RobustQNN: Noise-Aware Training for Robust Quantum Neural Networks

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ABSTRACT
Quantum Neural Network (QNN) is a promising application towards quantum advantage on near-term quantum hardware. However, due to the large quantum noises (errors), the performance of QNN models has a severe degradation on real quantum devices. For example, the accuracy gap between noise-free simulation and noisy results on IBMQ-Yorktown for MNIST-4 classification is over 60%. Existing noise mitigation methods are general ones without leveraging unique characteristics of QNN and are only applicable to inference; on the other hand, existing QNN work does not consider noise effect. To this end, we present RobustQNN, a QNN-specific framework to perform noise-aware optimizations in both training and inference stages to improve robustness. We experimentally observe that the effect of quantum noise to QNN measurement outcome is a linear map from noise-free outcome with a scaling and a shift factor. Motivated by that, we propose post-measurement normalization to mitigate the feature distribution differences between noise-free and noisy scenarios. Furthermore, to improve the robustness against noise, we propose noise injection to the training process by inserting quantum error gates to QNN according to realistic noise models of quantum hardware. Finally, post-measurement quantization is introduced to quantize the measurement outcomes to discrete values, achieving the denoising effect. Extensive experiments on 8 classification tasks using 6 quantum devices demonstrate that RobustQNN improves accuracy by up to 43%, and achieves over 94% 2-class, 80% 4-class, and 34% 10-class classification accuracy measured on real quantum computers. The code for construction and noise-aware training of QNN is available in the TorchQuantum library.

1 INTRODUCTION
Quantum Computing (QC) is a new computational paradigm that can be exponentially faster than classical counterparts in various domains such as cryptography and database search. Among various Quantum Machine Learning approaches, Quantum Neural Network (QNN) is a popular candidate in which a network of parameterized quantum gates are constructed and trained to embed data and perform certain ML tasks on a quantum computer, similar to the training and inference of classical neural networks.

Currently we are in the Noisy Intermediate Scale Quantum (NISQ) stage, in which quantum operations suffer from a high error rate of $10^{-2}$ to $10^{-3}$, much higher than CPUs/GPUs ($10^{-6}$ FT). The quantum errors unfortunately introduces detrimental influence on QNN accuracy. Figure 1 shows the single-qubit gate error rates and the measured accuracy of classification tasks on different hardware.

Three key observations are: (1) Quantum error rates ($10^{-3}$) are much larger than classical CMOS devices’ error rates ($10^{-10}$ failure per 10^9 device hours). (2) Accuracy on real hardware is significantly degraded (up to 64%) compared with noise-free simulation. (3) The same QNN on different hardware has distinct accuracy due to different gate error rates. IBMQ-Yorktown has a five times larger error rate than IBMQ-Santiago, and higher error causes lower accuracy.

Researchers have proposed noise mitigation techniques [25, 33] to reduce the noise impact. However, they are general methods without considering the unique characteristics of QNN, and can only be applied to QNN inference stage. On the other hand, existing QNN work [6, 12] does not consider the noise impact. This paper proposes a QNN-specific noise mitigation framework called RobustQNN that optimizes QNN robustness in both training and inference stages, boosts the intrinsic robustness of QNN parameters, and improves accuracy on real quantum machines.

RobustQNN comprises a three-stage pipeline. The first step, post-measurement normalization normalizes the measurement outcomes on each quantum bit (qubit) across data samples, thus removing the quantum error-induced distribution shift. Furthermore, we inject noise to the QNN training process by performing error gate insertion. The error gate types and probabilities are obtained from hardware-specific realistic quantum noise models provided by QC vendors. During training, we iteratively sample error gates, insert them to QNN, and updates weights. Finally, post-measurement quantization is further proposed to reduce the precision of measurement outcomes from each qubit and achieve a denoising effect.

Table 2

| Noise-Free Simulation | IBMQ-Yorktown | Lima | Santiago |
|-----------------------|---------------|------|----------|
| MNIST-4               |               |      |          |
| Accuracy              | 0.8666666667  | 0.23 | 0.5566666667 |
| Error Rate            | 2.03E-04      | 2.03E-04 | 1.11E-03 |
| Failure               | 0.14          | 0.31 | 0.64 |

Figure 1: Left: Current quantum hardware has much larger error rates ($10^{-3}$) than classical CPUs/GPUs. Right: Due to the errors, QNN models suffer from severe accuracy drops. Different devices have various error magnitudes, leading to distinct accuracy. These motivate RobustQNN, a hardware-specific noise-aware QNN training approach to improve robustness and accuracy.
The contributions of RobustQNN are as follows:

- We propose a systematic approach to mitigate the real QC noise impact on QNN accuracy, containing three techniques: post-measurement normalization matches the measurement distribution between noise-free and real QC processing; noise injection improves intrinsic noise-resilience of QNN parameters; post-measurement quantization reduces data precision and denoises the quantum error impacts.
- Extensive experiments on 8 ML tasks with 5 different design spaces on 6 quantum devices show that RobustQNN can improve accuracy by up to 42%, 43%, 23% for 2-class, 4-class and 10-class classification tasks and successfully demonstrates over 94%, 80% and 34% accuracy for 2-, 4-, and 10-classifications on real quantum hardware.
- The code for construction and noise-aware training of QNN is available at the TorchQuantum library. It is an easy-to-use infrastructure to query noise models from QC providers such as IBMQ, extract noise information, perform training on CPU/GPU and finally deploy on real QC.

3 NOISE-AWARE QNN TRAINING

Figure 2 shows the QNN architecture. The inputs are classical data such as image pixels, and the outputs are classification results. The QNN consists of multiple blocks. Each has three components: encoder encodes the classical values to quantum states with rotation gates such as \( R_y \); trainable quantum layers contain parameterized gates that can be trained to perform certain ML tasks; measurement outcomes of one block are passed to the next block. For the MNIST-4 example in Figure 2, the first encoder takes the pixels of a 4 image as rotation angles of 16 rotation gates.

