the training set and also randomly sampled 300 images as the validation set. The input images are all $28 \times 28$. We firstly center-crop them to $24 \times 24$ and
then down-sample them to 4 × 4 for MNIST and Fashion 2 and 4-class tasks. Vowel 4-class uses the front 100 samples as the training set and randomly sampled 300 samples as the validation set. For each sample, we perform principal component analysis (PCA) for the vowel features and take the 10 most significant dimensions.

All the tasks use four logical qubits. To embed classical image and vowel features to the quantum states, we first flatten them and then encode them with rotation gates. For down-sampled 4 × 4 images, we use 4RY, 4RZ, 4RX, and 4RY gates as the encoder. We put the 16 classical input values to the phases of 16 rotation gates, respectively. Therefore we can encode the classical values to quantum states. For 10 vowel features, we use 4RY, 4RZ, and 2RX gates for encoding. The encoding gates are our hand-designed circuits. Our circuits are composed of several layers. There are 7 kinds of layers used to construct our circuits. (i) RX layer: Add RX gates to all wires; (ii) RY layer: same structure as in RX layer; (iii) RZ layer: same structure as in RX layer; (iv) RZZ layer: add RZZ gates to all logical adjacent wires and the logical farthest wires to form a ring connection, for example, an RZZ layer in a 4-qubit circuit contains 4 RZZ gates which lie on wires 1, 2, 2, 3, 2, 3, 4, 4, 4, 4, and 1; (v) RXX layer: same structure as in RZZ layer; (vi) RZX layer: same structure as in RZZ layer; (vii) CZ layer: add CZ gates to all logical adjacent wires.

For MNIST and Fashion 2-class tasks, the circuit contains 1 RZZ layer followed by 1 RY layer. For MNIST 4-class task, the circuit contains 3 RX+RY+RZ+CZ layers (1 RX layer, 1 RY layer, 1 RZ layer, and 1 CZ layer in series). For Fashion 4-class task, the circuit contains 3 RZZ+RY layers (1 RZZ layer followed by 1 RY layer). For Vowel 4-class task, the circuit contains 2 RZZ+RXY layers (1 RZZ layer followed by 1 RXY layer).

For the output of our quantum circuits, we measure the expectation values on Pauli-Z basis and obtain a value [-1, 1] from each qubit. For 2-class, we sum the qubit 0 and 1, 2, and 3 respectively to get 2 output values. For 4-class, we just use the four expectation values as 4 output values. Then we process the output values by Softmax to get probabilities.

**Quantum devices and compiler configurations.** We use IBM quantum computers via qiskit API [7] to submit our circuits to real superconducting quantum devices and achieve quantum on-chip training. We set all the circuits to run 1024 shots.
size, \( w_a = 1 \) or 2 are suitable choices. When \( w_a \) is too large, the accumulated gradient magnitudes are similar among all parameters, leading to a nearly uniform sampling distribution. This will bring undifferentiated pruning, and the accuracy will drop as the Fashion-4 curve shows. The pruning window \( w_a \) should also not be too large. As \( w_p \) grows, the accumulated gradient magnitudes used to instruct our pruning become less reliable.

**Discussion on scalability.** Figure 8 shows the superior scalability of quantum on-chip training. Classical simulation runtime exponentially increases as \( q \)-qubits scales up, while the runtime on real quantum machines scales nearly linearly to \( q \)-qubits. The classical curve in Figure 8 represents runtime and memory cost of running 50 circuits of different \( q \)-qubits with 16 rotation gates and 32 RZZ gates. The curve before 22 qubits is measured on a single NVIDIA RTX 2080 Ti GPU; points after 24 qubits are extrapolated. The quantum curve before 27 qubits is tested on ibmq_toronto; the points after 30 qubits are extrapolated.

We can observe clear quantum advantages on circuits with more than 27 qubits. In terms of memory cost, classical simulation consumes thousands of Gigabits for storage which is intractable. In contrast, on quantum machines, the information is stored in the quantum state of the circuit itself with negligible memory cost.

**Probabilistic vs. deterministic gradient pruning.** Our pruning is decided by a random sampler based on the accumulated gradient magnitude. We call this probabilistic pruning. If the sampler only samples the parameters with the biggest accumulated gradient magnitude, this is called deterministic pruning. We adopt probabilistic pruning instead of deterministic pruning because deterministic pruning limits the degree of freedom and increases the gradient sampling bias. Table 2 shows that deterministic pruning has 1%-7% accuracy loss compared with probabilistic pruning.

**Different optimizers.** Table 3 shows the accuracy tested on classical devices trained with different optimizers. The learning rate is controlled by a cosine scheduler from 0.3 in the beginning to 0.03 in the end. We test SGD, SGD with a momentum factor of 0.8, and Adam on MNIST-4, MNIST-2, Fashion-4, and Fashion-2, and found that Adam always performs the best. Hence, all the experiments are done using Adam optimizers by default.

### 5 Conclusion

In this work, for the first time, we present an efficient and robust on-chip training framework for PQC and demonstrate its effectiveness on real quantum devices. By leveraging parameter shift, we can calculate the exact quantum gradients directly on quantum machines, thus achieving high scalability. To alleviate the negative impact of quantum noises on gradients, we further propose the probabilistic gradient pruning technique to avoid updating parameters with unreliable gradients. Experimental results on 5 classification tasks and 5 machines demonstrate that QOC achieves comparable accuracy with noise-free simulations. We hope QOC can open an avenue towards practical training of large PQC models for quantum advantage.

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### REFERENCES


