



TorchQuantum Tutorial

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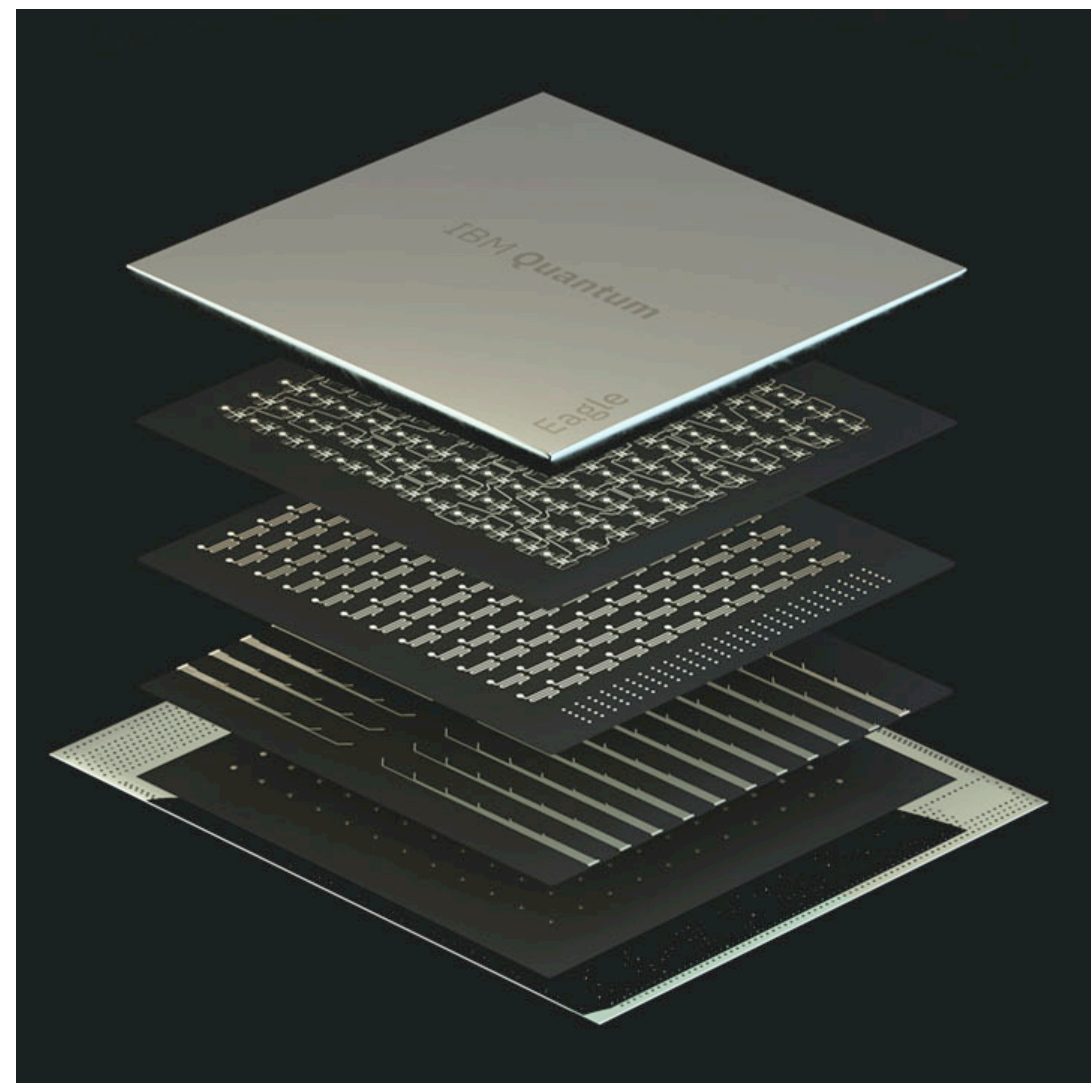
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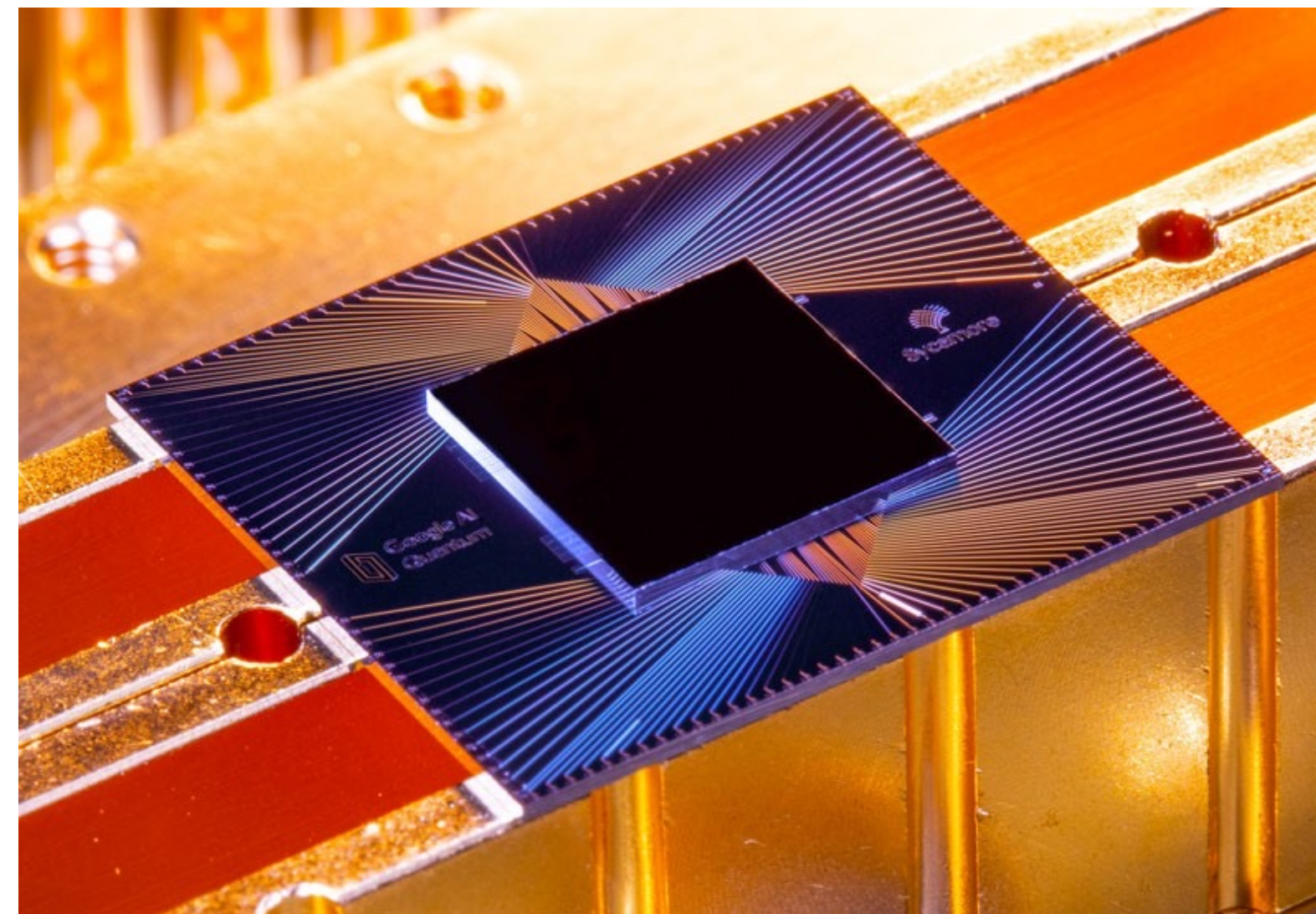
<https://torchquantum.org>

Quantum Computing

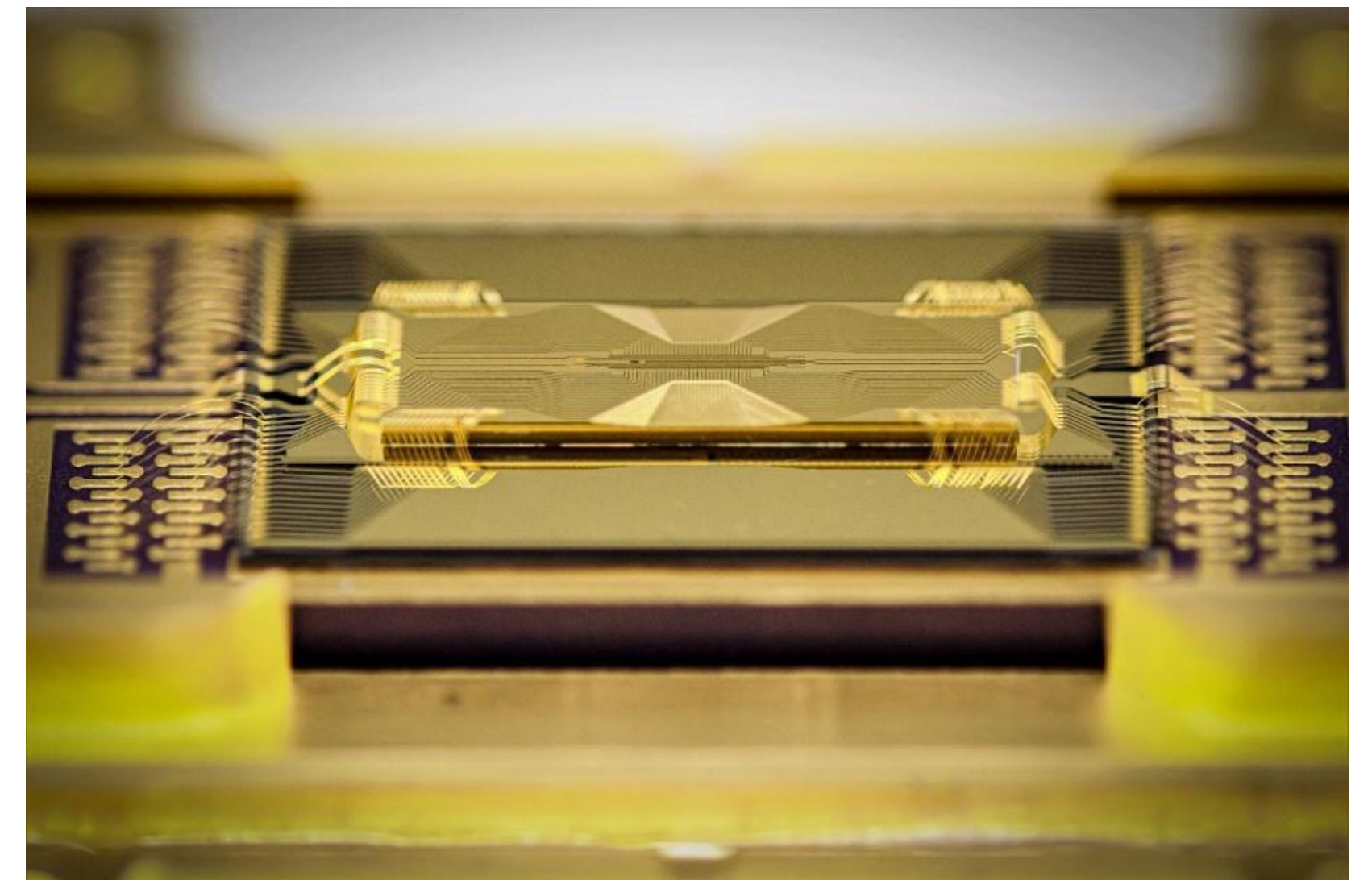
- Fast progress of quantum devices
- Different technologies
 - Superconducting, trapped ion, neutral atom, photonics, etc.



IBM
127 Qubit



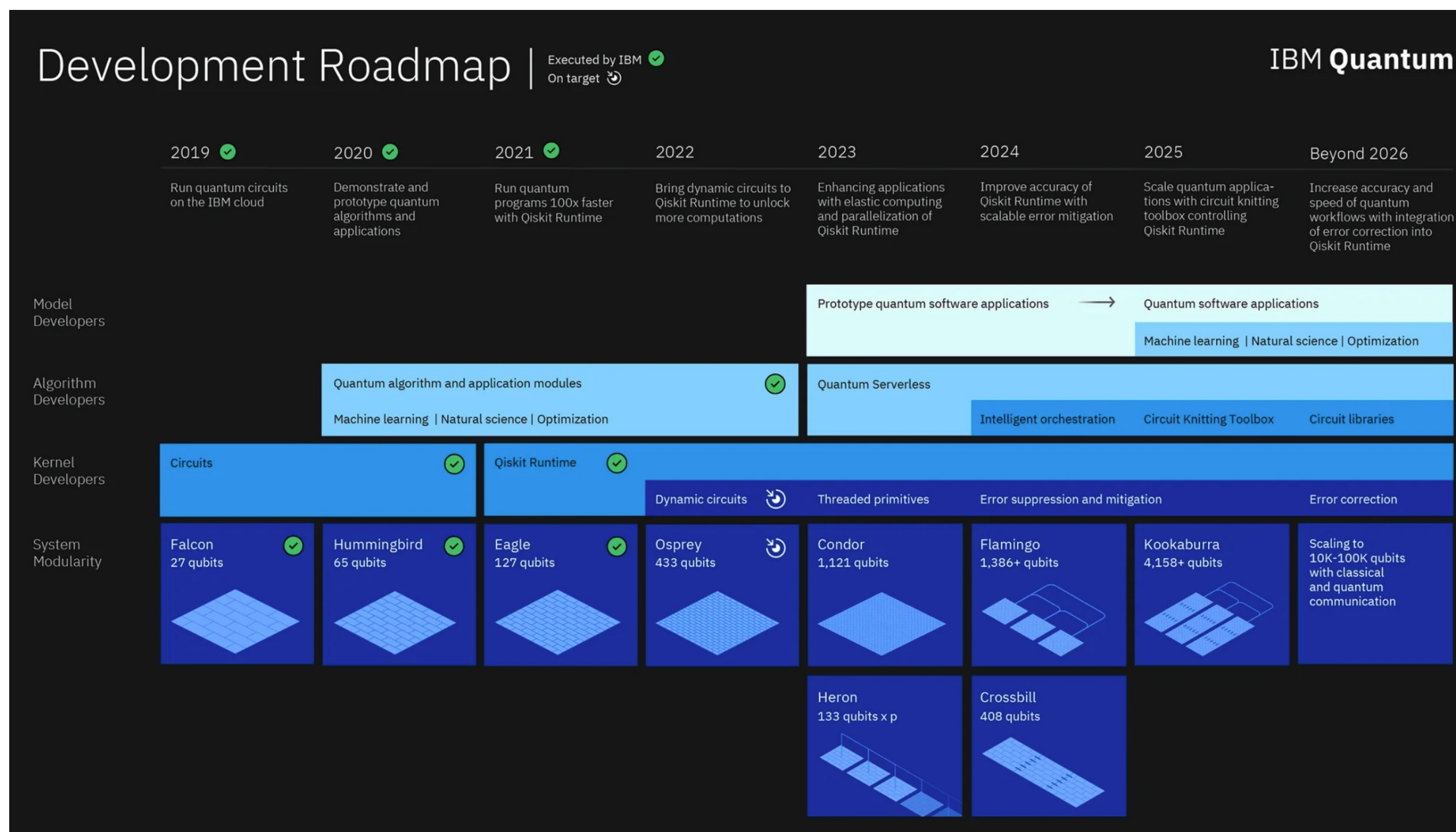
Google
53 Qubits



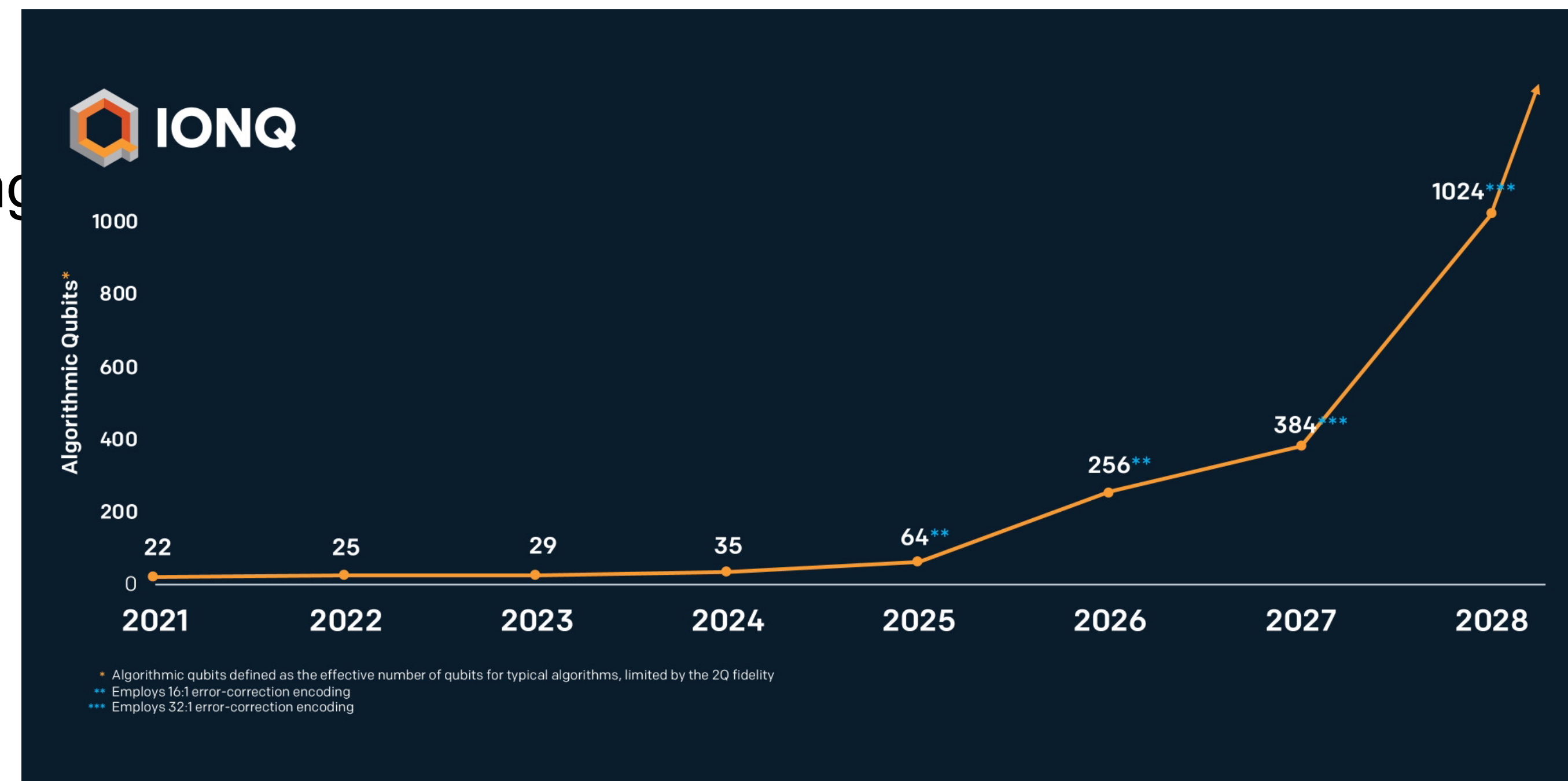
IonQ
32+ Qubits

Quantum Computing

- The number of qubits increases exponentially over time
- The computing power increases exponentially with the number of qubits
- => “doubly exponential” rate



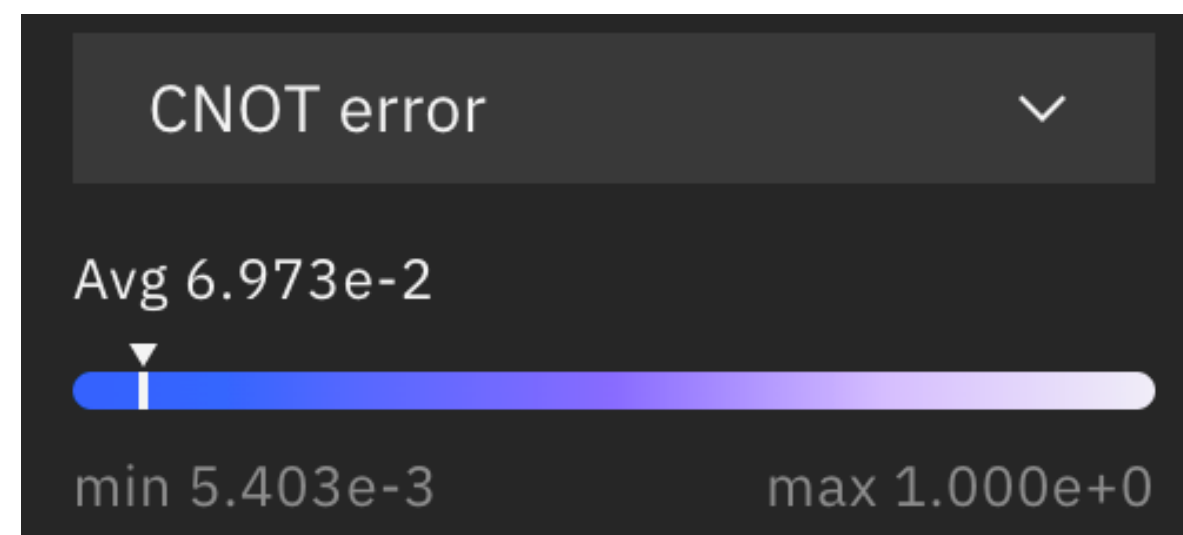
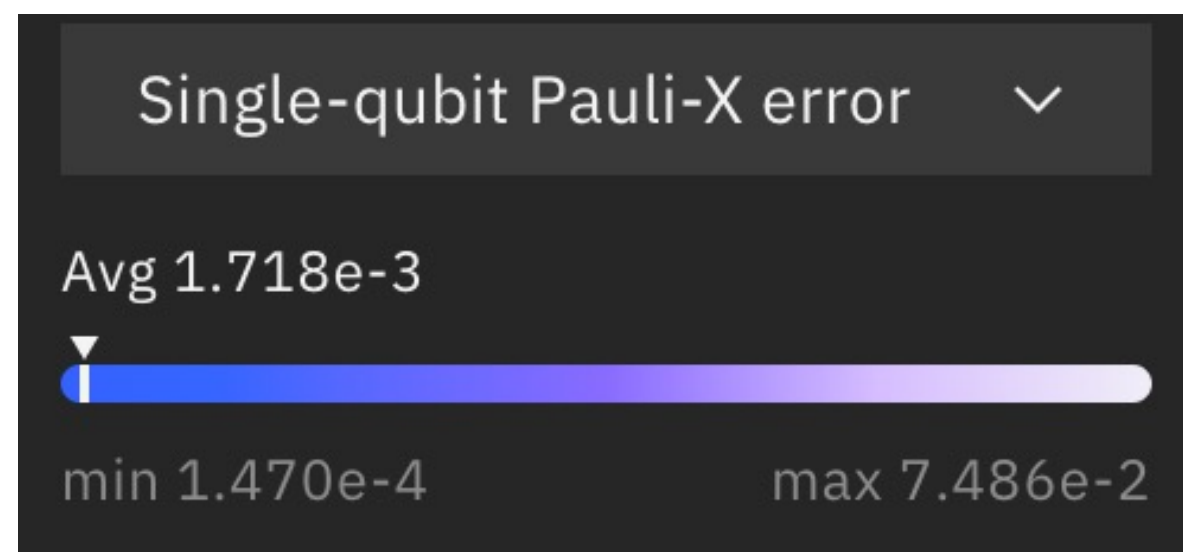
IBM Roadmap



IonQ Roadmap

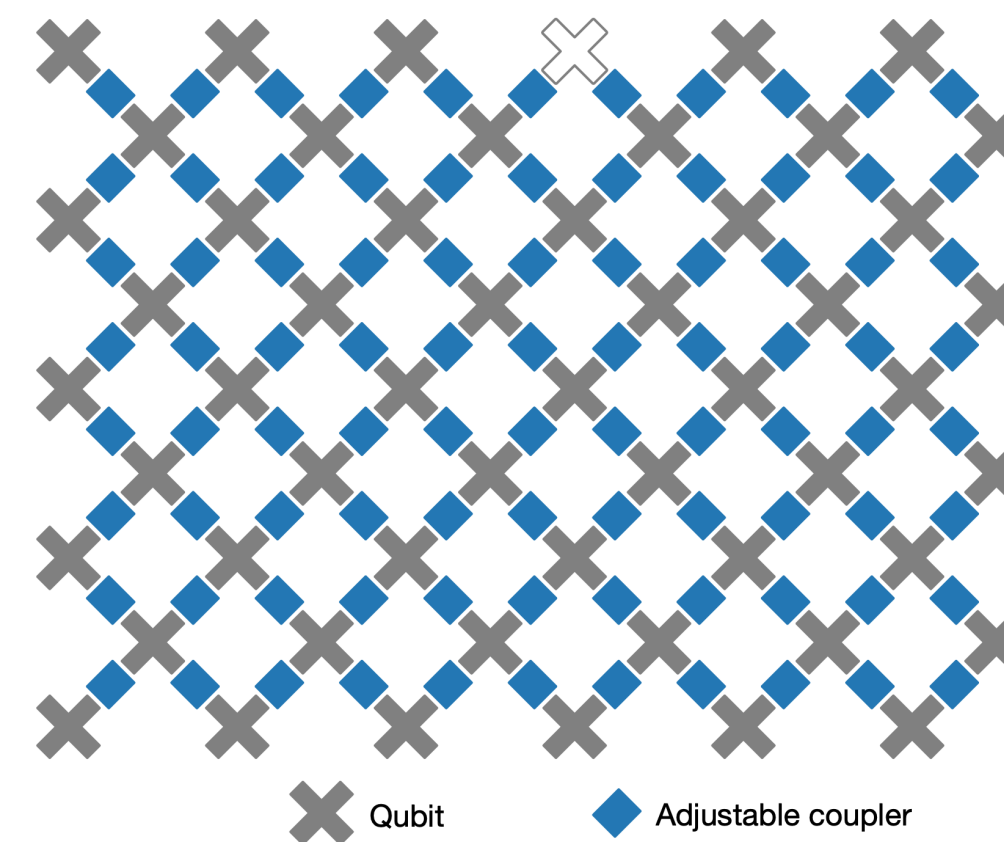
Quantum Computing in NISQ Era

- Noisy Intermediate-Scale Quantum (NISQ)
 - **Noisy**: qubits are sensitive to environment; quantum gates are unreliable
 - **Limited number of qubits**: tens to hundreds of qubits
 - **Limited connectivity**: no all-to-all connections



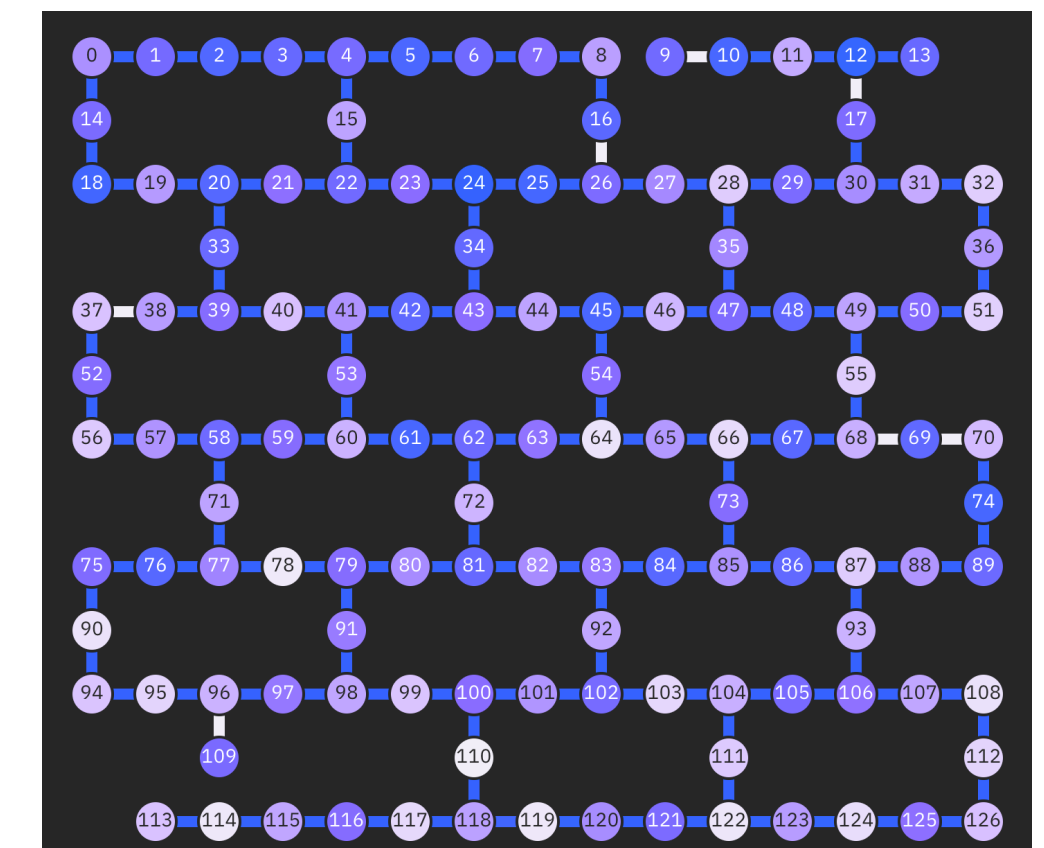
IBMQ Gate Error Rate

<https://quantum-computing.ibm.com/>



Google Sycamore 53Q

<https://www.nature.com/articles/s41586-019-1666-5>

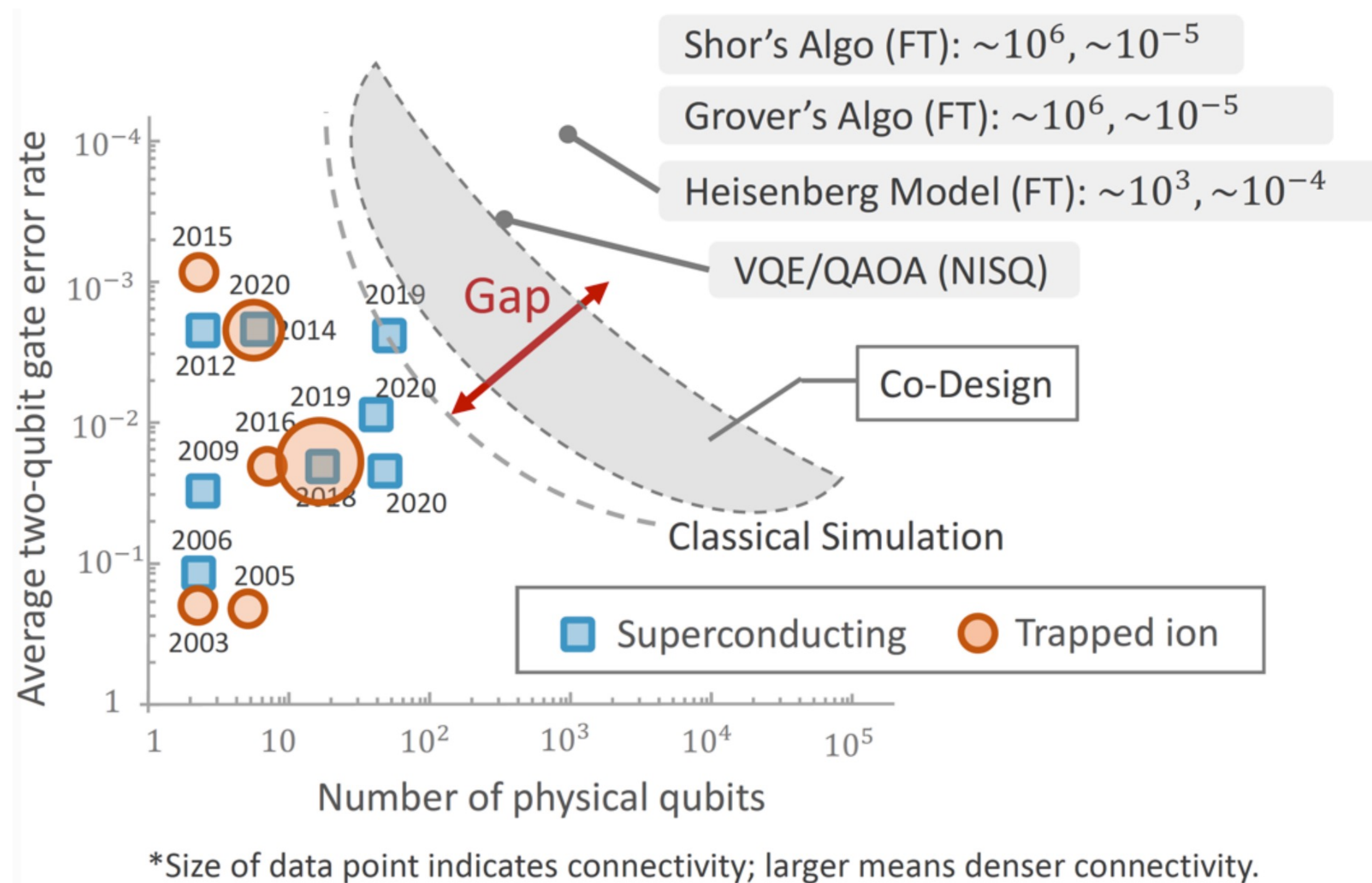


IBM Washington 127Q

<https://quantum-computing.ibm.com/>

A Large Gap between Powerful Quantum Algorithms and Current Devices

- Close the gap with **machine learning** and **hardware-aware algorithm design**



Good Infrastructure is Critical

- To enable ML-assisted hardware-aware quantum algorithm design
- Need a simulation framework on classical computer
 - Fast
 - PyTorch native
 - Portable
 - Scalable
 - Analyze circuit **behavior**
 - Study **noise** impact
 - Develop **ML model** for quantum optimization

TorchQuantum Library

- A fast library for classical simulation of quantum circuit in **PyTorch**
 - Automatic **gradient** computation for training parameterized quantum circuit
 - **GPU-accelerated** tensor processing with batch mode support
 - **Dynamic computation graph** for easy debugging
 - Easy construction of **hybrid classical and quantum** neural networks
 - **Gate** level and **pulse** level simulation support
 - **Converters** to other frameworks such as IBM Qiskit
 - And so on...

TorchQuantum Tutorial Outline

Section 1

TorchQuantum Basic Usage

1.1 Quantum Basics

1.2 TQ Operations 

1.3 TQ for State Prep 


1.4 TQ for VQE 

1.5 TQ for QNN 

Section 2

Use TorchQuantum on Gate Level Optimization

2.1 QuantumNAS: Ansatz
Search and Gate Pruning 

2.2 QuantumNAT: Noise
Injection and Quantization 

2.3 QOC: On-Chip Training 

2.4 Transformer for Quantum
Circuit Reliability Prediction

2.5 QNN Compression 

Section 3

Use TorchQuantum on Pulse Level Optimization

3.1 Quantum Optimal Control 

3.2 Variational Pulse Learning 

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Quantum Bit

- Quantum Bit (Qubit)

- Statevector: contains 2^n complex numbers for n qubit system

- The square sum of magnitude of 2^n numbers are 1

- 1 qubit:

$$\begin{bmatrix} a_0 \\ a_1 \end{bmatrix} \quad \begin{aligned} a_0, a_1 &\in \mathbb{C} \\ |a_0|^2 + |a_1|^2 &= 1 \end{aligned}$$

- 2 qubits:

$$\begin{bmatrix} a_0 \\ a_1 \\ a_2 \\ a_3 \end{bmatrix} \quad \begin{aligned} a_0, a_1, a_2, a_3 &\in \mathbb{C} \\ |a_0|^2 + |a_1|^2 + |a_2|^2 + |a_3|^2 &= 1 \end{aligned}$$

Quantum Bit

- Classical bits represented in statevector

- Classical 0: $\begin{bmatrix} 1 \\ 0 \end{bmatrix}$

- Classical 1: $\begin{bmatrix} 0 \\ 1 \end{bmatrix}$

- An arbitrary quantum states: $\begin{bmatrix} a_0 \\ a_1 \end{bmatrix} = a_0 \cdot \begin{bmatrix} 1 \\ 0 \end{bmatrix} + a_1 \cdot \begin{bmatrix} 0 \\ 1 \end{bmatrix}$

Quantum Gates

- Qubit gates: operations on one qubit or multiple qubits
- The qubit gates can be represented with matrix format with dimension $2^n \times 2^n$
- All gate matrices are unitary matrices: the conjugate transpose is the same as its inverse
- Single qubit gates:

- Not (X) gate:

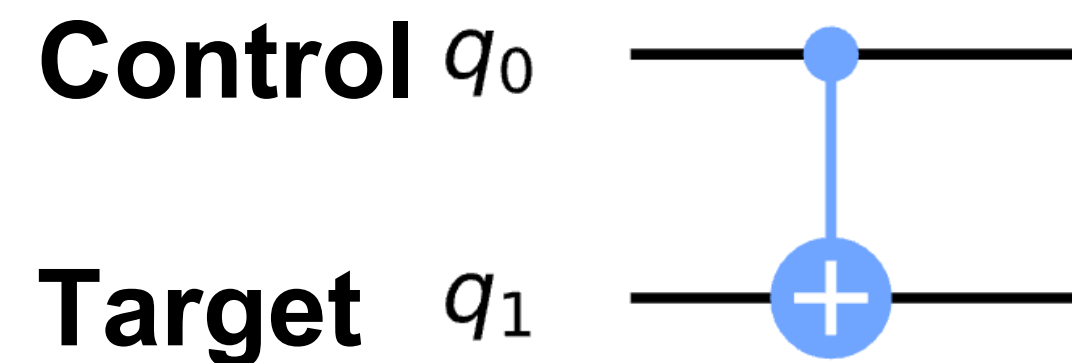
$$X = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$$

- Parameterized gate: Rotation X (RX) with parameter theta

$$RX(\theta) = \begin{bmatrix} \cos \frac{\theta}{2} & -i \sin \frac{\theta}{2} \\ -i \sin \frac{\theta}{2} & \cos \frac{\theta}{2} \end{bmatrix}$$

Quantum Gates

- 2-qubit gates:
 - Controlled Not (CNOT) gate:



$$CNOT = \begin{matrix} & \text{Input} & \begin{matrix} 00 & 01 & 10 & 11 \end{matrix} \\ \begin{matrix} 00 \\ 01 \\ 10 \\ 11 \end{matrix} & \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix} \end{matrix}$$

- Controlled Rotation X (CRX) gate

$$CRX(\theta) = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & \cos \frac{\theta}{2} & -i \sin \frac{\theta}{2} \\ 0 & 0 & -i \sin \frac{\theta}{2} & \cos \frac{\theta}{2} \end{bmatrix}$$

Quantum Gates

- Applying a gate to qubits is performing matrix-vector multiplication between the gate matrix and statevector
 - Apply an X gate to classical state 0, we get 1

$$X \begin{bmatrix} 1 \\ 0 \end{bmatrix} = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \begin{bmatrix} 1 \\ 0 \end{bmatrix} = \begin{bmatrix} 0 \\ 1 \end{bmatrix}$$

- Apply an CNOT gate to state 10, we get 11

$$CNOT \begin{bmatrix} 0 \\ 0 \\ 1 \\ 0 \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix} \begin{bmatrix} 0 \\ 0 \\ 1 \\ 0 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 1 \end{bmatrix}$$

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TQ for Statevector simulation

- Performing matrix-vector multiplication between the gate matrix and statevector
 - The `tq.QuantumDevice` stores the statevectors
 - `q_dev = tq.QuantumDevice(n_wires=5)`
 - Two ways of applying quantum gates: method 1:
 - `import torchquantum.functional as tqf`
 - `tqf.h(q_dev, wires=1)`

TQ for Statevector simulation

- Performing matrix-vector multiplication between the gate matrix and statevector
 - The `tq.QuantumDevice` stores the statevectors
 - `q_dev = tq.QuantumDevice(n_wires=5)`
 - Two ways of applying quantum gates: method 2:
 - `h_gate = tq.H()`
 - `h_gate(q_dev, wires=3)`

TQ for Statevector simulation

- Performing matrix-vector multiplication between the gate matrix and statevector
 - The `tq.QuantumState` class can also store the statevectors
 - `q_state = tq.QuantumState(n_wires=5)`
 - Three ways of applying quantum gates
 - `import torchquantum.functional as tqf`
 - `tqf.h(q_state, wires=1)`
 - `h_gate = tq.H()`
 - `h_gate(q_state)`
 - `q_state.h()`
 - `q_state.rx(wires=1, params=0.2 * np.pi)`

TQ for Statevector simulation

- Performing matrix-vector multiplication between the gate matrix and statevector
- The implementation of statevector and quantum gates are using the native data structure in PyTorch

```
_state = torch.zeros(2 ** self.n_wires, dtype=C_DTYPE)
```

```
_state[0] = 1 + 0j
```

```
'cnot': torch.tensor([[1, 0, 0, 0],  
                      [0, 1, 0, 0],  
                      [0, 0, 0, 1],  
                      [0, 0, 1, 0]], dtype=C_DTYPE),
```

Dynamic computation graph

- Performing matrix-vector multiplication between the gate matrix and statevector
 - The `tq.QuantumState` class can also store the statevectors
 - `q_state = tq.QuantumState(n_wires=5)`
 - `q_state.h(wires=1)`
 - `print(q_state)`
 - `q_state.sx(wires=3)`
 - `print(q_state)`

Batch Mode Tensorized Processing

- Performing matrix-vector multiplication between the gate matrix and statevector
 - The `tq.QuantumState` class can also store the statevectors
 - `q_state = tq.QuantumState(n_wires=5, bsz=64)`

GPU Support

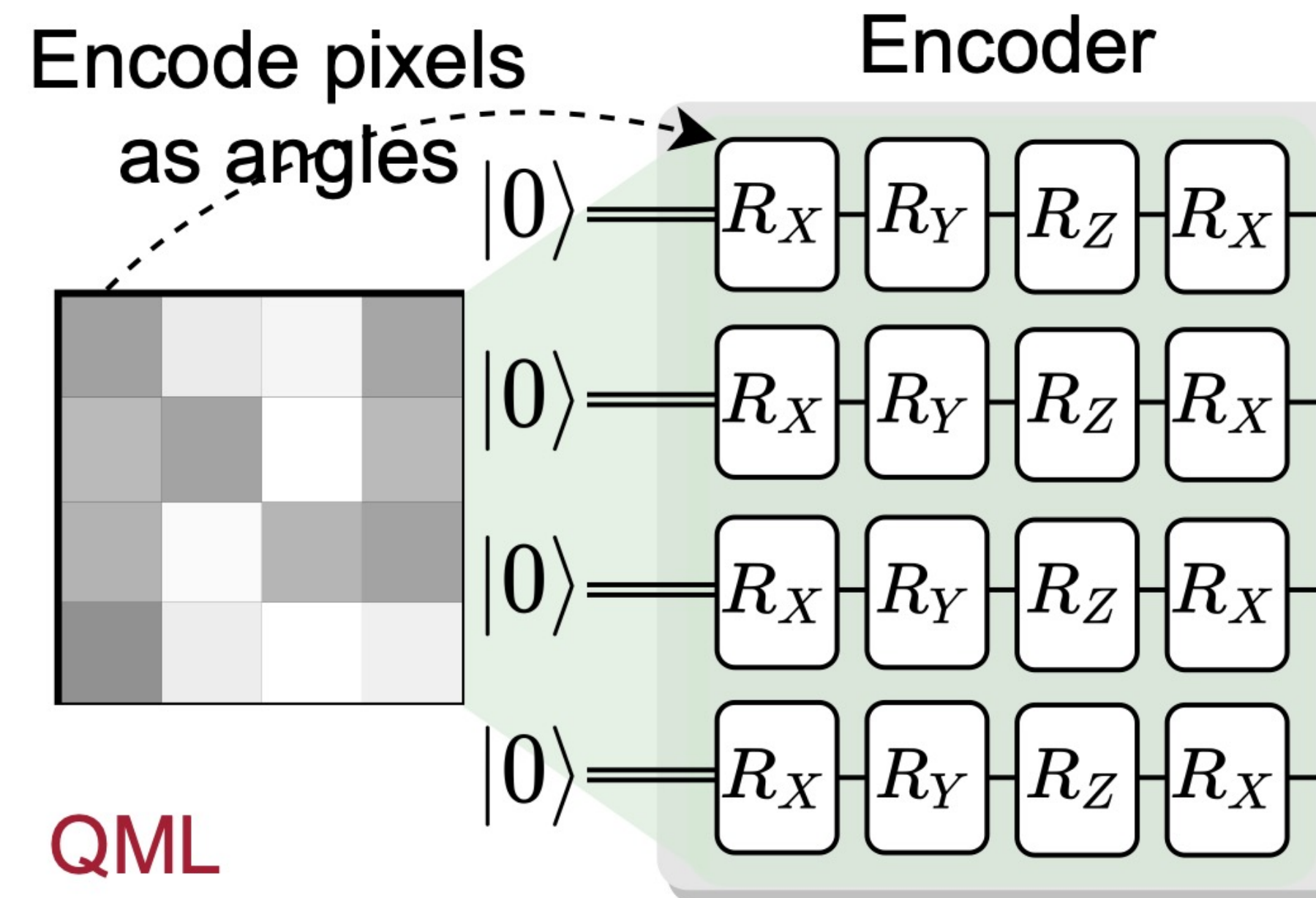
- Performing matrix-vector multiplication between the gate matrix and statevector
 - The `tq.QuantumState` class can also store the statevectors
 - `q_state = tq.QuantumState(n_wires=5, bsz=64)`
 - `q_state.to(torch.device('cuda'))`
 - Leverage the fast GPU support

Automatic Gradient Computation

- Performing matrix-vector multiplication between the gate matrix and statevector
 - The `tq.QuantumState` class can also store the statevectors
 - `q_state = tq.QuantumState(n_wires=2)`
 - `target_quantum_state = torch.tensor([0, 0, 0, 1])`
 - `loss = 1 - (q_state.get_states_1d()[0] @ target_quantum_state).abs()`
 - `loss.backward()`

Encoding Classical Data to Quantum various encoder support

- `tq.AmplitudeEncoder()` encodes the classical values to the amplitude of quantum statevector
- `tq.PhaseEncoder()` encodes the classical values using the rotation gates



Construct a Circuit Class

- Construct a class for circuit model
- `tq.QuantumModule` class
- In the `__init__` function, create all the gates that will be used
- In the forward function, specify how the gates will be used in the circuit

```
• Class q_model(tq.QuantumModule)  
    def __init__():  
        self.n_wires = 2  
        self.rx_0 = tq.RX(has_params=True, trainable=True)  
        self.ry_0 = tq.RY(has_params=True, trainable=True)  
  
    def forward(q_dev):  
        self.rx_0(q_dev)  
        self.ry_0(q_dev)
```