Figure 2: Quantum Neural Networks Architecture. QNN has multiple blocks, each has an encoder to encode classical values to quantum domain, quantum layers with trainable weights, and a measurement layer that obtains classical values.
Theorem 3.1. (informal version). The measurement outcome $y$ of a quantum neural network for the training input data $x$ is transformed by the quantum noise that the system undergoes with a linear map $f(y_x) = y_y + \beta_x$, where the translation $\beta_x$ depends on the input $x$ and quantum noises, while scaling factor $y$ is input independent.

We refer to Appendix Section A.2.2 for background and a complete proof. The main theoretical contribution of this theorem equips our proposed normalization methodology with robustness guarantees. Most importantly, we observe that the changes in measurement results can often be compensated by proper post-measurement normalization across input batches. For simplicity, we restrict our analysis on $Z$-basis single-qubit measurement outcome $y$. Similar analytical results for multi-qubit general-basis measurement will follow if we apply the same analysis qubit by qubit. Theorem 3.1 is most powerful when applied on a small batch of input data $x = \{x_1, \ldots, x_m\}$ where each $x_i$ is a set of classical input values for the encoder of the QNN and $m$ is the size of the batch. In an ideal noiseless scenario, the QNN model outputs measurement result $y_i$ for each input $x_i$. For a noisy QNN, the measurement result undergoes a composition of two transformations: (1) a constant scaling by $\gamma$; (2) an input-specific shift by $\beta_i$, i.e., $f(y) = \gamma y + \beta_i$. In the realistic noise regime, the scaling constant $\gamma \in [-1, 1]$. However, for small noises, $\gamma$ is close to 1, and $\beta_i$ is close to 0. Therefore, the distribution of noisy measurement outcomes undergoes a constant scaling by $\gamma \leq 1$ and a small shift by each $\beta_i$. In the small-batch regime when $\beta = \{\beta_1, \ldots, \beta_m\}$ has small variance, the distribution is shifted by its mean $\beta = E[\beta]$. Thus $f(y_i) \approx \gamma y_i + \beta$.

Post-measurement normalization. Based on the analysis above, we propose post-measurement normalization to offset the distribution scaling and shift. For each qubit, we collect its measurement results on a batch of input samples, compute their mean and std., then make the distribution of each qubit across the batch zero-centered and of unit variance. This is performed during both training and inference. During training, for a batch of measurement results: $y = \{y_1, \ldots, y_m\}$, the normalized results are $\hat{y}_i = (y_i - E[y]) / \sqrt{\text{Var}(y)}$. For noisy inference, we correct the error as $f(\hat{y}_i) = (f(y_i) - E[f(y_i)]) / \sqrt{\text{Var}(f(y_i))} = ((\gamma y_i + \beta) - (\gamma E[y] + \beta)) / \sqrt{\gamma^2 \text{Var}(y)} = \hat{y}_i$.

Figure 3 compares the noise-free measurement result distribution of 4 qubits (blue) with their noisy counterparts (yellow) for MNIST-F-4. Qualitatively, we can clearly observe that the post-measurement normalization reduces the mismatch between two distributions. Quantitatively, we adopt signal-to-noise ratio, $\text{SNR} = \|A\|^2 / \|A - \hat{A}\|^2$.

Figure 4: Post-measurement normalization reduces the distribution mismatch between noise-free simulation and noisy results on real hardware, thus improving the Signal-to-Noise Ratio (SNR).

3.2 Quantum Noise Injection

Although the normalization above mitigates error impacts, we can still observe small discrepancies on each individual measurement outcome, which degrade the accuracy. Therefore, to make the QNN model robust to those errors, we propose noise injection to the training process.

Quantum error gate insertion. As introduced in Section 2, different quantum errors can be approximated by Pauli errors via Pauli Twirling. The effect of Pauli errors is the random insertion of Pauli gates to the model with a probability distribution $E$. How to compute $E$ is out of the scope of this work. But fortunately, we can directly obtain it from the realistic device noise model provided by quantum hardware manufacturers such as IBMQ. The noise model specifies the probability $E$ for different gates on each qubit. For single-qubit gates, the error gates are inserted after the original gate. For two-qubit gates, error gates are inserted after the gate on one or both qubits. For example, the $\text{SX}$ gate on qubit 1 on IBMQ-Yorktown device has $E$ as $[X: 0.00096, Y: 0.00096, Z: 0.00096, \text{None}: 0.99712]$. When ‘None’ is sampled, we will not insert any gate. The same gate
Figure 5: Noise injection via error gate insertion. X, Y, Z are sampled Pauli error gates. R is the injected readout error. Probabilities for gate insertion are obtained from real device noise models.

Figure 6: Left: Error maps before and after post-measurement quantization. Most errors can be corrected. Right: 5-level quantization buckets with a quadratic penalty loss.

Errors Before Quantize
MSE=0.235, SNR=4.256
Errors After Quantize
MSE=0.167, SNR=6.455

Compiled Quantum Circuits
(Noise-free)
Sample Quantum
Gate Error
Readout
Error
ProbError Type
QC-backed
Noise Model
Sample ... Type
QC-backed
Noise Model
Compiled Quantum Circuits
(Noise-free)
Sample Quantum
Gate Error
Readout
Error
ProbError Type
QC-backed
Noise Model
Sample ... Type
QC-backed
Noise Model

Table 1: Noise injection results. MSE and SNR are used to compare the performance of different quantization schemes. The best results are highlighted in bold.

| Noise Model | MSE (Error) | SNR (Error) |
|-------------|-------------|-------------|
| QC-backed   | 0.167       | 6.455       |
| Noise Model | 0.235       | 4.256       |

3.3 Post-Measurement Quantization

Finally, we propose post-measurement quantization on the normalized results to further denoise the measurement outcomes. We first clip the outcomes to \( [p_{min}, p_{max}] \), where \( p \) are pre-defined thresholds, and then perform uniform quantization. The quantized values are later passed to the next block’s encoder. Figure 6 shows one real example from Fashion-4 on IBMQ-Santiago with five quantization levels and \( p_{min} = -2, p_{max} = 2 \). The left/middle matrices show the error maps between noise-free and noisy outcomes before/after quantization. Most errors can be corrected back to zero with few exceptions of being quantized to a wrong centroid. The MSE is reduced from 0.235 to 0.167, and the SNR is increased from 4.256 to 6.455. We also add a loss term \( \|y - Q(y)\|^2 \) to the training loss, as shown on the right side, to encourage outcomes to be near to the quantization centroids to improve error tolerance and reduce the chance of being quantized to a wrong centroid. Besides improving robustness, quantization also brings an additional benefit: the control complexity of rotation gates using those quantized values can be largely reduced.

4 EXPERIMENTS

4.1 Experiment Setup

Datasets. We conduct experiments on 8 classification tasks including MNIST [15] 10-class, 4-class (θ, 1, 2, 3), and 2-class (3, 6); Vowel [4] 4-class (hi, hiD, had, hoD); Fashion [34] 10-class, 4-class (t-shirt/top, trouser, pullover, dress), and 2-class (dress, shirt), and CIFAR [14] 2-class (frog, ship). MNIST, Fashion, and CIFAR use 95% images in ‘train’ split as training set and 5% as the validation set. Due to the limited real QC resources, we use the first 300 images of ‘test’ split as test set. Vowel-4 dataset (990 samples) is separated to train/validation:test = 6:1:3 and test with the whole test set. MNIST and Fashion images are center-cropped to 24 × 24; and then down-sample to 4×4 for 2- and 4-class, and 6×6 for 10-class; CIFAR images are converted to grayscale, center-cropped to 28×28, and down-sampled to 4×4. All down-samplings are performed with average pooling. For vowel-4, we perform feature principal component analysis (PCA) and take 10 most significant dimensions.

QNN models. QNN models for 2 and 4-class use 4 qubits; 10-class uses 10. The first quantum block’s encoder embeds images and features. For 4×4 images, we use 4 qubits and 4 layers with 4 RY, 4 RX, 4 RZ, and 4 RY gates in each layer, respectively. There are in total 16 gates to encode the 16 classical values as the rotation angles. For 6×6 images, 10 qubits and 4 layers are used with 10 RY, 10 RX, 10 RZ, and 6 RY gates in each layer, respectively. 10 vowel features, uses 4 qubits and 3 layers with 4 RY, 4 RX, and 2 RZ gates on each layer for encoding. For trainable quantum layers, we use U3 and CU3 layers interleaved as in Figure 2 except for Table 2. For measurement, we measure the expectation values on Pauli-Z basis and obtain a value [-1, 1] from each qubit. The measurement outcome goes through post-measurement normalization and quantization and is used as rotation angles for RY gates in the next block’s encoder.
After the last block, for two-classifications, we sum the qubit 0 and 1, 2 and 3 measurement outcomes, respectively, and use Softmax to get probabilities. For 4 and 10-class, Softmax is directly applied to measurement outcomes.

The number of parameters can be computed as $N_{\text{Block}} \times N_{\text{params_per_block}}$. For instance, for QNN using 4 qubits, 1 U3, and 1 CU3 layer in each block, since one U3 and CU3 gates both have 3 parameters, $N_{\text{params_per_block}} = 3 \times 4 \times 1 \times 2 = 24$. A model with 5 blocks has 120 parameters. We implement a library for construction and noise-aware training of QNN models in PyTorch [23], and all model training in this work is performed with it. For baselines and RobustQNN, we use Adam optimizer with a linear learning rate warm-up from 0 to 5e-3 in the first 30 epochs then cosine decay and weight decay $\lambda = 1e - 4$. We train 200 epochs with batch size 256 for image classification and 4 for vowel. For 4-qubit QNN models, the overall training time is typically less than 2 hours on an Nvidia TITAN RTX 2080 ti GPU machine.

**Quantum hardware and compiler configurations.** We use IBMQ quantum computers via Qiskit [9] APIs. We study 6 devices, with #qubits from 5 to 15 and Quantum Volume from 8 to 32. We also employ Qiskit for compilation. The optimization level is set to 2 for all experiments. All experiments run 8192 shots. The noise models we used are off-the-shelf ones updated by IBMQ team.

### 4.2 Main Results

**QNN results.** We experiment with four different QNN architectures on 8 tasks running on 5 quantum devices to demonstrate RobustQNN’s effectiveness. For each benchmark, we experiment with noise factor $T = \{0.1, 0.5, 1, 1.5\}$ and quantization level among [3, 4, 5, 6] and select one out of 16 combinations with the lowest loss on the validation set and test on the test set. Normalization and quantization are not applied to the last block’s measurement outcomes as they are directly used for classification. As in Table 1, RobustQNN consistently achieves the highest accuracy on 26 benchmarks. The third bars of Athens are unavailable due to its retirement. On average, normalization, noise injection and quantization improve accuracy by 10%, 9%, and 3%, respectively. A larger model does not necessarily have higher accuracy. For example, Athens’ QNN model is 7.5x larger than Yorktown with higher noise-free accuracy. However, because of more gate errors introduced by the larger model, the real accuracy is lower.

**Performance on different design spaces.** In Table 2, we evaluate RobustQNN on different QNN design spaces. Specifically, the trainable quantum layers in one block of ‘ZZ+RY’ [15] space contains one layer of ZZ gate, with ring connections, and one RY layer. ‘RXYZ’ [21] space has five layers: RX, RX, RY, RZ, and CZ. ‘ZX+XX’ [6] space has two layers: ZX and XX. ‘RXYZ+U1+CU3’ [8] space, according to their random circuit basis gate set, has 11 layers in the order of RX, S, CNOT, RY, T, SWAP, RZ, H, √SWAP, U1 and CU3. We conduct experiments on MNIST-4 and Fashion-2 on 2 devices. In 13 settings out of 16, RobustQNN achieves better accuracy. Thus, RobustQNN is a general technique agnostic to QNN model size and design space.