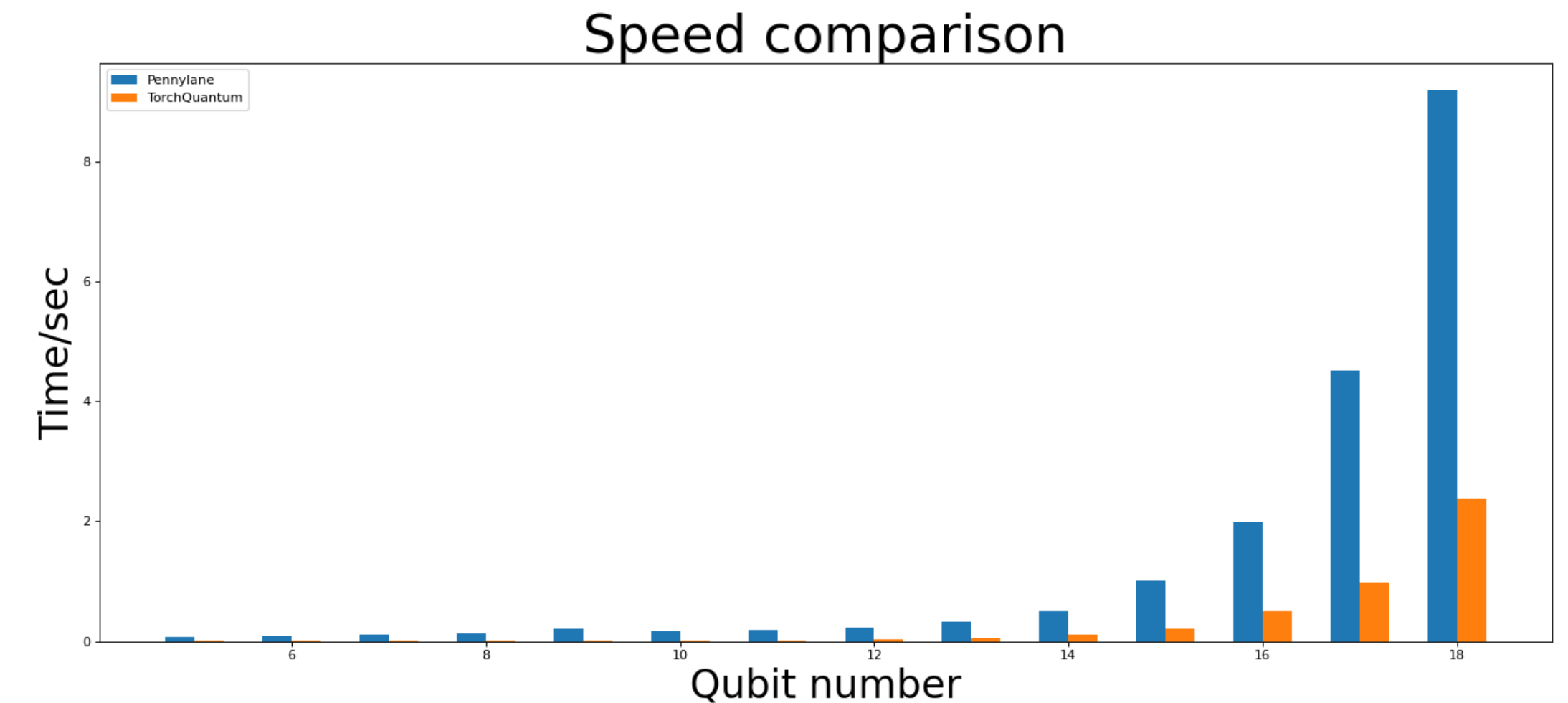
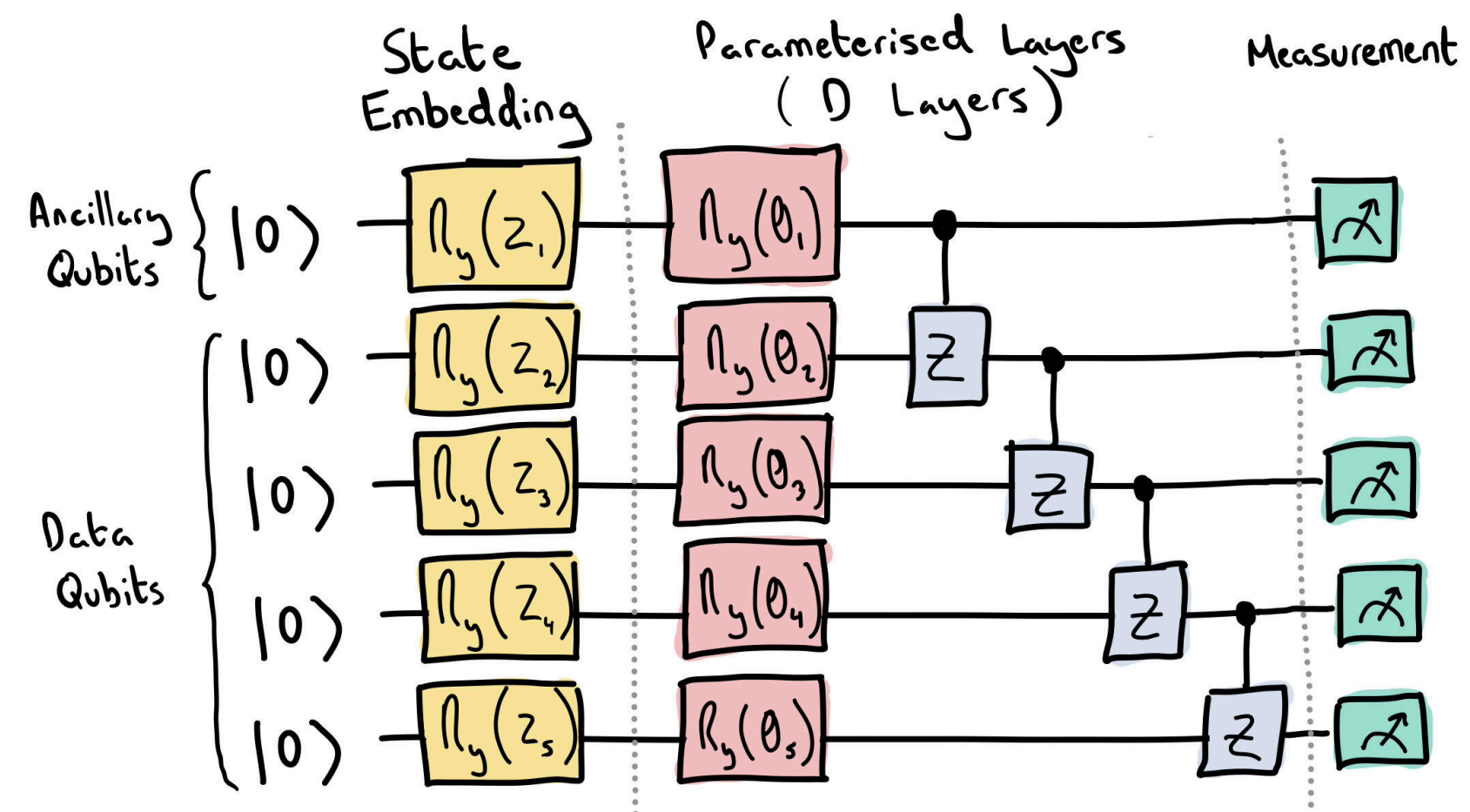
Conversion tq model to other frameworks

- Convert the `tq.QuantumModule` to other frameworks such as Qiskit
- `from torchquantum.plugins.qiskit_plugin import tq2qiskit`
- `circ = tq2qiskit(q_dev, q_model)`
- `circ.draw('mpl')`

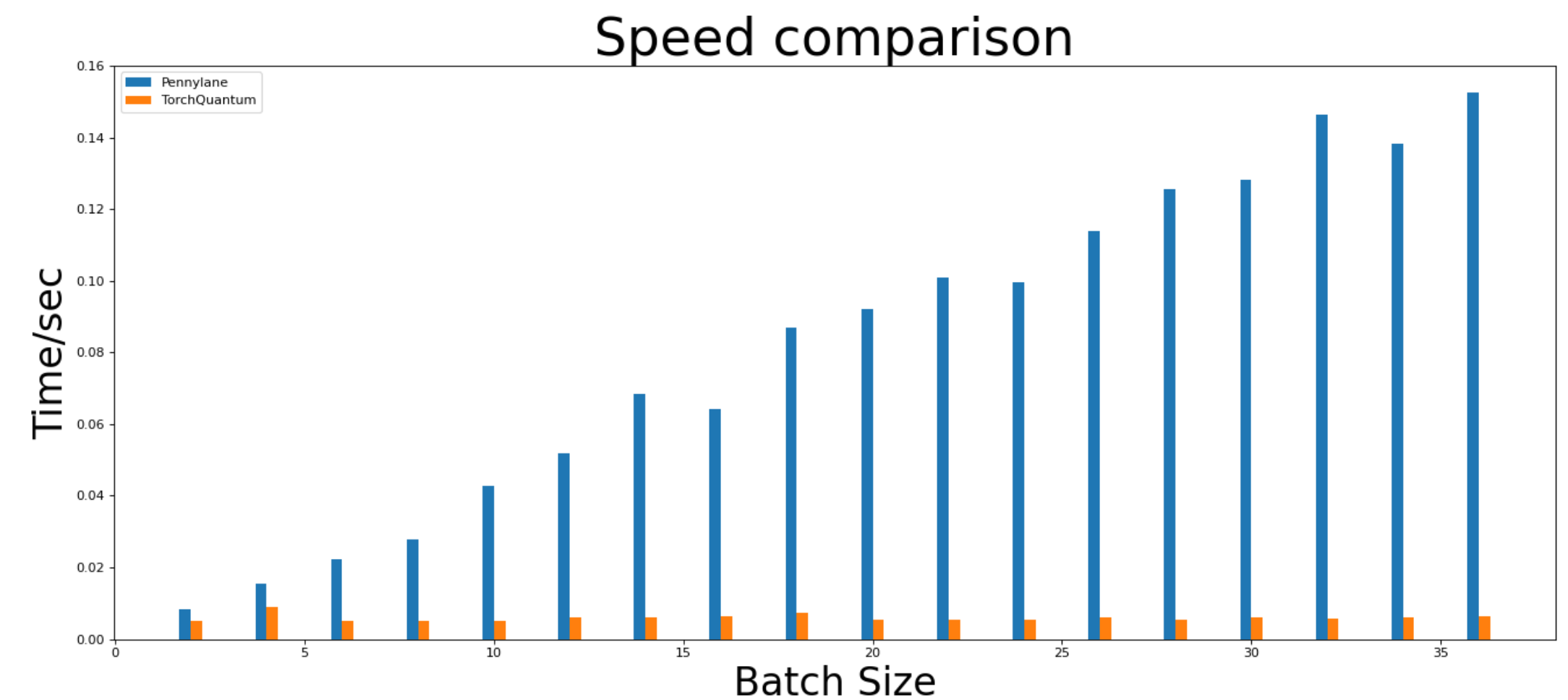
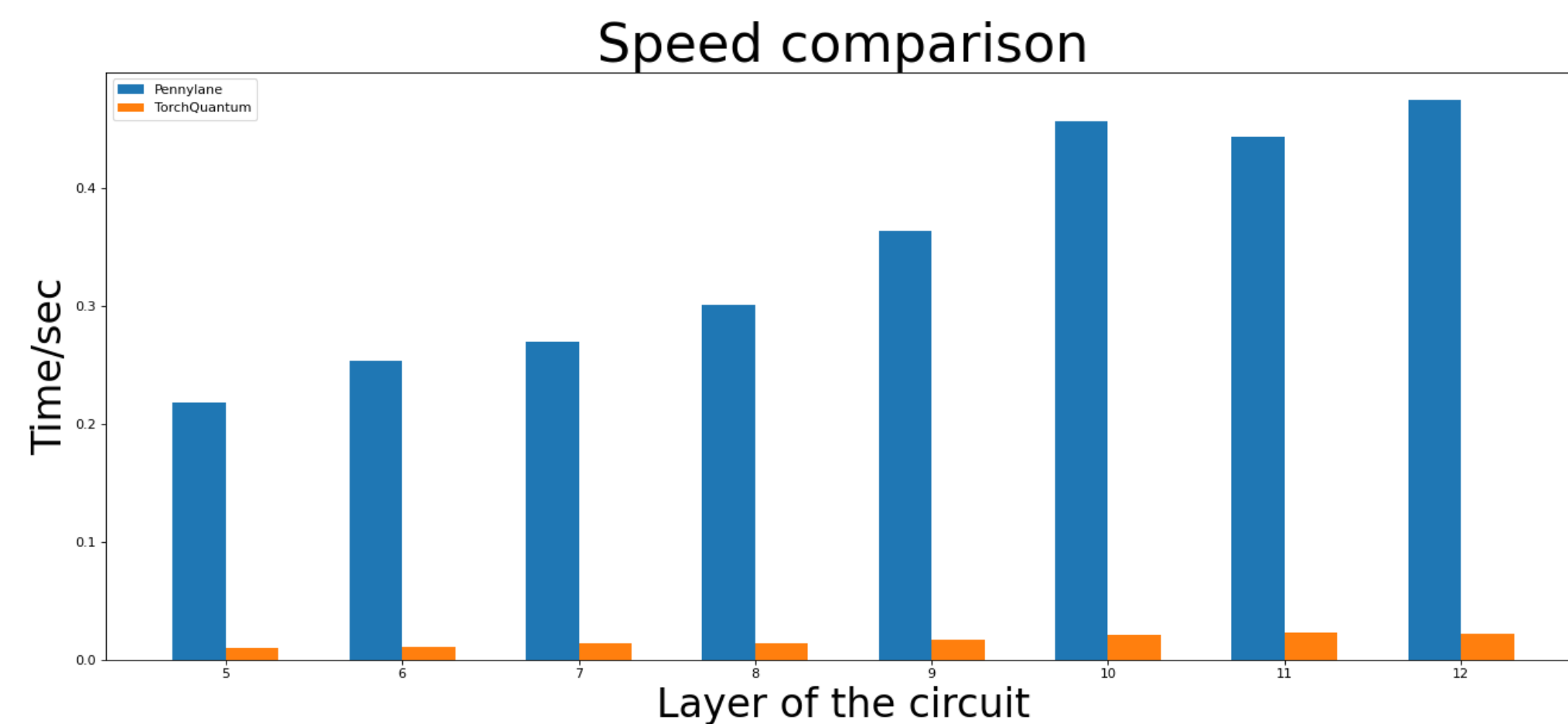
Easy Deployment on Real Quantum Machines

- Convert the `tq.QuantumModule` to other frameworks such as Qiskit
- `from torchquantum.plugins.qiskit_plugin import tq2qiskit`
- `from torchquantum.plugins.qiskit_processor import QiskitProcessor`
- `processor = QiskitProcessor(use_real_qc=False, max_jobs=1)`
- `circ = tq2qiskit(q_dev, model)`
- `circ.measure_all()`
- `res = processor.process_ready_circs(q_dev, [circ])`

Compare the Speed of TQ and Pennylane

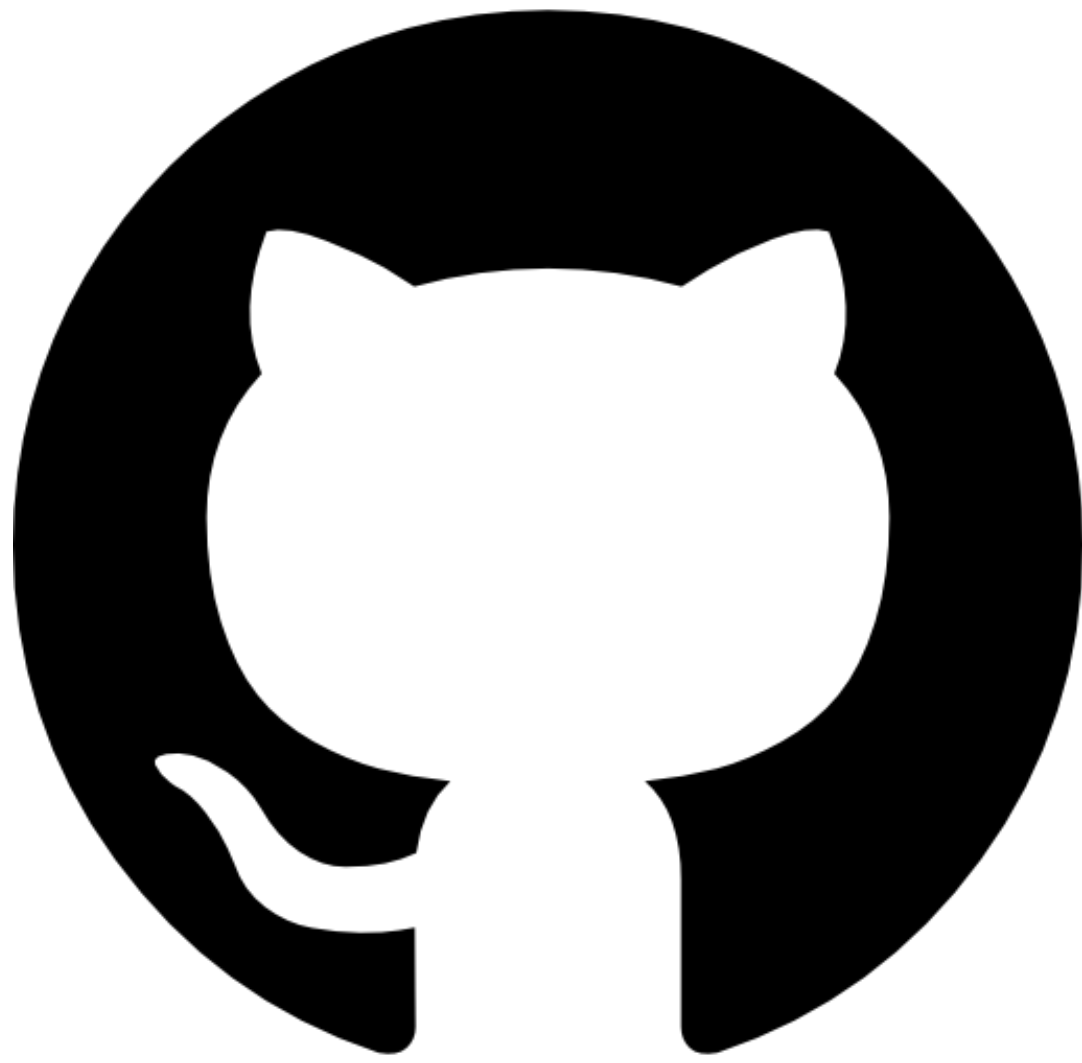


https://pennyLane.ai/qml/_images/qcircuit.jpeg



Hands-On Section

1.2 TorchQuantum Operations



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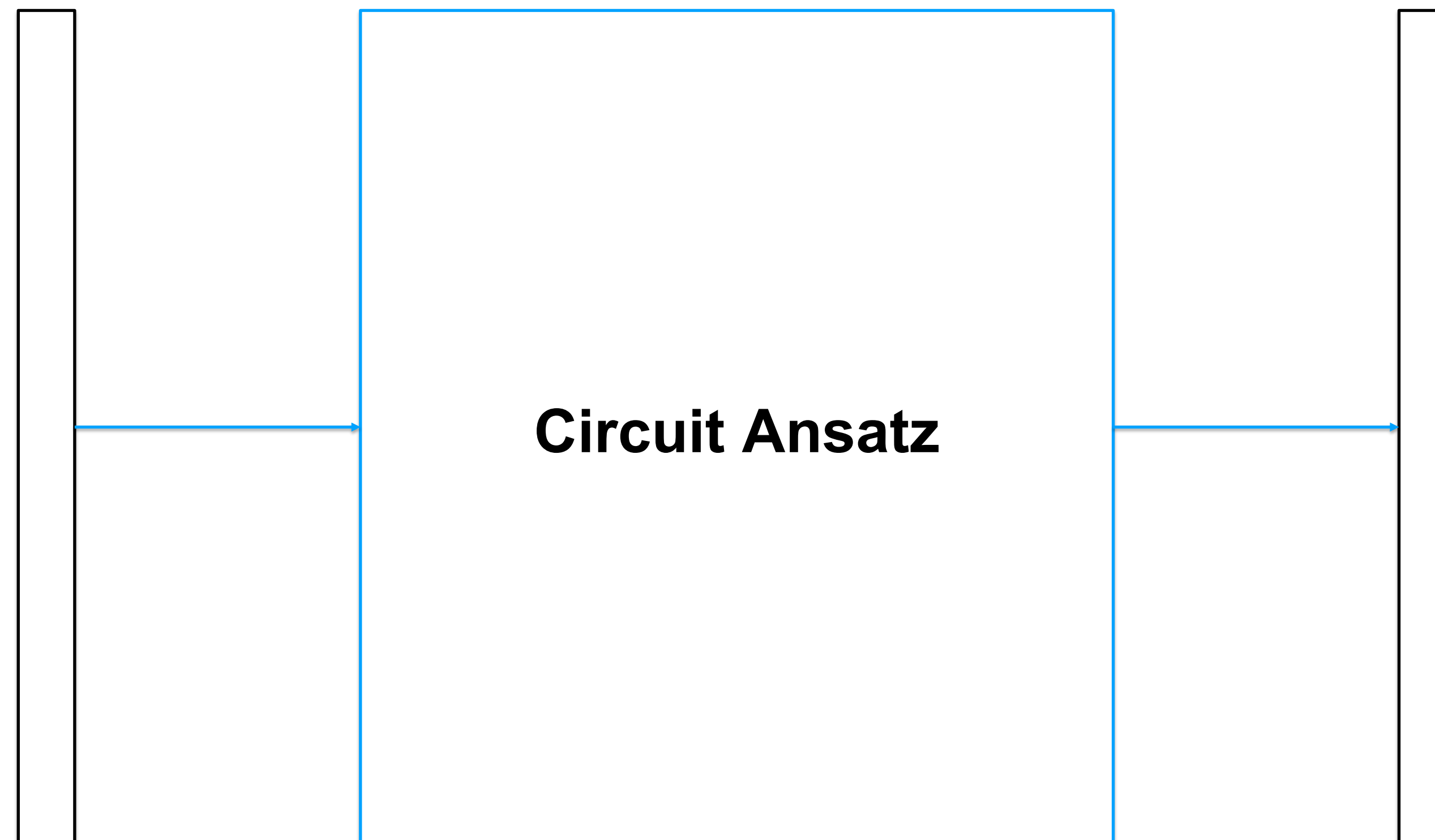
Use TorchQuantum on Pulse level

3.1 Quantum Optimal Control 

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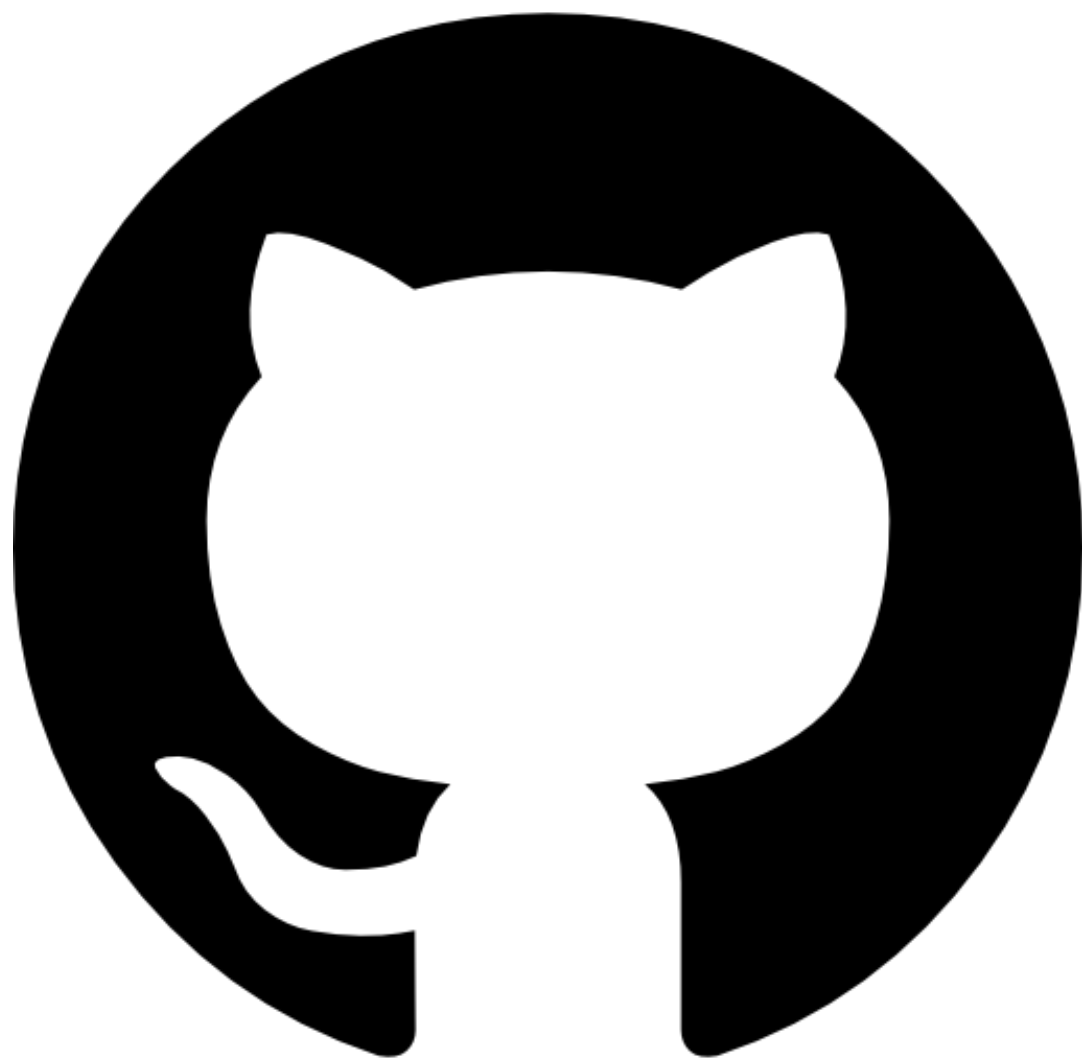
State Preparation with Parameterized Circuit

- Use parameterized circuit to prepare initial quantum states



Hands-On Section

1.3 TQ for State Preparation



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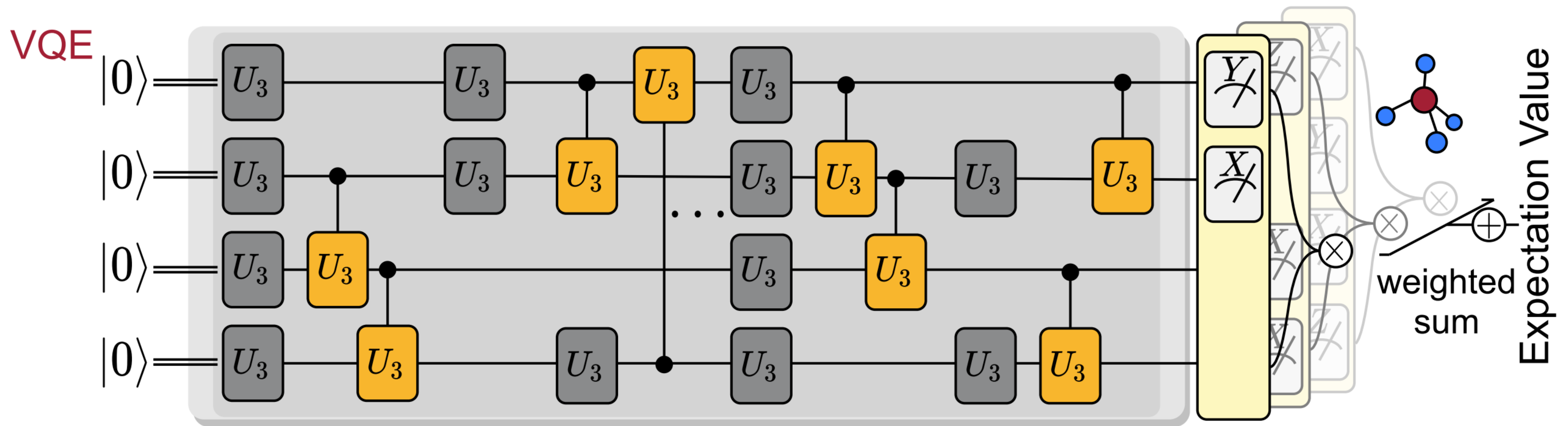
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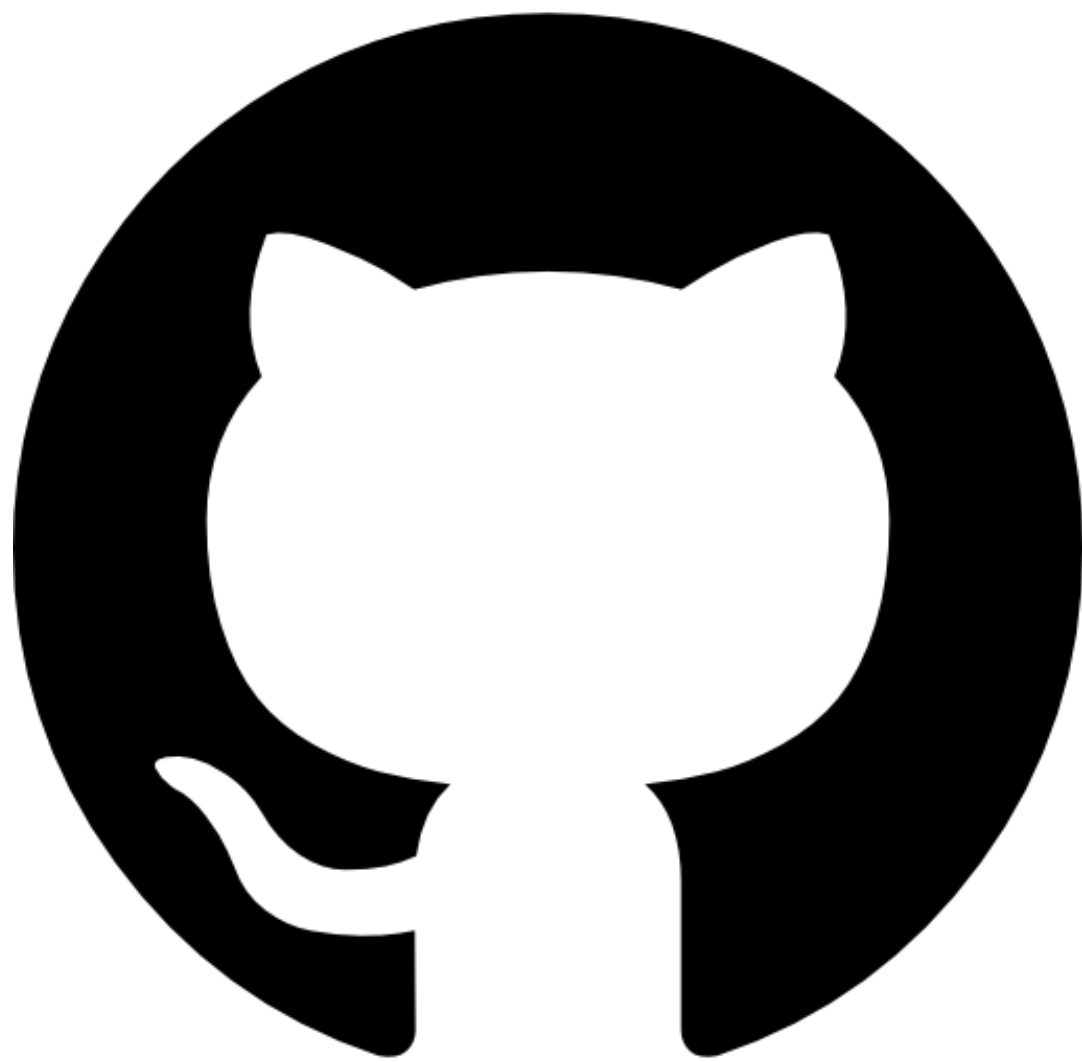
Variational Quantum Eigensolver

- VQE: Finds the ground state energy of molecule Hamiltonian



Hands-On Section

1.4 TQ for VQE



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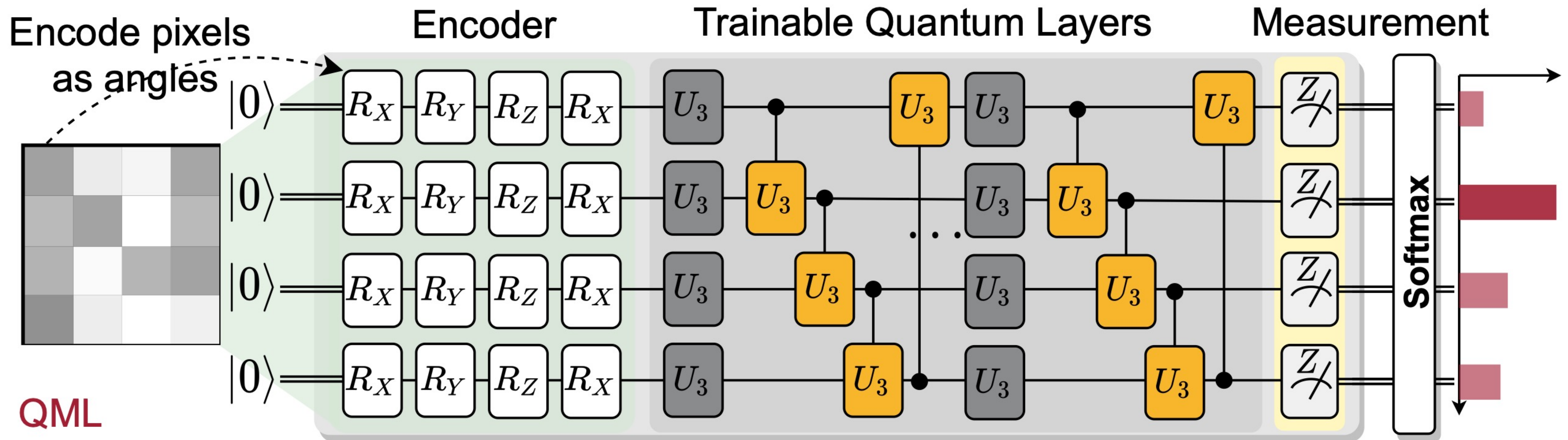
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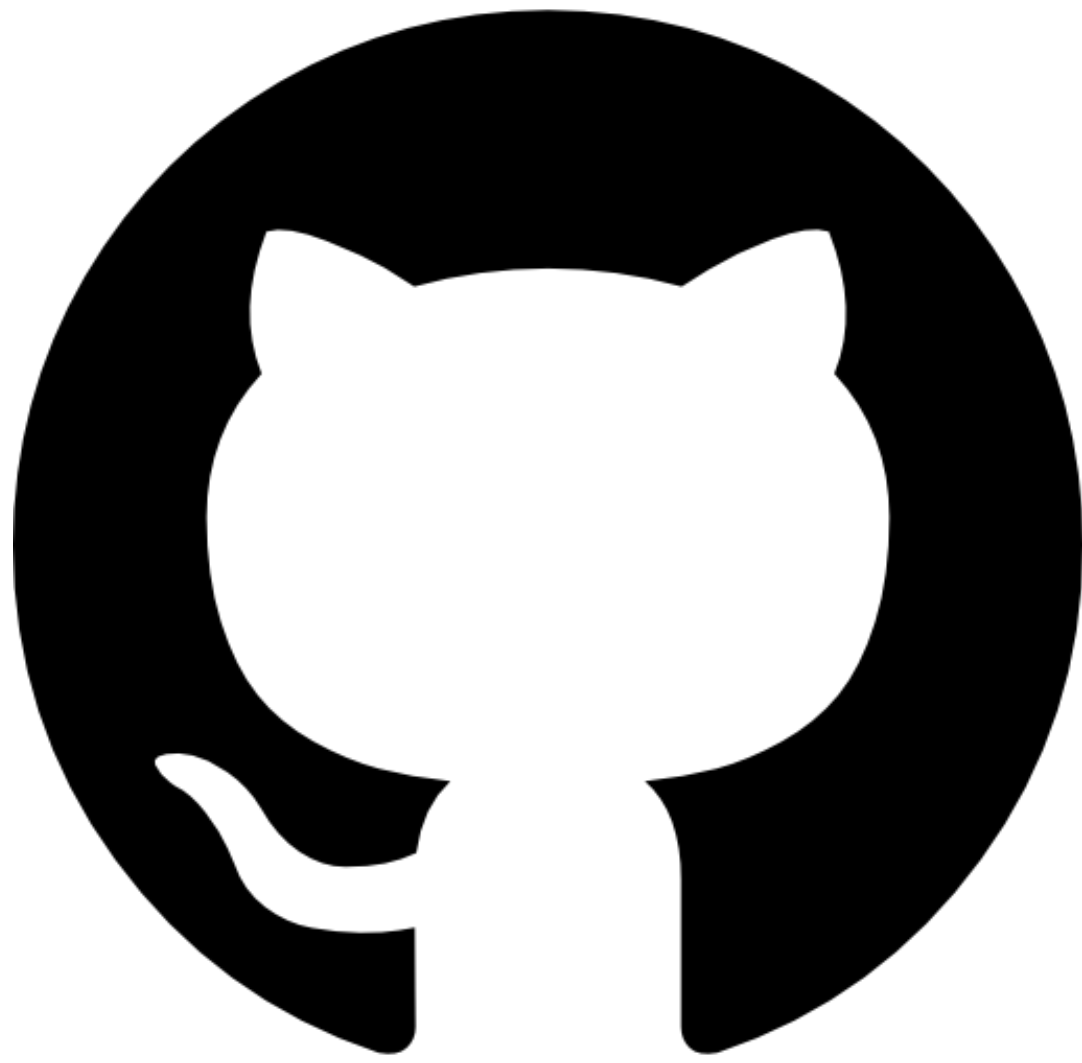
Quantum Neural Networks for MNIST Classification

- Encode the classical values using phase encoding
- Then trainable quantum layers
- Finally measurement layers



Hands-On Section

1.5 TQ for QNN



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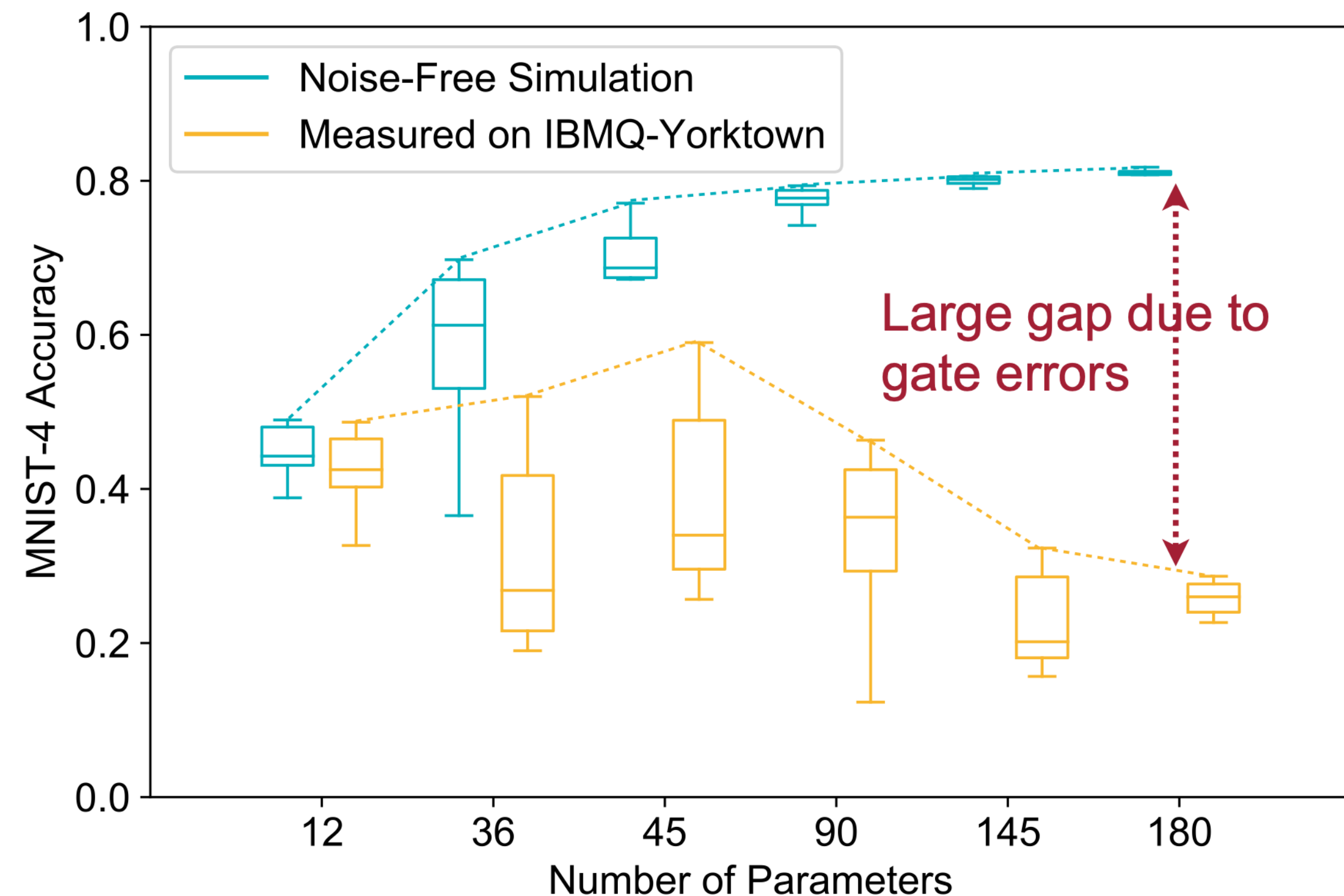
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Challenges of PQC — Noise

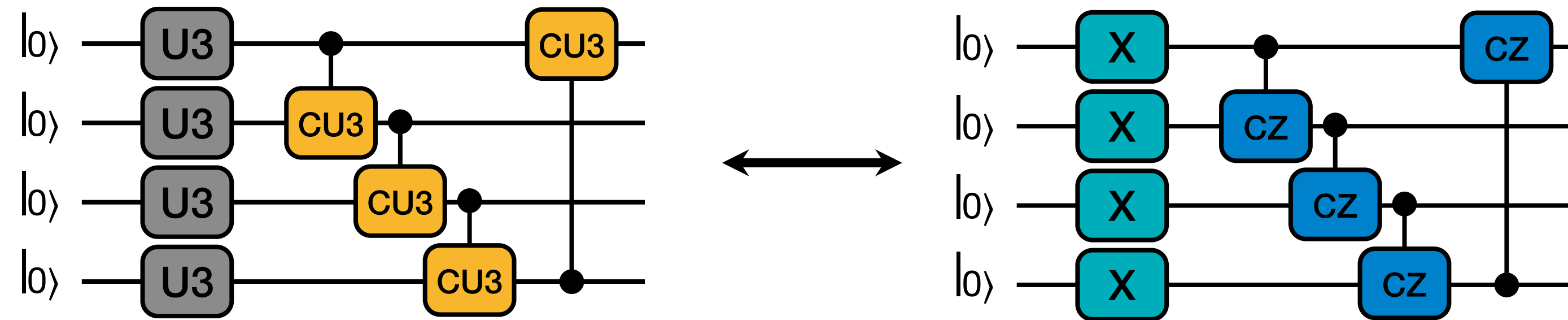
- Noise **degrades** PQC reliability
- More parameters increase the noise-free accuracy but degrade the measured accuracy
- Therefore, circuit architecture is critical



Challenges of PQC — Large Design Space

- Large design space for circuit architecture

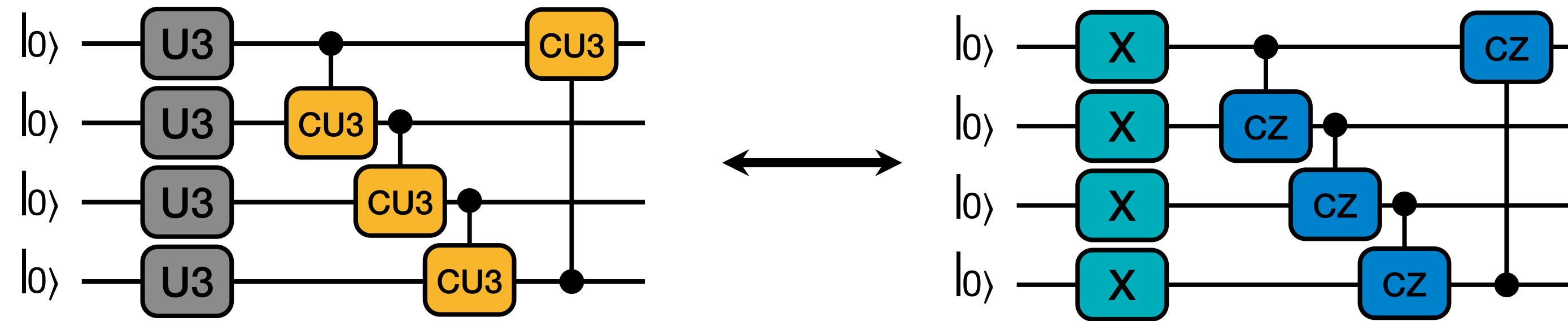
- Type of gates



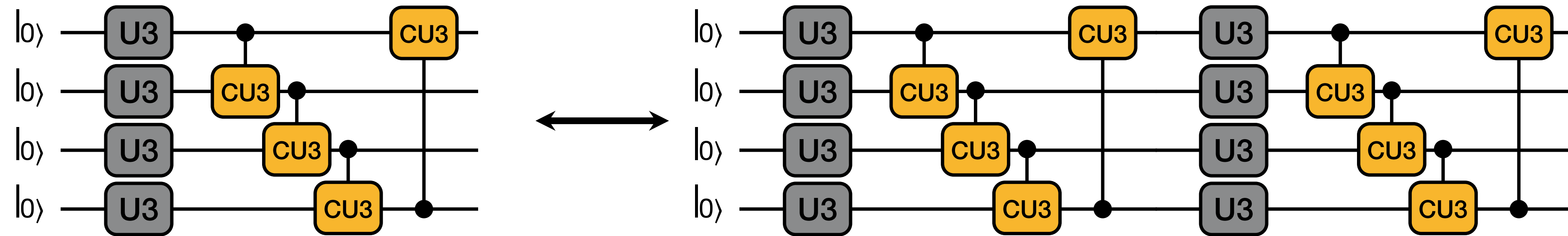
Challenges of PQC — Large Design Space

- Large design space for circuit architecture

- Type of gates



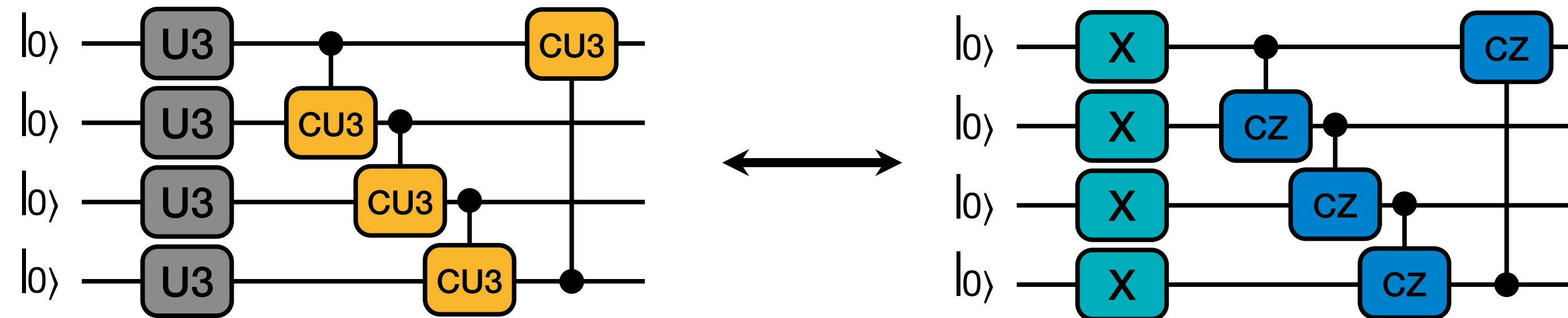
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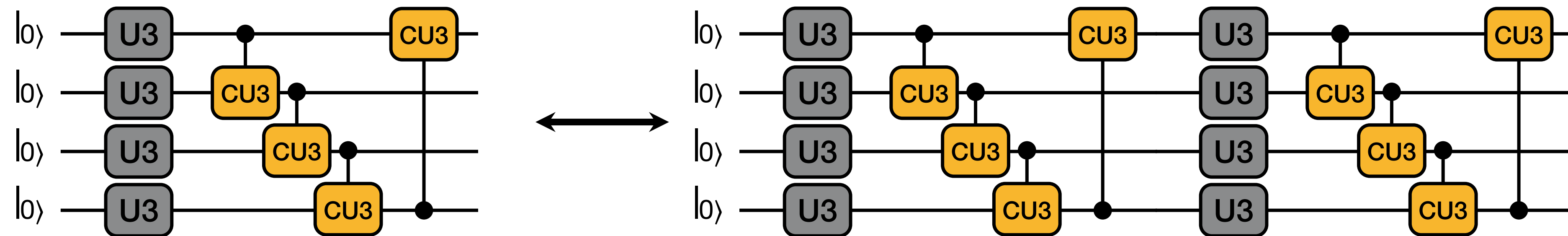
Challenges of PQC — Large Design Space

- Large design space for circuit architecture

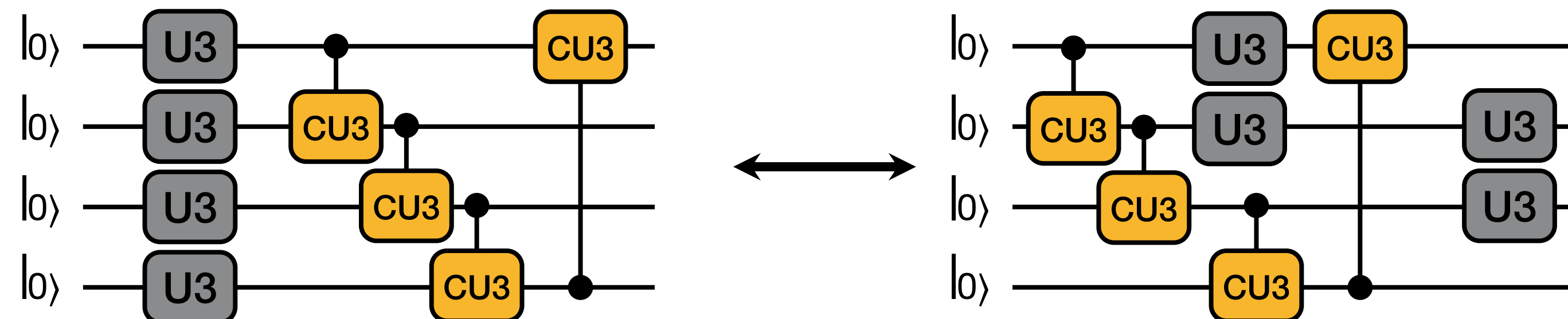
- Type of gates



- Number of gates



- Position of gates



Goal of QuantumNAS

Automatically & efficiently search for noise-robust quantum circuit

Train one “SuperCircuit”,
providing parameters to
many “SubCircuits”

Solve the challenge of large
design space

(1) Quantum noise feedback in
the search loop
(2) Co-search the circuit
architecture and qubit mapping

Solve the challenge of large
quantum noise

QuantumNAS

- SuperCircuit Construction and Training
- Noise-Adaptive Evolutionary Co-Search of SubCircuit and Qubit Mapping
- Train the Searched SubCircuit
- Iterative Quantum Gate Pruning

QuantumNAS

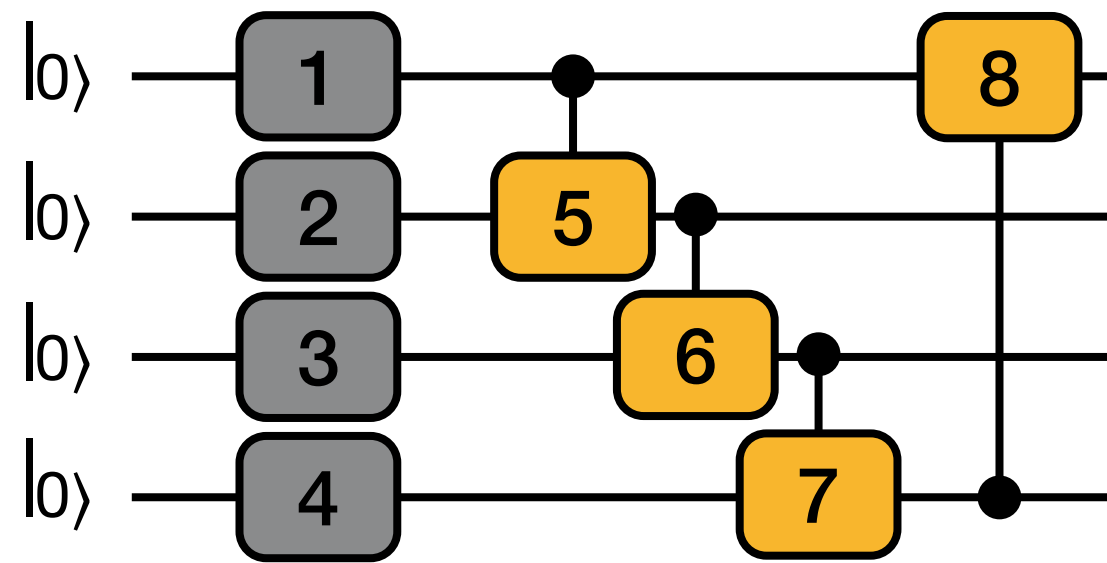
- SuperCircuit Construction and Training
- Noise-Adaptive Evolutionary Co-Search of SubCircuit and Qubit Mapping
- Train the Searched SubCircuit
- Iterative Quantum Gate Pruning

SuperCircuit & SubCircuit

- Firstly construct a design space. For example, a design space of maximum 4 U3 in the first layer and 4 CU3 gates in the second layer

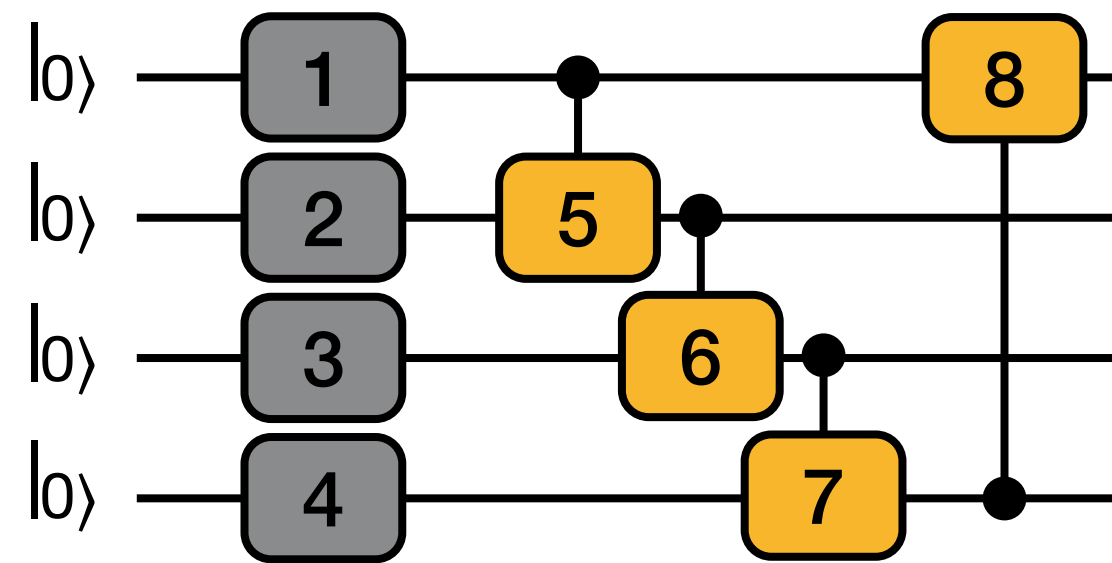
SuperCircuit & SubCircuit

- Firstly construct a design space. For example, a design space of maximum 4 U3 in the first layer and 4 CU3 gates in the second layer
- SuperCircuit: the circuit with the **largest** number of gates in the design space
 - Example: SuperCircuit in U3+CU3 space

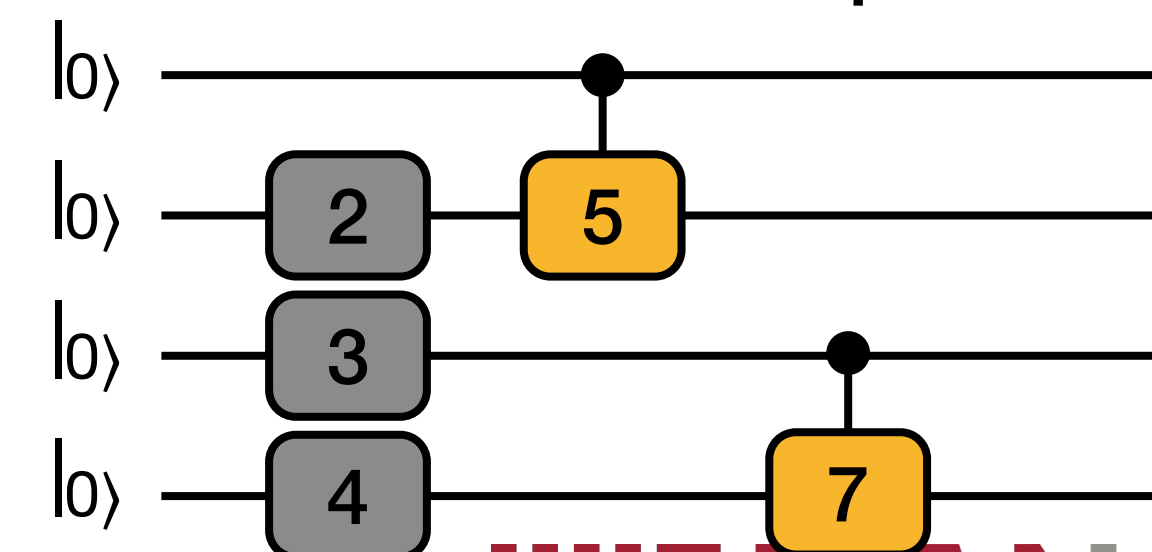
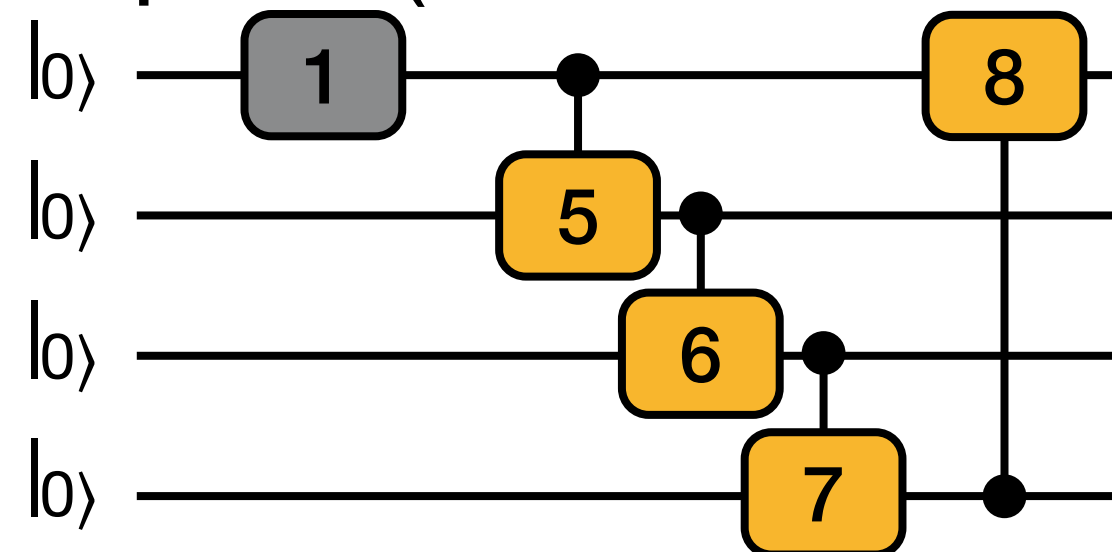
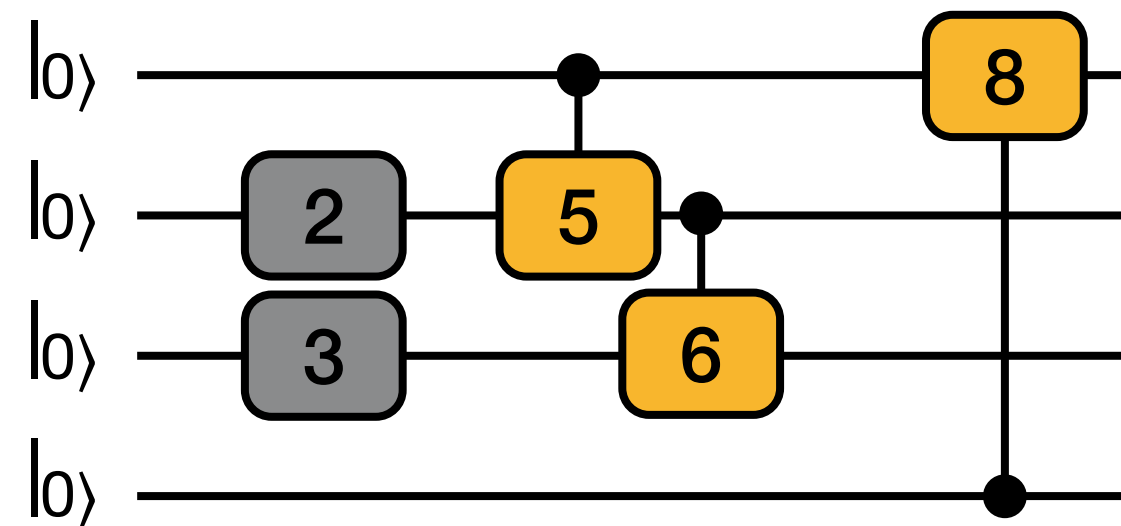


SuperCircuit & SubCircuit

- Firstly construct a design space. For example, a design space of maximum 4 U3 in the first layer and 4 CU3 gates in the second layer
- SuperCircuit: the circuit with the **largest** number of gates in the design space
 - Example: SuperCircuit in U3+CU3 space



- Each candidate circuit in the design space (called SubCircuit) is a **subset** of the SuperCircuit



SuperCircuit Construction

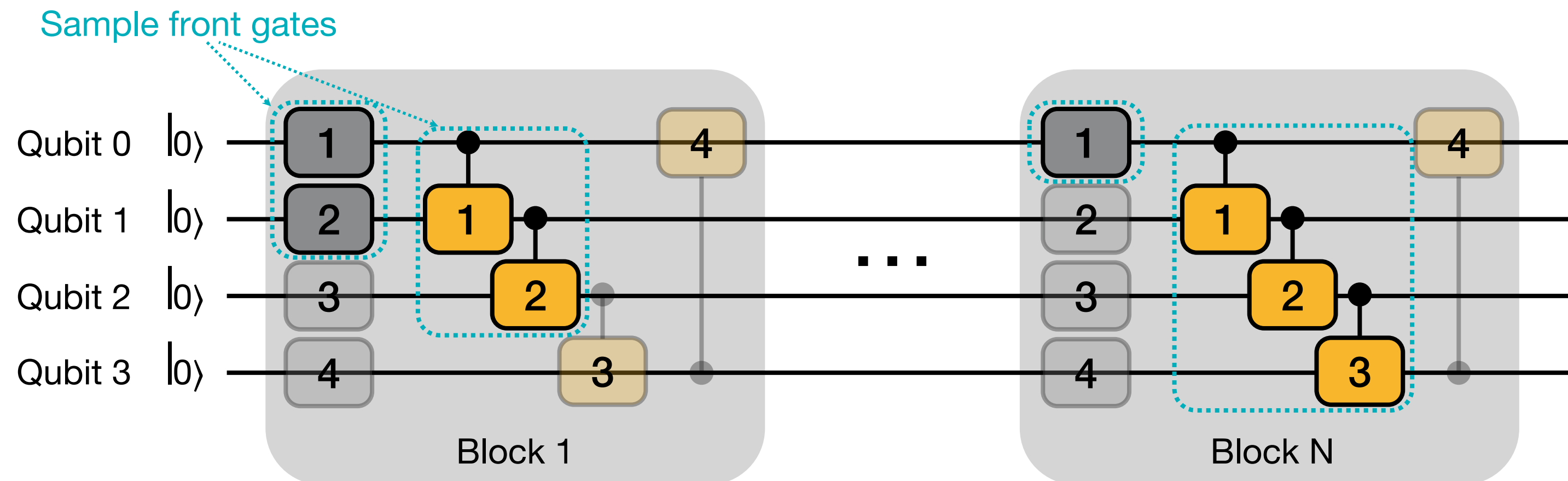
- Why use a SuperCircuit?
 - Enables **efficient** search of architecture candidates without training each
 - SubCircuit inherits parameters from SuperCircuit
 - With **inherited** parameters, we find some good SubCircuits, we find that they are **also good SubCircuits** with parameters **trained from-scratch** individually

SuperCircuit Training

- In one SuperCircuit Training step:
 - Sample a gate subset of SuperCircuit (a SubCircuit)
 - Front Sampling and Restricted Sampling
 - Only use the subset to perform the task and updates the parameters in the subset
 - Parameter updates are cumulative across steps

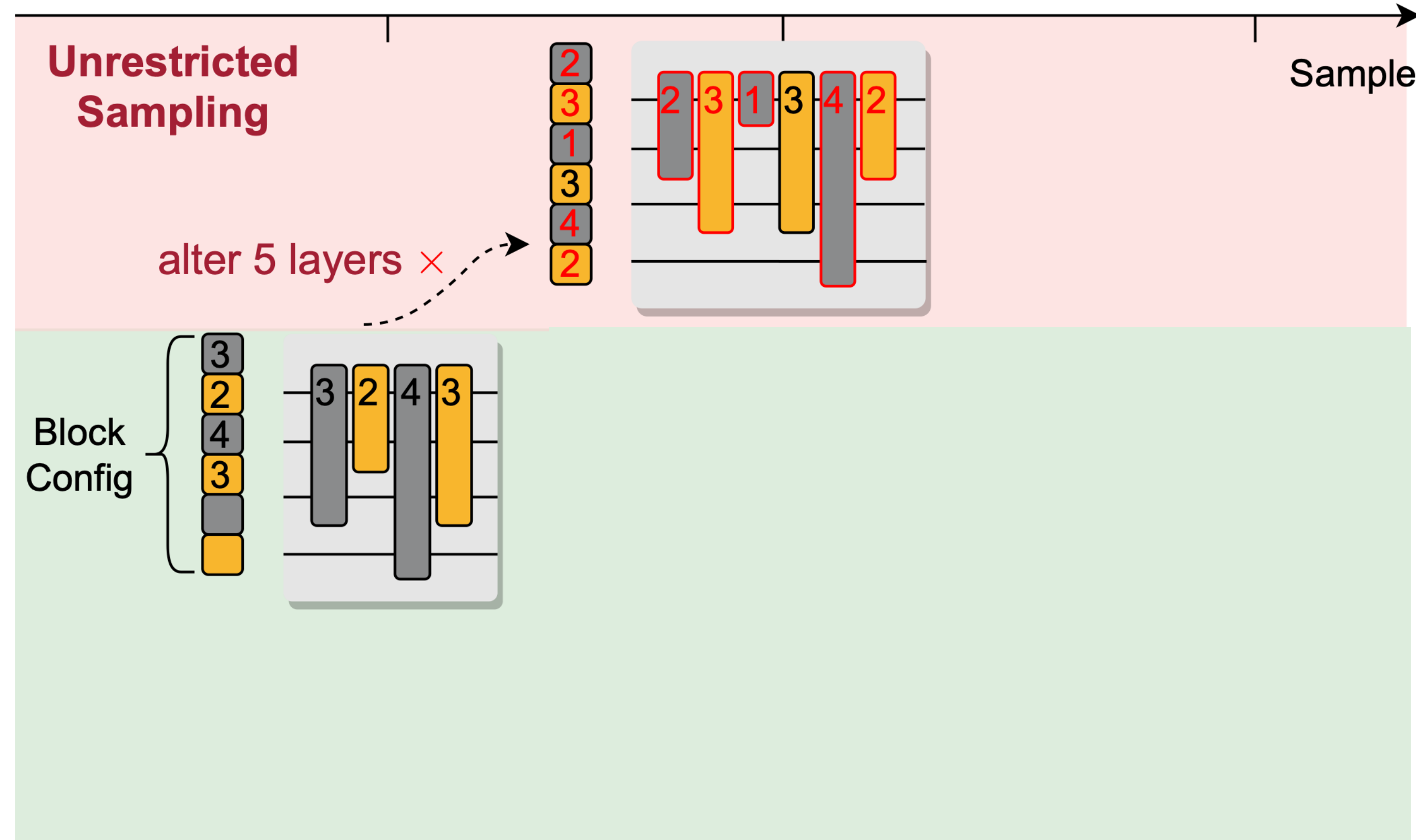
Front Sampling

- During sampling, we first sample total number of blocks, then sample gates within each block
 - Front sampling: Only the **front** several blocks and **front** several gates can be sampled to make SuperCircuit training more stable



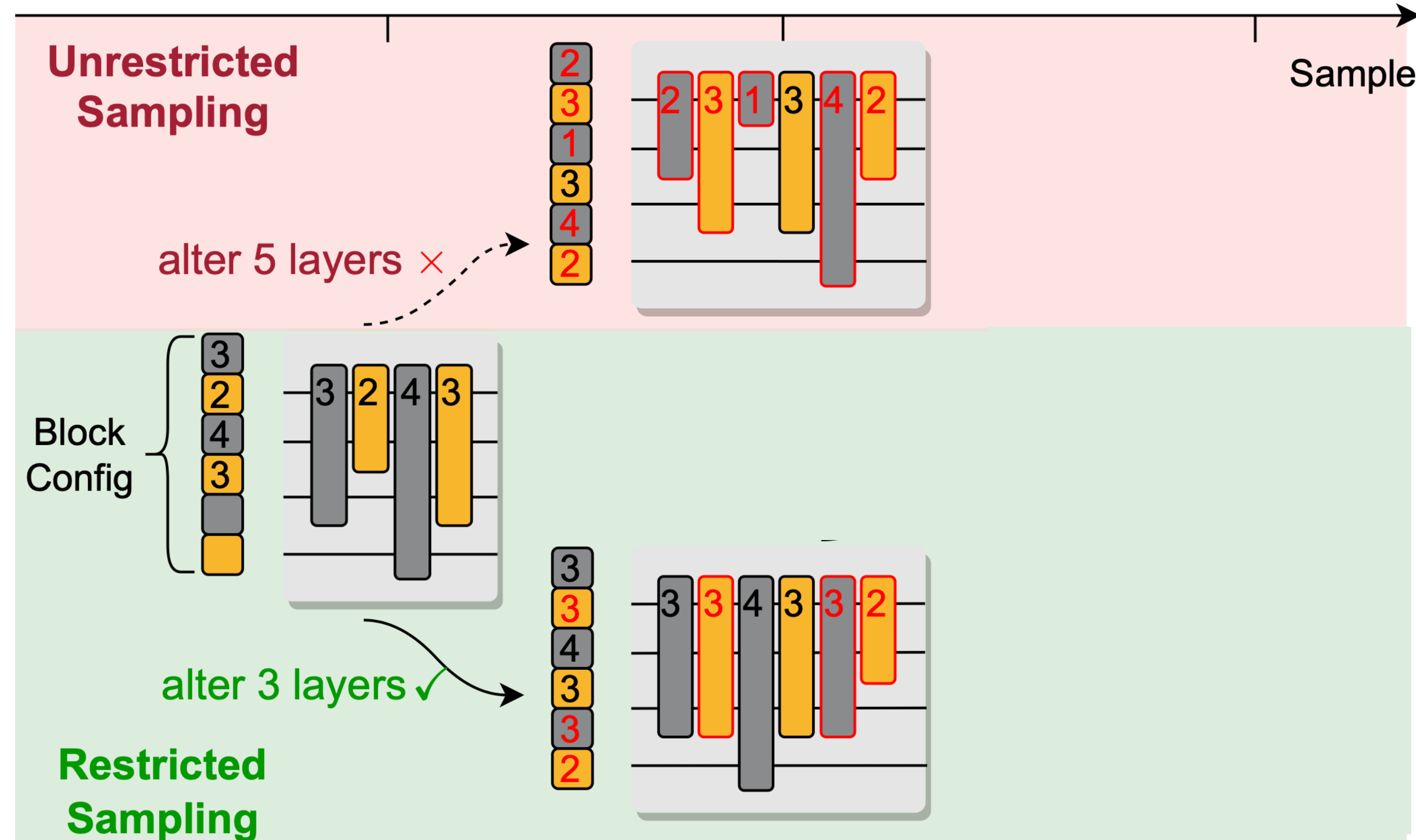
Restricted Sampling

- Restricted Sampling:
 - Restrict the difference between SubCircuits of two consecutive steps
 - For example: restrict to at most 4 different layers



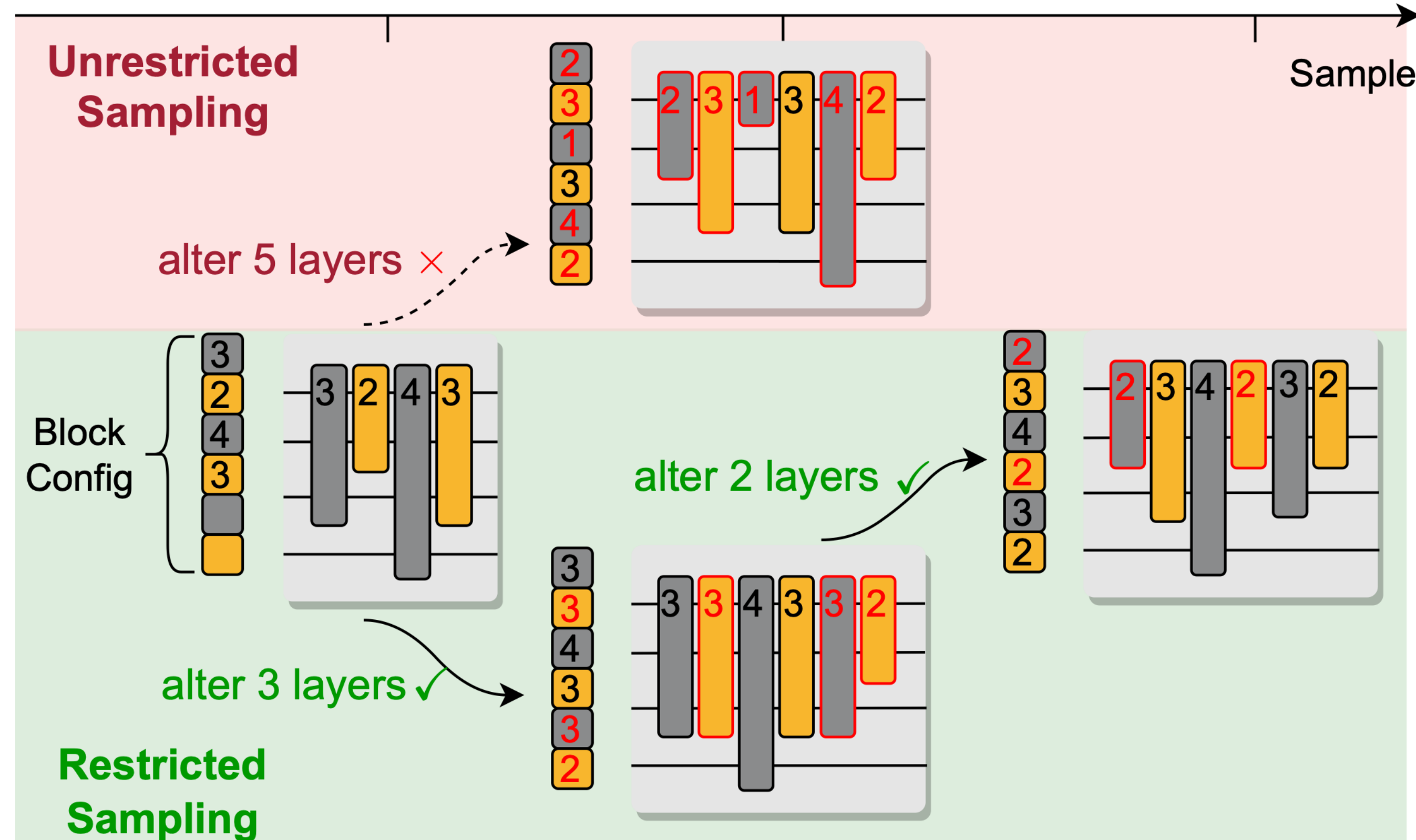
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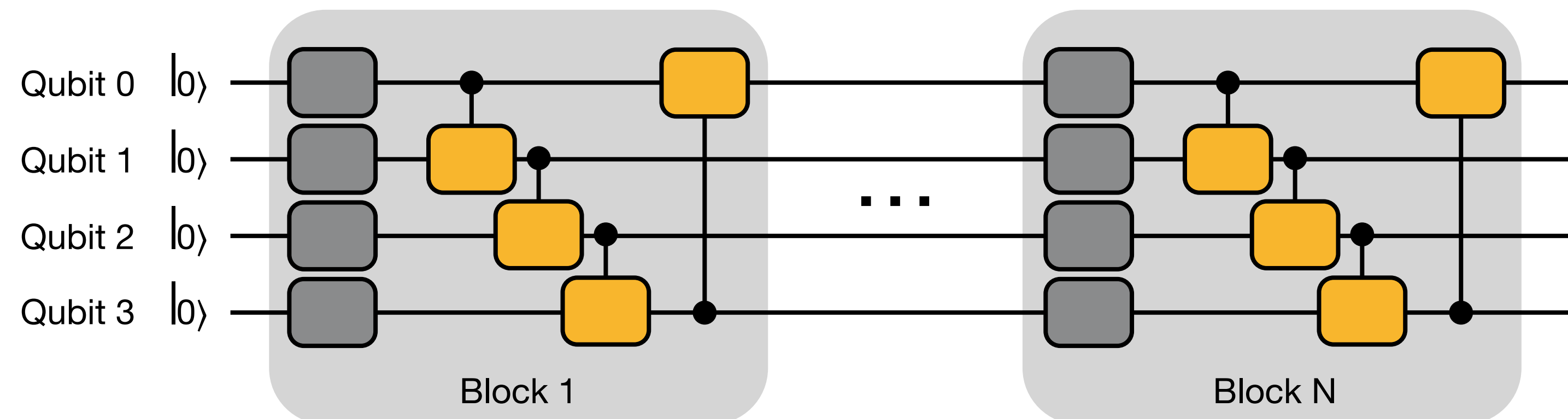
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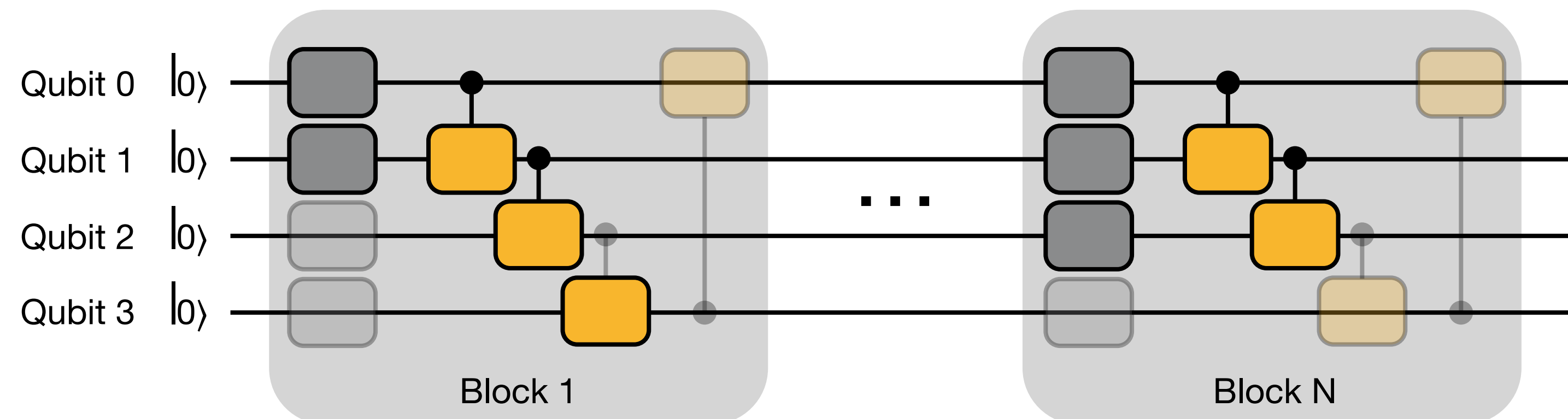
Train SuperCircuit for Multiple Steps

- In one SuperCircuit Training step: Sample and Train



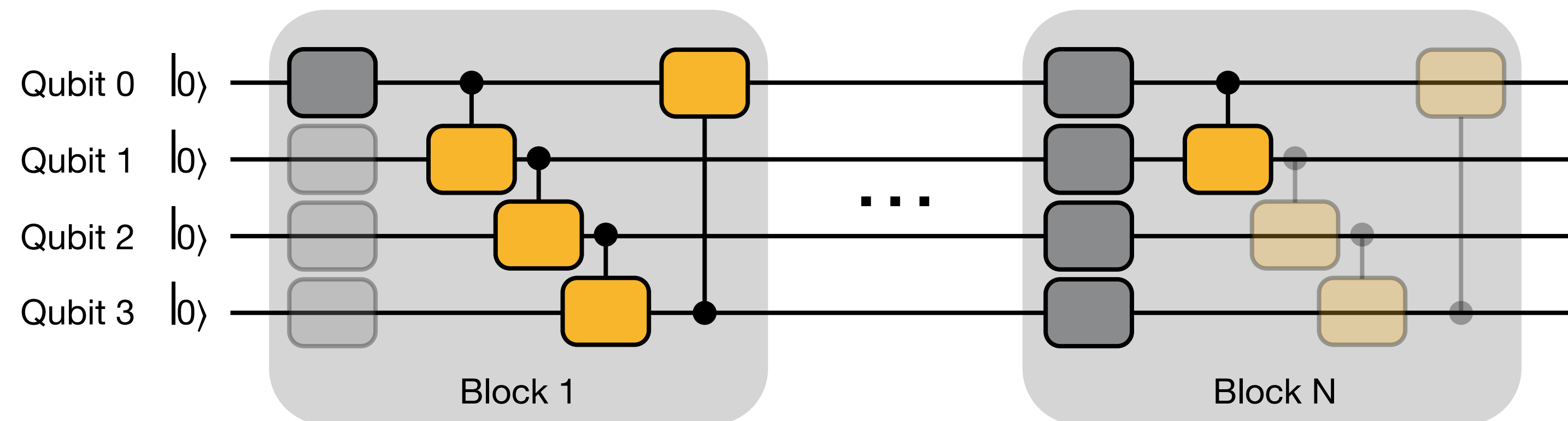
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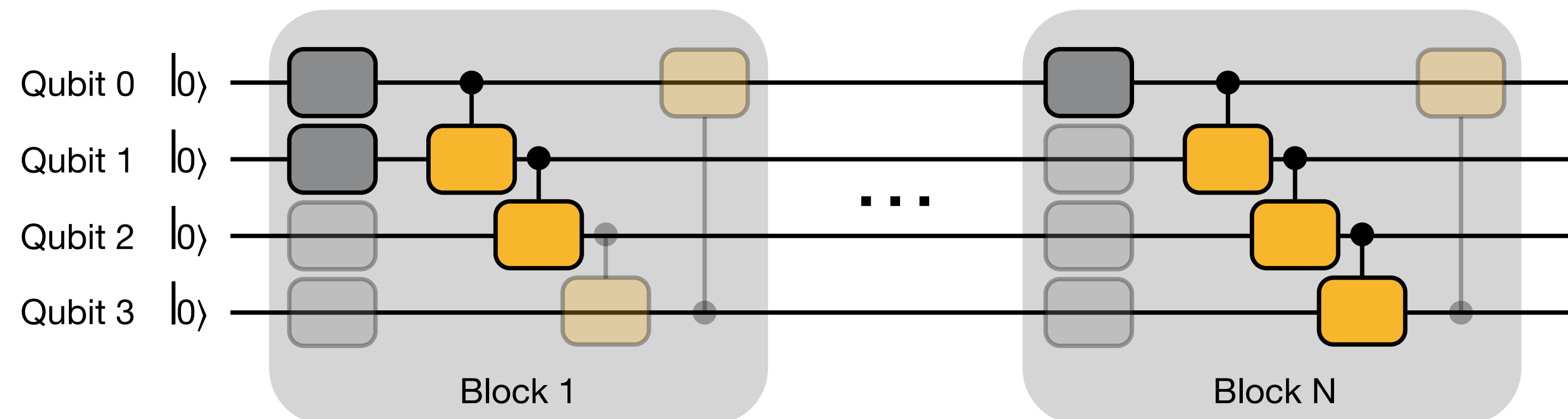
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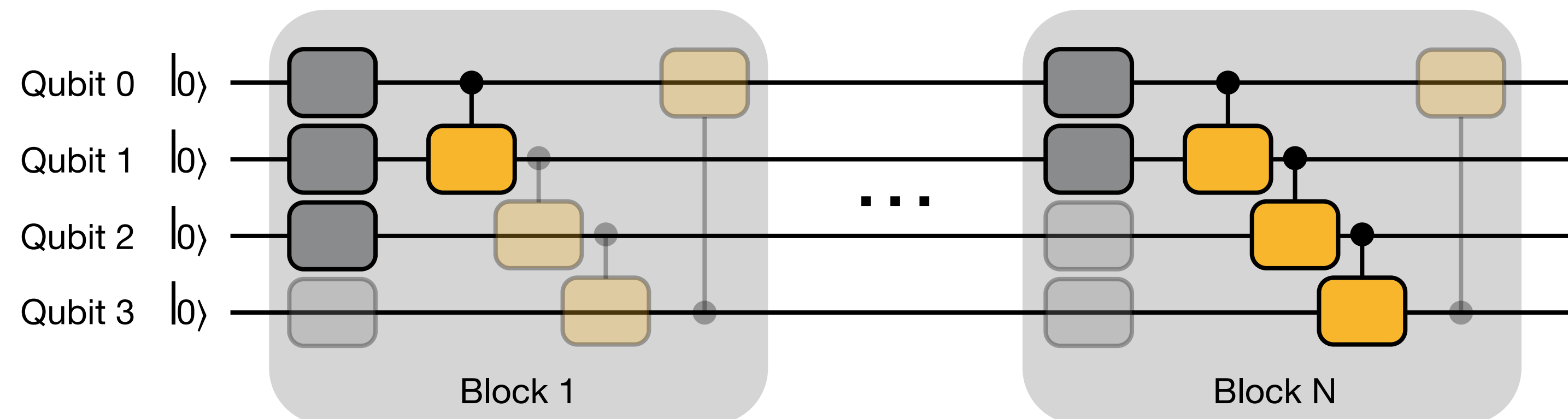
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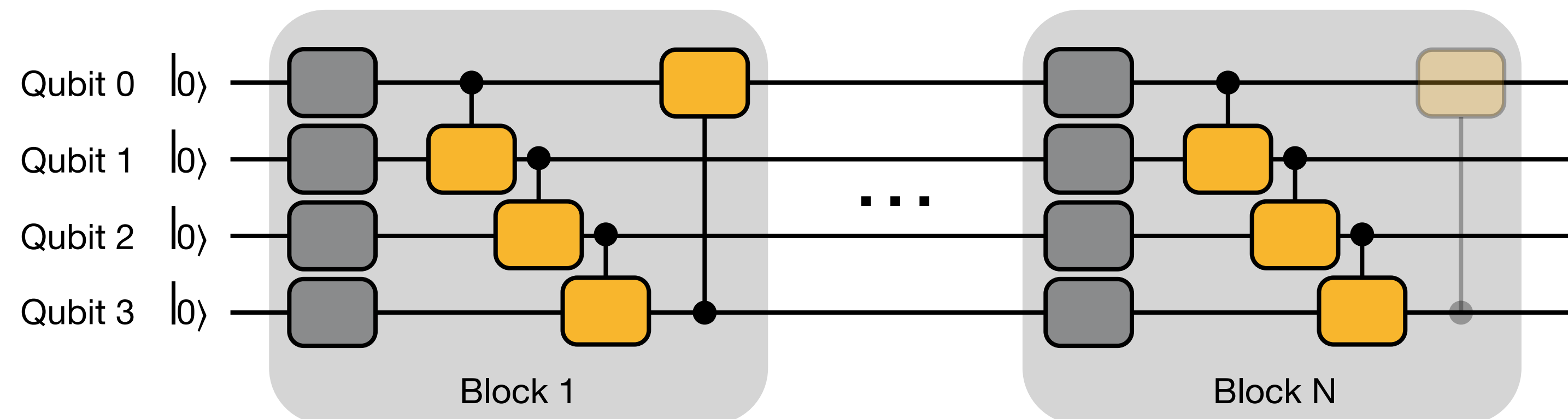
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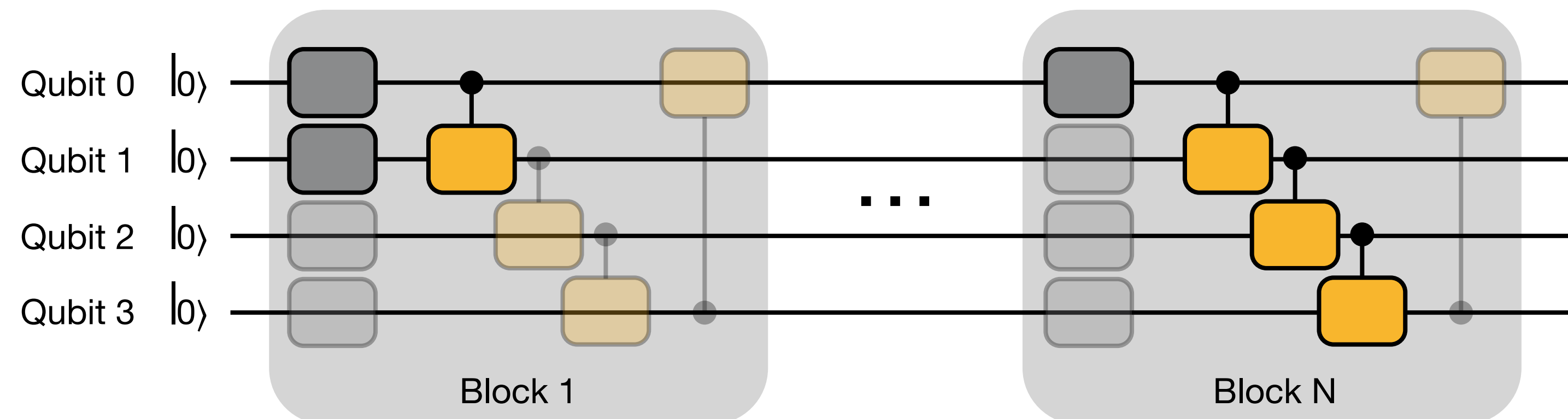
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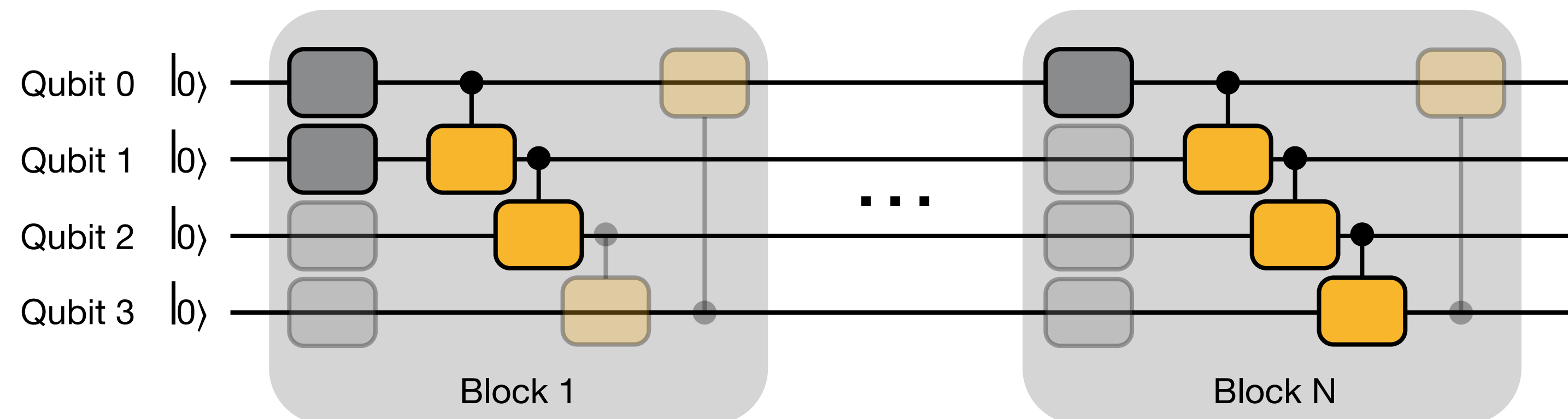
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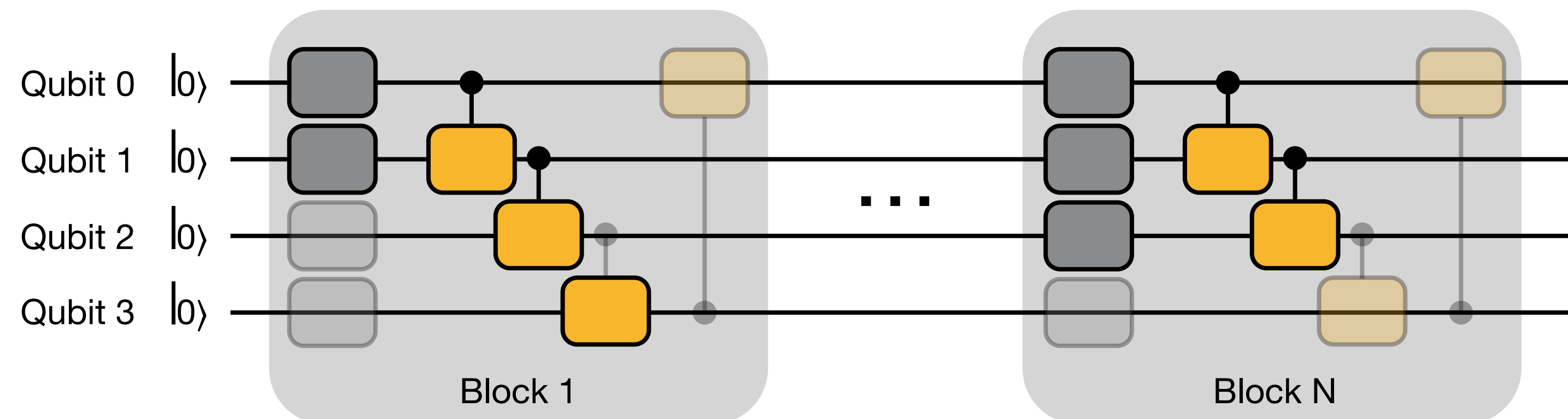
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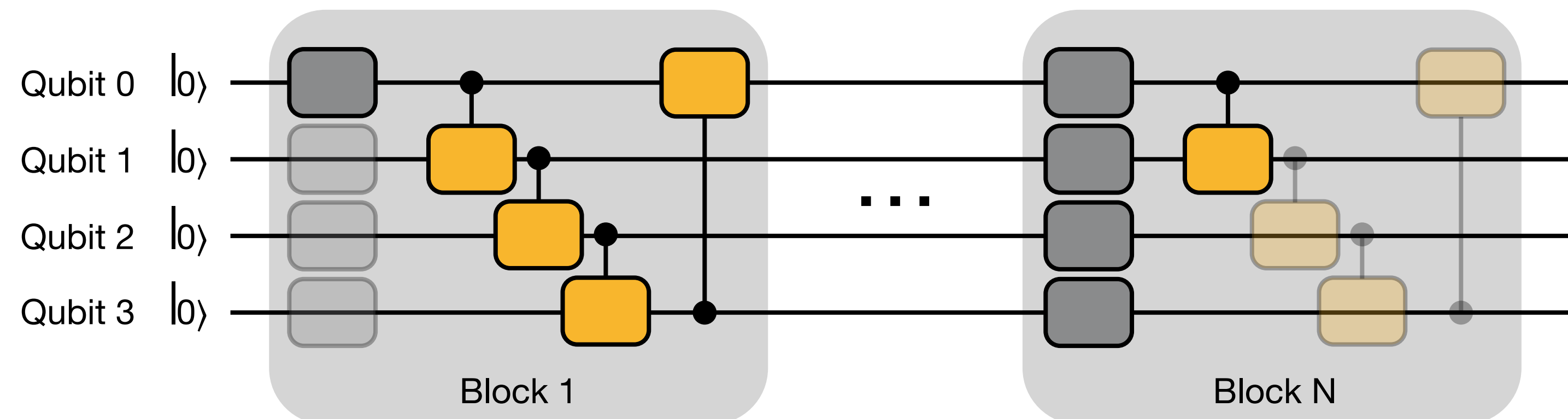
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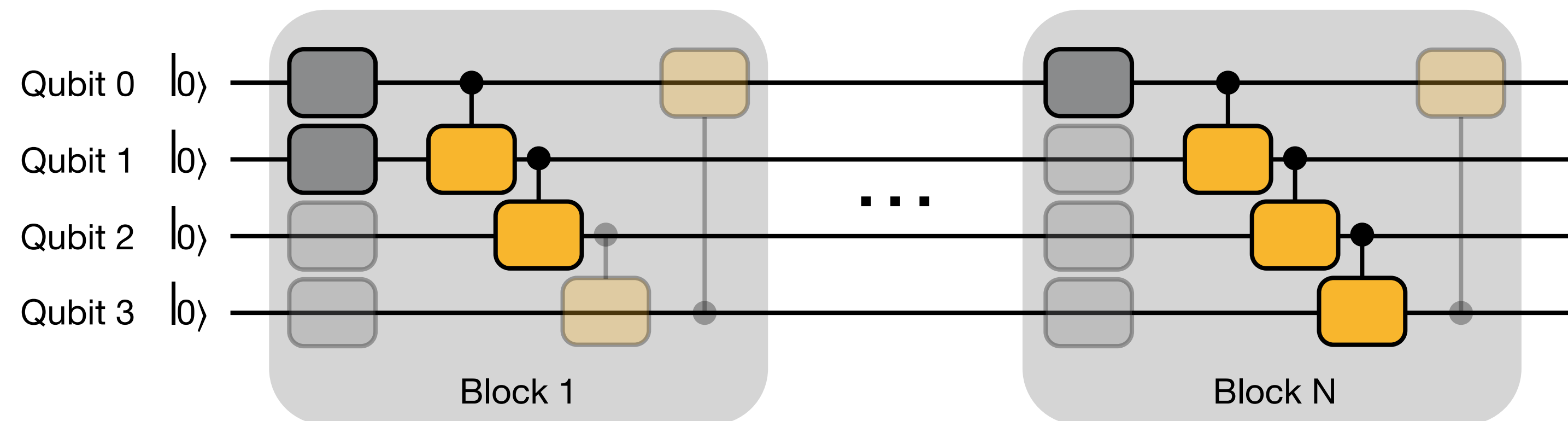
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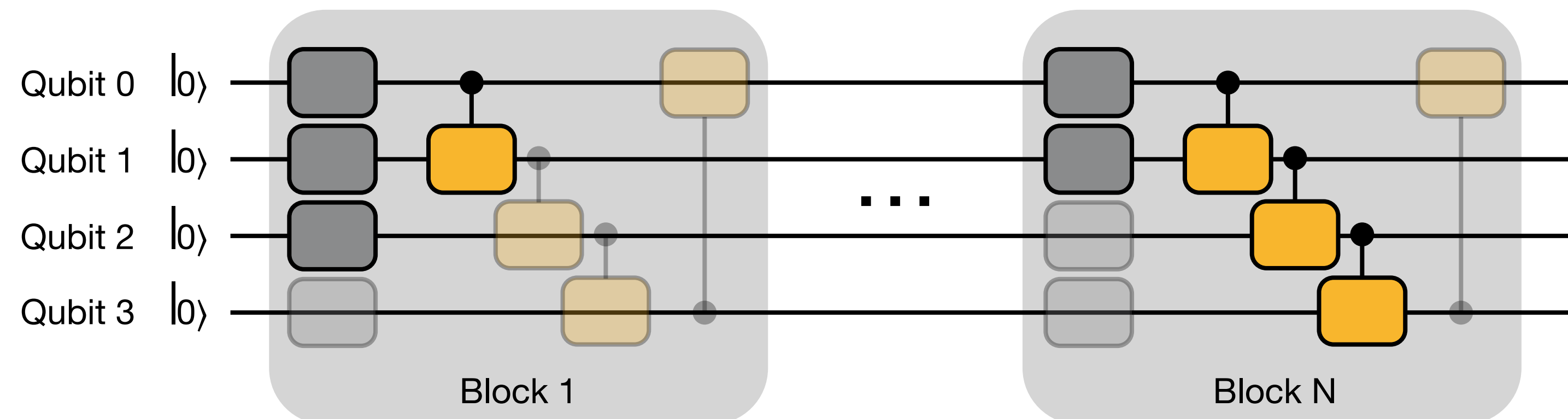
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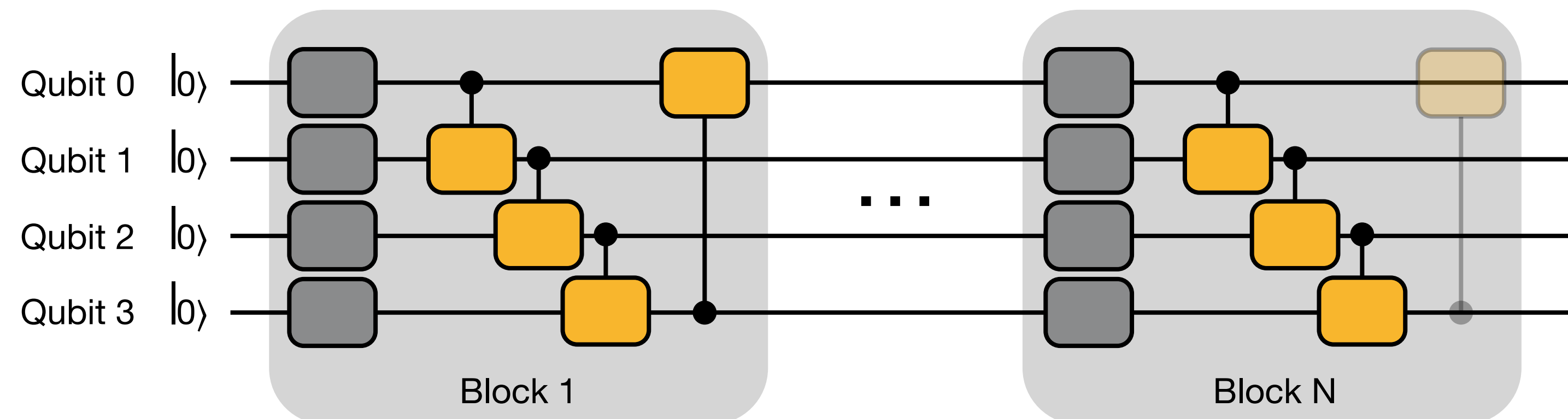
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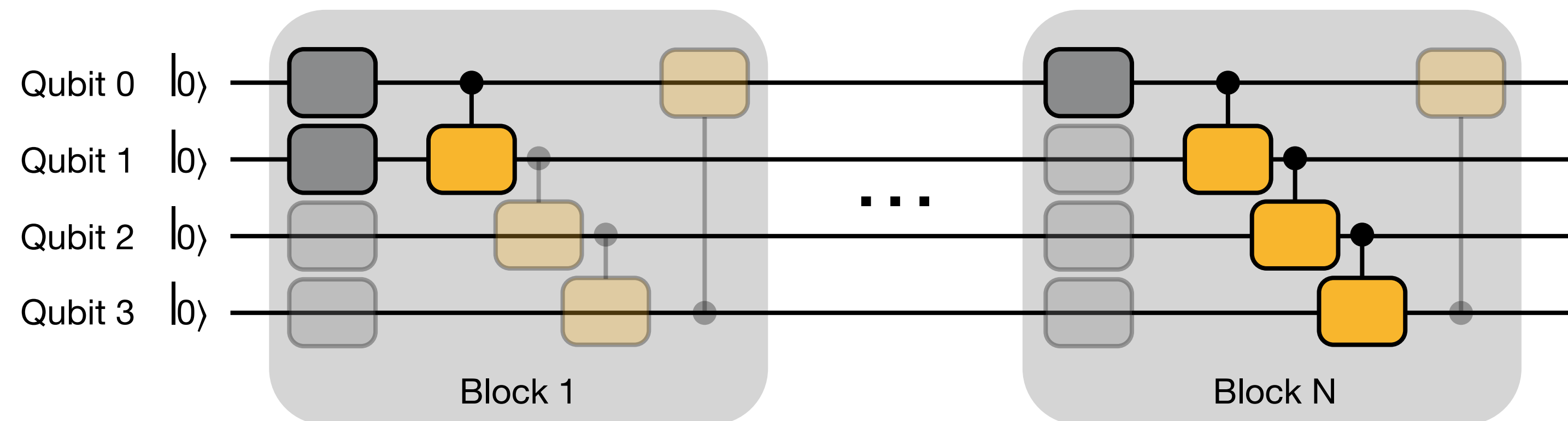
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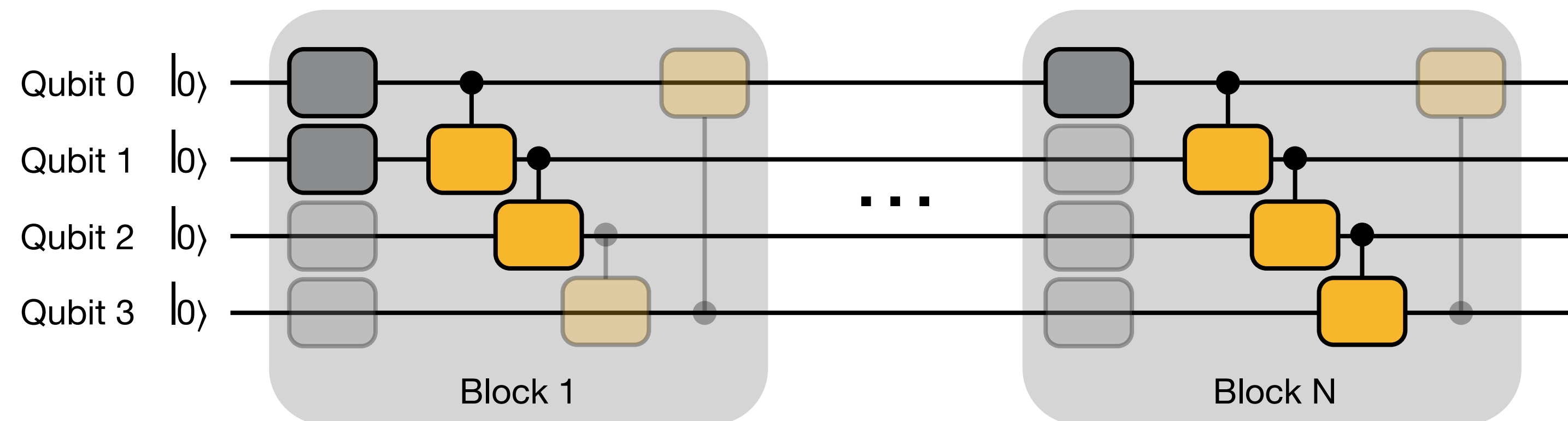
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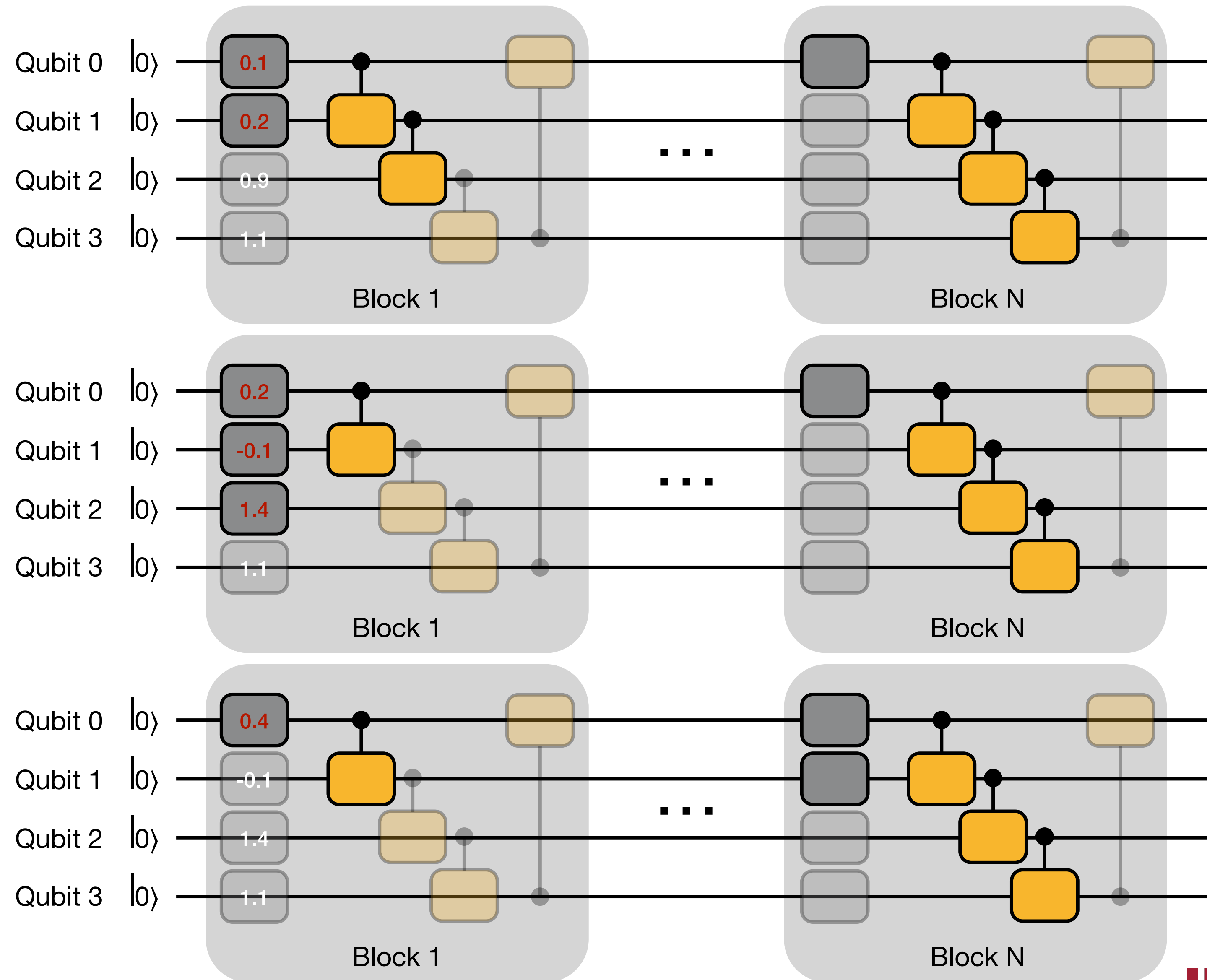