**Scalability.** When classical simulation is infeasible, we can move the noise-injected training to real QC using techniques such as parameter shift [3]. In this case, the training cost is linearly scaled with qubit number. Post-measurement normalization and quantization are also linearly scalable because they are performed on the measurement outcomes. Gradients obtained with real QC are naturally noise-aware because they are directly influenced by quantum noise. To demonstrate the practicality, we train a 2-class task with two numbers as input features [12] (Table 3). The QNN has 2 blocks; each with 2 RY and a CNOT gates. The noise-unaware baseline trains the model on classical part and test on real QC. In RobustQNN, we train the model with parameter shift and test, both on real QC. We consistently outperform noise-unaware baselines.

**Compatibility with existing noise mitigation.** RobustQNN is orthogonal to existing noise mitigation such as extrapolation method. It can be combined with post-measurement normalization (Table 4). The QNN model has 2 blocks, each with three U3+CU3 layers. For

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**Table 1: RobustQNN consistently achieves the highest accuracy, with on average 22% better. ’B’ for Block, ’L’ for Layer.**

| Model Method | MNIST-4 | Fash.-4 | Vow.-4 | MNIST-2 | Fash.-2 | Cifar-2 |
|--------------|---------|---------|--------|---------|---------|---------|
| Baseline     | 0.30    | 0.32    | 0.28   | 0.84    | 0.78    | 0.51    |
| 2B×2L        | 0.41    | 0.61    | 0.29   | 0.87    | 0.68    | 0.36    |
| 2B×2L + Post Norm. | 0.41    | 0.61    | 0.29   | 0.87    | 0.68    | 0.36    |
| 2B×2L + Gate Insert. | 0.61    | 0.70    | 0.44   | 0.93    | 0.86    | 0.57    |
| 2B×2L + Post Quant. | 0.68    | 0.75    | 0.48   | 0.94    | 0.88    | 0.59    |
| 2B×4L        | 0.57    | 0.60    | 0.38   | 0.86    | 0.72    | 0.56    |
| 2B×4L + Post Norm. | 0.57    | 0.60    | 0.38   | 0.86    | 0.72    | 0.56    |
| 2B×4L + Gate Insert. | 0.58    | 0.60    | 0.45   | 0.91    | 0.85    | 0.57    |
| 2B×4L + Post Quant. | 0.62    | 0.65    | 0.44   | 0.93    | 0.86    | 0.60    |
| 3B×10L       | 0.57    | 0.60    | 0.37   | 0.84    | 0.82    | 0.57    |
| 3B×10L + Post Norm. | 0.58    | 0.62    | 0.41   | 0.88    | 0.80    | 0.61    |
| 3B×10L + Gate Insert. | 0.59    | 0.64    | 0.41   | 0.87    | 0.64    | 0.53    |
| 3B×10L + Post Quant. | 0.66    | 0.64    | 0.41   | 0.87    | 0.64    | 0.53    |

**Table 2: Accuracy on different design spaces.**

| Design Space | MNIST-4 | Fashion-2 |
|--------------|---------|-----------|
| ‘ZZ+RY’      | 0.43    | 0.57      |
| ‘RY’         | 0.34    | 0.60      |
| ‘RX’         | 0.43    | 0.57      |
| ‘RY’         | 0.34    | 0.60      |
| ‘RX’         | 0.43    | 0.57      |
| ‘RY’         | 0.34    | 0.60      |
| ‘RX’         | 0.43    | 0.57      |
| ‘RY’         | 0.34    | 0.60      |

**Table 3: Scalable noise-aware training.**

| Machine | Bogota | Santiago | Lima |
|---------|--------|----------|------|
| Noise-unaware | 0.74 | 0.97 | 0.87 |
| RobustQNN | 0.79 | 0.99 | 0.90 |

**Table 4: Compatible with existing noise mitigation.**

| Method | MNIST-4 | Fashion-4 |
|--------|---------|-----------|
| Normalization only | 0.78 | 0.81 |
| Normalization + Extrapolation | 0.81 | 0.83 |
### 4.3 Ablation Studies

**Ablation on post-measurement normalization.** Table 5 compares the accuracy and signal-to-noise ratio (SNR) before and after post-measurement normalization on MNIST-4. We study 4 different QNN architectures and evaluate on 3 devices. The normalization can significantly and consistently increase SNR.

**Ablation on different noise injection methods.** Figure 7 compares different noise injection methods. Gaussian noise statistics for perturbations are obtained from error benchmarking. The left side shows accuracy without quantization. With different noise factors $\mathcal{T}$, the gate insertion and measurement outcome perturbation have similar accuracy, both better than rotation angle perturbation. A possible explanation is that the rotation angle perturbation does not consider non-rotation gates such as $\mathcal{T}$ and $\mathcal{X}$. The right side further investigates the first two methods' performance with quantization. We set noise factor $\mathcal{T} = 0.5$ and alter quantization levels. Gate insertion outperforms perturbation by 11% on average on 3 different devices and QNN models. The reason is: directly added perturbation on measurement outcomes can be easily canceled by quantization, and thus it is harder for noise injection to take effect.

**Noise factor and post-measurement quantization level analysis.** We visualize the QNN accuracy contours on Fashion-4 on IBMQ-Athens with different noise factors and quantization levels in Figure 8 left. The best accuracy occurs for factor 0.2 and 5 levels. Horizontal-wise, the accuracy first goes up and then goes down. This is because too few quantization levels hurt the QNN model capacity; too many levels cannot bring sufficient denoising effect. Vertical-wise, the accuracy also goes up and then down. Reason: when the noise is too small, the noise-injection effect is weak, thus cannot improve the model robustness; while too large noise makes the training process unstable and hurts accuracy.