Train SuperCircuit for Multiple Steps

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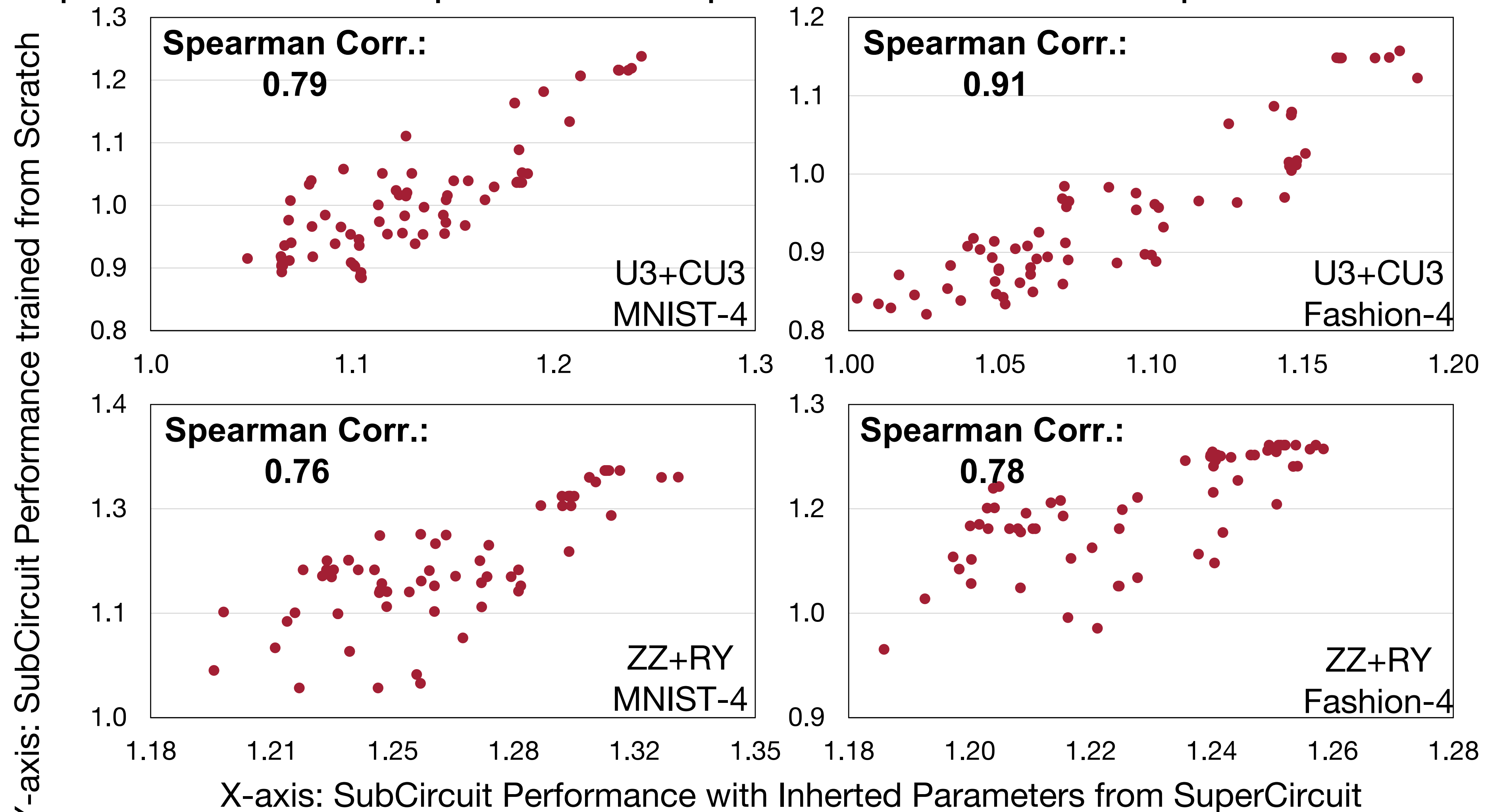


Train SuperCircuit for Multiple Steps



How Reliable is the SuperCircuit?

- Inherited parameters from SuperCircuit can provide accurate relative performance

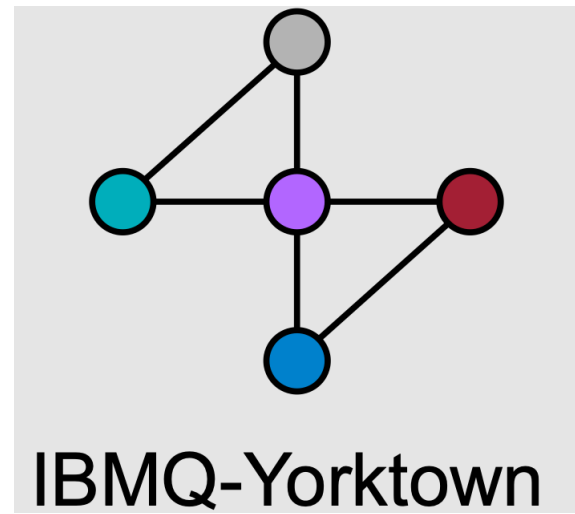


QuantumNAS

- SuperCircuit Construction and Training
- **Noise-Adaptive Evolutionary Co-Search of SubCircuit and Qubit Mapping**
- Train the Searched SubCircuit
- Iterative Quantum Gate Pruning

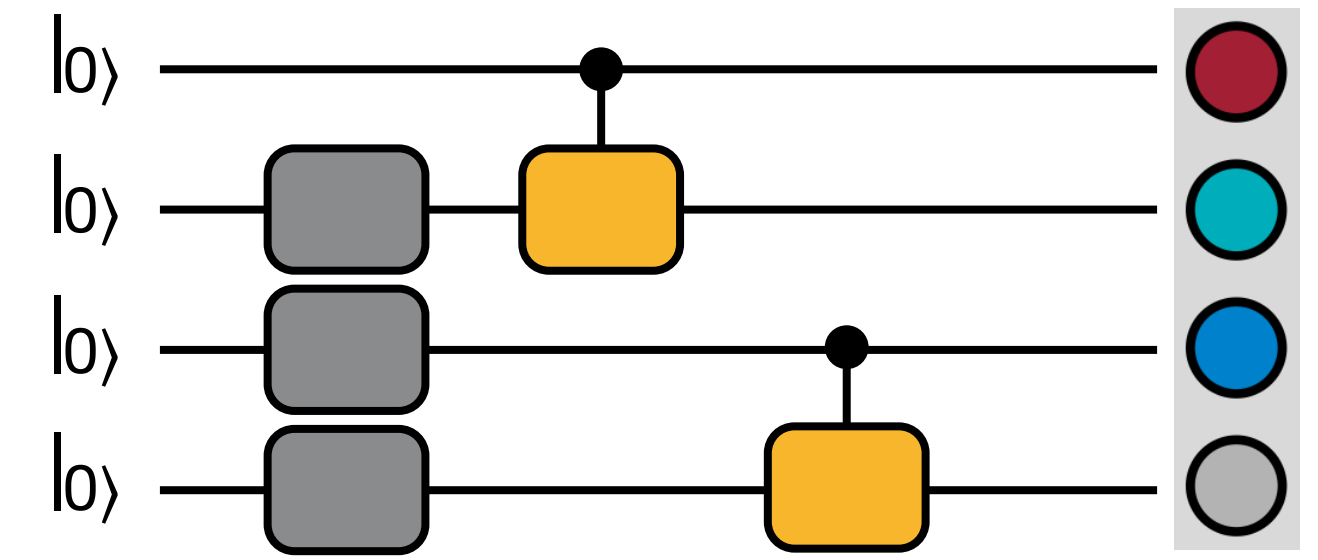
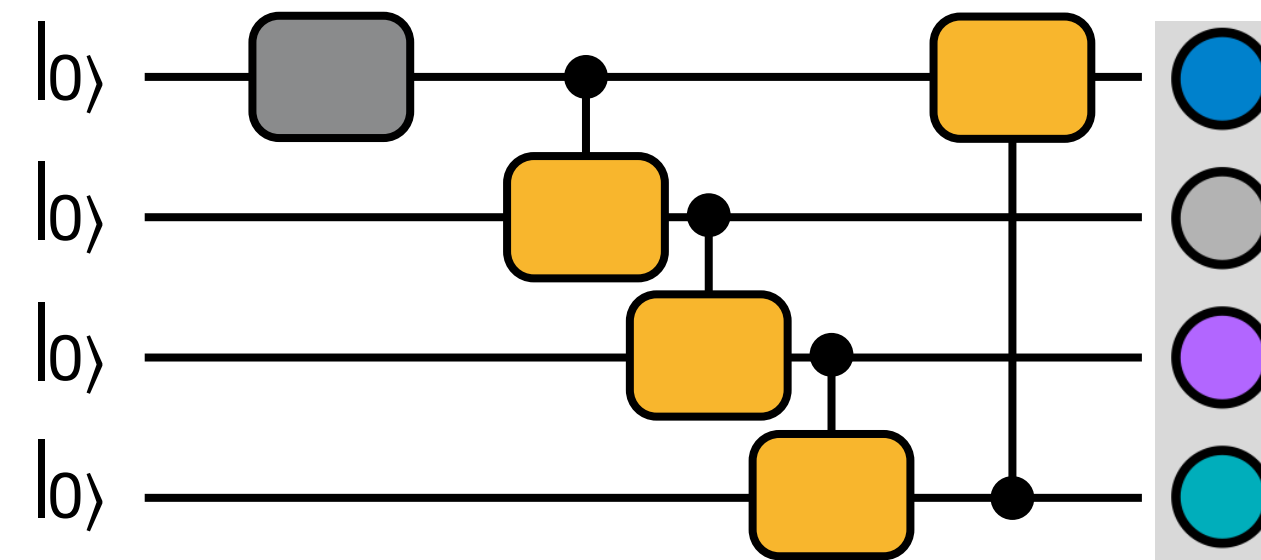
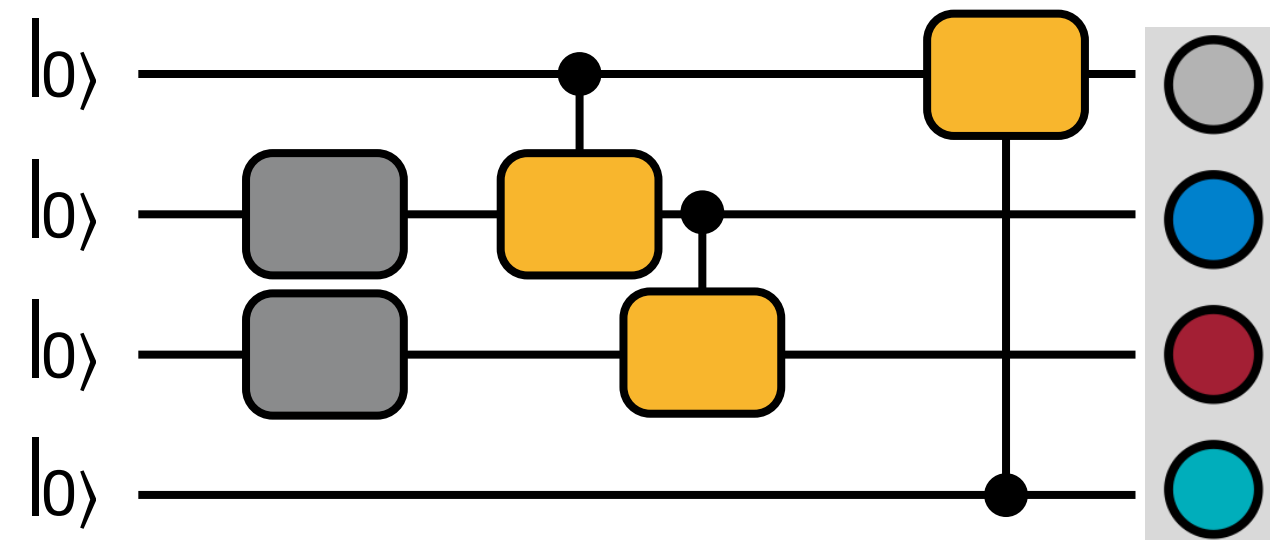
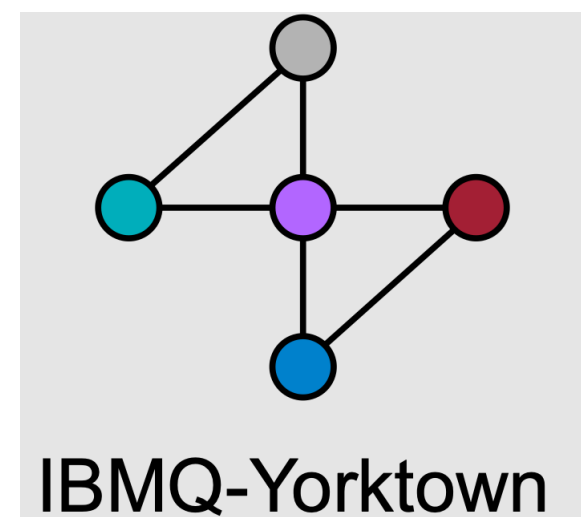
Noise-Adaptive Evolutionary Co-Search

- Search the best SubCircuit and its qubit mapping on target device



Noise-Adaptive Evolutionary Co-Search

- Search the best SubCircuit and its qubit mapping on target device



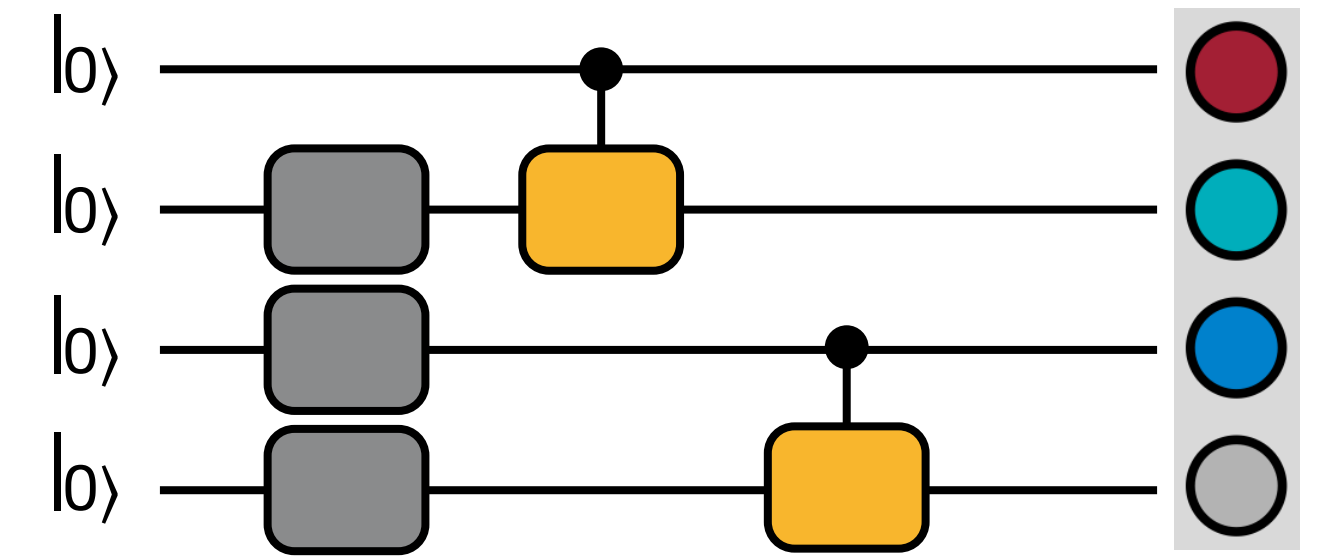
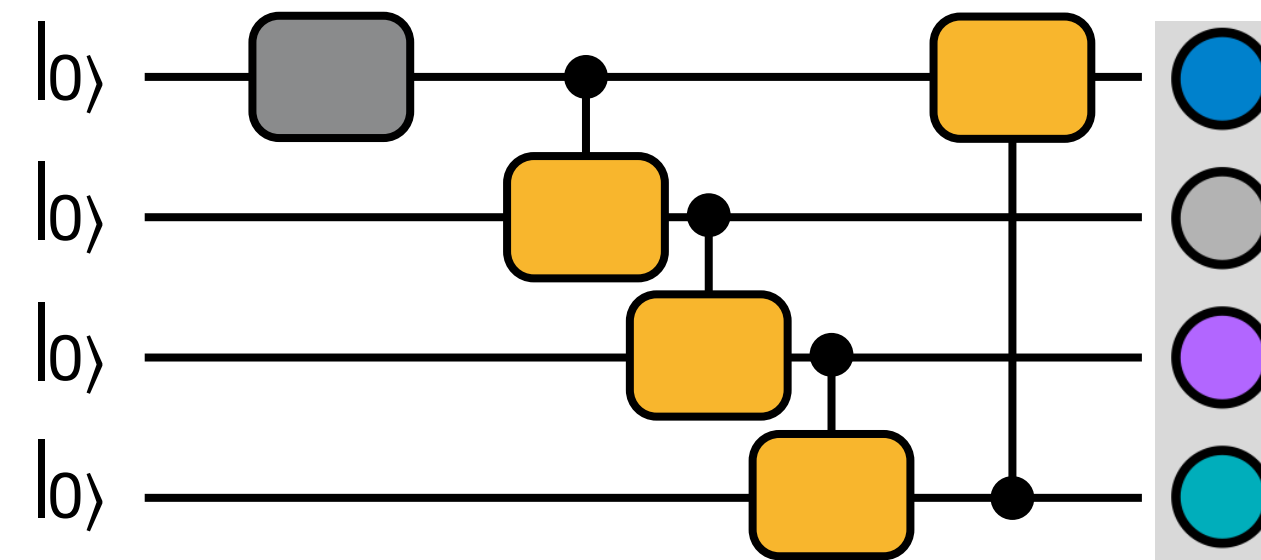
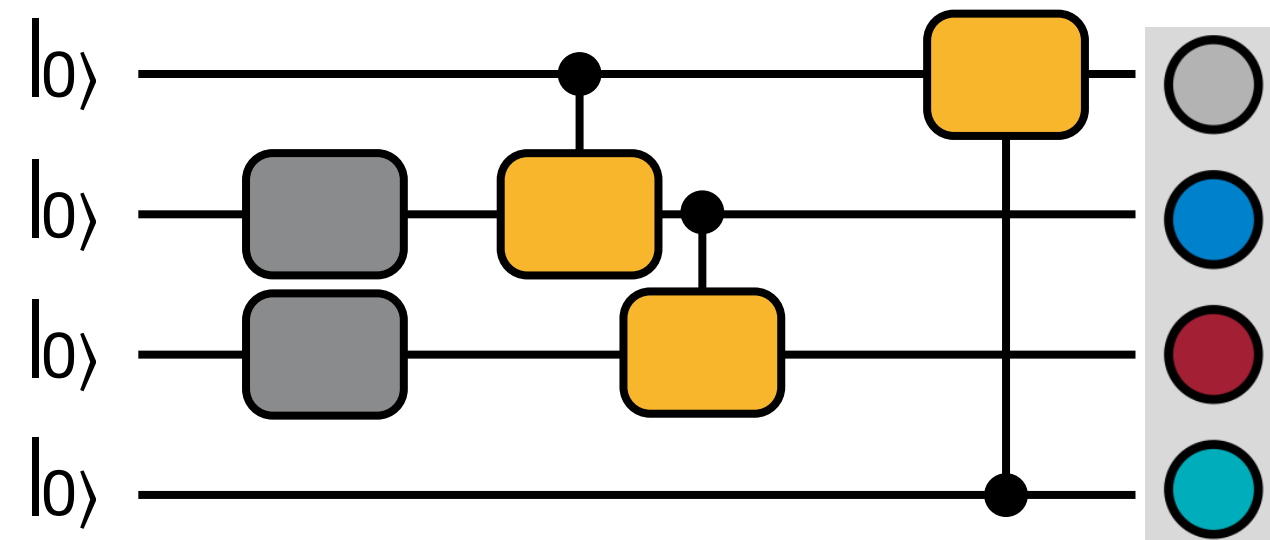
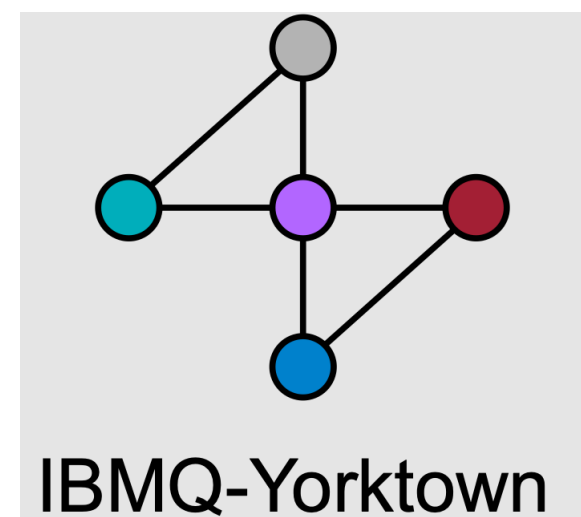
Evolutionary Search Engine
Mutation
Crossover

SubCircuit and Qubit Mapping pairs

Parameters from SuperCircuit
Simulate with noise model
Or
Directly run on real QC device

Noise-Adaptive Evolutionary Co-Search

- Search the best SubCircuit and its qubit mapping on target device



Evolutionary Search Engine
Mutation
Crossover

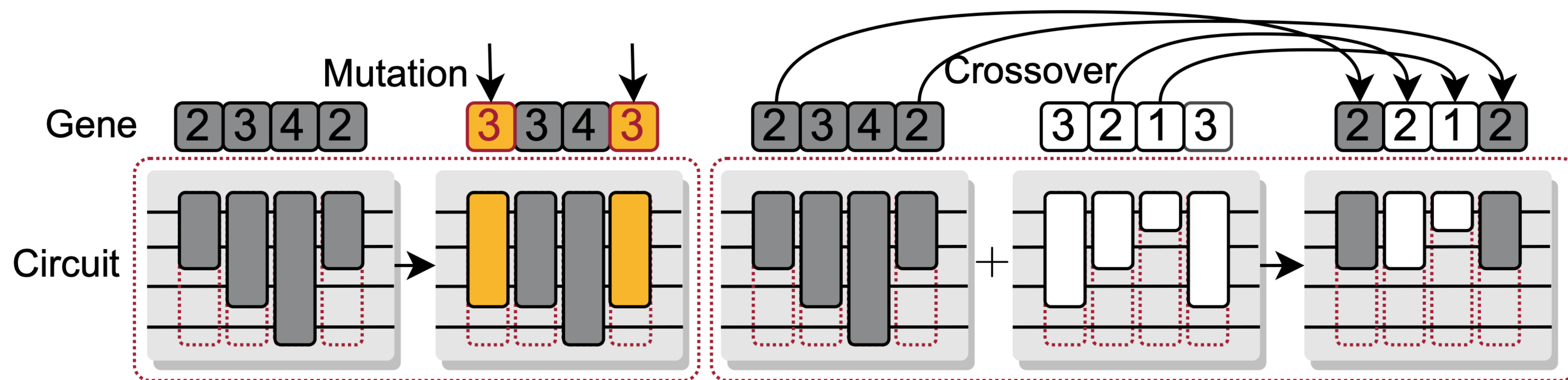
SubCircuit and Qubit Mapping pairs

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Simulate with noise model
Or
Directly run on real QC device

Performance of SubCircuit and Qubit Mapping pairs

Mutation and Crossover

- Mutation and crossover create new SubCircuit candidates



QuantumNAS

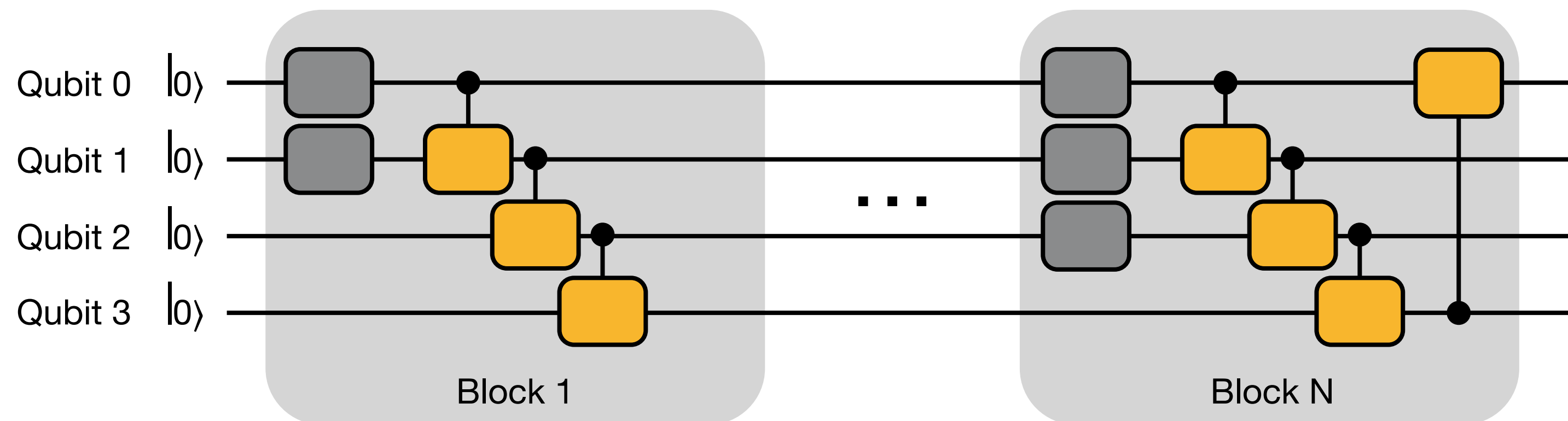
- SuperCircuit Construction and Training
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- **Train the Searched SubCircuit**
- Iterative Quantum Gate Pruning

QuantumNAS

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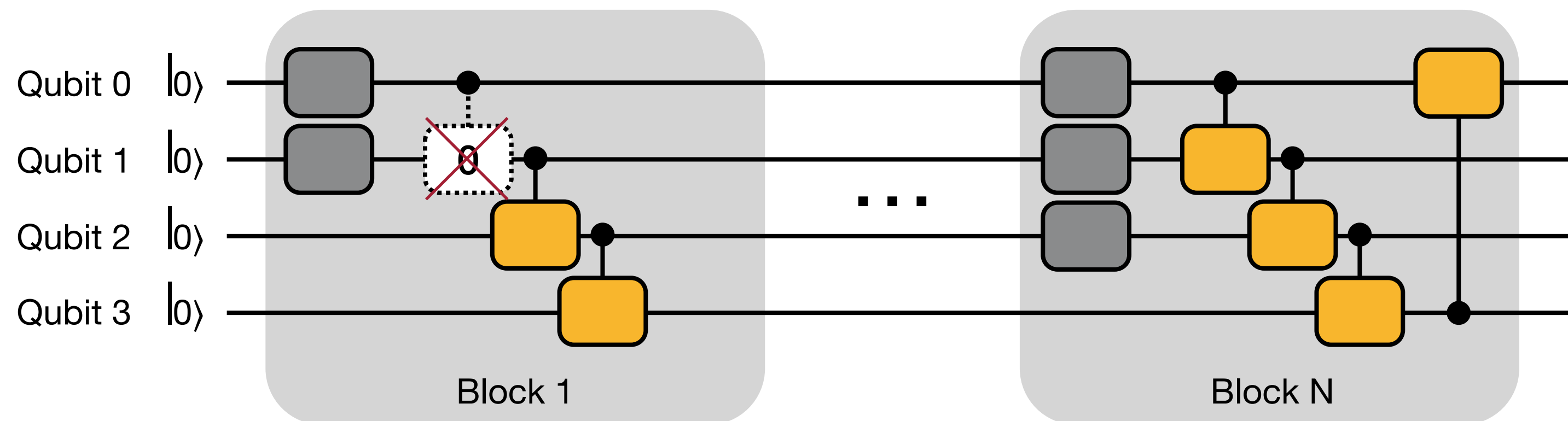
Iterative Pruning

- Some gates have parameters close to 0
 - Rotation gate with angle close to 0 has small impact on the results
- Iteratively prune small-magnitude gates and fine-tune the remaining parameters



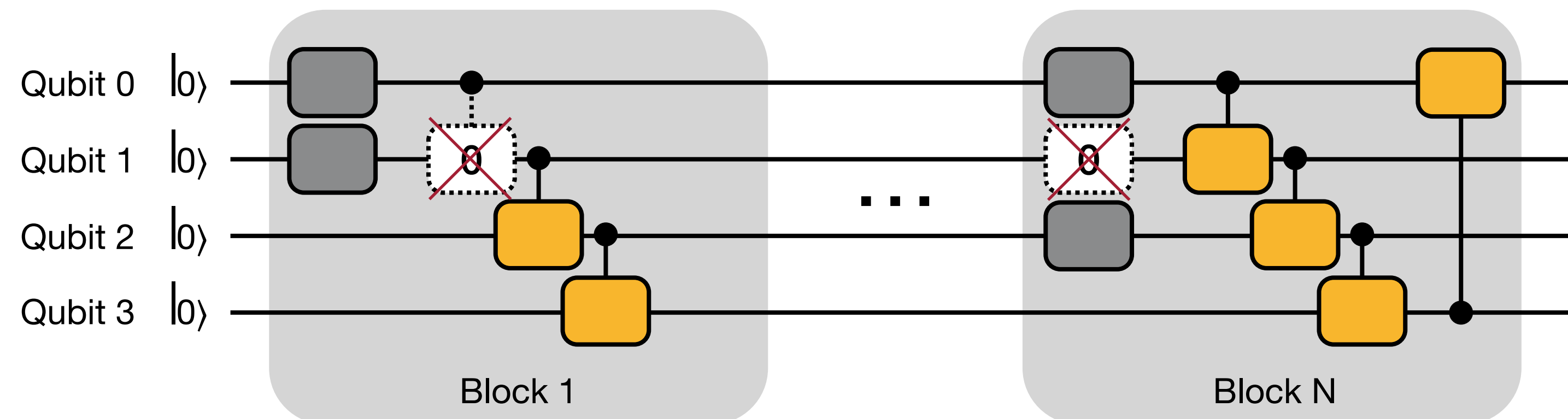
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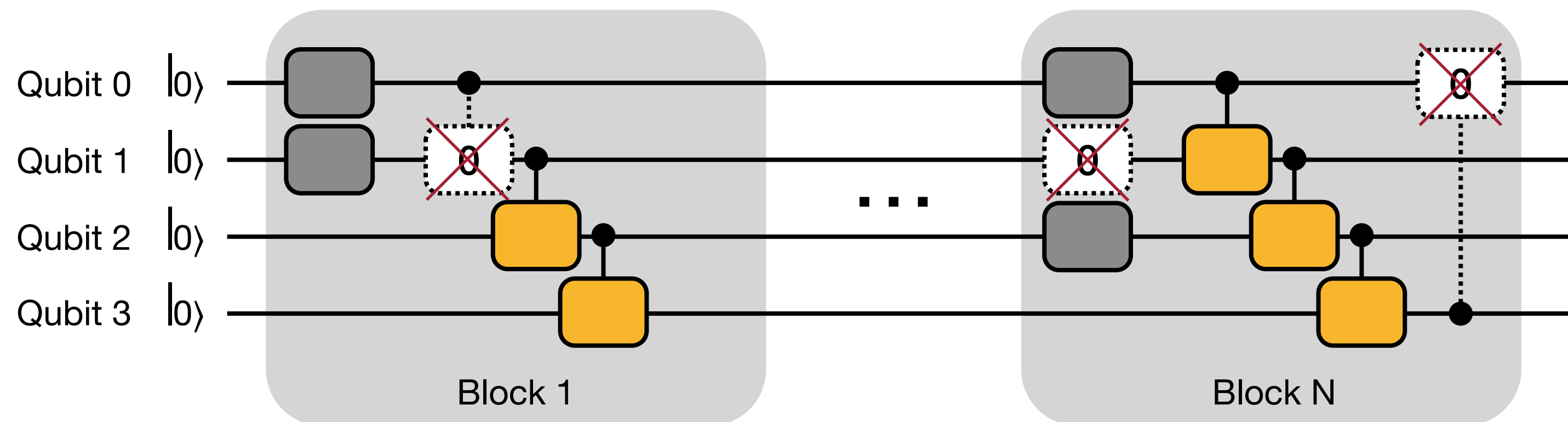
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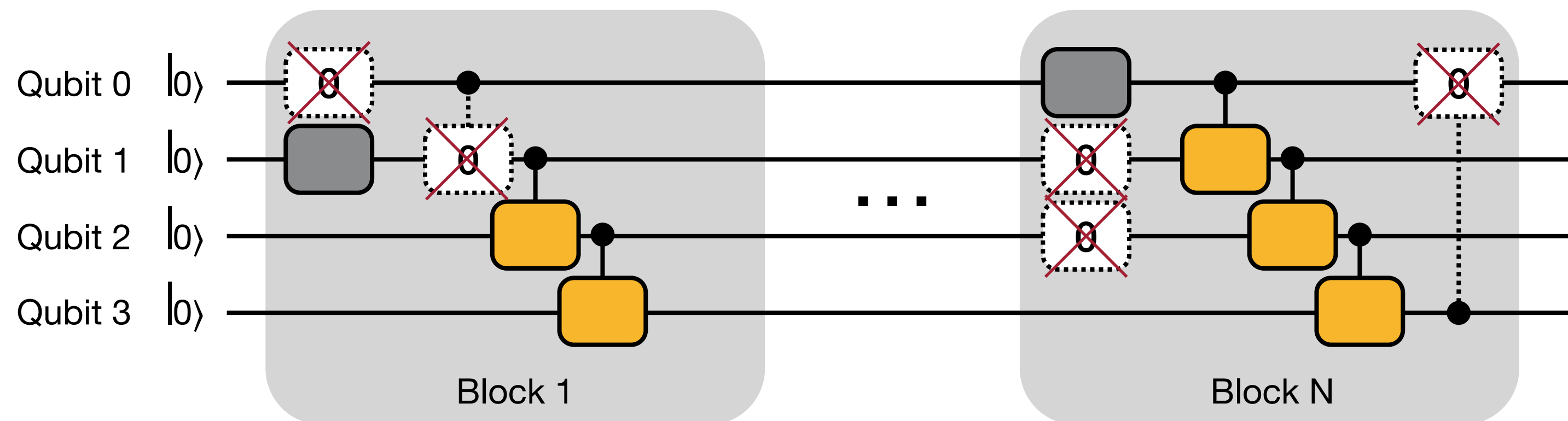
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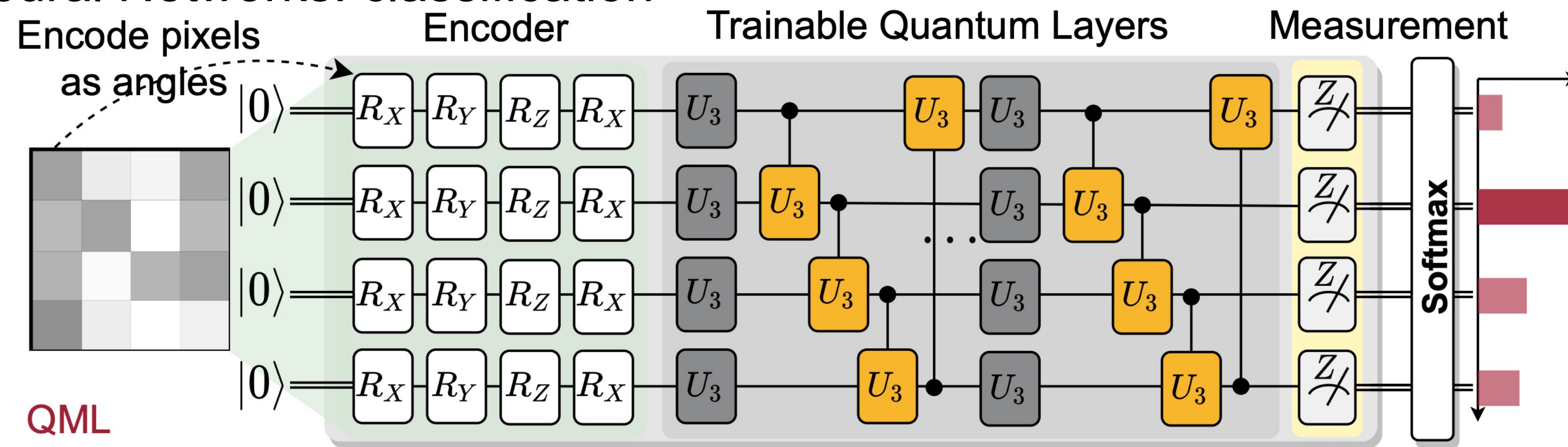


Evaluation Setups: Benchmarks and Devices

- Benchmarks
 - QML classification tasks: MNIST 10-class, 4-class, 2-class, Fashion 4-class, 2-class, Vowel 4-class
 - VQE task molecules: H₂, H₂O, LiH, CH₄, BeH₂
- Quantum Devices
 - IBMQ
 - #Qubits: 5 to 65
 - Quantum Volume: 8 to 128

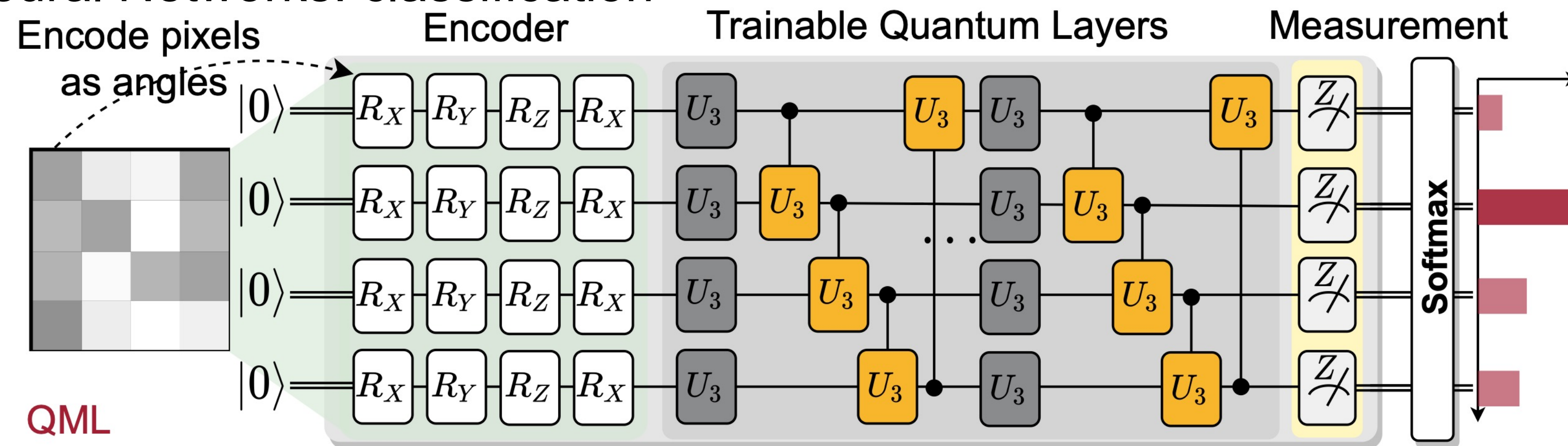
Benchmarks: QNN and VQE

- Quantum Neural Networks: classification

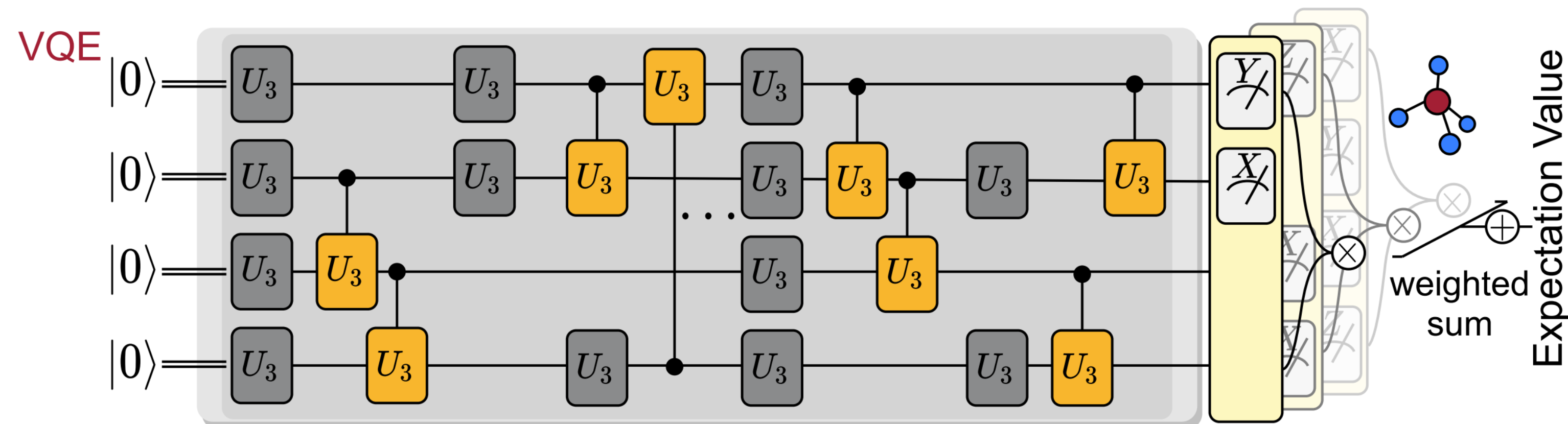


Benchmarks: QNN and VQE

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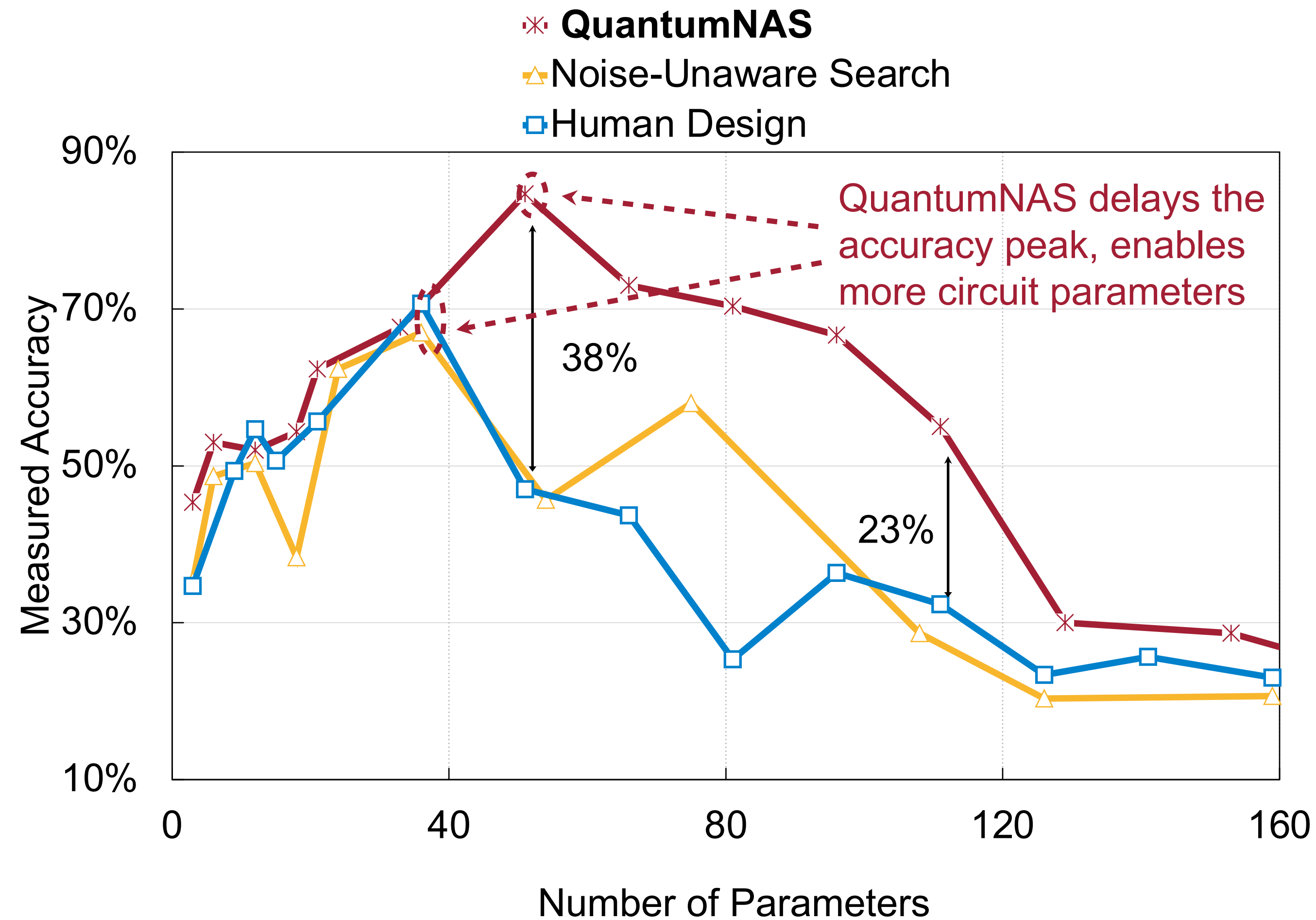


- Variational Quantum Eigensolver: finds the ground state energy of molecule Hamiltonian



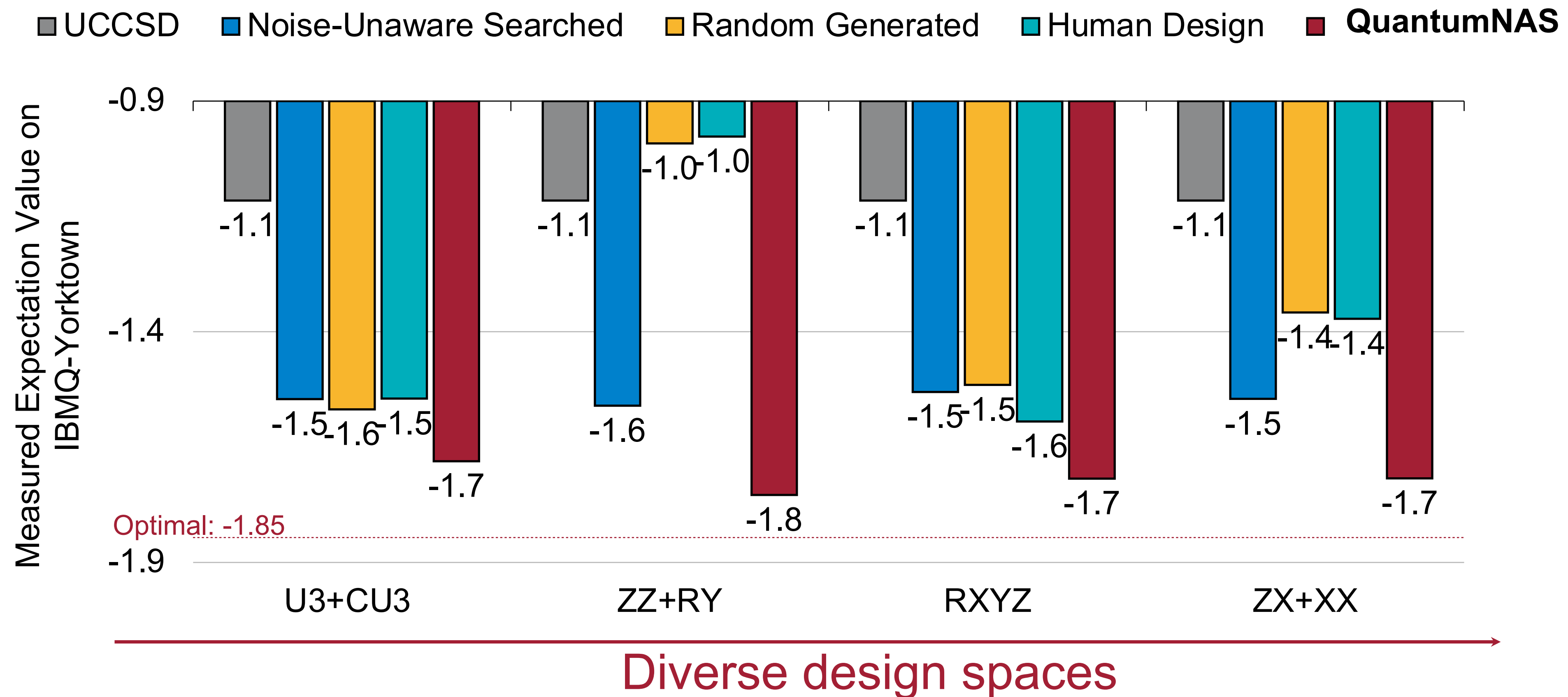
QML Results

- 4-classification: MNIST-4 U3+CU3 on IBMQ-Yorktown



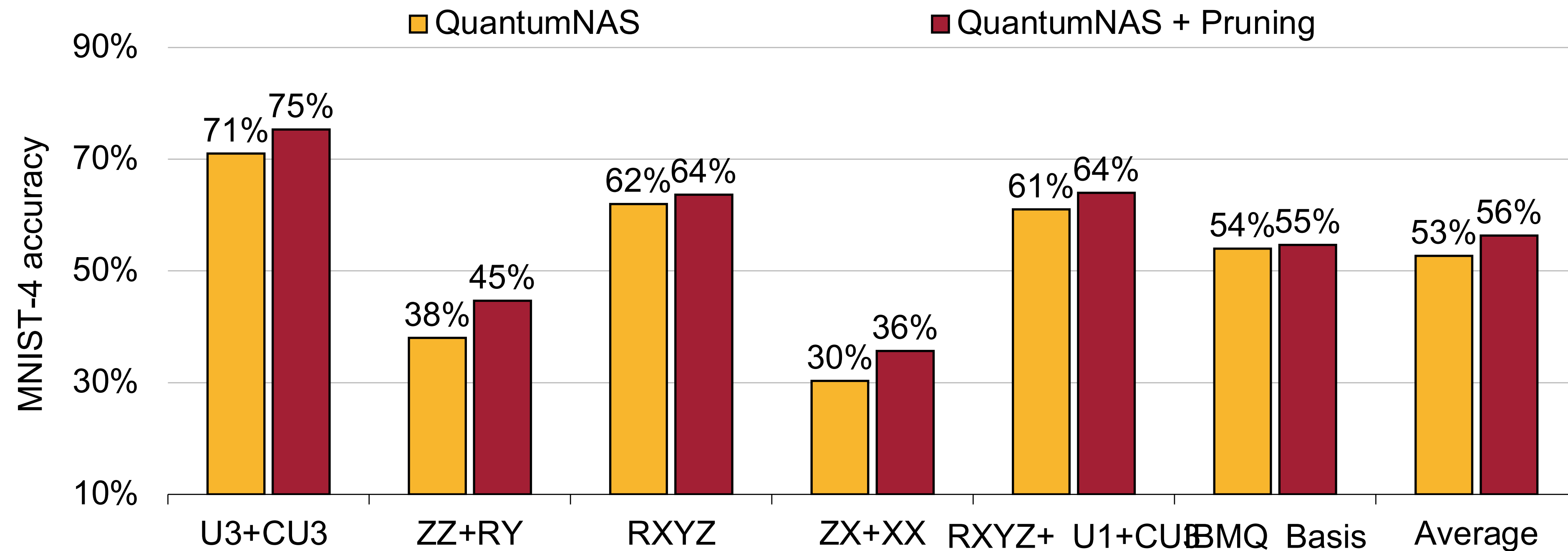
Consistent Improvements on Diverse Design Spaces

- H2 in different design spaces on IBMQ-Yorktown



Effective of Quantum Gate Pruning

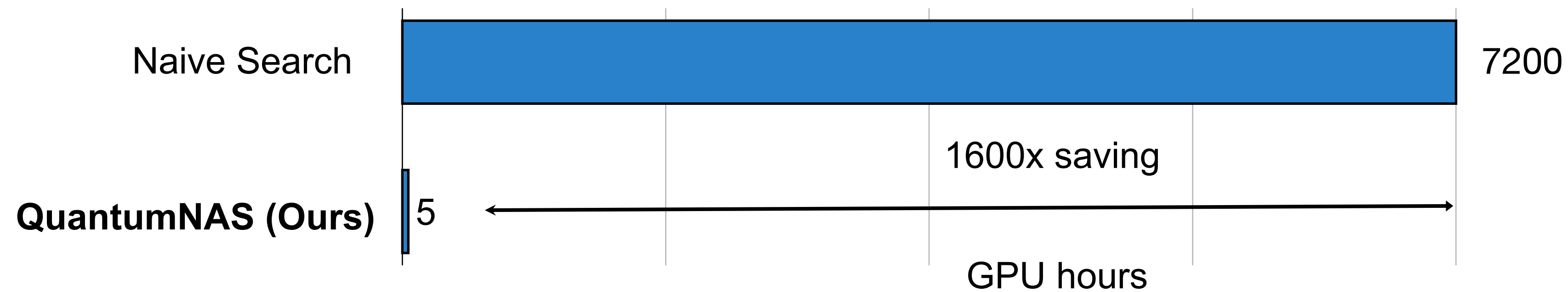
- For MNIST-4, Quantum gate pruning improves accuracy by 3% on average



Time Cost with TorchQuantum

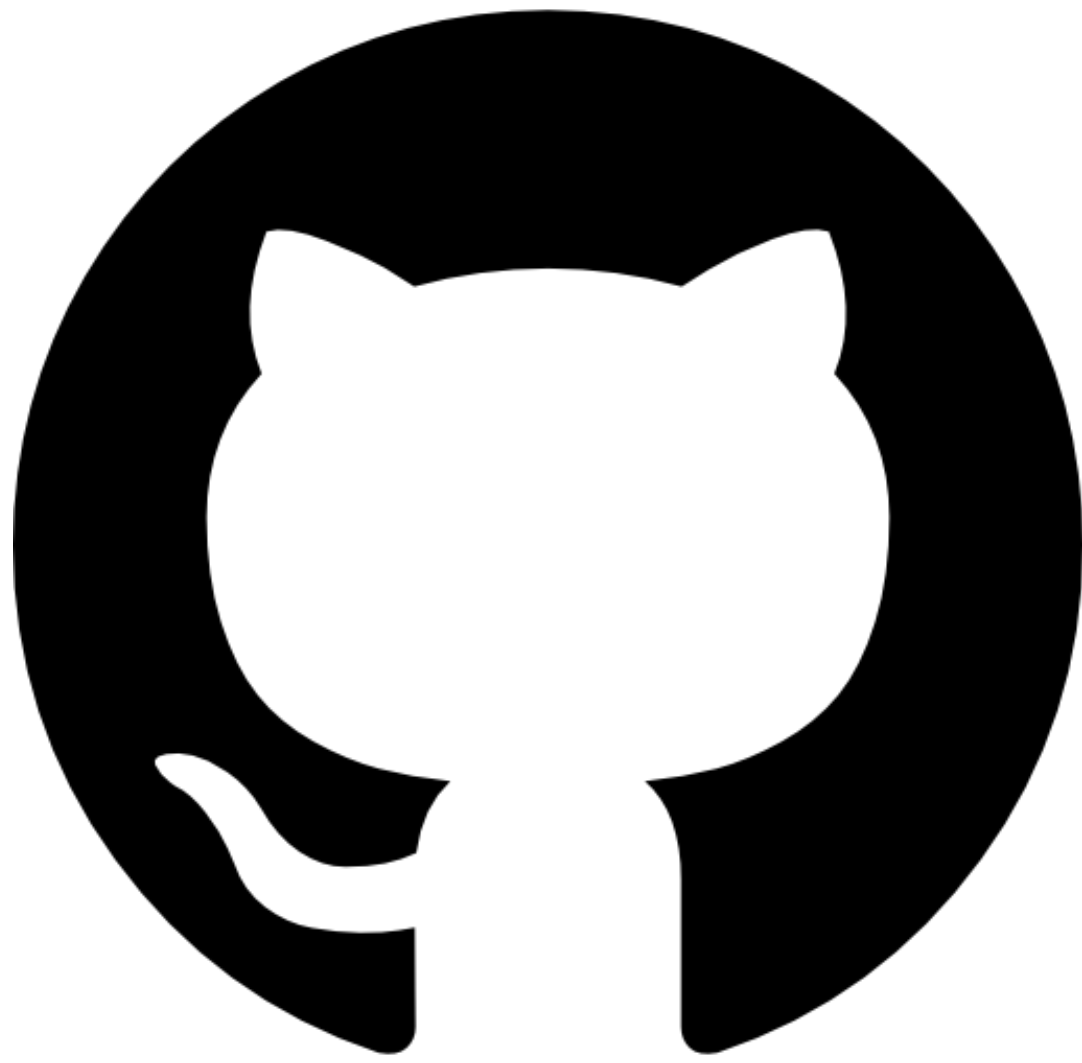
- On 1 Nvidia Titan RTX 2080 ti GPU

#qubits \ Step	Step			
	SuperCircuit Training	Noise-Adaptive Co-search	SubCircuit Training	Deployment on Real QC
4 Qubits	0.5h	3h	0.5h	0.5h
15 Qubits	5h	5h	5h	1h
21 Qubits	20h	10h	15h	1h



Hands-On Section

2.1 QuantumNAS



TorchQuantum Tutorial Outline

Section 1

TorchQuantum Basic Usage

1.1 Quantum Basics

1.2 TQ operations 

1.3 TQ for State Prep 


1.4 TQ for VQE 

1.4 TQ for QNN 

Section 2

Use TorchQuantum on Gate level

2.1 QuantumNAS: Ansatz
Search and Gate Pruning 

2.2 QuantumNAT: Noise
Injection and Quantization 

2.3 QOC: On-Chip Training 

2.4 Transformer for Quantum
Circuit Reliability Prediction

2.5 QNN Compression 

Section 3

Use TorchQuantum on Pulse level

3.1 Quantum Optimal Control 

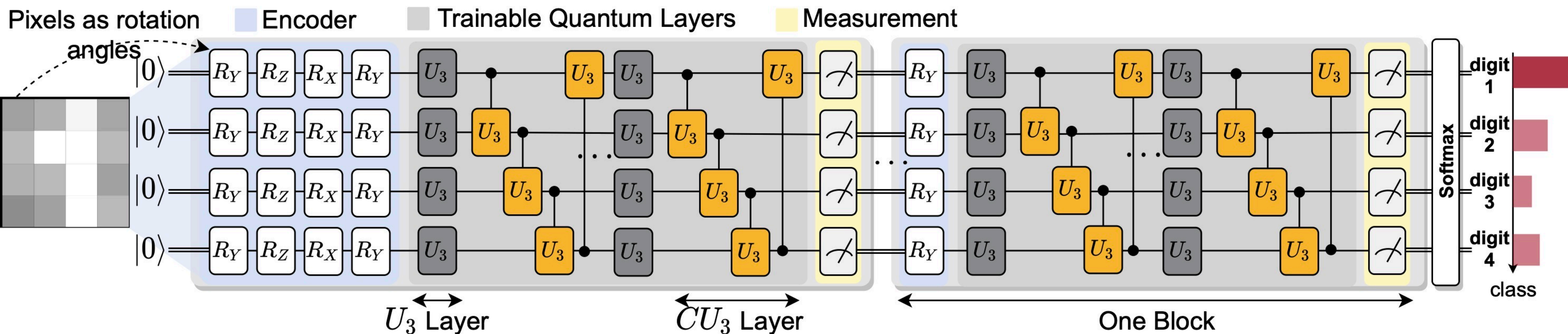
3.2 Variational Pulse Learning 

QuantumNAS vs. QuantumNAT

- **QuantumNAS** finds noise robust circuit **architecture**
- **QuantumNAT** finds noise robust circuit **parameters**

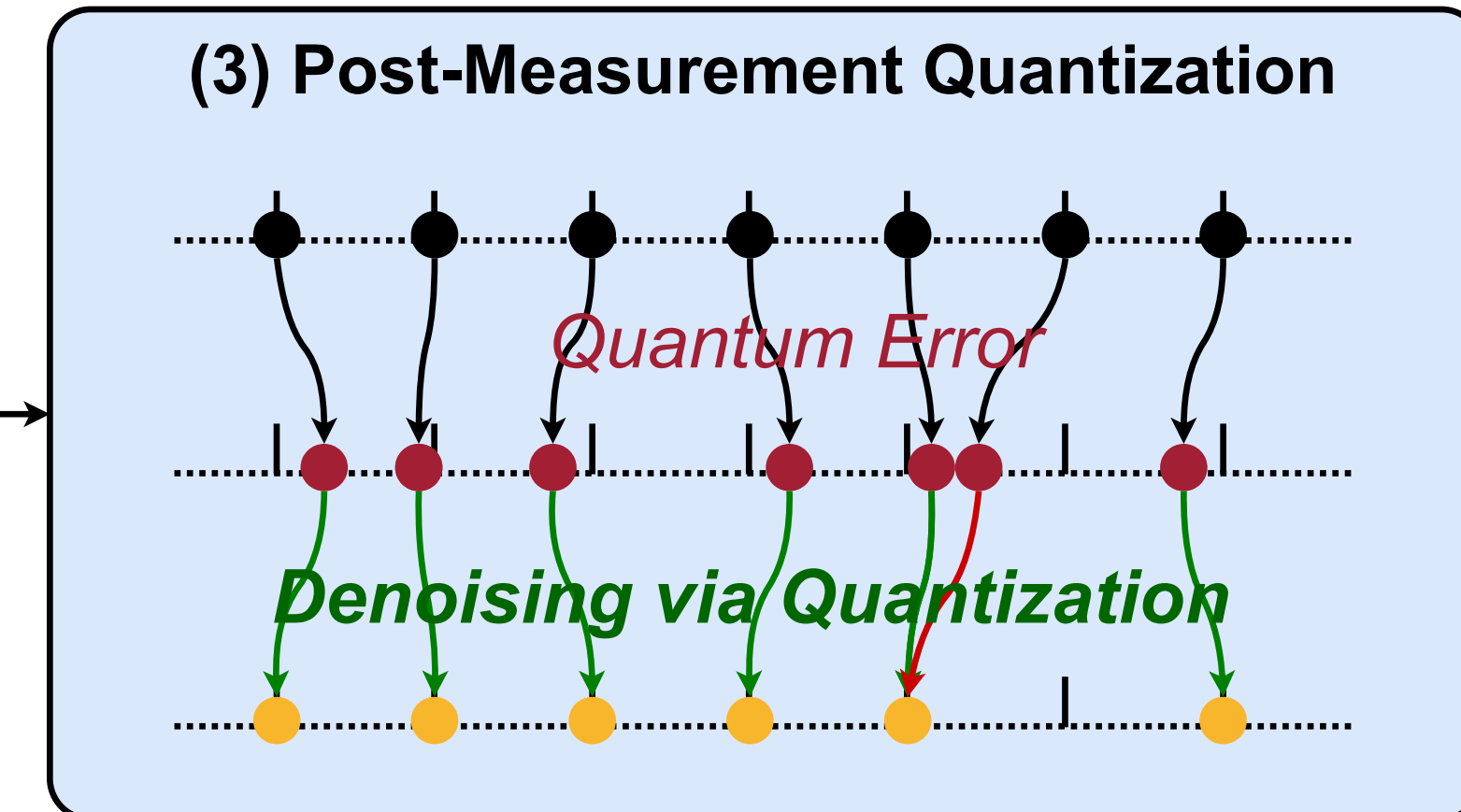
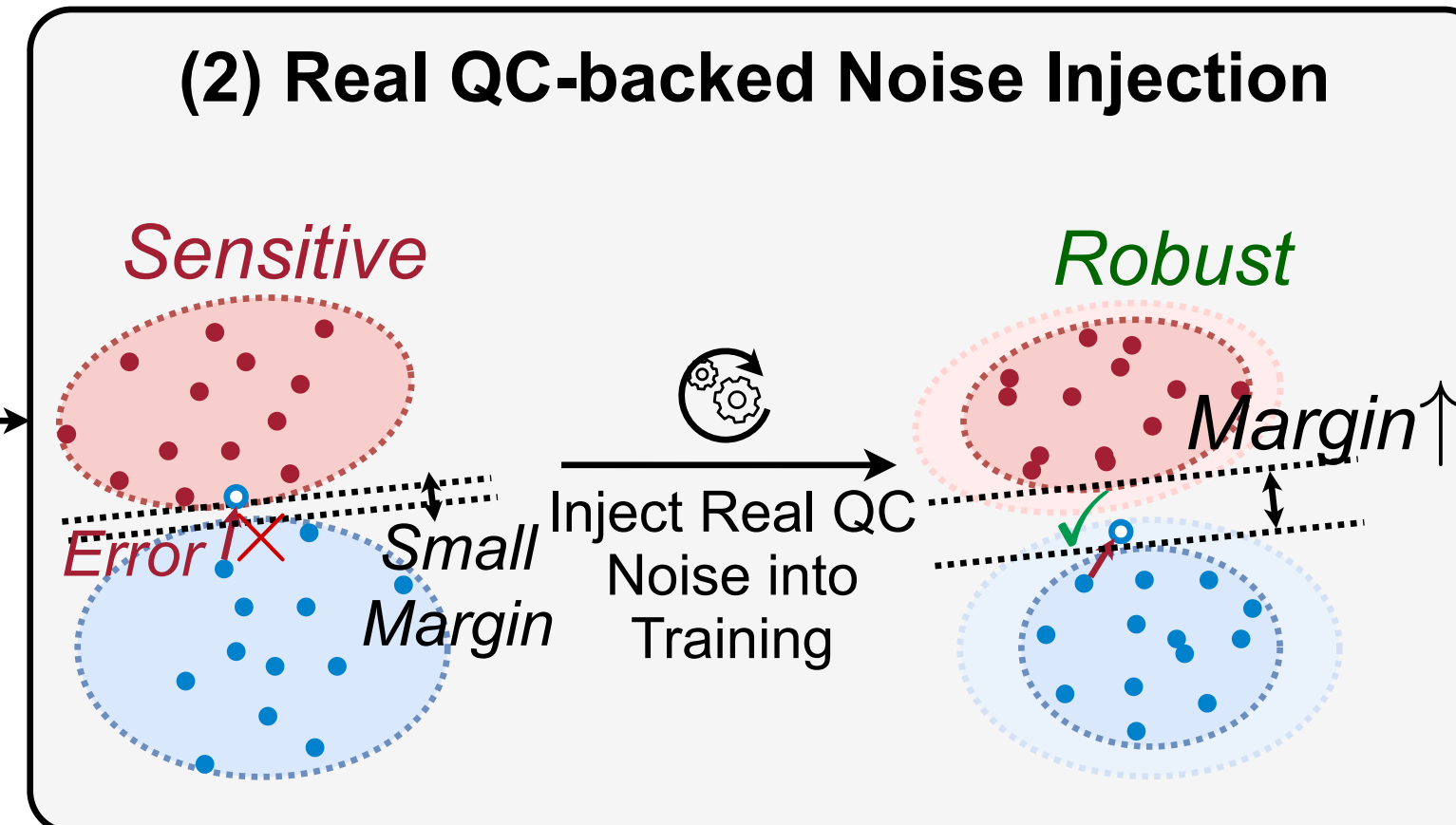
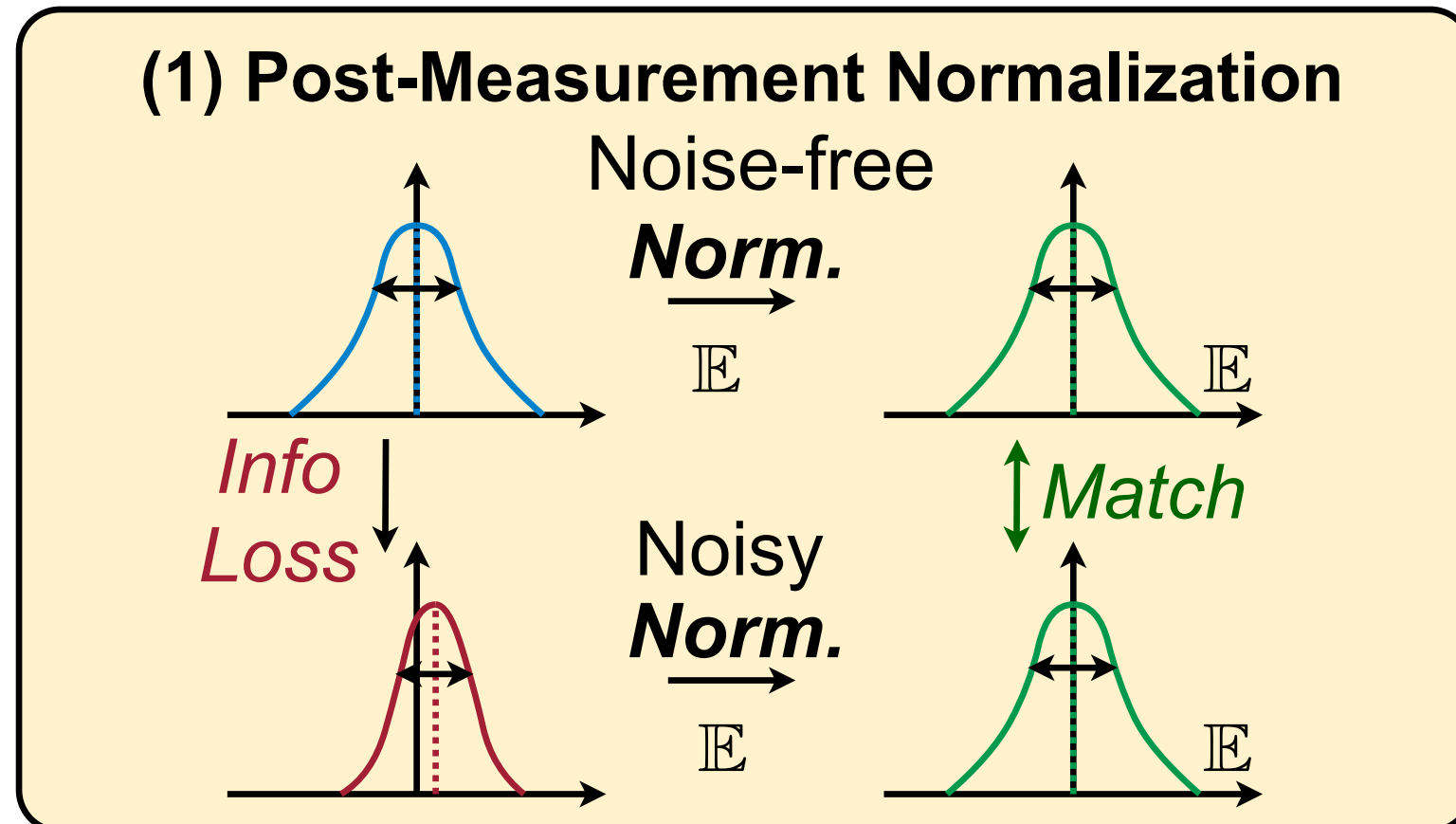
PQC Circuit in QuantumNAT

- QNN with multiple nodes
 - Encoder
 - Trainable Quantum Layers
 - Measurements

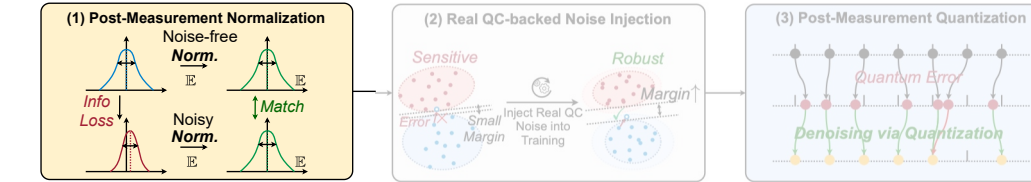


Three Techniques in QuantumNAT

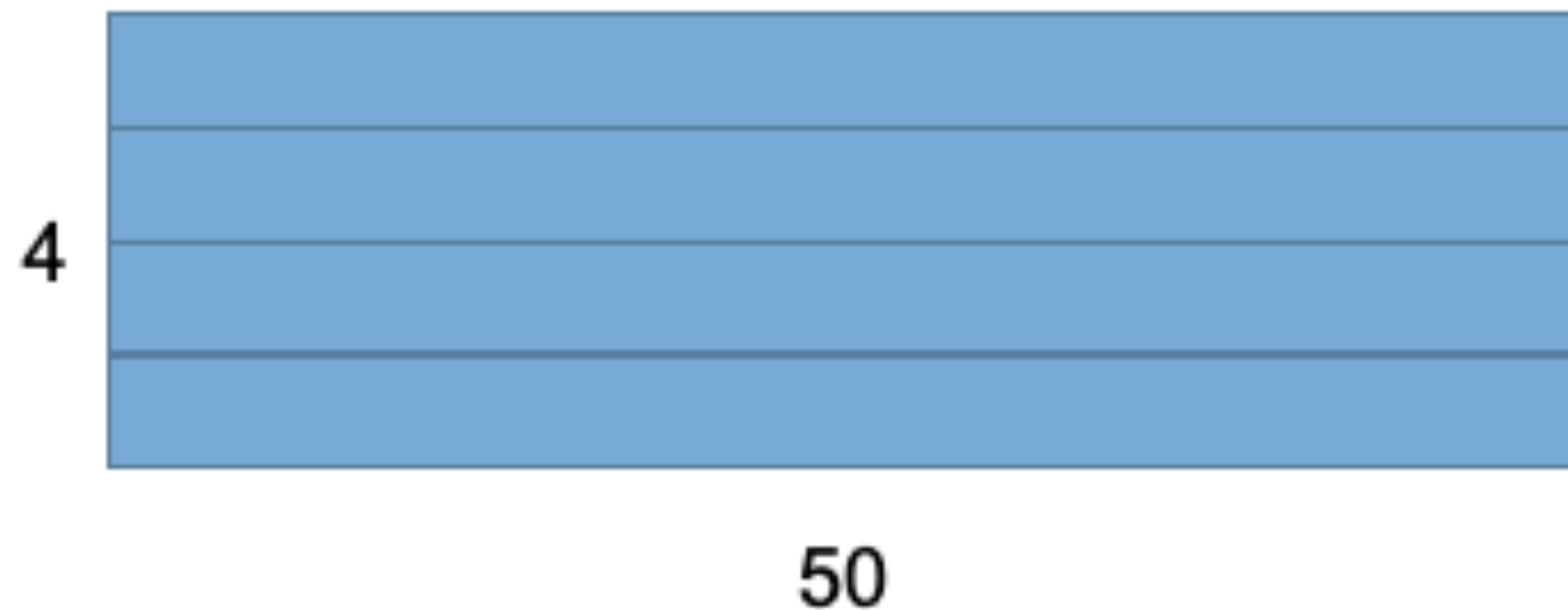
- QuantumNAT:
 - Normalization: mitigate noise impact
 - Noise injection: make the parameters aware of noise
 - Quantization: mitigate noise impact



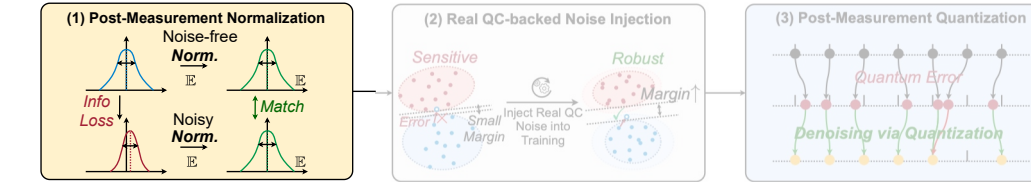
Post-Measurement Normalization



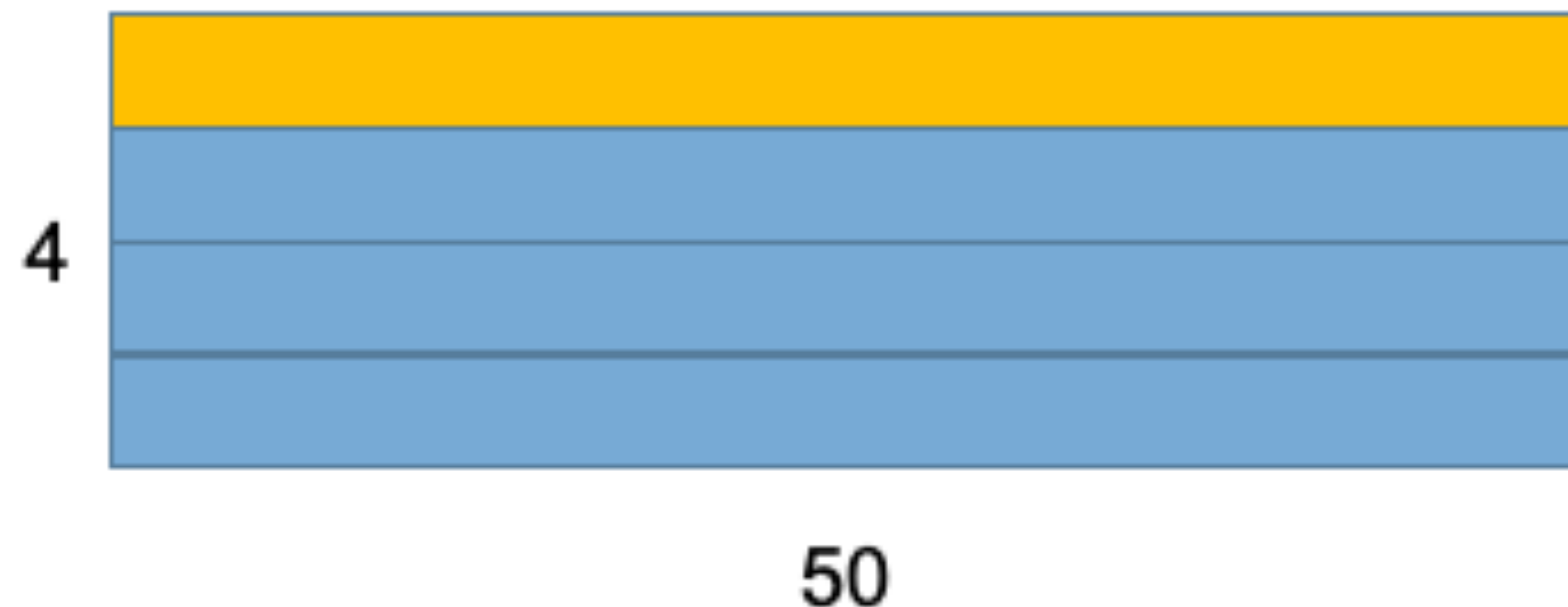
- Normalize the measurement outcome
 - Along the **batch** dimension
 - For example, we train the 4-qubit PQC with batch=50 then we have results as $50 * 4$ values



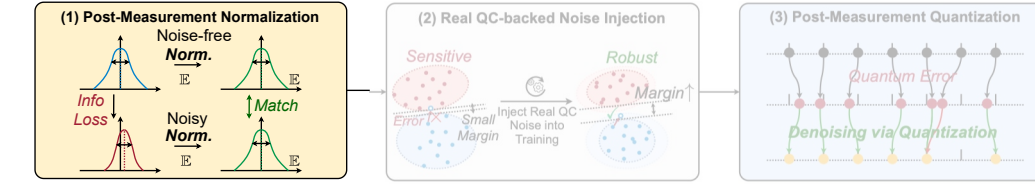
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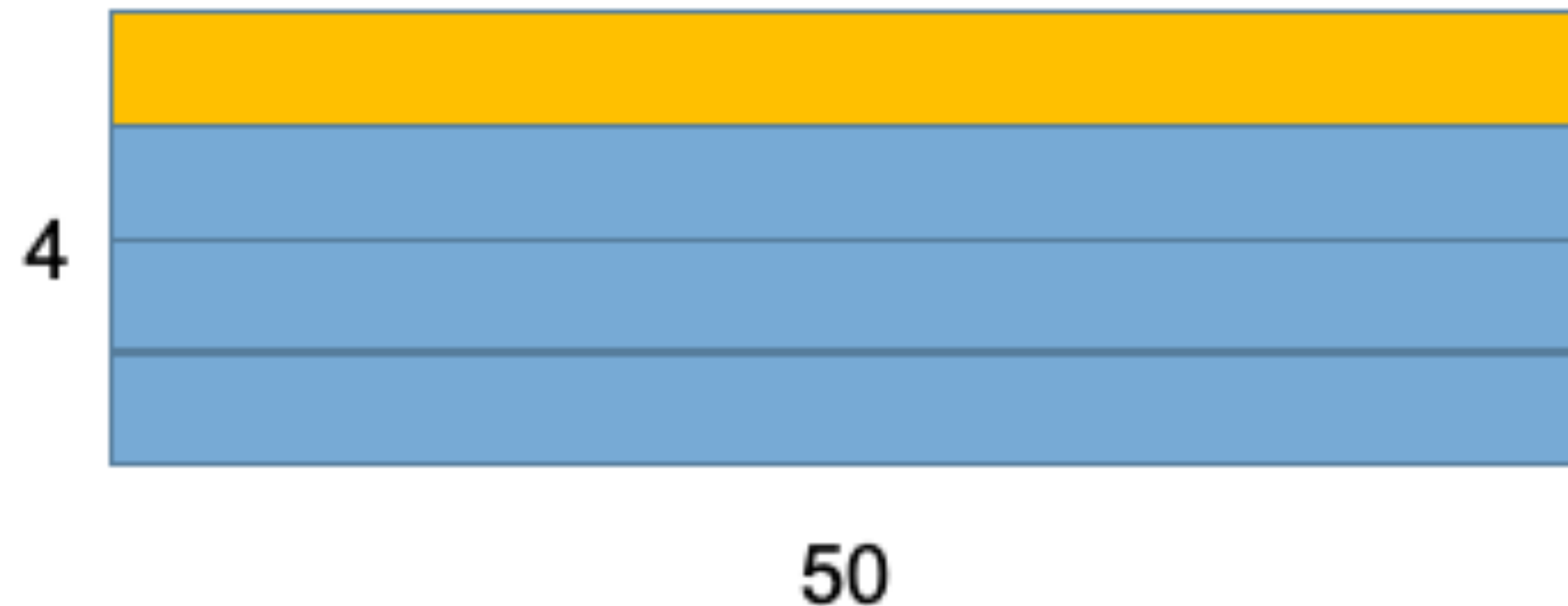
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 - Compute the mean and std on of the measurement outcome on each qubit across batch dim