**Visualization of QNN extracted features.** MNIST-2 classification result is determined by which feature is larger between the two: feature one is the sum of measurement outcomes of qubit 0 and 1; feature 2 is that of qubit 2 and 3. We visualize the two features obtained from experiments on Belem in a 2-D plane as in Figure 8 right. The blue dash line is the classification boundary. The circles/stars are samples of digit '3' and '6'. All the baseline points (yellow) huddled together, indicating a good classification performance.
together, and all digit ‘3’ samples are misclassified. With normalization (green), the distribution is significantly expanded, and the majority of ‘3’ is correctly classified. Finally, after noise injection (red), the margin between the two classes is further enlarged, and the samples are farther away from the classification boundary, thus becoming more robust.

**Breakdown of accuracy gain.** Figure 9 shows the performance of only applying noise-injection, only applying quantization, and both. Using two techniques individually can both improve accuracy by 9%. Combining two techniques delivers better performance with a 17% accuracy gain. This indicates the benefits of synergistically applying three techniques in RobustQNN.

**5 CONCLUSION**

QNN is a promising candidate to demonstrate practical quantum advantages over classical approaches. The road to such advantage relies on: (1) the discovery of novel feature embedding that encodes classical data non-linearly, and (2) overcome the impact of quantum noise. This work focuses on the latter and show that a noise-aware training pipeline with post-measurement normalization, noise injection, and post-measurement quantization can elevate the QNN robustness against arbitrary, realistic quantum noises. We anticipate such robust QNN being useful in exploring QML applications.

**A APPENDIX**

**A.1 Quantum Basics and Quantum Noise**

A quantum circuit uses quantum bit (qubit) to carry information, which is a linear combination of two basis state: \(|\psi\rangle = \alpha |0\rangle + \beta |1\rangle\), for \(\alpha, \beta \in \mathbb{C}\), satisfying \(|\alpha|^2 + |\beta|^2 = 1\). An \(n\)-qubit system can represent a linear combination of \(2^n\) basis states. A \(2^n\)-length complex state vector of all combination coefficients is used to describe the circuit state. In quantum computations, a sequence of quantum gates are applied to perform unitary transformation on the statevector, i.e., \(|\psi(x, \theta)\rangle = \cdots U_2(x, \theta_2)U_1(x, \theta_1) |0\rangle\), where \(x\) is the input data and \(\theta\) is the trainable parameters of rotation quantum gates. As such, the input data and trainable parameters are embedded in the quantum state \(|\psi(x, \theta)\rangle\). Finally, the computation results are obtained by qubit readout/measurement which measures the probability of a qubit state \(|\psi\rangle\) collapsing to either \(|0\rangle\) (i.e., output \(y = +1\)) or \(|1\rangle\) (i.e., output \(y = -1\)) according to \(|\alpha|^2\) and \(|\beta|^2\). With sufficient samples, we can compute the expectation value: \(E[y] = (+1)|\alpha|^2 + (-1)|\beta|^2\). By cascading multiple blocks of quantum gates and measurements, a non-linear network can be constructed to perform ML tasks.

In real quantum computer systems, errors would likely occur due to imperfect control signals, unwanted interactions between qubits, or interference from the environment [2, 13]. As a result, qubits undergo decoherence error (spontaneous loss of its stored information) over time, and quantum gates introduce operation errors (e.g., coherent errors and stochastic errors) into the system. These noisy systems need to be characterized [19] and calibrated [10] frequently to mitigate the impact of noise on computation. Noise modeling helps to paint a realistic picture of the behavior and performance of a quantum computer and enables noisy simulations [5]. While exact modeling and simulation is challenging, many approximate strategies [19, 26] have been developed based on Pauli/Clifford Twirling [22, 24].

**A.2 General Framework for Quantum Noise Analysis**

In this work, we examine how to characterize and mitigate the impact of quantum noises on quantum neural networks. We observe that the trainable quantum gates and post-measurement information processing play a huge role in boosting the algorithmic robustness to realistic quantum noises. In the following analysis, we restrict attention to: (1) a general (mixed) quantum state \(\rho(x, \theta)\) resulting from a QNN for input data \(x\) and trainable parameters \(\theta\), (2) single-qubit measurement output, and (3) any fixed but unknown quantum noise. For multi-qubit quantum neural networks, similar analysis follows when considered qubit by qubit.

**A.2.1 Measurement of Quantum Neural Networks.**

**Definition A.1.** (Measurement procedure). We measure a quantum state \(\rho\) in the computational basis \(|b\rangle : b \in \{0, 1\}\) and output \(z = +1\) if we obtain \(|0\rangle\) \(|0\rangle\) and \(z = -1\) if we obtain \(|1\rangle\) \(|1\rangle\). The expectation value of such measurement contains useful information about the quantum state \(\rho\):

\[
E_Z \equiv E[z] = \text{tr}(Z\rho),
\]

where \(Z\) is the Pauli-Z matrix: \(Z = (+1) |0\rangle \langle 0| + (-1) |1\rangle \langle 1|\) and \(\text{tr}(\cdot)\) is the trace. We can estimate the expectation value by repeating the experiment by \(s\) times, obtaining \(z_1, \ldots, z_s\), with each \(z_j \in \{+1, -1\}\), and calculate their empirical mean: \(\bar{y} = \frac{1}{s} \sum_{j=1}^{s} z_j\). Throughout this work, we use \(s = 8192\) shots for the experiments to keep the variance low.

**Definition A.2.** (Noise processes). A physical process (such as quantum noises) that can happen to a mixed quantum state \(\rho\) can be described as a linear map: \(\rho \rightarrow E(\rho)\), such that

\[
E(\rho) = \sum_k O_k \rho O_k^\dagger.
\]

The \(O_k\)'s are Kraus operators satisfying \(\sum_k O_k^\dagger O_k = I\). The noise process for a quantum neural network can be challenging to characterize, as it depends not only on the input to the network but also on the qubits and quantum gates used in the network. We wish to analyze this noise process by decoupling its dependence on the input data. We assume that each \(O_k\) has no explicit dependence on the classical input data; this is reasonable when we fix the model architecture.