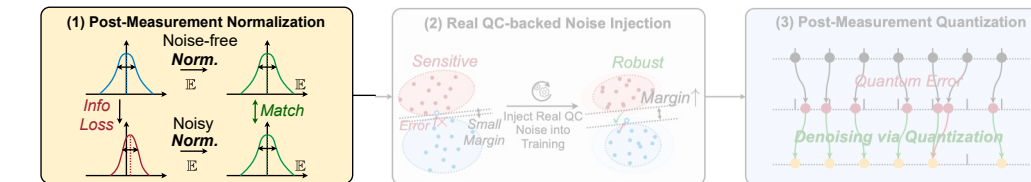
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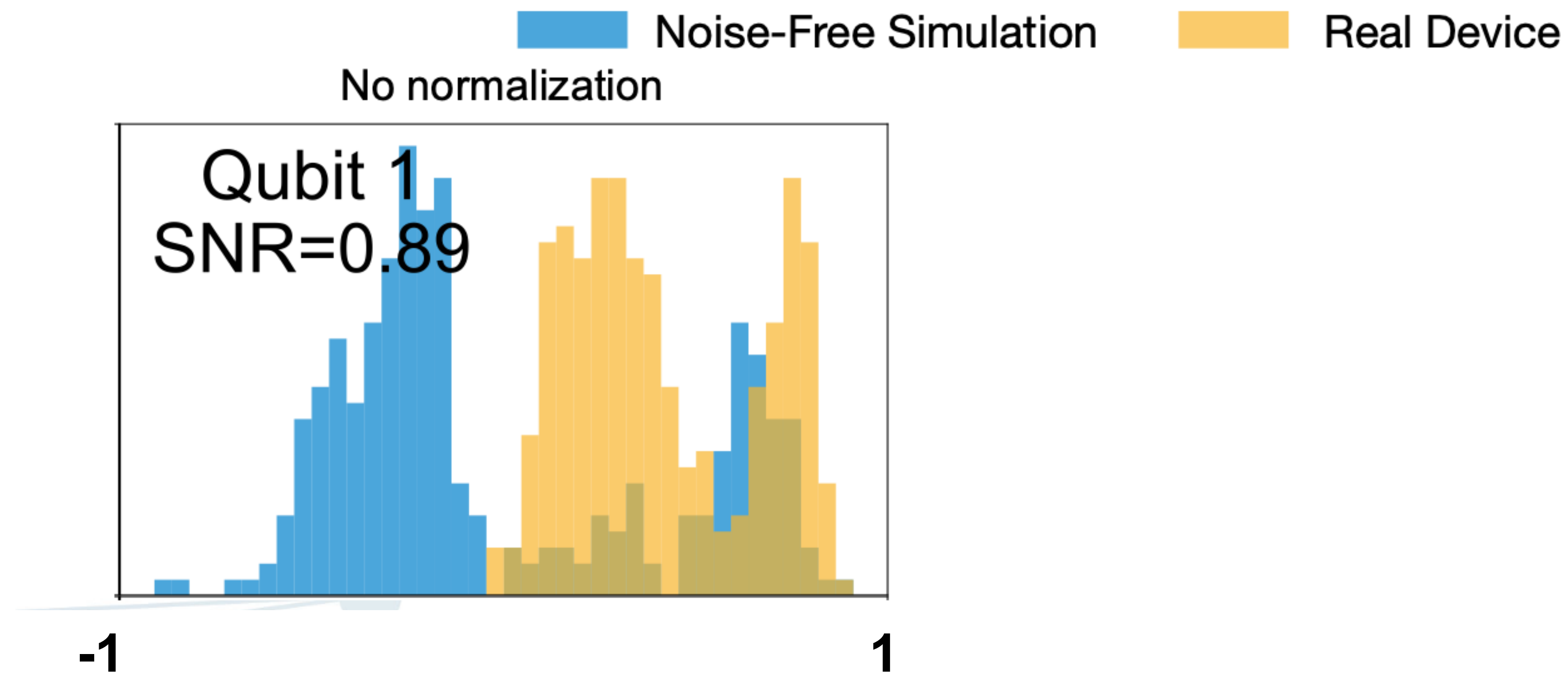
- Normalize the measurement outcome
 - Along the **batch** dimension
 - For example, we train the 4-qubit PQC with batch=50 then we have results as $50 * 4$ values
 - Compute the mean and std on of the measurement outcome on each qubit across batch dim
 - Normalize the measurement outcome with the computed mean and std



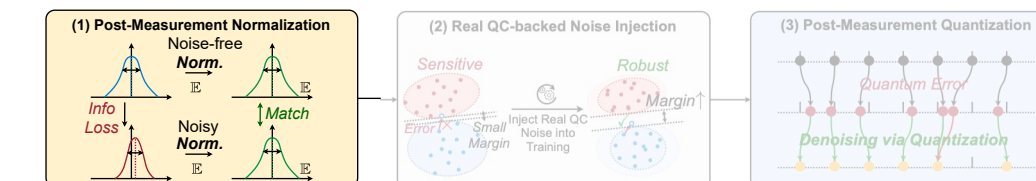
Post-Measurement Normalization



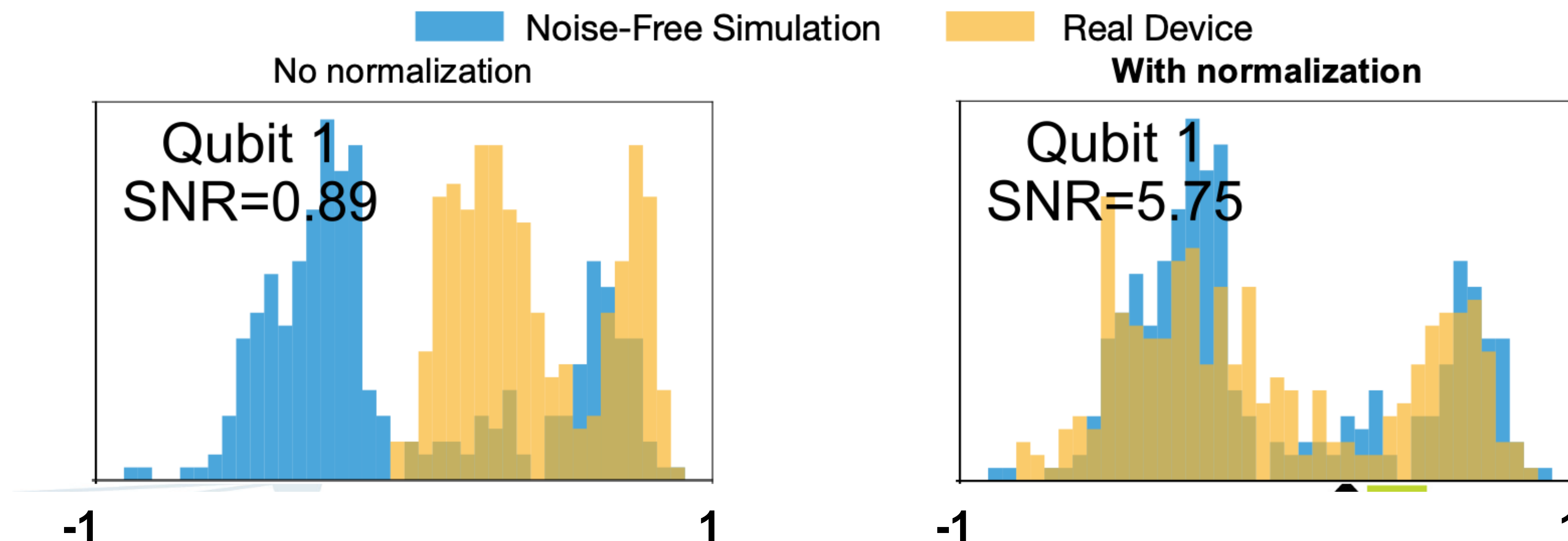
- Normalize the measurement outcome
 - Along the **batch** dimension
- Measurement outcome distribution of 50 quantum circuits:



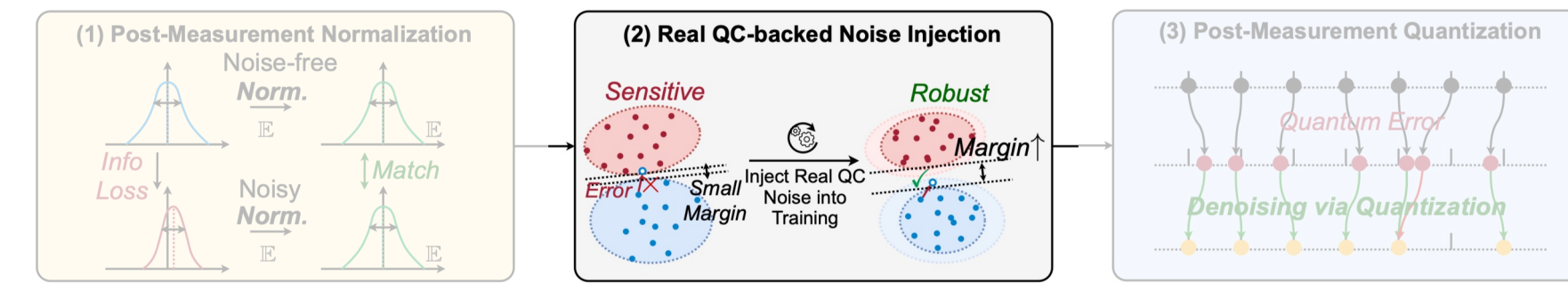
Post-Measurement Normalization



- Normalize the measurement outcome
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- Measurement outcome distribution of 50 quantum circuits:

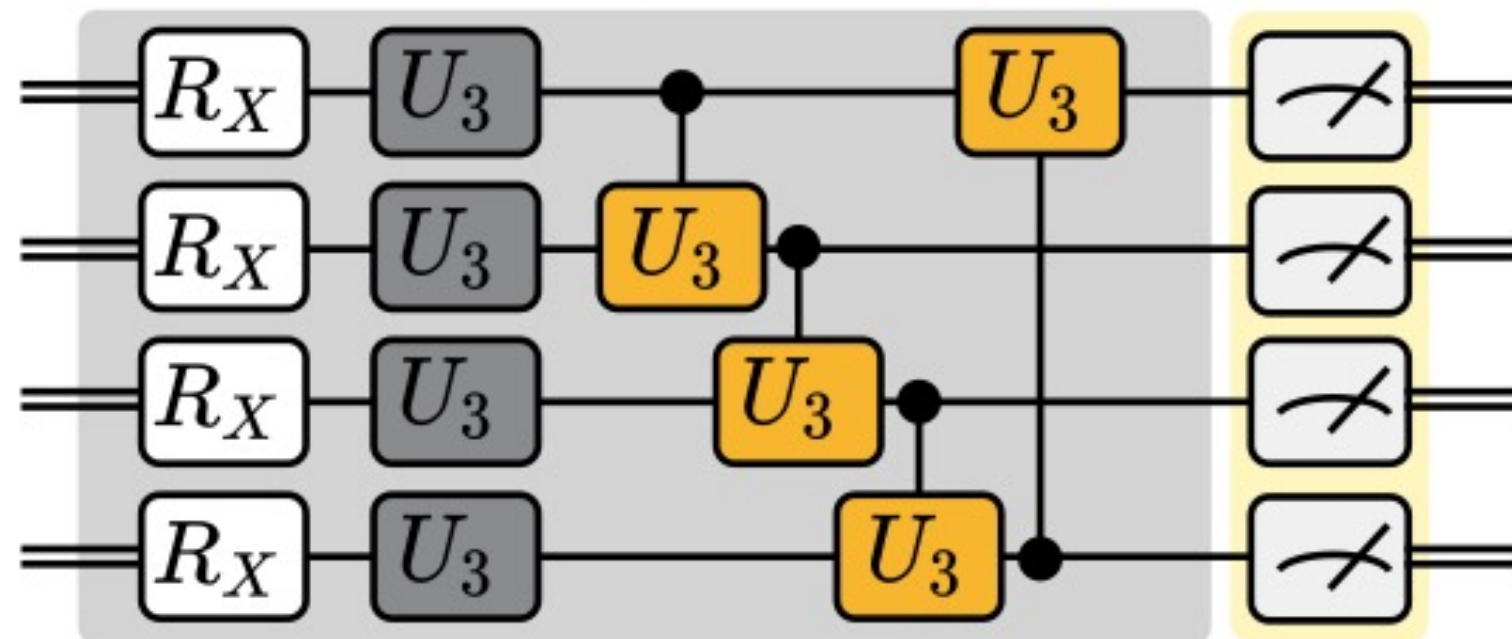


Noise Injection

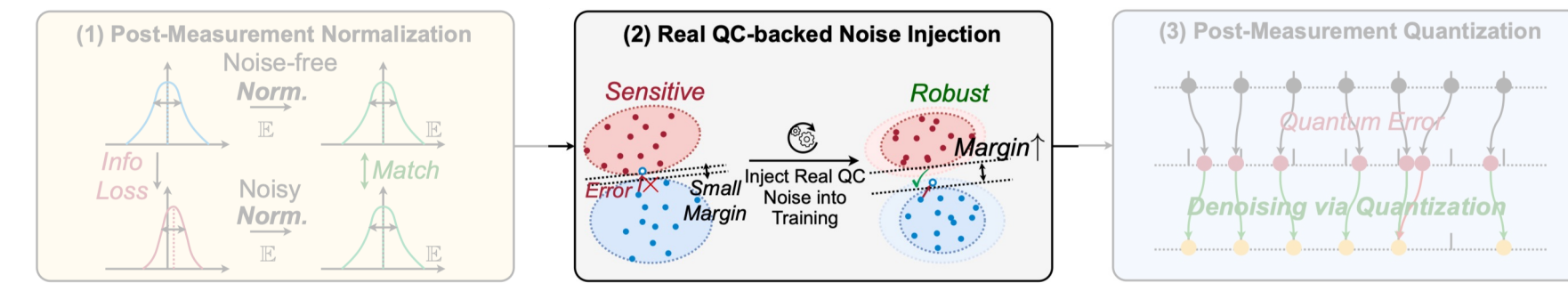


- Inject noise during training on classical simulator
 - Pauli error
 - Readout error

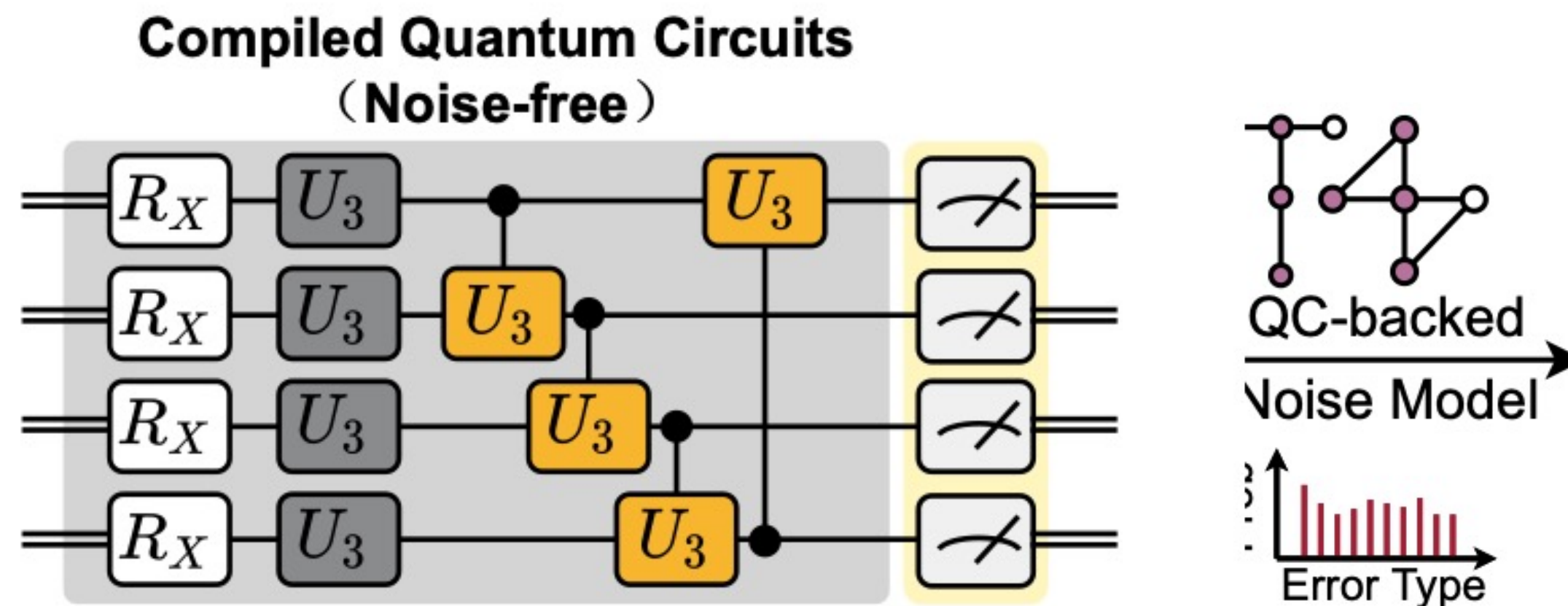
Compiled Quantum Circuits
(Noise-free)



Noise Injection



- Inject noise during training on classical simulator
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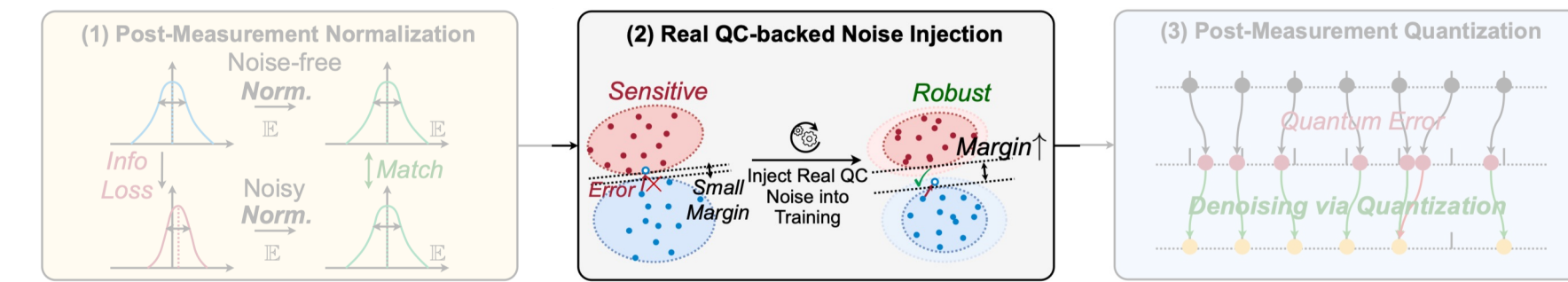


Pauli error: SX gate: {X: 0.00096, Y: 0.00096, Z: 0.00096, None: 0.99712}

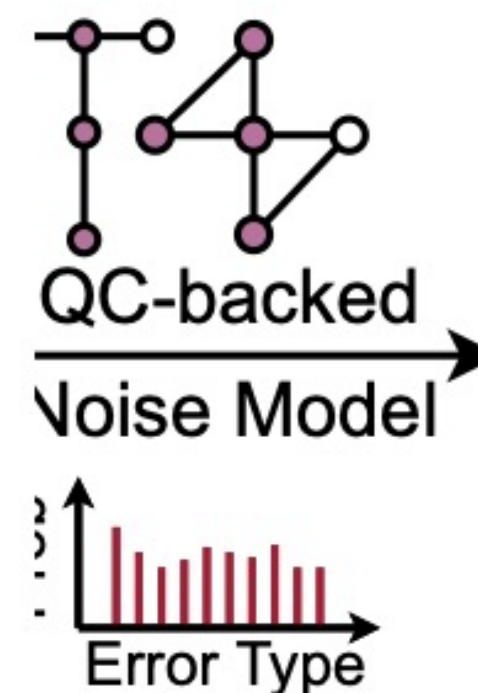
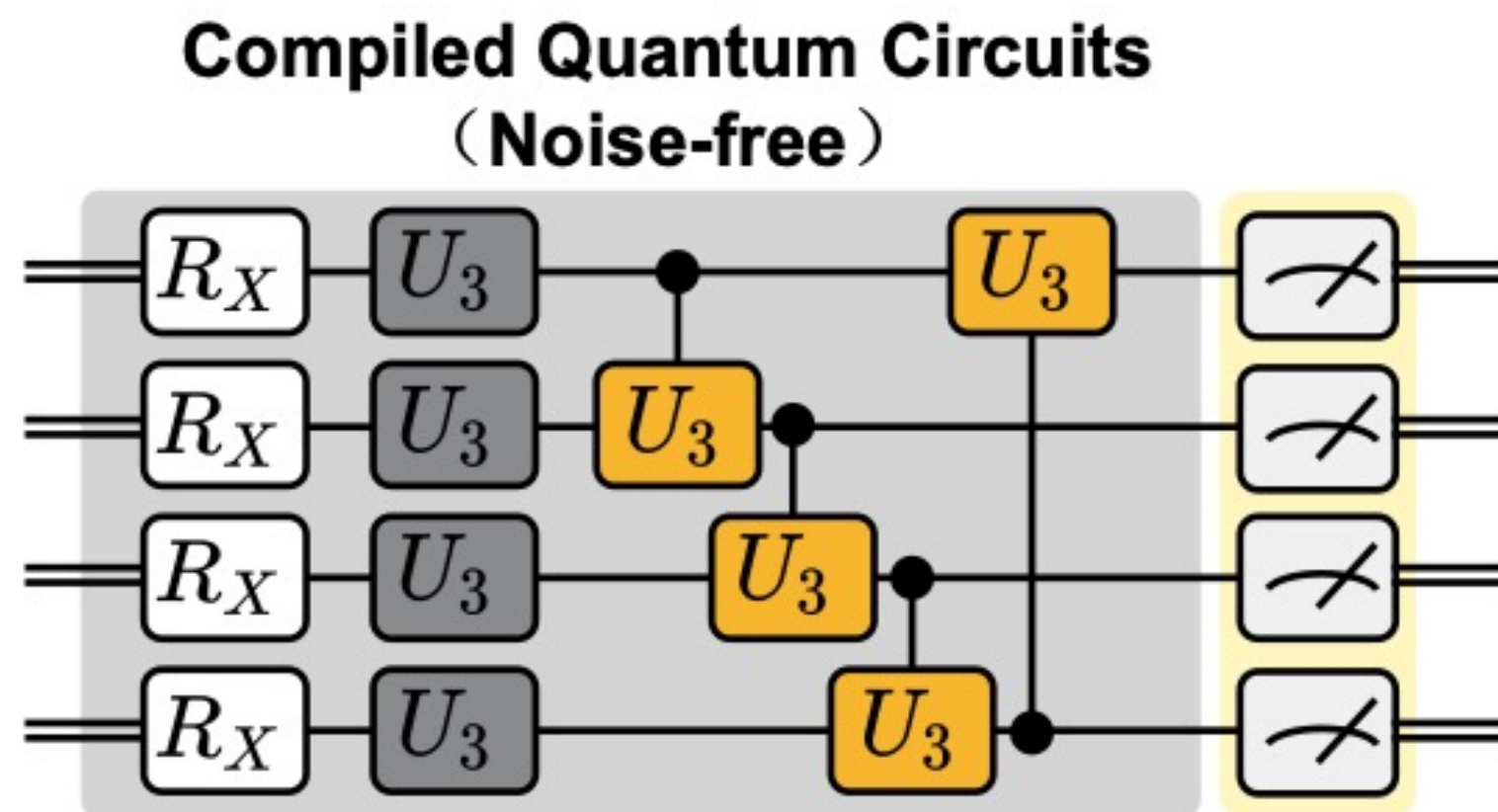
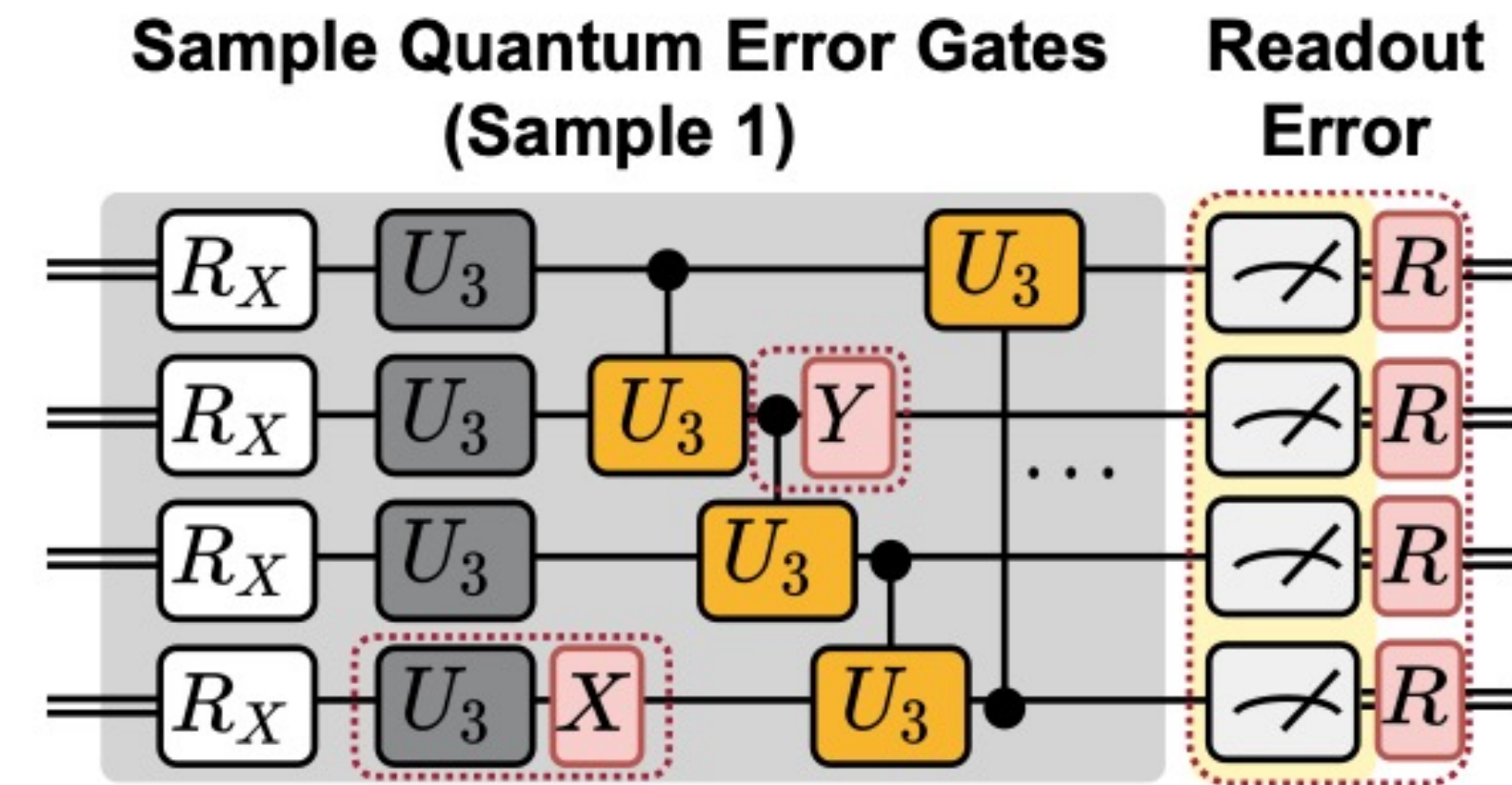
Readout Error Matrix:
0.984, 0.016
0.022, 0.978

Materials at: <https://torchquantum.org>

Noise Injection



- Inject noise during training on classical simulator
 - Pauli error
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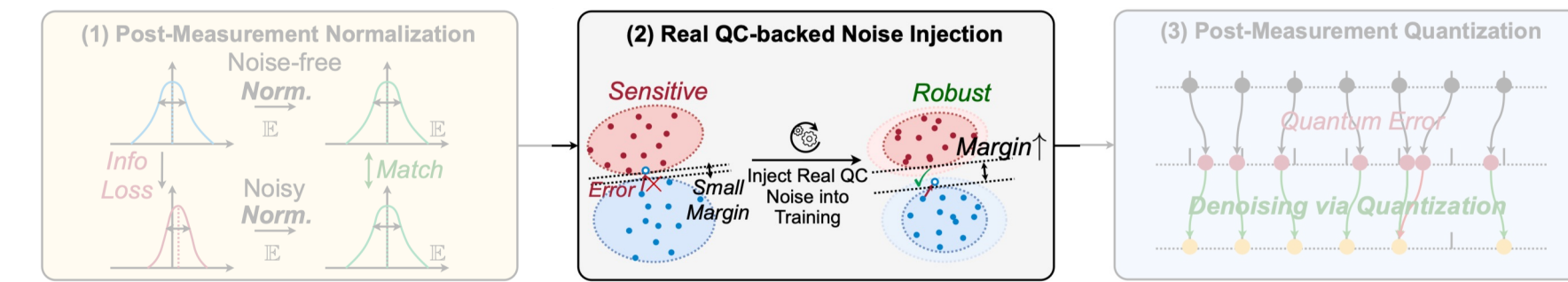


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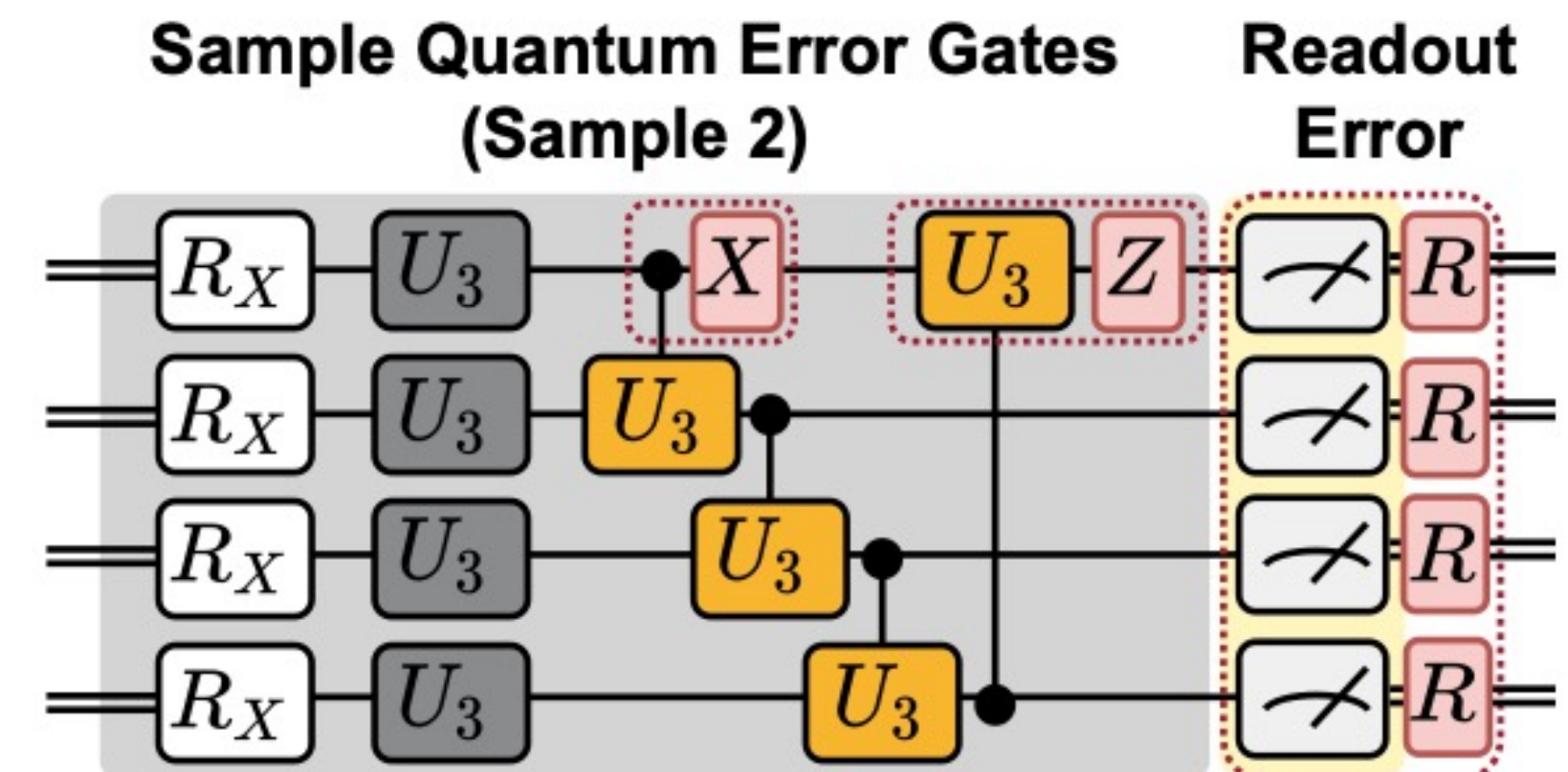
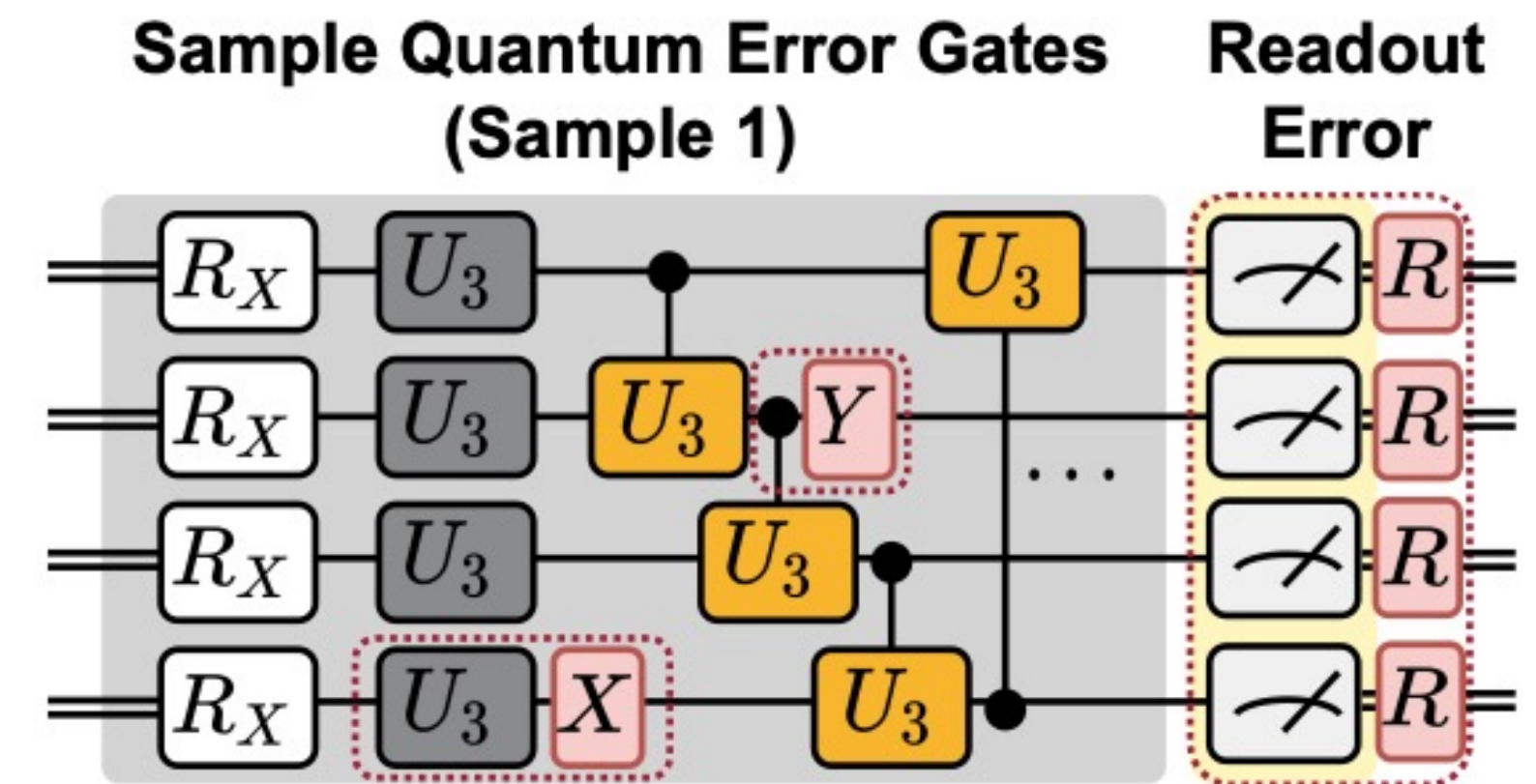
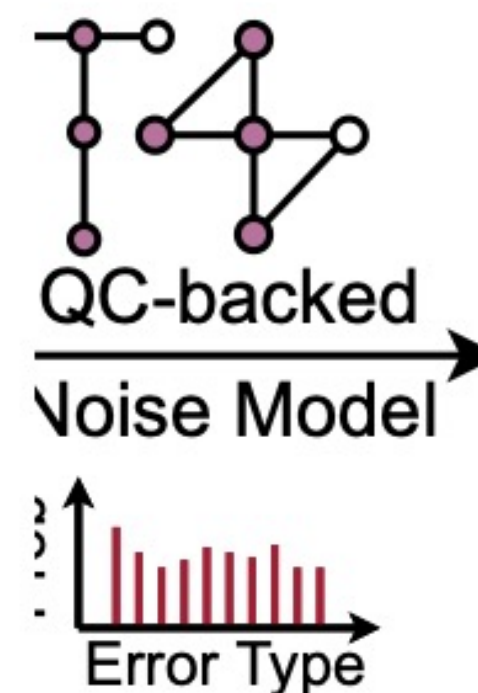
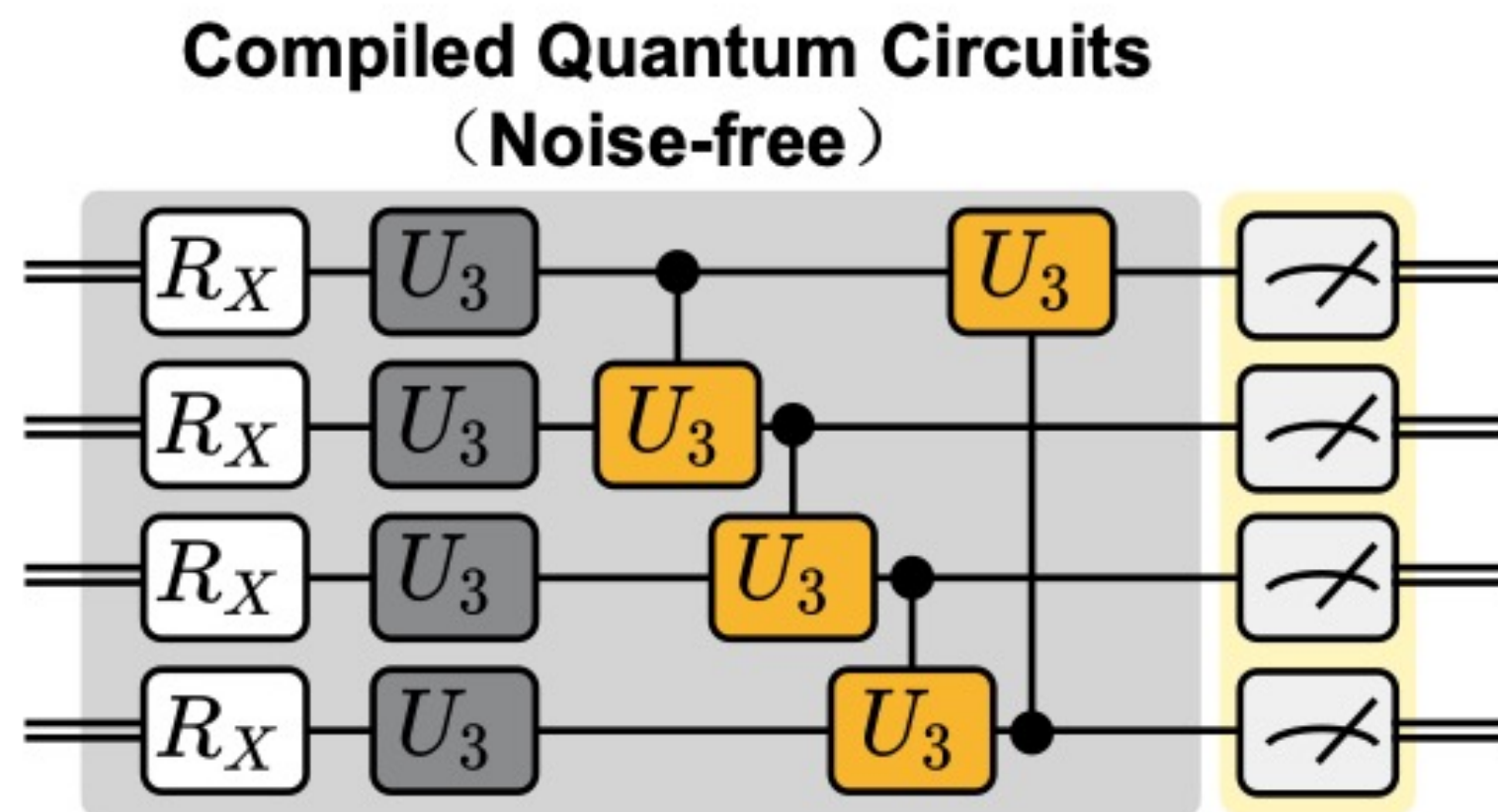
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Noise Injection



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 - Pauli error
 - Readout error

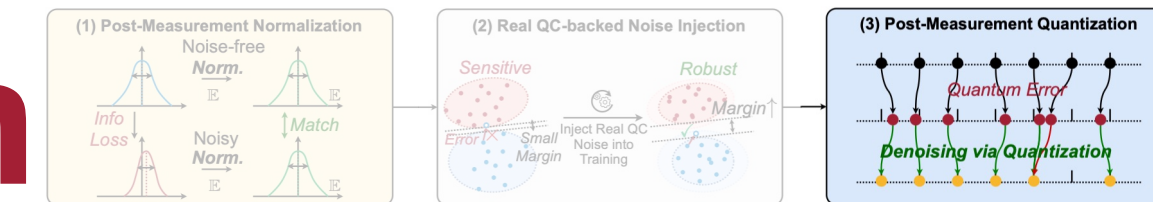


Pauli error: SX gate: {X: 0.00096, Y: 0.00096, Z: 0.00096, None: 0.99712}

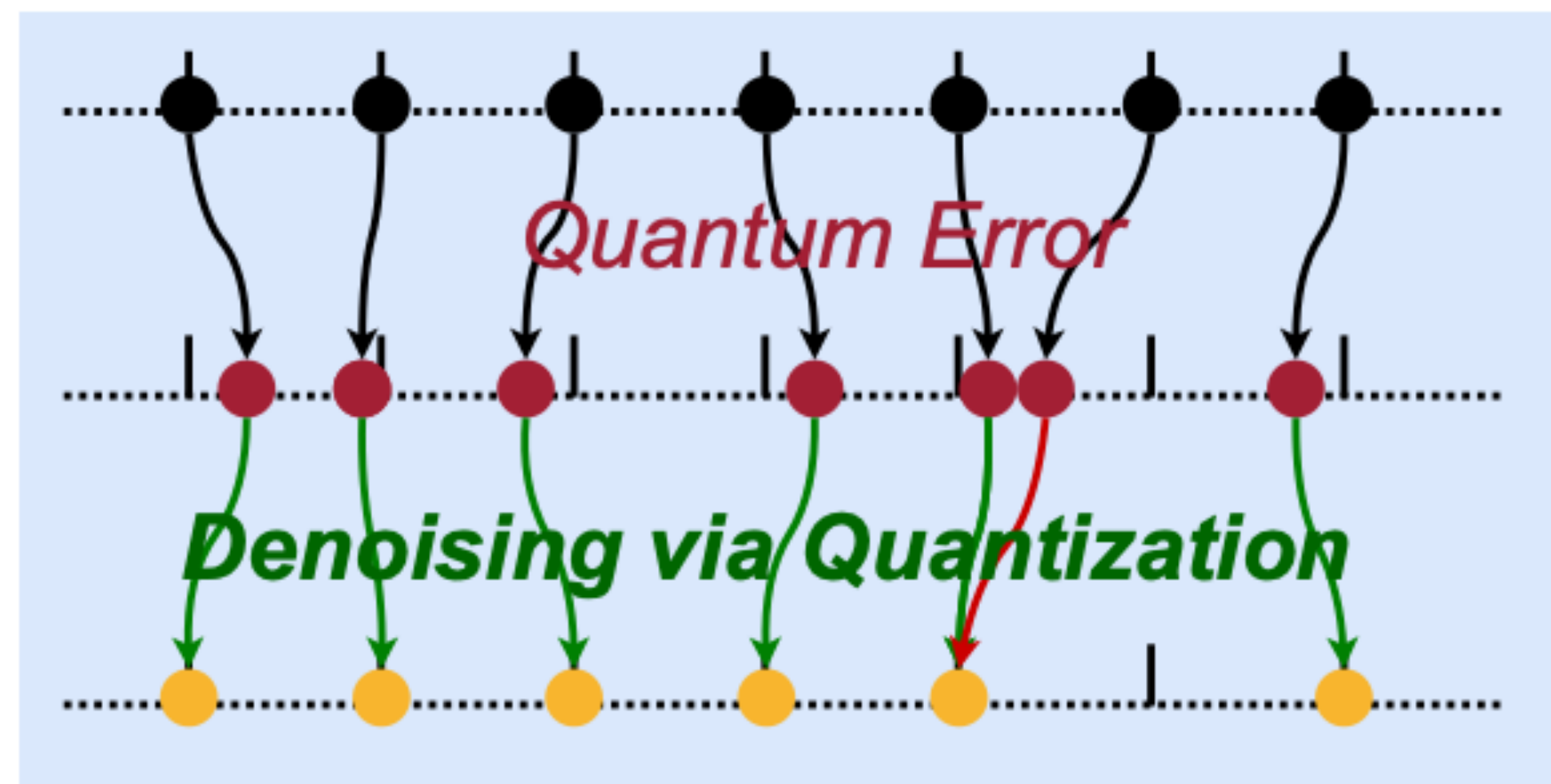
Readout Error Matrix:
0.984, 0.016
0.022, 0.978

Materials at: <https://torchquantum.org>

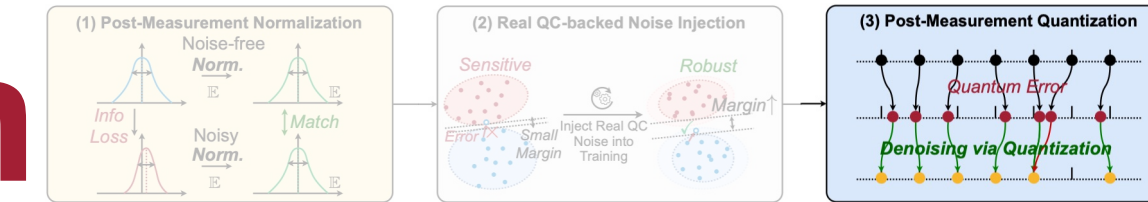
Post-Measurement Quantization



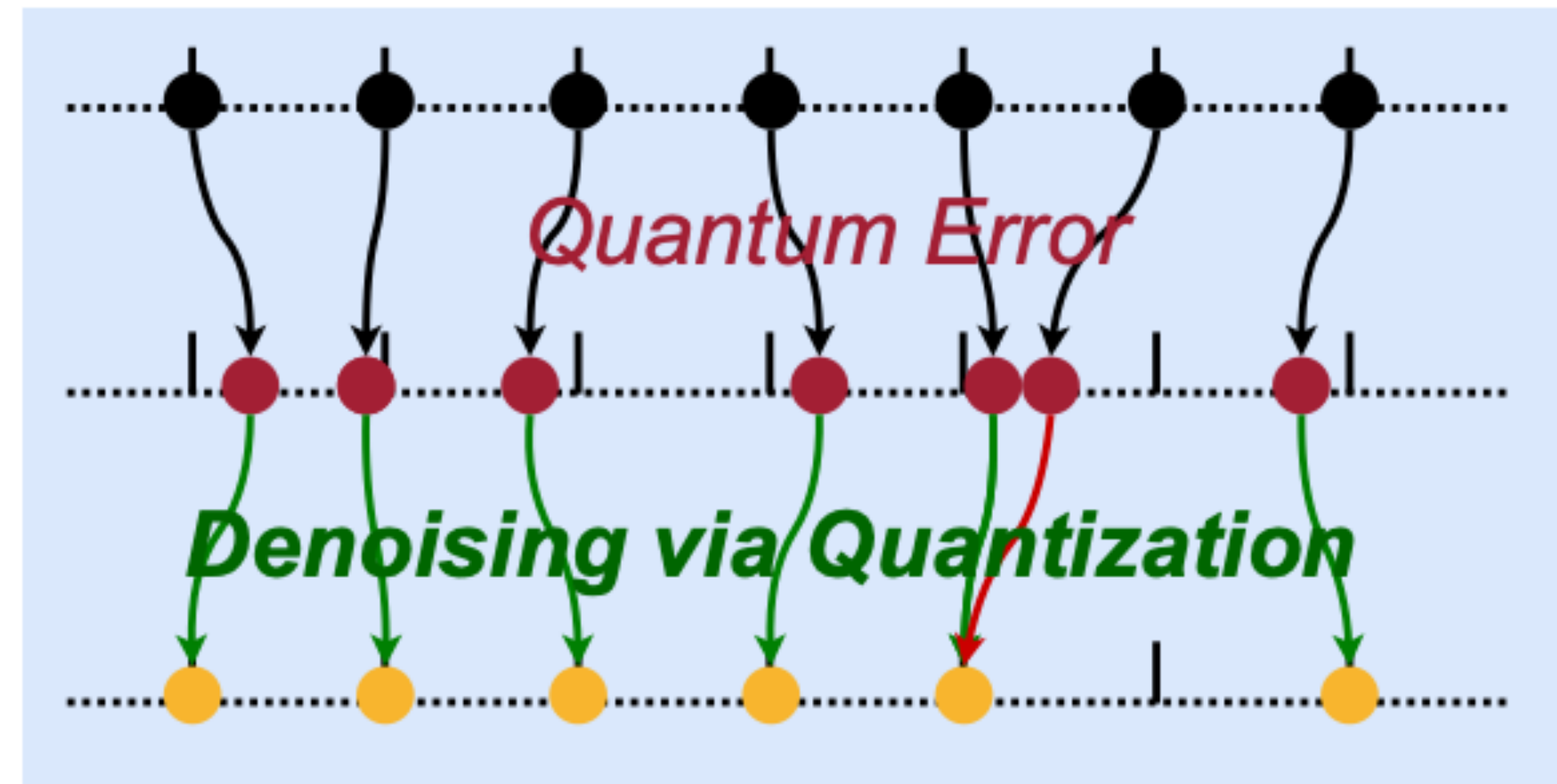
- Quantize measurement outcomes
 - Denoising effect
 - Small errors will be mitigated



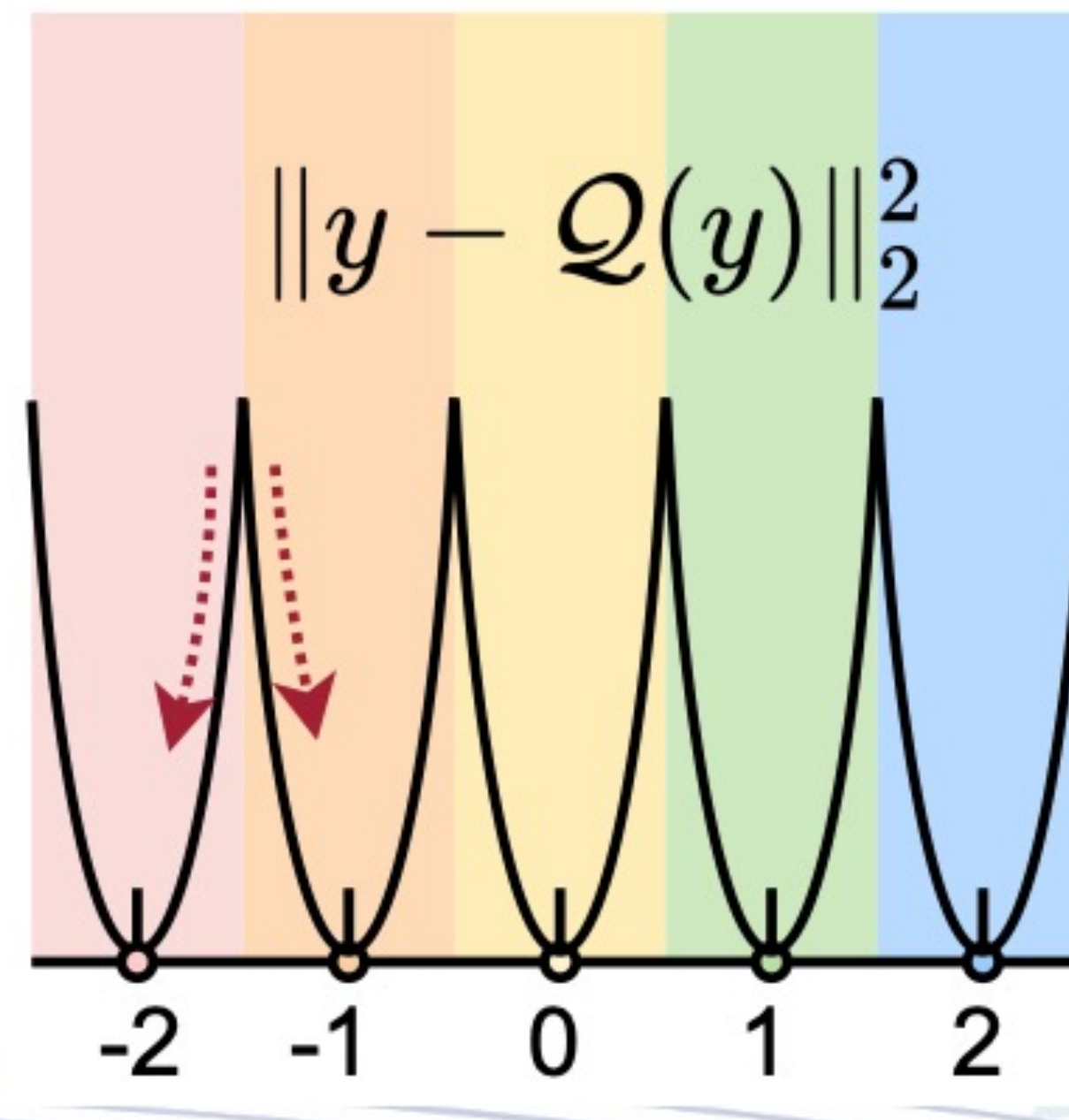
Post-Measurement Quantization



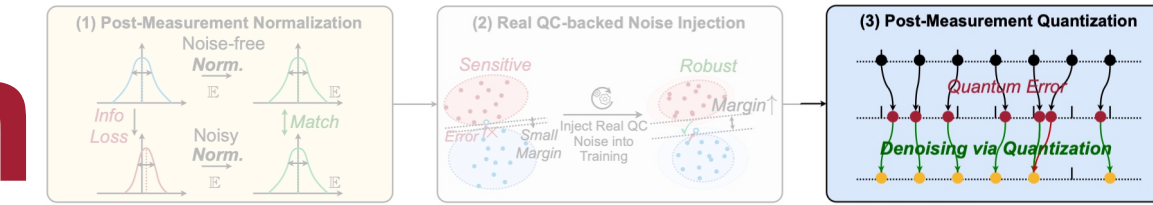
- Quantize measurement outcomes
 - Denoising effect
 - Small errors will be mitigated



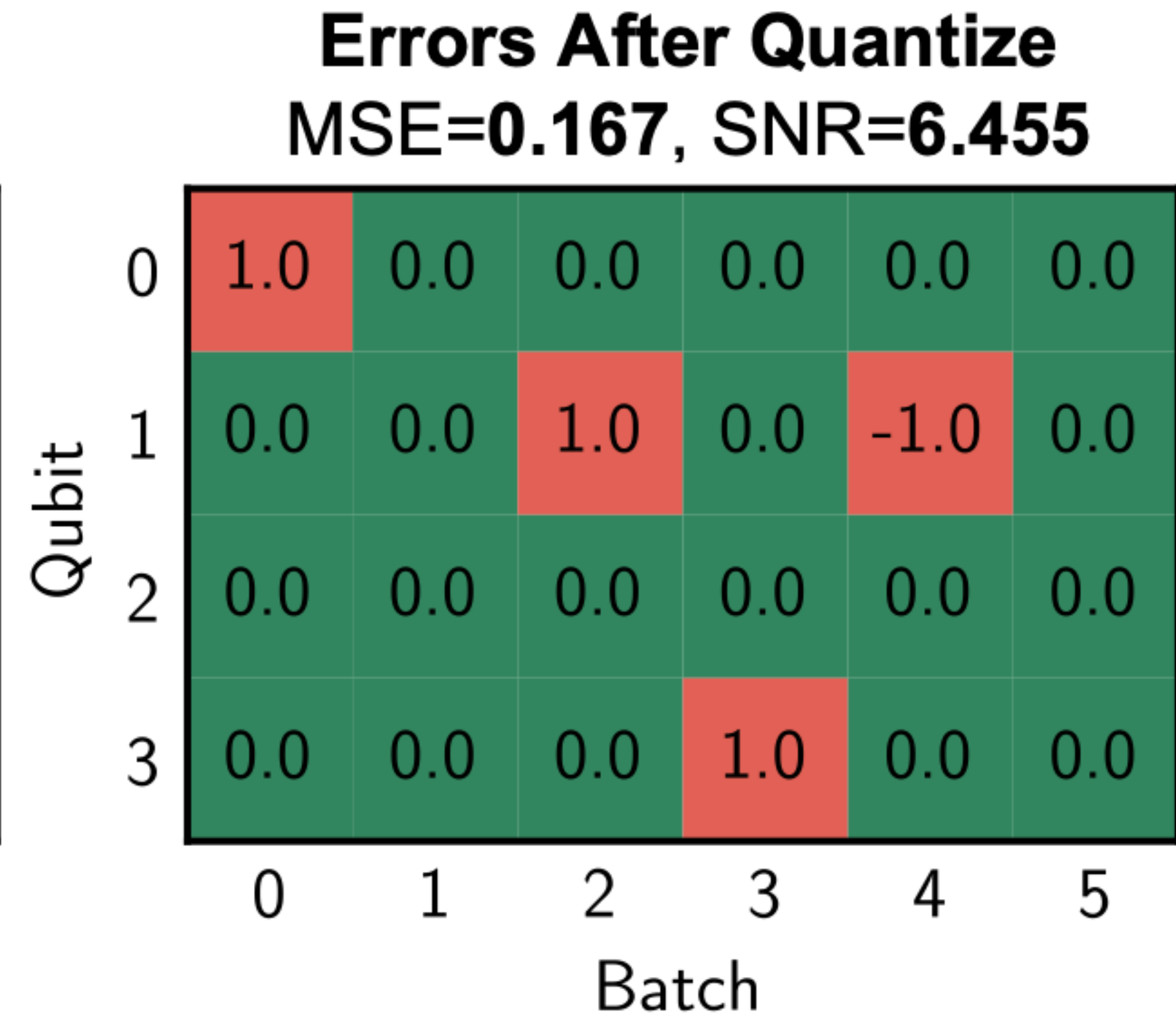
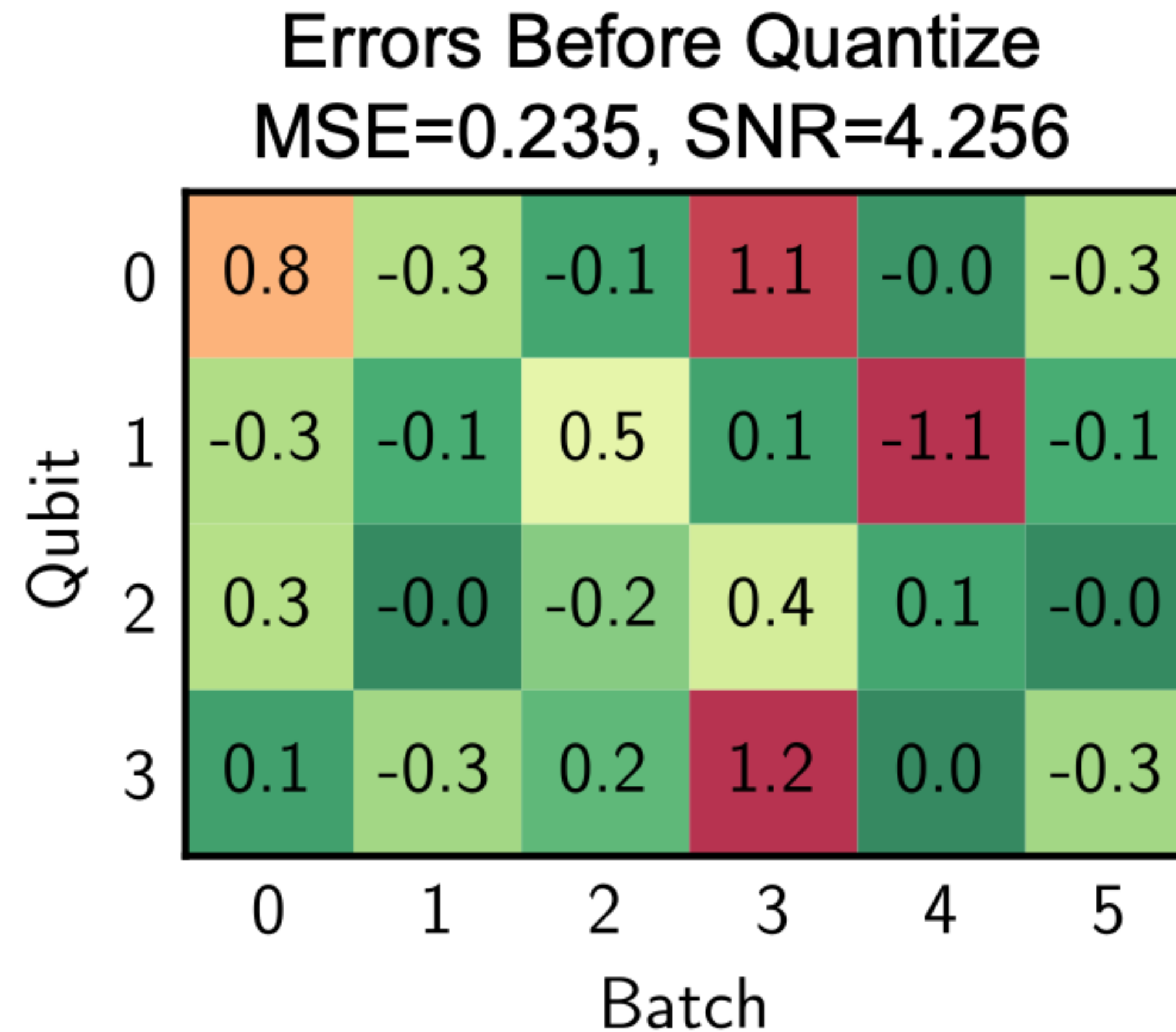
- **Loss** term to encourage measurement outcomes to be close to **centroids**



Post-Measurement Quantization



- Quantization reduces errors and improves SNR

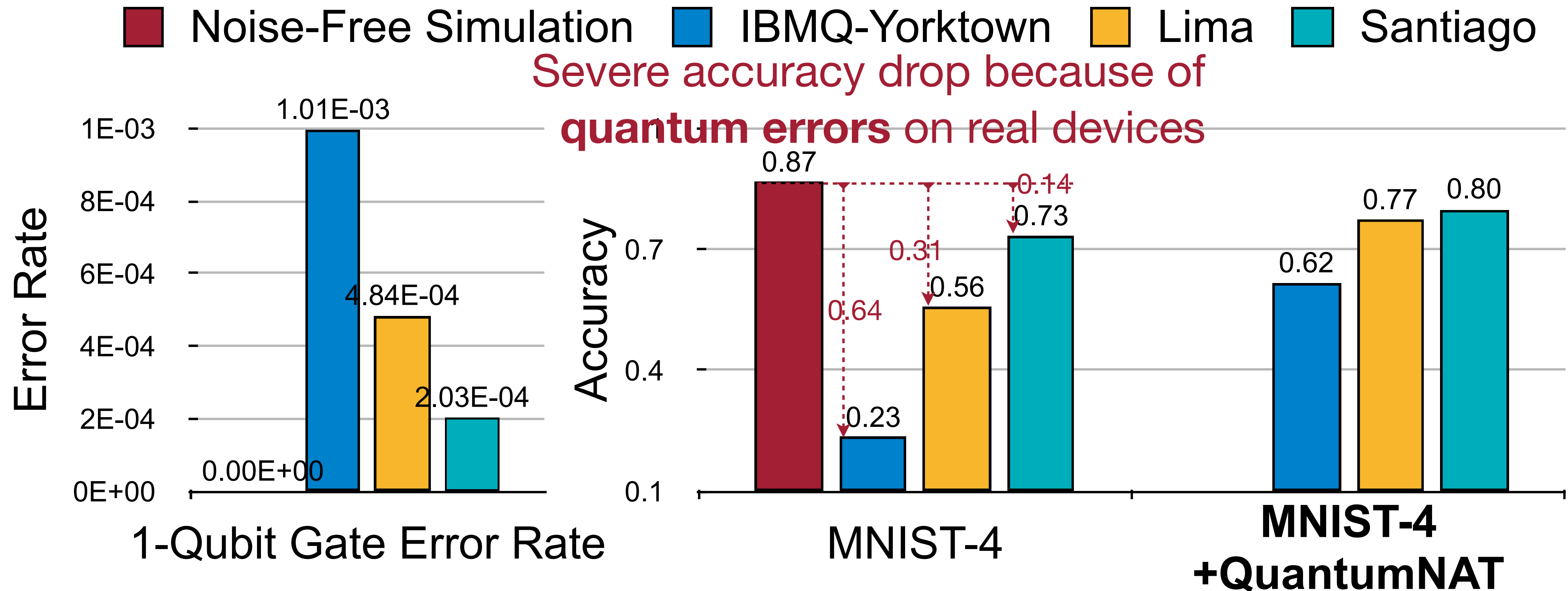


Evaluation

- Benchmarks
 - Quantum Machine Learning task:
 - MNIST 10-class, 4-class, 2-class
 - Fashion MNIST 10-class, 4-class, 2-class
 - Vowel 4-class
 - Cifar-2 class
- Quantum Devices
 - IBMQ
 - #Qubits: 5 to 15
 - Quantum Volume: 8 to 32

Evaluation

- QuantumNAT significantly improves real measurement accuracy



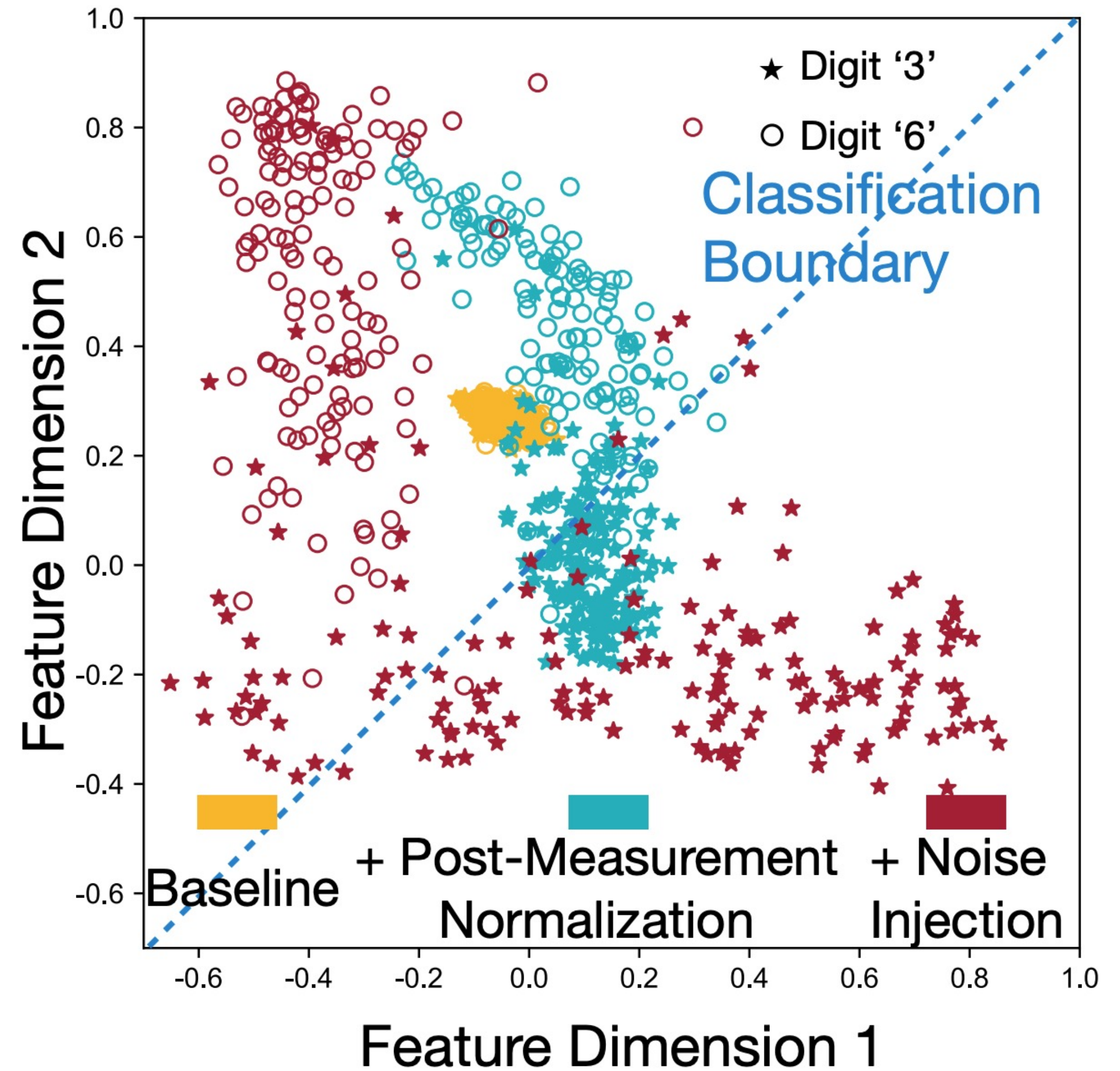
Consistent Improvements on Various Benchmarks

- On IBMQ santiago

Method	MNIST-4	FMNIST-4	Vowel-4	MNIST-2	FMNIST-2	Cifar-2
Baseline	0.30	0.32	0.28	0.84	0.78	0.51
+ Normalization	0.41	0.61	0.29	0.87	0.68	0.56
+Noise Injection	0.61	0.70	0.44	0.93	0.86	0.57
+ Quantization	0.68	0.75	0.48	0.94	0.88	0.59

Visualization

- QuantumNAT stretches the distribution of features
 - MNIST-2 classification task

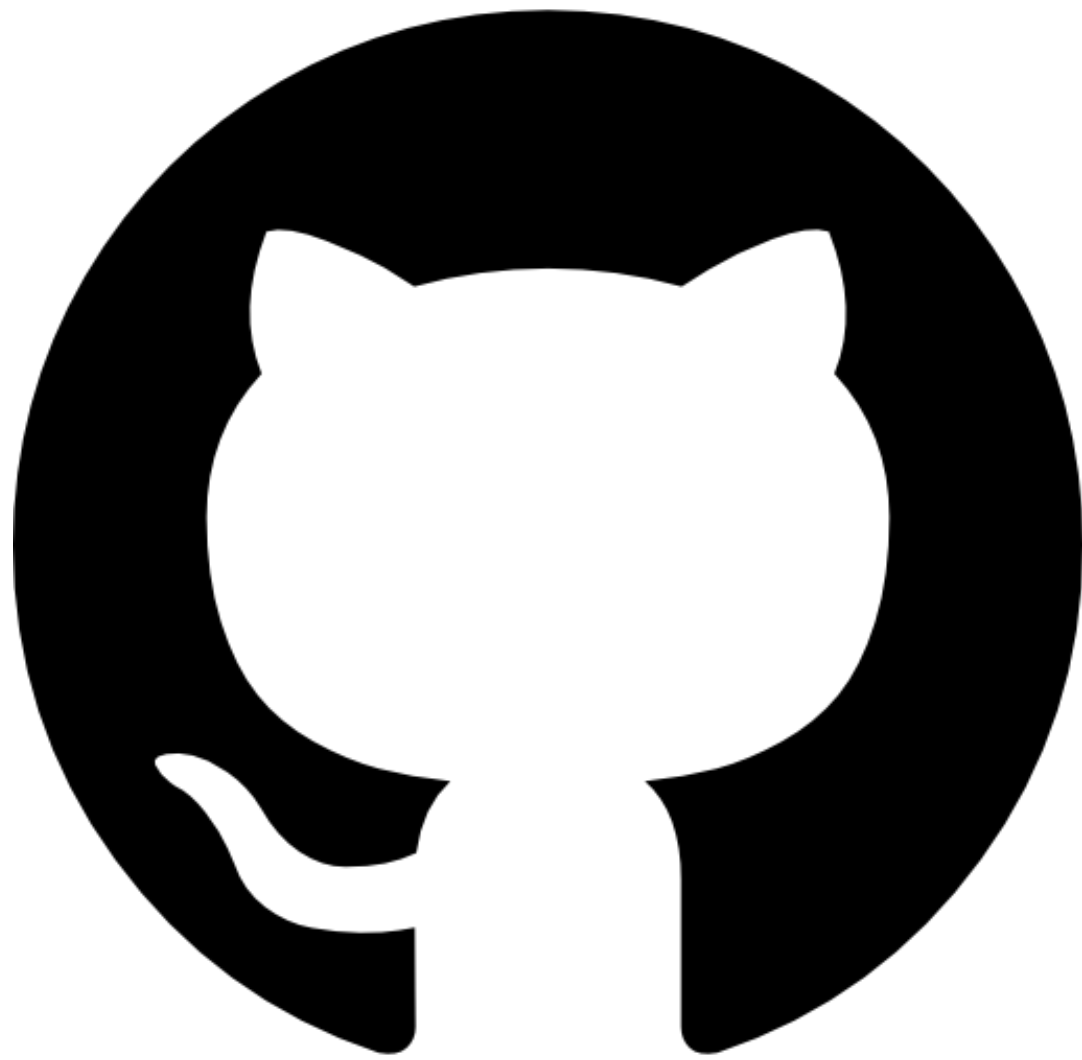


Noise Model in TQ

- `noise_model_tq = tq.NoiseModelTQ(`
- `noise_model_name='ibmq_quito',`
- `factor=10,`
- `add_thermal=True`
- `)`

Hands-On Section

2.2 QuantumNAT



TorchQuantum Tutorial Outline

Section 1

TorchQuantum Basic Usage

1.1 Quantum Basics

1.2 TQ operations 

1.3 TQ for State Prep 


1.4 TQ for VQE 

1.4 TQ for QNN 

Section 2

Use TorchQuantum on Gate level

2.1 QuantumNAS: Ansatz
Search and Gate Pruning 

2.2 QuantumNAT: Noise
Injection and Quantization 

2.3 QOC: On-Chip Training 

2.4 Transformer for Quantum
Circuit Reliability Prediction

2.5 QNN Compression 

Section 3

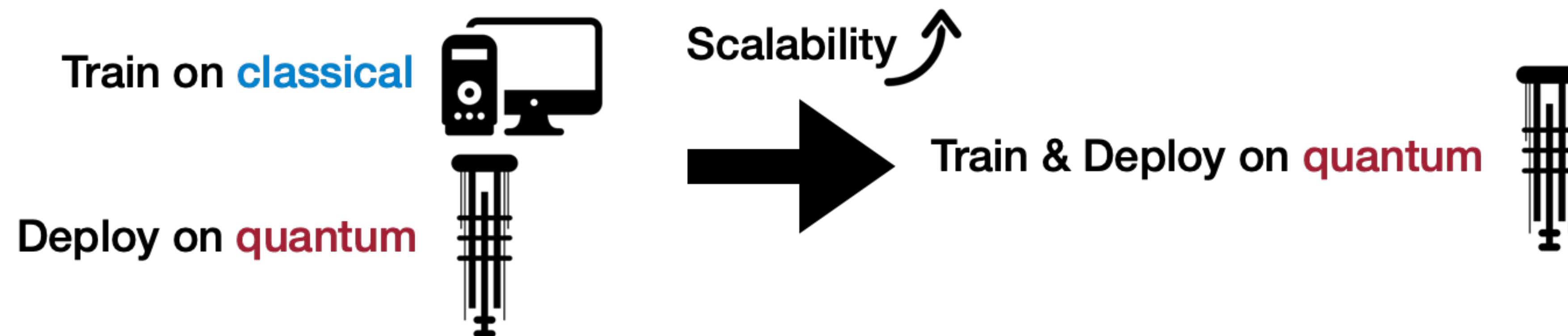
Use TorchQuantum on Pulse level

3.1 Quantum Optimal Control 

3.2 Variational Pulse Learning 

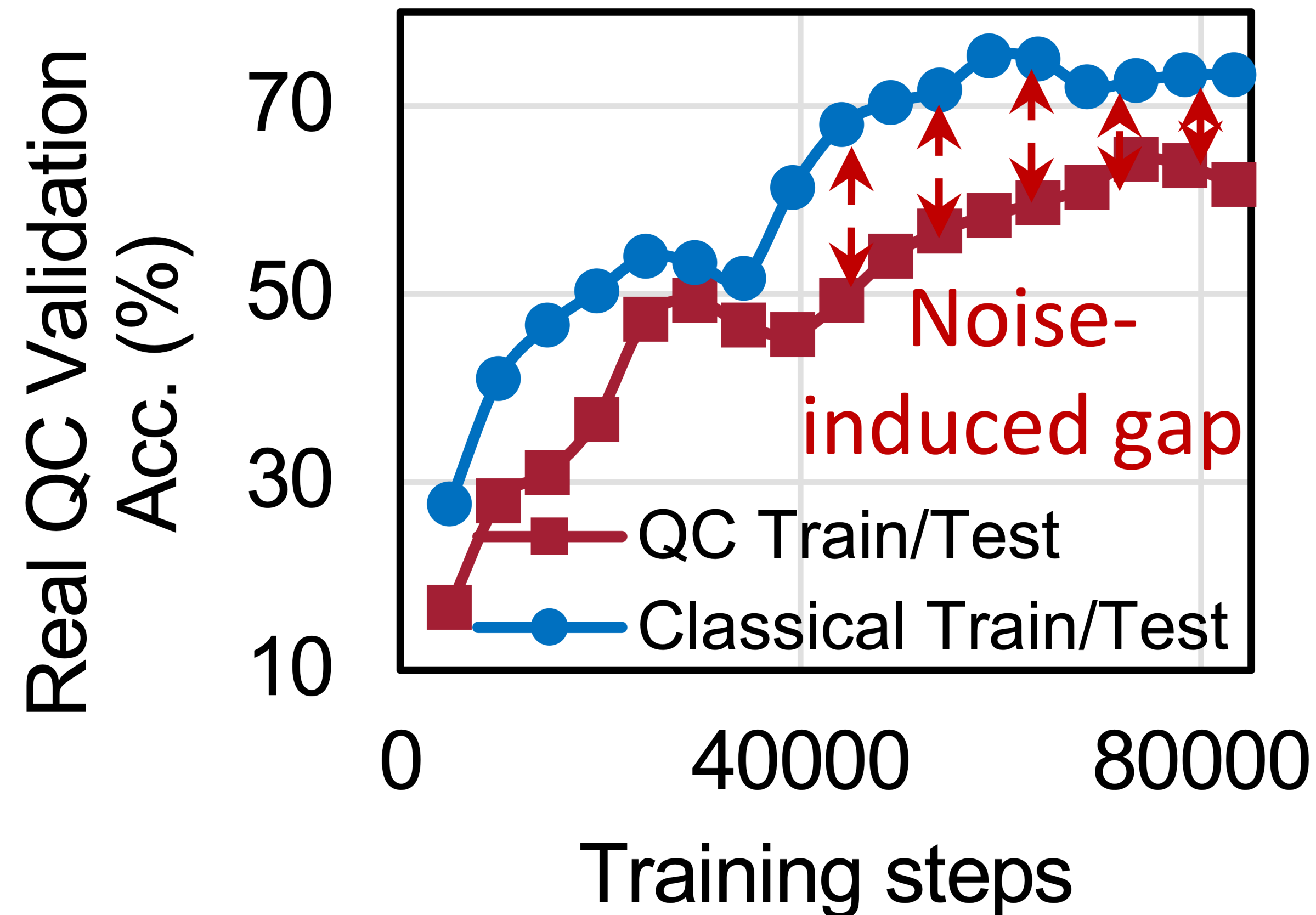
QOC for High Scalability

- How to further improve the scalability of PQC training?
- Train the parameters directly on real quantum machine



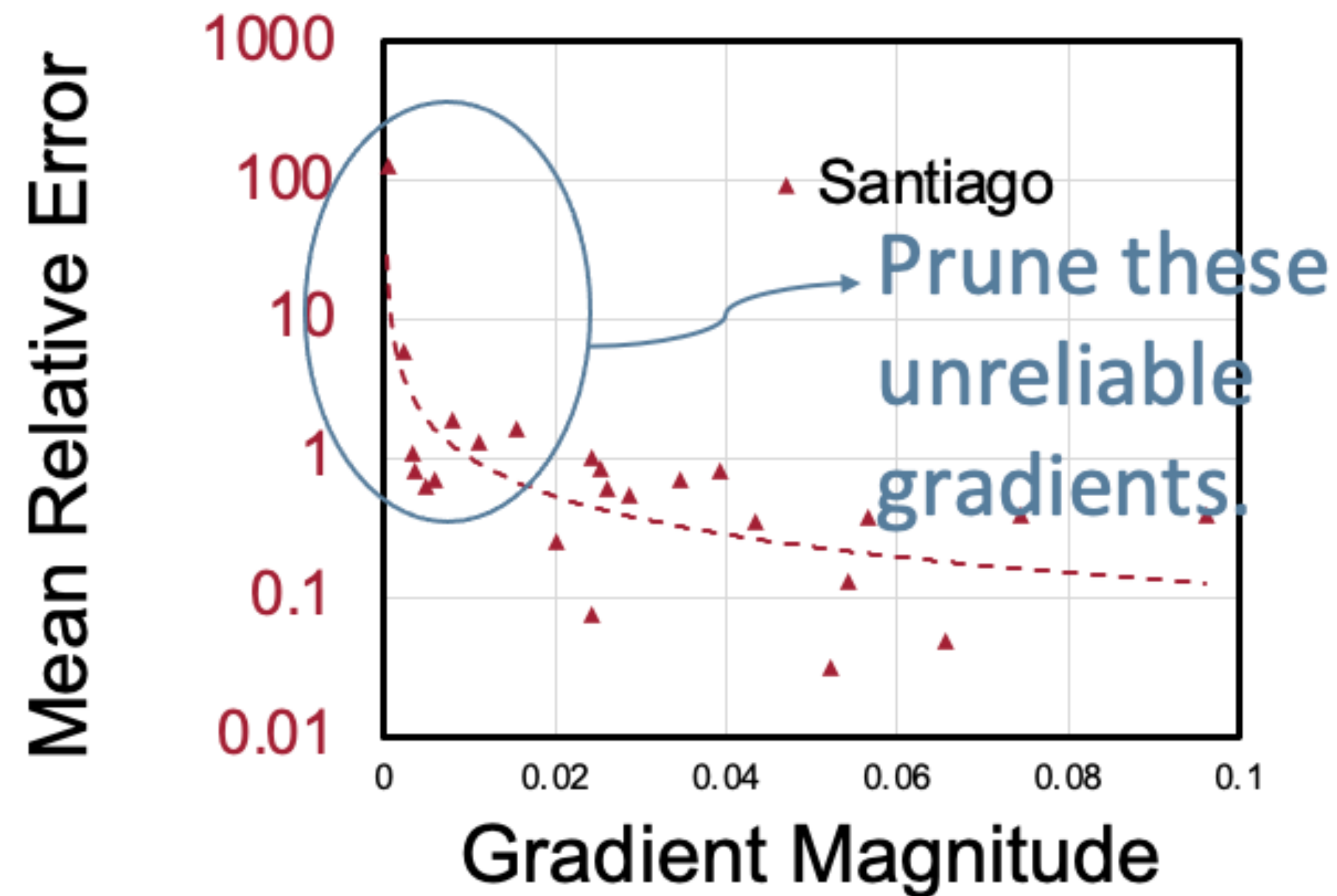
Challenge of On-chip Training: noise

- Noise **reduces reliability** of on-chip computed gradients



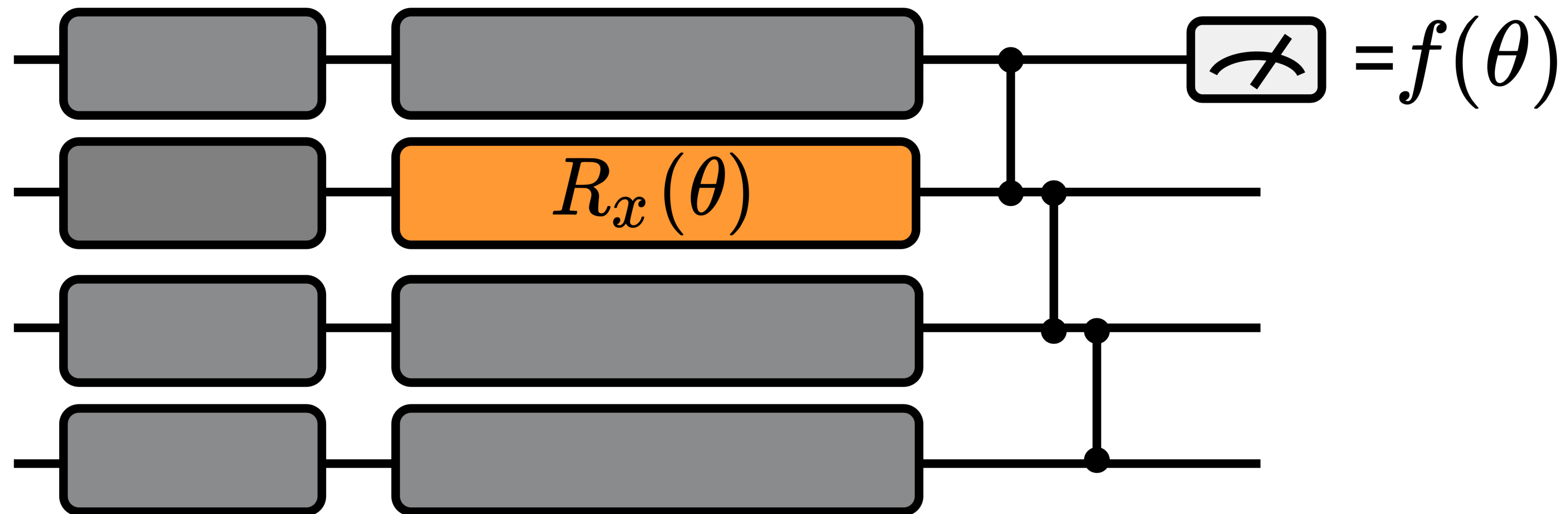
Challenge of On-chip Training: noise

- Noise **reduces reliability** of on-chip computed gradients
- **Small** magnitude gradients have **large** relative errors



Parameter Shift Rules

- Calculate the gradient of θ w.r.t. $f(\theta)$.

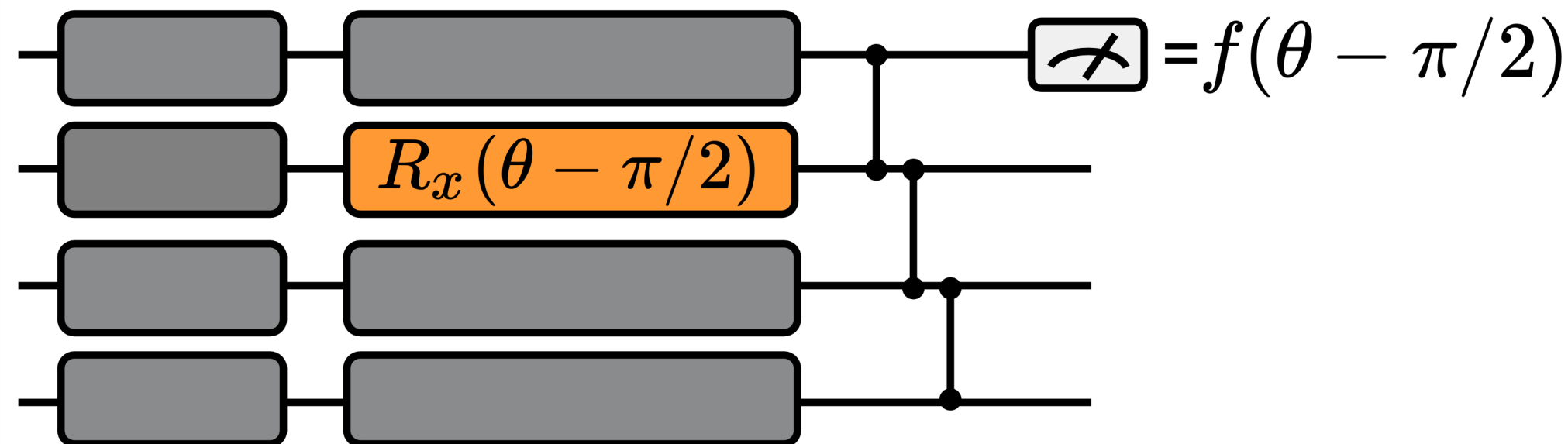
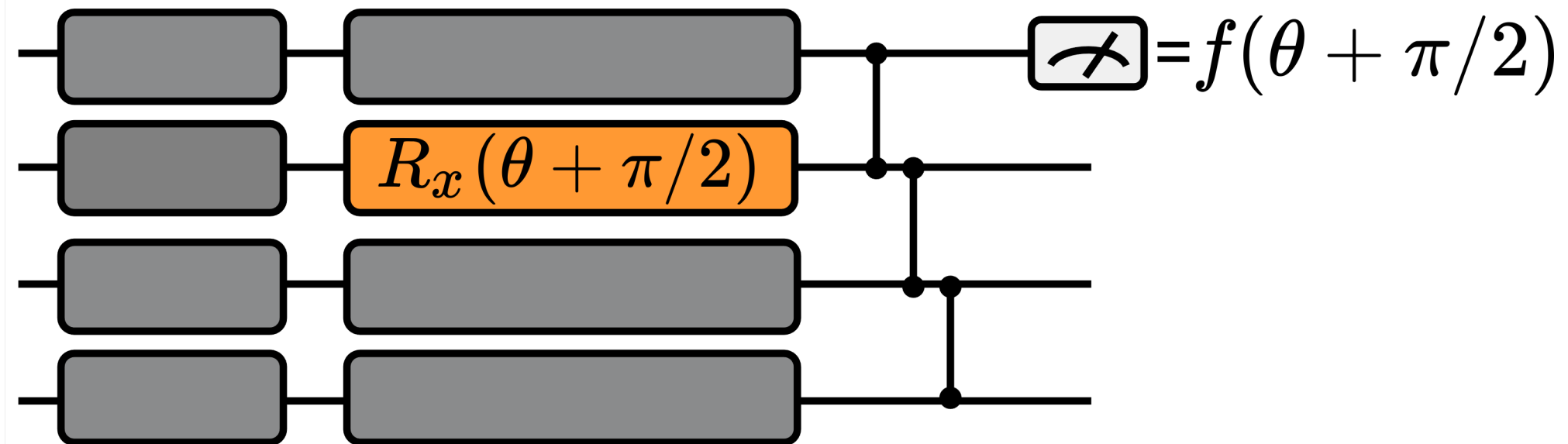


Parameter Shift Rules

- Calculate the gradient of θ w.r.t. $f(\theta)$.