**A.2.2 Proof of Theorem 3.1.** Now we are ready to analyze the effect of quantum noise on the measurement result from a quantum neural network. For classical data \(x_i\) from the input data set \(x\), we construct a quantum neural network that embeds the classical data in the quantum state \(\rho_i \equiv \rho(x_i, \theta_i)\) where \(\theta_i\) is some training parameters. The output of the network is the expectation value of the measurement outcome \(E_{z,i}^x \equiv \text{tr}(Z\rho_i)\). However, in reality, the results are transformed by some unknown process \(\rho_i \rightarrow E(\rho_i)\). The goal is to quantify the impact of the quantum noise on the expectation value.

**Theorem 3.1.** (Formal version). There exists some real parameters \(\beta_i\) and \(\gamma\), such that the expectation value of the measurement results \(E_{z,i}^x\) for input data \(x_i\) with the presence of any valid quantum noise \(E(\rho)\) can be described as a linear map from the noiseless value \(E_{z,i}^x\):

\[
E_{z,i} = \gamma E_{z,i}^x + \beta_i.
\]


We can further utilize the fact that an arbitrary quantum state can undergo some quantum noise processes $E(\rho) = \sum_k O_k \rho O_k^\dagger$. Therefore, in the presence of noise, the expectation value becomes:

$$E_z = \mathbb{E}[E(\rho)] = tr(E(\rho)Z) = \sum_k tr(O_k \rho O_k^\dagger Z) = \sum_k tr(\rho O_k^\dagger Z O_k),$$

where the third and fourth equality is from the properties of trace.

We can further utilize the fact that an arbitrary quantum state can be expanded as:

$$\rho = \frac{1}{2} (tr(\rho) I + tr(X\rho)X + tr(Y\rho)Y + tr(Z\rho)Z).$$

If we denote $\Omega = \sum_k O_k^\dagger Z O_k$, we obtain

$$E_z = \frac{1}{2}tr(\Omega) + \frac{1}{2}tr(X\Omega)tr(X) + \frac{1}{2}tr(Y\Omega)tr(Y) + \frac{1}{2}tr(Z\Omega)tr(Z).$$

Notice that $tr(\Omega) = 0$ and $tr(Z\rho) = E_2^\star$. We can set $\gamma = \frac{1}{2}tr(Z\Omega) \in [-1, 1]$ and $\beta_\rho = \frac{1}{2}tr(X\Omega)tr(X) + \frac{1}{2}tr(Y\Omega)tr(Y)$. We arrive at the linear map as desired. \qed

## A.3 Additional Experiments

### A.3.1 Importance of hardware-specific noise model.

We train three QNN models for Fashion-2 with the same architecture but different noise models from 3 devices and then deploy each model. Results in Table 6 show a diagonal pattern: the best accuracy is achieved when the noise model and inference device are the same. This is due to various noise magnitude and distribution on different devices. For instance, the gate error of Yorktown is 5× larger than Santiago, so using Yorktown noise information for model running on Santiago is too large. Therefore, a hardware-specific noise model is necessary for proper noise injection. However, this also marks the limitation of this work, as repeated training may be required when the noise model is updated. A future direction is to explore how to finetune already trained QNN for fast adaption to a new noise setting, thus reducing the marginal cost.

### A.3.2 Compatibility with existing noise-adaptive compilation.

We further show the compatibility of RobustQNN with state-of-the-art noise-adaptive quantum compilation techniques. Specifically, we set the optimization level of Qiskit compiler to the highest 3, which enables noise-adaptive qubit mapping and instruction scheduling. Then we inference the RobustQNN trained model and compare the accuracy of MNIST-2 in Table 7. With noise-adaptive compilation, the accuracy of baseline models is improved. While on top of that, the RobustQNN can still provide over 10% accuracy improvements, demonstrating the extensive applicability of our methods.

### A.3.3 Experiments on Fully Quantum Models.

For the results in Section 4, the QNN models contain multiple blocks. Here we further experiment on fully quantum models which only contains one single block to show the strong generality of RobustQNN as in Table 8. We select two fully quantum models, with three and six U3+CU3 layers, respectively, and experiment with six tasks on two machines. We apply the post-measurement normalization and quantization to the measurement outcomes of the last layer and use noise factor 0.5 and quantization level 6. No intermediate measurements are required. Our methods can still outperform baselines by 7.4% on average. Therefore, The noise injection can be applied to different kinds of variational quantum circuits, no matter whether the output of one layer is measured and passed to the next layer. Furthermore, the post-measurement normalization and quantization can also benefit various quantum circuits because they reduce the noise impact on measurement outcomes.

### A.3.4 Experiments on Effect of Number of Intermediate Measurements.

We also explore under the same number of parameters whether a fully quantum model is the best choice in the NISQ era. There exists a tradeoff on the number of intermediate measurements as in Table 9. More measurements mean less noise impact because we can perform post-measurement normalization and quantization on measurement outcomes. However, measurements will collapse the state vector in the large Hilbert space back to the small classical space, hurting the model capacity. We perform experiments on the IBMQ-Santiago machine and find there exists a sweet spot to achieve the highest deployment accuracy: the best model contains 2 blocks and each has 3 layers.

Furthermore, we show direct accuracy comparisons between the original (with measurements in between) QNN and fully-quantum QNN in Table 10. In each row, they have exactly the same dataset, same hardware. They have nearly the same architecture: same encoder/measurement, same gate sets, same layers, same number of parameters; the only difference is whether being measured and encoded back to quantum in the middle.

From the experimental results, we can see that under the total 6-layer setting, the 2 Block x 3 Layer can have better accuracy in most cases. This is because we perform normalization and quantization in the middle that can mitigate the noise impacts.

We also would like to emphasize that how to design the best architecture is not the main focus of our work. RobustQNN is architecture-agnostic and can be applied to various architectures to improve their robustness on real QC devices, as illustrated in paper Table 2.

### A.3.5 Accuracy Gap between Using Noise Model and Real QC.

To demonstrate the reliability of noise models, we show the accuracy of Baseline 0.68 0.83 0.83 0.54 +Norm 0.87 0.86 0.91 0.51 +Noise & Quant 0.92 0.92 0.91 0.93

| Method          | Santiago | Yorktown | Belem | Athens |
|-----------------|----------|----------|-------|--------|
| Baseline        | 0.68     | 0.83     | 0.83  | 0.54   |
| +Norm           | 0.87     | 0.86     | 0.91  | 0.51   |
| +Noise & Quant  | 0.92     | 0.92     | 0.91  | 0.93   |

Table 7: MNIST-2 accuracy with noise-adaptive compilation enabled (Qiskit optimization level=3).
We experiment with three tasks, each on three quantum devices. We show the mean and std of measurement outcomes of each qubit on the validation set and test set as in Table 13. We can see that the statistics of validation and test sets are similar. The last column of Table 13 shows the accuracy of test set using statistics of the test set itself and validation set, respectively. In 9 benchmarks, the accuracy of two settings is very close. The average accuracy of using test set stats is 0.67; using validation set stats is 0.65.

Therefore, using the statistics of validation set can bring similar accuracy to using statistics of test set itself; thus the RobustQNN can support small test batch size using validation set stats.

### A.4 Hyperparameters for main results

Table 14 shows the detailed noise factor and quantization level for all the tasks in Table 1.

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Table 8: Effect of RobustQNN on fully quantum models.

| IBMQ Machine | Model | Method  | MNIST-4 | Fashion-4 | Vowel-4 | MNIST-2 | Fashion-2 | Cifar-2 |
|--------------|-------|---------|---------|-----------|---------|---------|-----------|---------|
| Santiago     | 3 Layer | Baseline | 0.64    | 0.78      | 0.41    | 0.94    | 0.89      | 0.59    |
|              |       | RobustQNN | 0.78    | 0.82      | 0.53    | 0.96    | 0.90      | 0.58    |
| Santiago     | 6 Layer | Baseline | 0.61    | 0.37      | 0.22    | 0.51    | 0.52      | 0.52    |
|              |       | RobustQNN | 0.62    | 0.69      | 0.22    | 0.84    | 0.89      | 0.56    |
| Yorktown     | 3 Layer | Baseline | 0.49    | 0.53      | 0.4     | 0.88    | 0.85      | 0.51    |
|              |       | RobustQNN | 0.55    | 0.66      | 0.42    | 0.9     | 0.91      | 0.55    |
| Yorktown     | 6 Layer | Baseline | 0.22    | 0.33      | 0.26    | 0.73    | 0.80      | 0.54    |
|              |       | RobustQNN | 0.42    | 0.35      | 0.25    | 0.78    | 0.80      | 0.52    |
| Belem        | 3 Layer | Baseline | 0.53    | 0.60      | 0.37    | 0.64    | 0.81      | 0.51    |
|              |       | RobustQNN | 0.58    | 0.42      | 0.39    | 0.93    | 0.85      | 0.55    |
| Belem        | 6 Layer | Baseline | 0.27    | 0.18      | 0.21    | 0.54    | 0.48      | 0.43    |
|              |       | RobustQNN | 0.43    | 0.31      | 0.22    | 0.54    | 0.54      | 0.52    |

Table 9: Effect of number of intermediate measurements.

| Task  | 1 Block × 6 Layers | 2 Blocks × 3 Layers | 3 Blocks × 2 Layers | 6 Blocks × 1 Layer |
|-------|-------------------|--------------------|--------------------|-------------------|
| MNIST-4 | 0.62 | 0.74 | 0.71 | 0.66 |
| Fashion-4 | 0.69 | 0.82 | 0.78 | 0.68 |

Table 10: Direct comparison between QNN models with measurement in between and fully-quantum QNN models.

| Machine | Task  | Fully-Quantum (6L) | Original (2B × 3L) |
|---------|-------|--------------------|--------------------|
| Santiago | MNIST-4 | 0.62 | 0.74 |
| Santiago | Fashion-4 | 0.69 | 0.82 |
| Santiago | MNIST-2 | 0.84 | 0.86 |
| Belem | MNIST-4 | 0.43 | 0.37 |
| Belem | Fashion-4 | 0.31 | 0.34 |
| Belem | MNIST-2 | 0.54 | 0.60 |

---

A.3.6 Accuracy improvements comparison as number of classes increases. Since we have different tasks with various number of classes, we compare the average accuracy improvements between them in Table 12. We can see that the relative accuracy improvement on 10-class (230%) is significantly higher than 4-class and 2-class. That of 4-class is also higher than 2-class. To improve the same absolute accuracy, it is clearly more difficult on a 10-class task than on a 2-class task. So RobustQNN is highly effective on 10-class tasks.

A.3.7 Experiments on Using Validation Set Statistics for Test Set. If the test batch size is small for the deployment on real QC hardware, then the statistics may not be accurate enough for post-measurement normalization. In this case, we can profile the statistics of the validation set on real hardware ahead of time and then use the validation set mean and std to normalize the test set measurement outcomes.

We experiment with three tasks, each on three quantum devices. We show the mean and std of measurement outcomes of each qubit on the validation set and test set as in Table 13. We can see that the statistics of validation and test sets are similar. The last column of Table 13 shows the accuracy of test set using statistics of the test set itself and validation set, respectively. In 9 benchmarks, the accuracy of two settings is very close. The average accuracy of using test set stats is 0.67; using validation set stats is 0.65.

Therefore, using the statistics of validation set can bring similar accuracy to using statistics of test set itself; thus the RobustQNN can support small test batch size using validation set stats.
Table 11: Accuracy gap between evaluation using noise model and real QC.

| Machine | Model     | Method       | MNIST-4 | Fashion-4 | Vowel-4 | MNIST-2 | Fashion-2 | Cifar-2 |
|---------|-----------|--------------|---------|-----------|---------|---------|-----------|---------|
| Santiago | 2 Blocks  | Noise model  | 0.73    | 0.74      | 0.51    | 0.95    | 0.92      | 0.65    |
|         | × 12 Layer| Real QC      | 0.68    | 0.75      | 0.48    | 0.94    | 0.88      | 0.59    |
| Yorktown | 2 Blocks  | Noise model  | 0.68    | 0.7       | 0.44    | 0.92    | 0.90      | 0.59    |
|         | × 2 Layer | Real QC      | 0.62    | 0.65      | 0.44    | 0.93    | 0.86      | 0.60    |
| Belem    | 2 Blocks  | Noise model  | 0.64    | 0.72      | 0.41    | 0.96    | 0.82      | 0.64    |
|         | × 6 Layer | Real QC      | 0.58    | 0.62      | 0.41    | 0.88    | 0.8       | 0.61    |

Table 12: Improvements are still significant as the number of classes increases.

| Task       | Average Accuracy | Baseline | RobustQNN | Absolute Improvement | Relative Improvement |
|------------|------------------|----------|-----------|----------------------|----------------------|
| 2-classification | 0.58          | 0.76     | 0.28      | 48%                  |
| 4-classification | 0.31          | 0.57     | 0.26      | 84%                  |
| 10-classification | 0.1           | 0.33     | 0.23      | 230%                 |

Table 13: Statistics of test and validation set; Accuracy of test set using test stats and validation stats.

| Task       | Stats      | MEAN | STD | Accuracy |
|------------|------------|------|-----|----------|
| Fashion-4-Santiago | Test Stats | [0.0469, 0.0025, -0.0581, -0.0191] | 0.0868, 0.0496, 0.1021, 0.1152 | 0.75 |
|             | Valid Stats| [0.0679, 0.0025, -0.0519, -0.0473] | 0.0915, 0.0448, 0.0884, 0.1114 | 0.70 |
| Fashion-4-Yorktown | Test Stats | [-0.0396, 0.0478, 0.0995, 0.1375] | 0.1279, 0.3368, 0.1761, 0.1538 | 0.65 |
|             | Valid Stats| [-0.0362, 0.0771, 0.0965, 0.1535] | 0.1230, 0.3232, 0.1835, 0.1584 | 0.65 |
| Fashion-4-Belem  | Test Stats | [0.1118, 0.0075, 0.0901, -0.0005] | 0.0868, 0.1511, 0.1391, 0.2039 | 0.62 |
|             | Valid Stats| [0.1508, -0.0130, 0.0533, 0.0478] | 0.0882, 0.1298, 0.1315, 0.1401 | 0.53 |
| Vowel-4-Santiago | Test Stats | [0.1091, 0.0526, 0.0290, 0.2172] | 0.0551, 0.0260, 0.0554, 0.0422 | 0.48 |
|             | Valid Stats| [0.1042, 0.0698, 0.0458, 0.1951] | 0.0418, 0.0226, 0.0443, 0.0362 | 0.43 |
| Vowel-4-Yorktown | Test Stats | [0.0900, -0.3700, -0.2524, 0.1645] | 0.0997, 0.0580, 0.0663, 0.1198 | 0.44 |
|             | Valid Stats| [0.0841, -0.3869, -0.2948, 0.1736] | 0.0946, 0.0651, 0.0615, 0.1199 | 0.41 |
| Vowel-4-Belem  | Test Stats | [0.0115, 0.0800, 0.1703, 0.1775] | 0.0171, 0.0411, 0.0518, 0.0293 | 0.41 |
|             | Valid Stats| [0.0223, 0.0459, 0.1930, 0.1628] | 0.0145, 0.0335, 0.0478, 0.0263 | 0.40 |
| MNIST-2-Santiago | Test Stats | [-0.0581, -0.0657, 0.0088, 0.0170] | 0.0737, 0.1090, 0.1561, 0.1351 | 0.94 |
|             | Valid Stats| [-0.0739, 0.0001, -0.0113, 0.00239] | 0.0666, 0.0840, 0.1468, 0.1167 | 0.95 |
| MNIST-2-Yorktown | Test Stats | [0.0892, -0.0007, 0.0548, 0.0485] | 0.1281, 0.3501, 0.2100, 0.2975 | 0.99 |
|             | Valid Stats| [0.0704, 0.0536, 0.0204, 0.1043] | 0.1377, 0.3813, 0.2596, 0.2955 | 0.91 |
| MNIST-2-Belem  | Test Stats | [-0.0549, 0.1949, 0.0540, 0.1313] | 0.0856, 0.1137, 0.1553, 0.1688 | 0.88 |
|             | Valid Stats| [-0.0540, 0.2074, 0.0744, 0.1872] | 0.0561, 0.1008, 0.1345, 0.1103 | 0.91 |
| Average     | Test Stats  | —      | —   | —        | 0.67     |
|             | Valid Stats | —      | —   | —        | 0.65     |

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Table 14: Hyperparameters of Table 1.

| Task, (noise-factor, quantization level) | MNIST-4 | Fashion-4 | Vowel-4 | MNIST-2 | Fashion-2 | Cifar-2 |
|----------------------------------------|---------|-----------|---------|---------|-----------|---------|
| QNN (2 Blocks × 12 Layers) on Santiago | (1, 3)  | (0.5, 6)  | (0.5, 6) | (1, 4)  | (1, 6)    | (0.5, 6) |
| QNN (2 Blocks x 2 Layers) on Yorktown  | (0.5, 6)| (1, 5)    | (0.1, 5) | (0.5, 5)| (0.1, 6)  | (0.1, 3) |
| QNN (2 Blocks x 6 Layers) on Belem     | (0.5, 5)| (1.5, 6)  | (0.5, 3) | (0.5, 5)| (0.1, 4)  | (0.5, 6) |
| QNN (3 Blocks x 10 Layers) on Athens   | (0.1, 6)| (0.1, 5)  | (0.5, 6) | (0.1, 6)| (0.5, 6)  | (0.1, 6) |

| Task, (noise-factor, quantization level) | MNIST-10 | Fashion-10 |
|----------------------------------------|-----------|------------|
| QNN (2 Blocks x 2 Layers) on Melbourne | (0.1, 6)  | (0.1, 5)   |