Parameter Shift Rules

- Shift θ twice



$$\frac{\partial}{\partial \theta} f(\theta) = \frac{1}{2} \left(f\left(\theta + \frac{\pi}{2}\right) - f\left(\theta - \frac{\pi}{2}\right) \right)$$

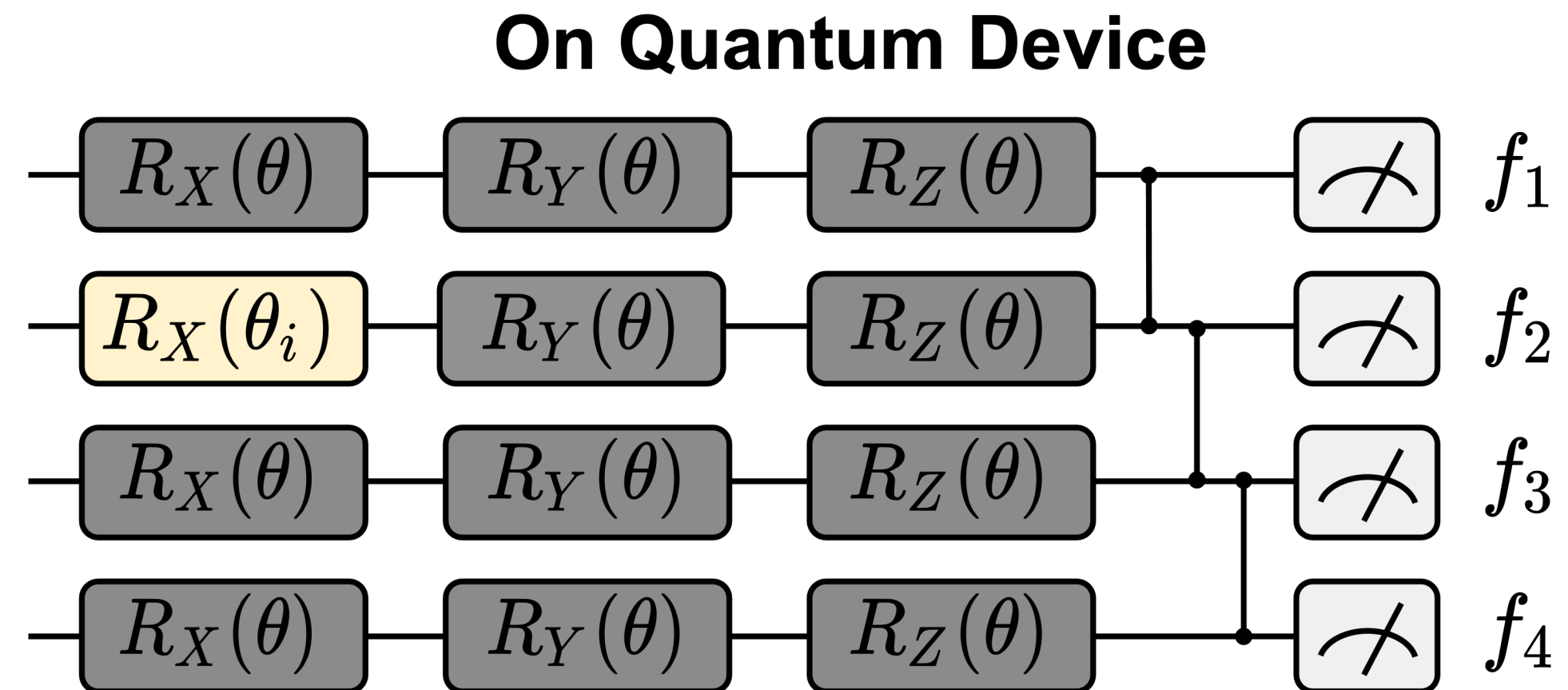
Parameter Shift Rules

- This formula is valid to all rotation gates
 - RZ, RY, RX, RXX, RZZ
- One gradient requires two runs on real quantum machine

$$\frac{\partial}{\partial \theta} f(\theta) = \frac{1}{2} \left(f\left(\theta + \frac{\pi}{2}\right) - f\left(\theta - \frac{\pi}{2}\right) \right)$$

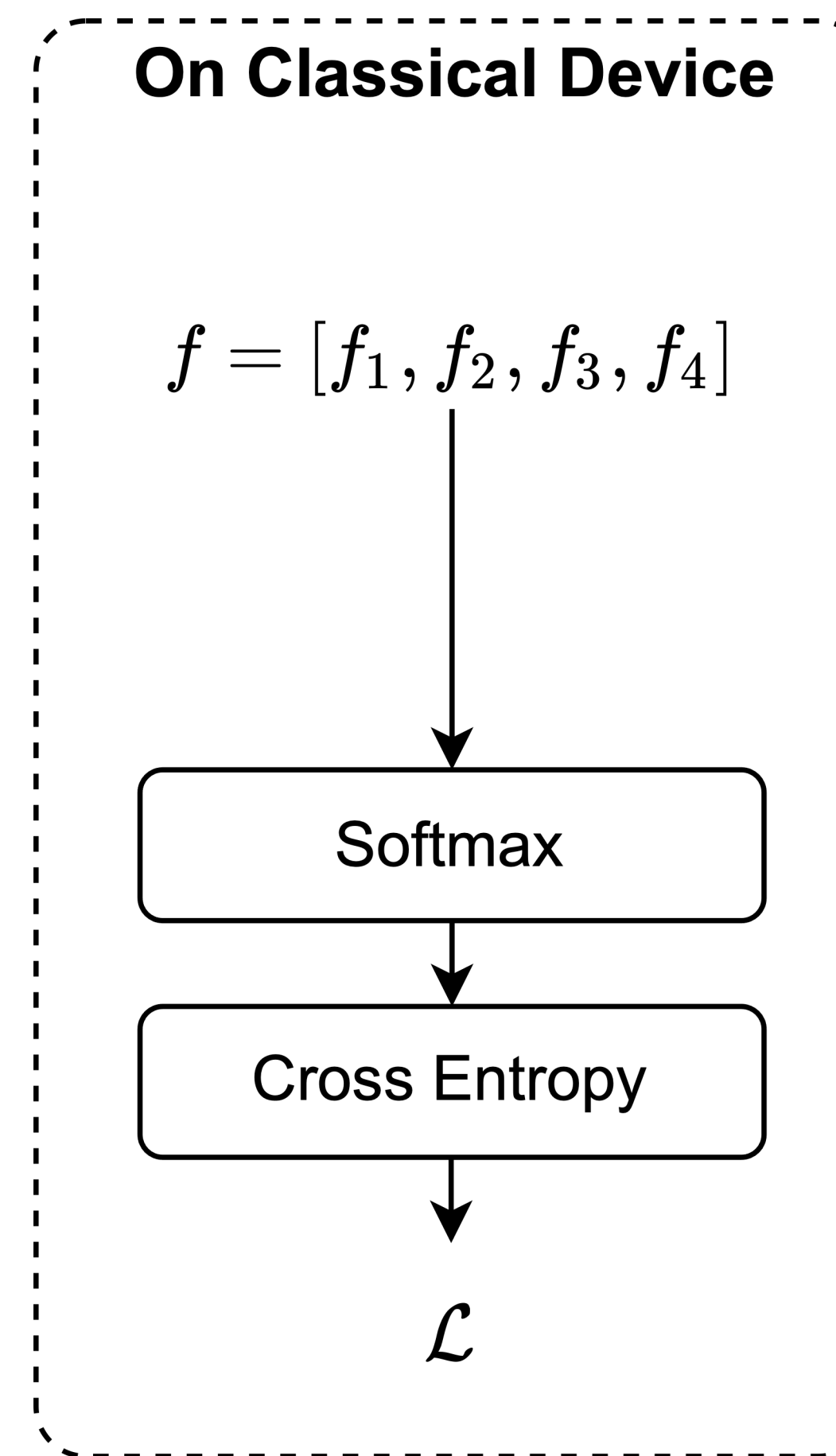
Calculate Gradients of PQC

- Step 1: Run on QC without shift to obtain f



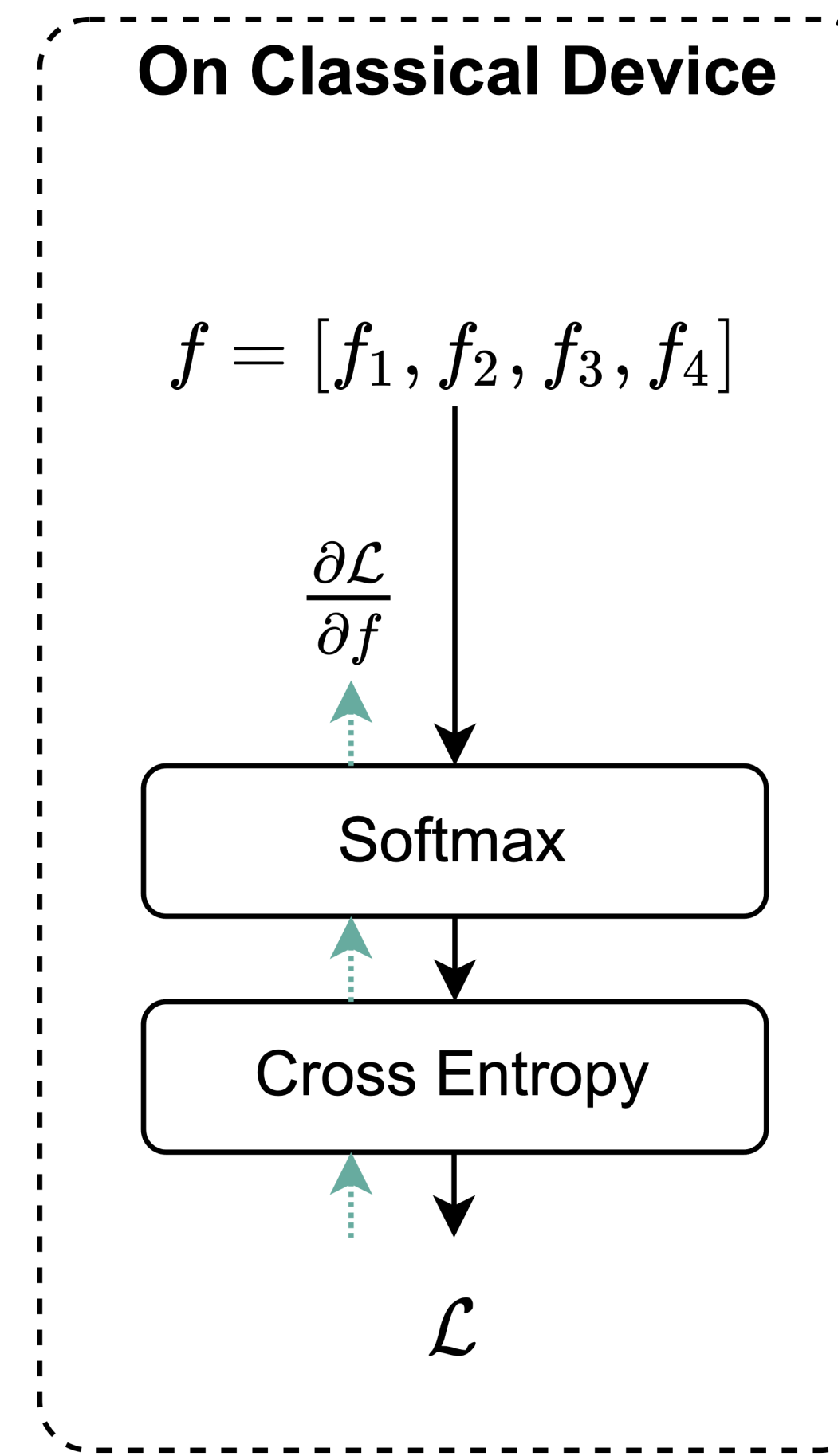
Calculate Gradients of PQC

- Step 2: Further forward to get $Loss$



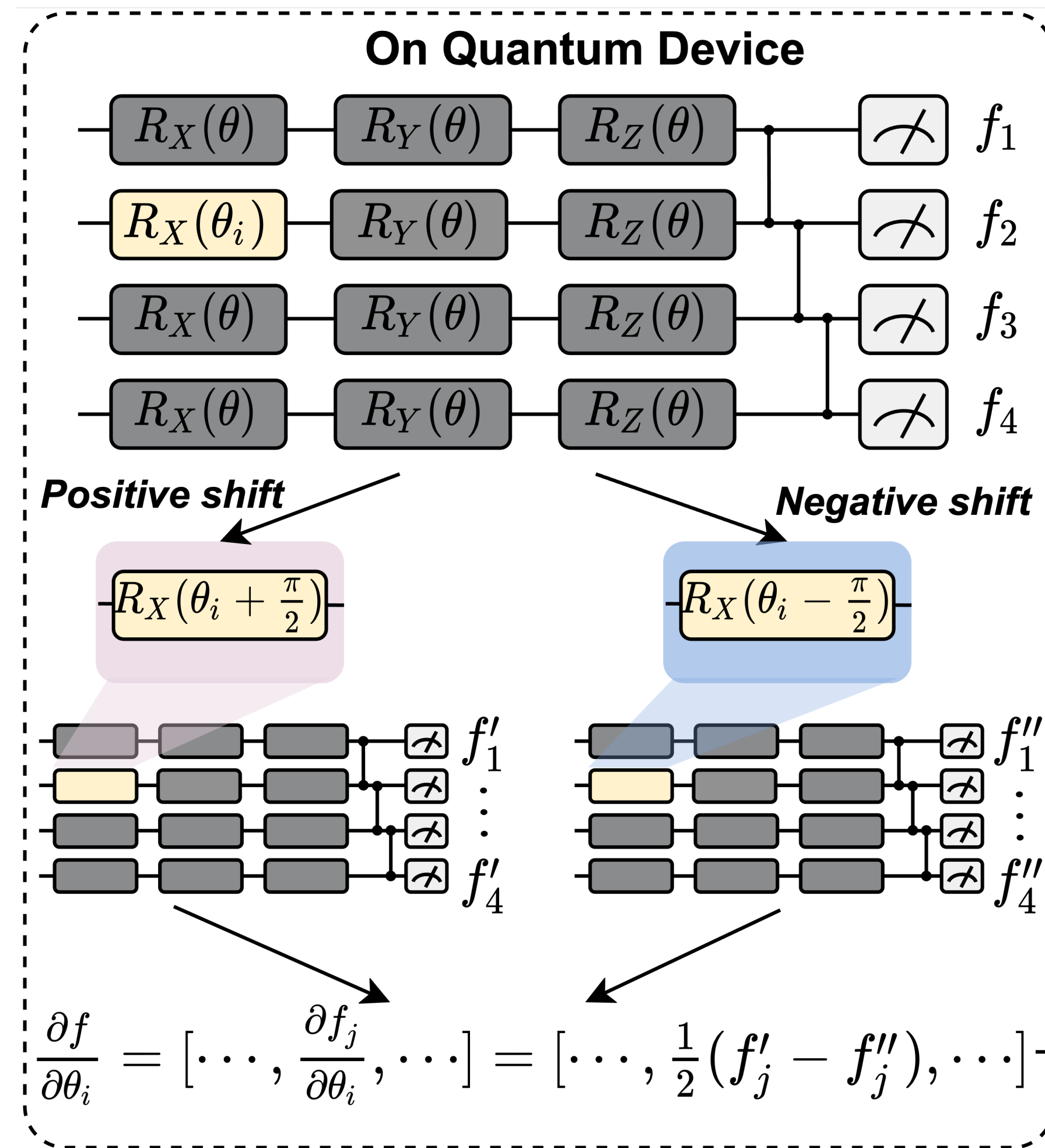
Calculate Gradients of PQC

- Step 3: Backpropagation to calculate $\frac{\partial \text{Loss}}{\partial f(\theta)}$



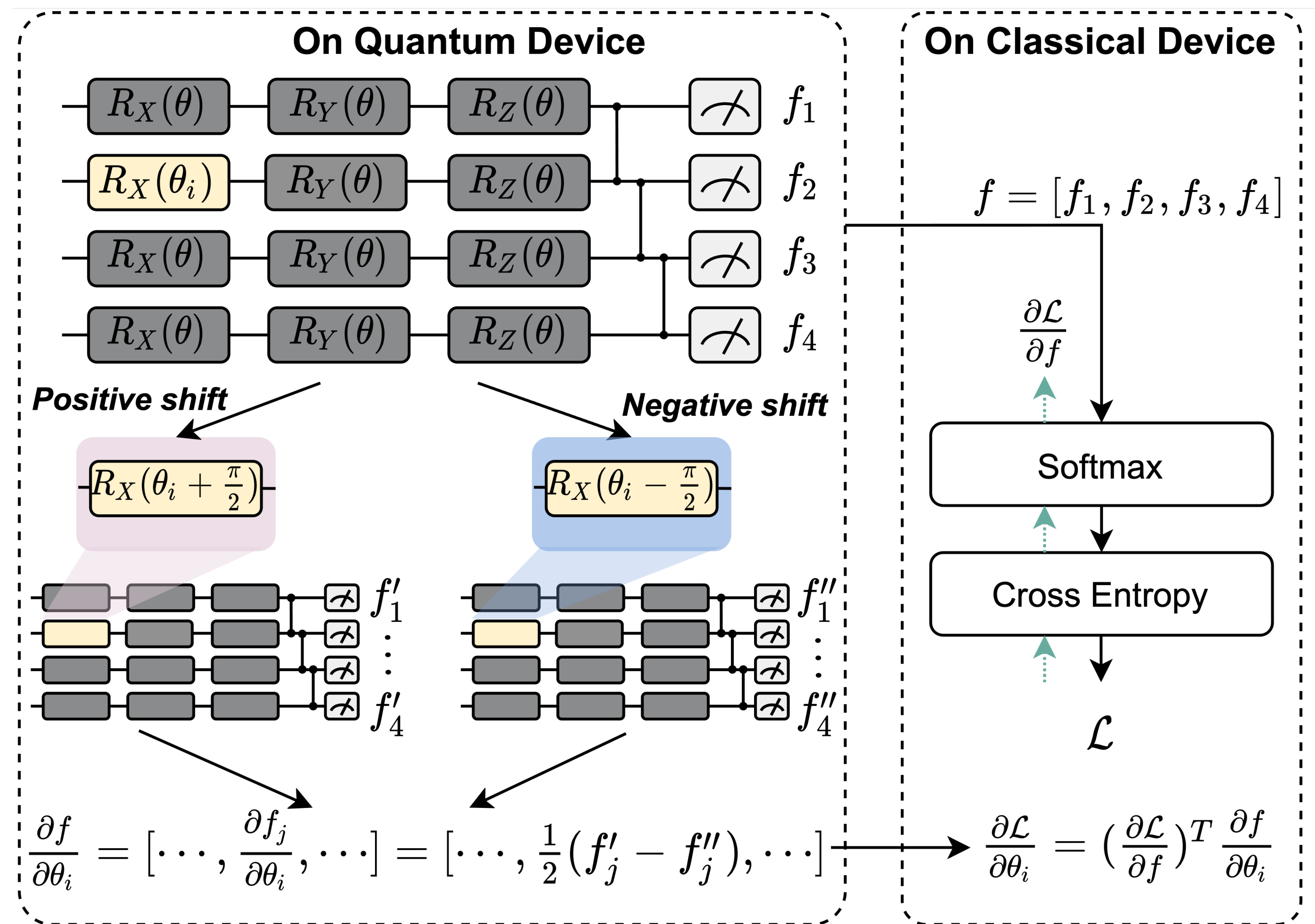
Calculate Gradients of PQC

- Step 4: Shift twice and run on QC to calculate $\frac{\partial f(\theta)}{\partial \theta_i}$



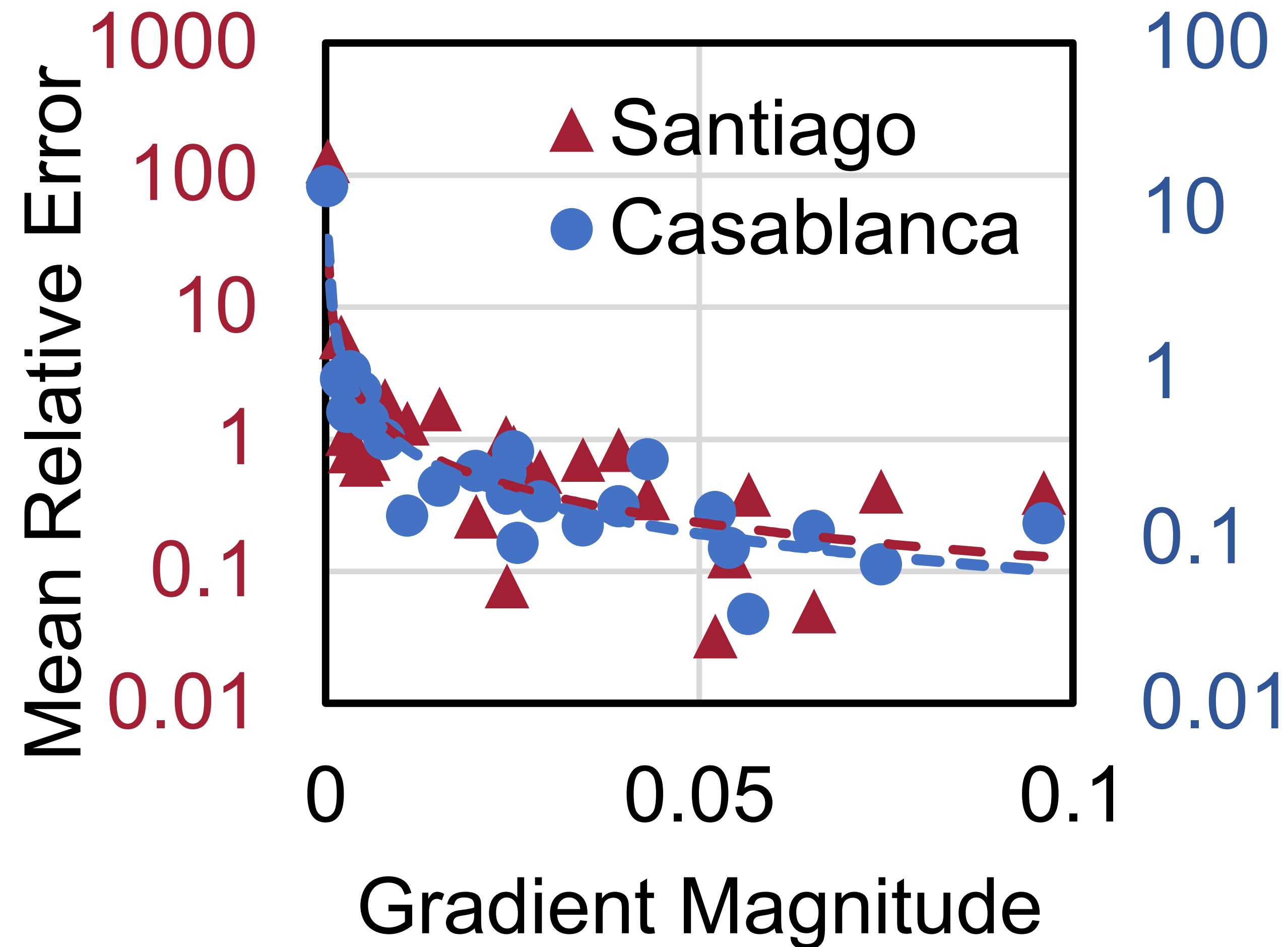
Calculate Gradients of PQC

- Step 5: By Chain Rule: $\frac{\partial \text{Loss}}{\partial f(\theta)} \frac{\partial f(\theta)}{\partial \theta_i} = \frac{\partial \text{Loss}}{\partial \theta_i}$, sum over 4 passes (4 qubits)
- Only **forward** on quantum device

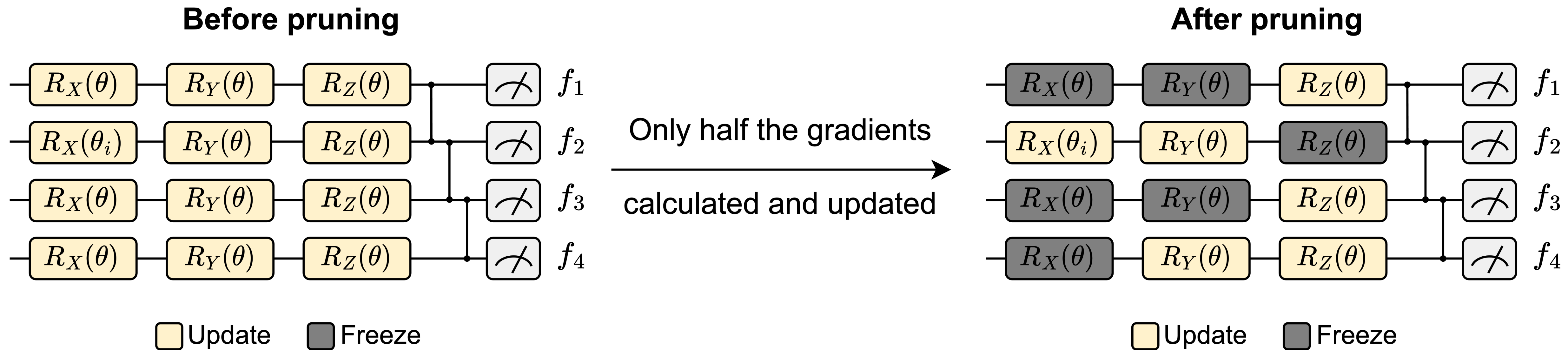


Probabilistic Gradient Pruning

- **Small** magnitude gradients have **large** relative errors

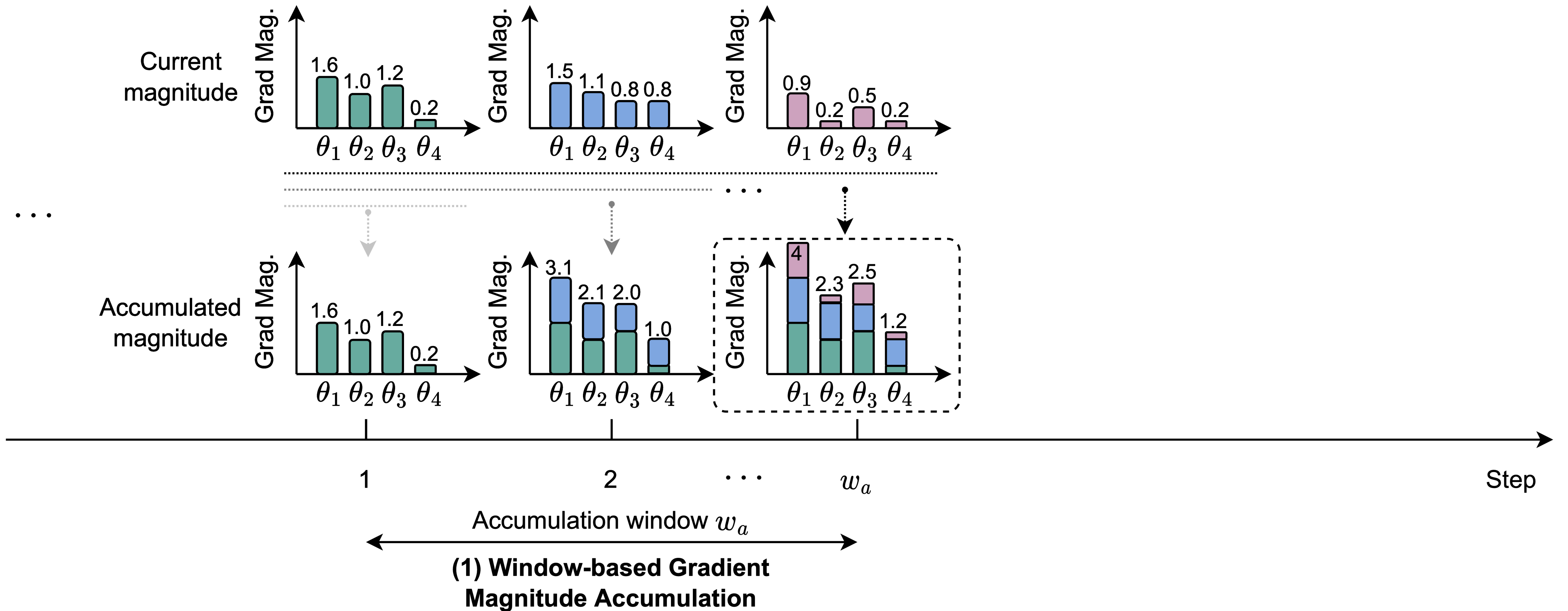


Probabilistic Gradient Pruning



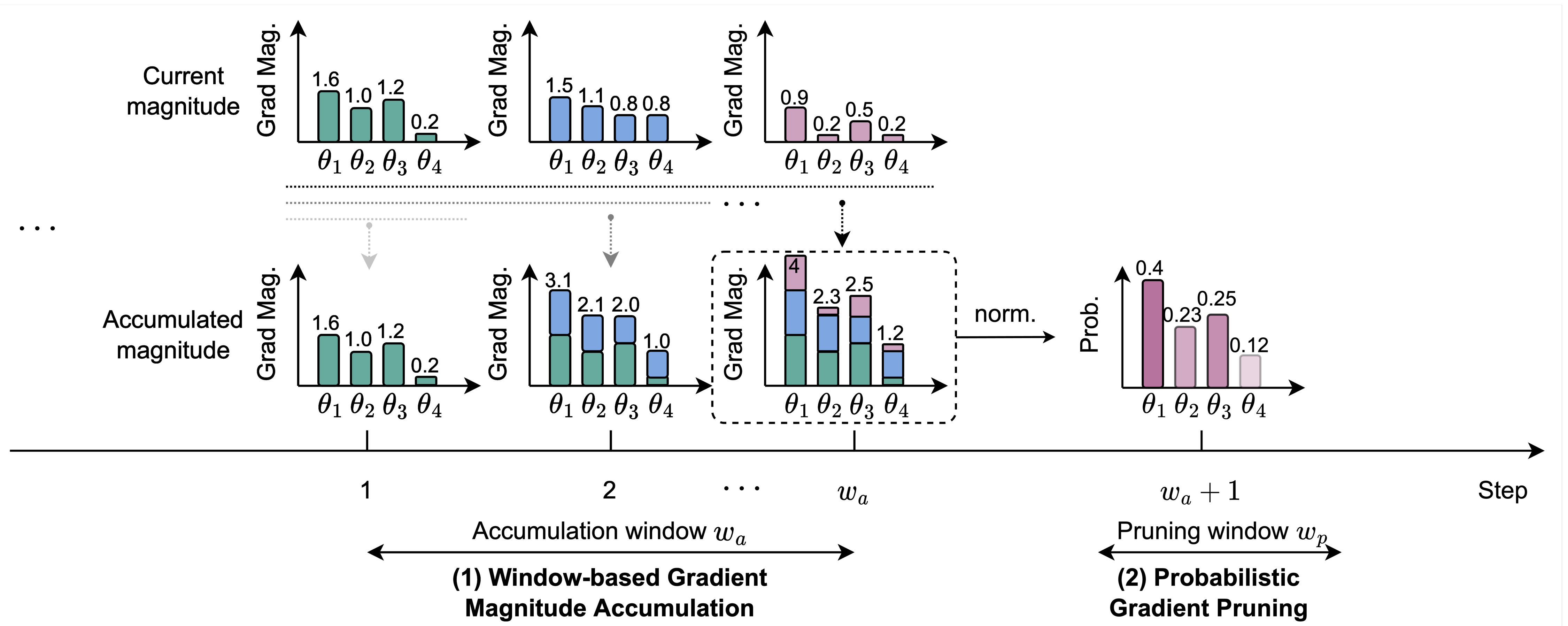
Accumulation Window

- Keep a record of accumulated gradient magnitude



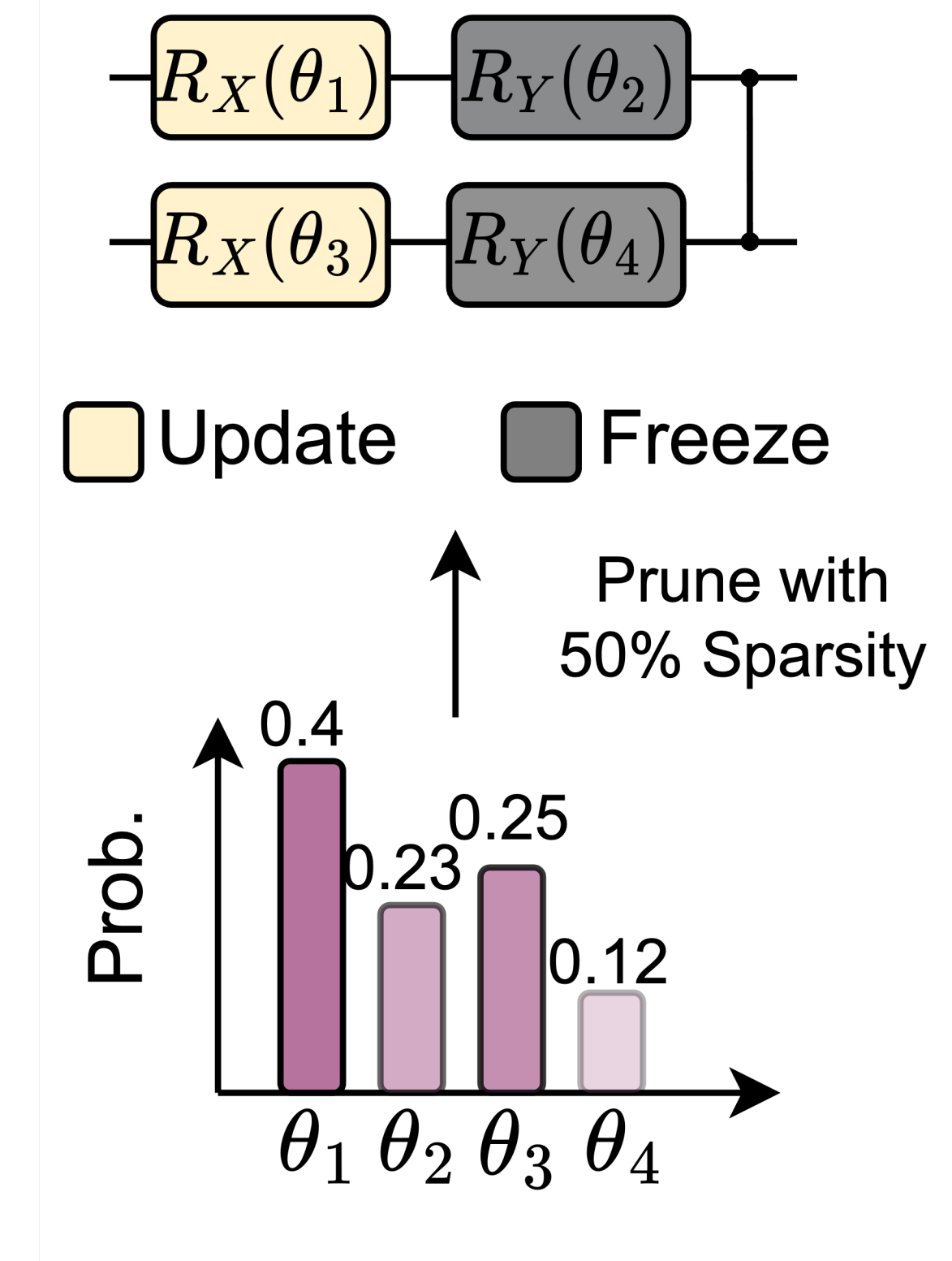
Accumulation Window

- Normalize the accumulated gradient magnitude to a probability distribution



Accumulation Window

- Prune the calculation of some gradients according to the probability distribution



Evaluation

- Benchmarks
 - Quantum Machine Learning task: MNIST 4-class, 2-class, Fashion MNIST 4-class, 2-class, Vowel 4-class
 - Variational Quantum Eigensolver task: H2 molecule
- Quantum Devices
 - IBMQ
 - #Qubits: 5 to 7
 - Quantum Volume: 8 to 32
- Circuit architecture
 - RZZ+RY, RXYZ+CZ, RZX+RXX

Evaluation

- Benchmarks
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- Circuit architecture
 - RZZ+RY, RXYZ+CZ, RZX+RXX

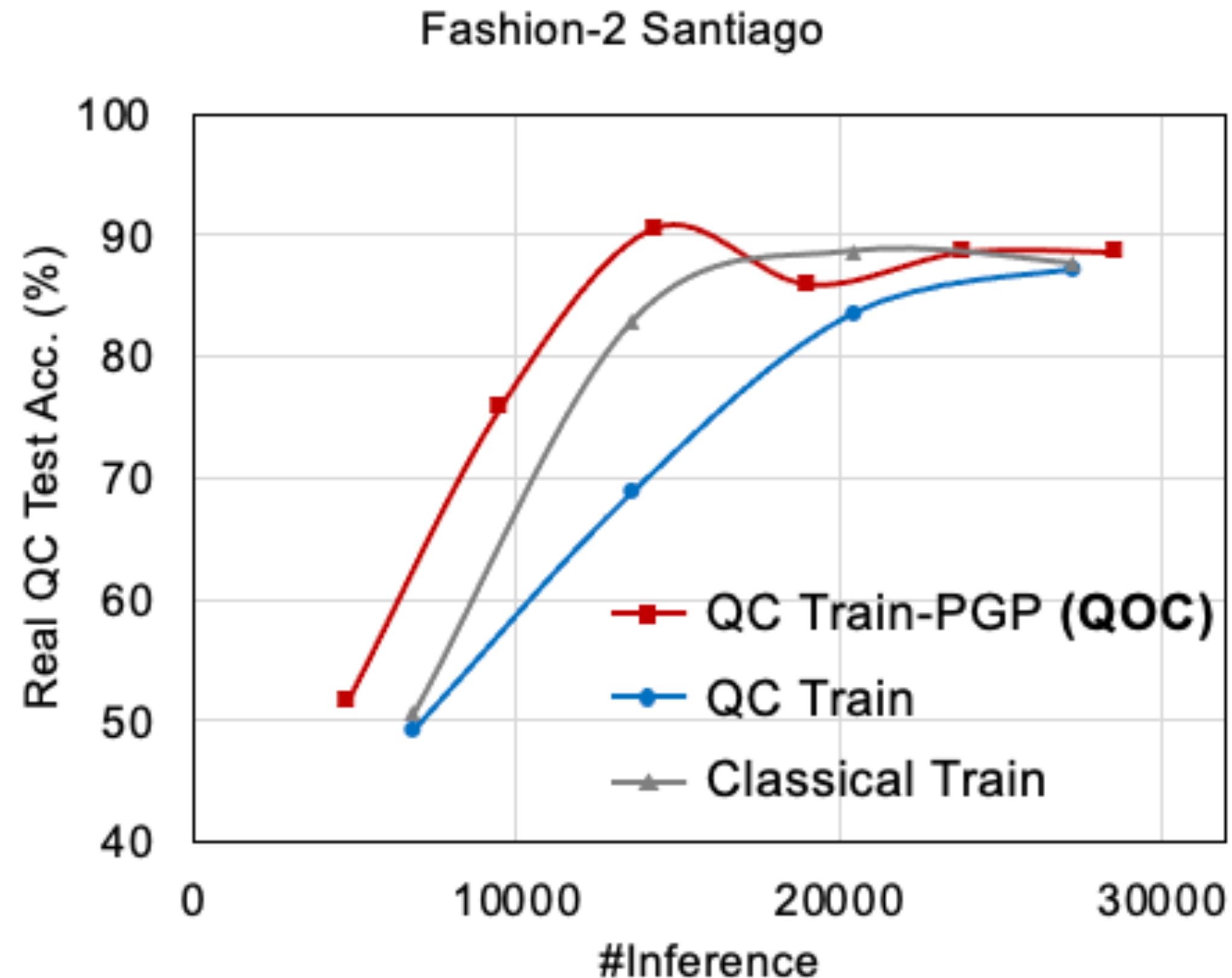
QNN results

- QOC achieved similar results to classical simulation

Method	Acc.	MNIST-4 Jarkata	MNIST-2 Jarkata	Fashion-4 Manila	Fashion-2 Santiago	Vowel-4 Lima
Classical-Train	Simu.	0.61	0.88	0.73	0.89	0.37
Classical-Train	QC	0.59	0.79	0.54	0.89	0.31
QC-Train		0.59	0.83	0.49	0.84	0.34
QC-Train-PGP		0.64	0.86	0.57	0.91	0.36

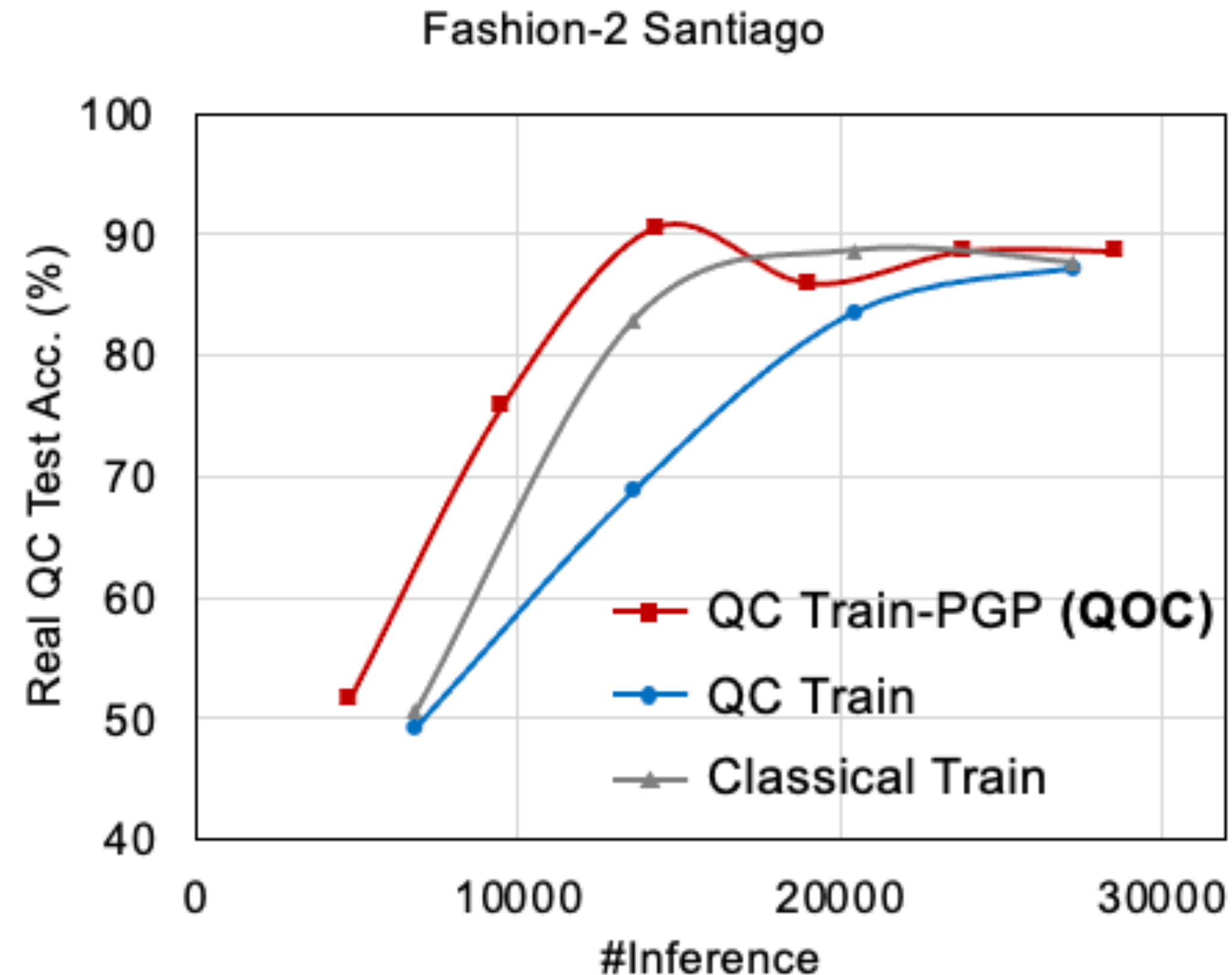
QNN Training Curves

- Classical Train: Train on classical simulator and test on real QC
- QC Train: Train and test the model on real QC
- QC Train-PGP (**QOC**): Train and test on real QC with gradient pruning



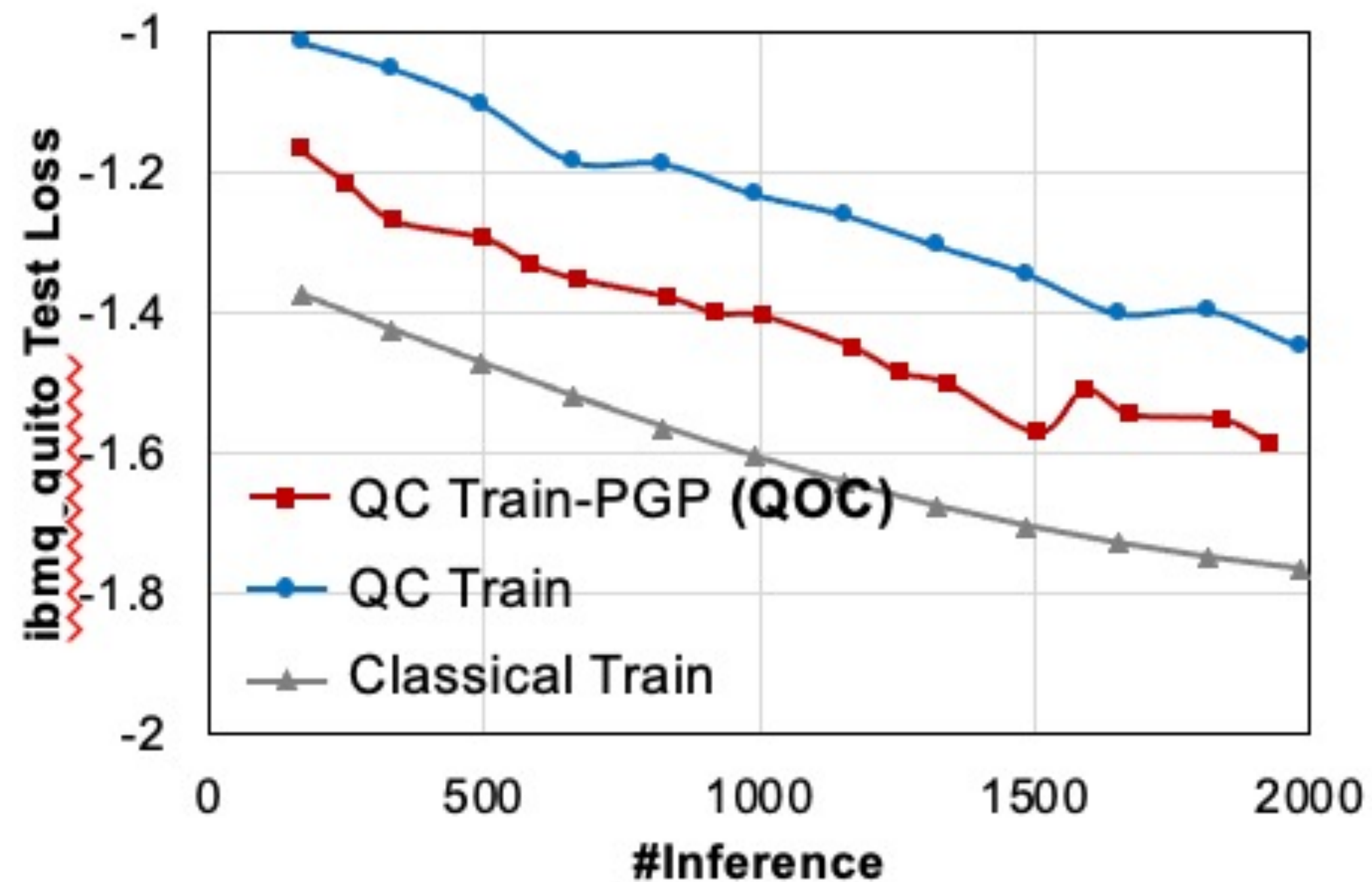
QNN Training Curves

- Gradient pruning can brings **2%~4%** accuracy improvements
- Pruning **accelerates convergence** with **2x** training time reduction



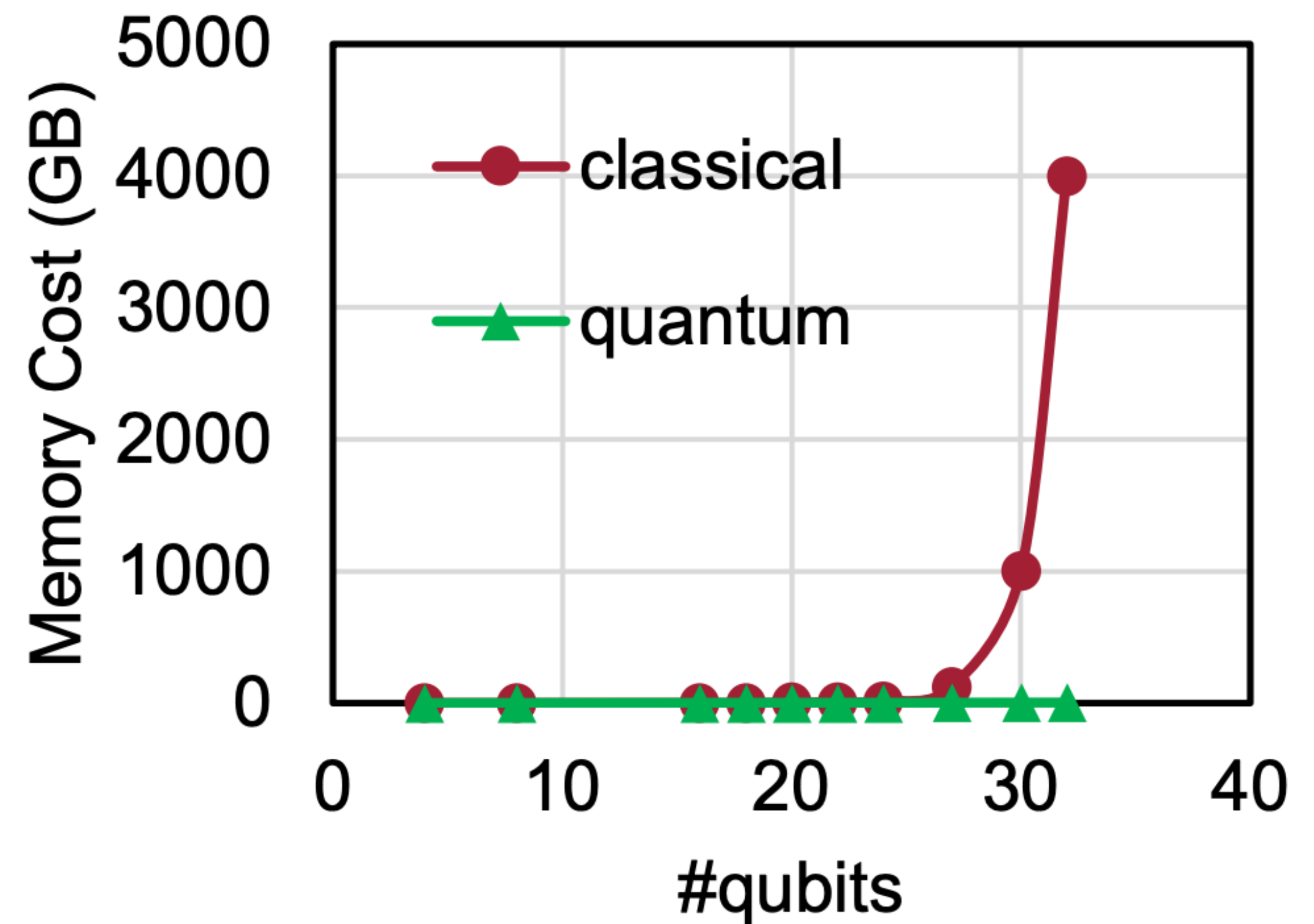
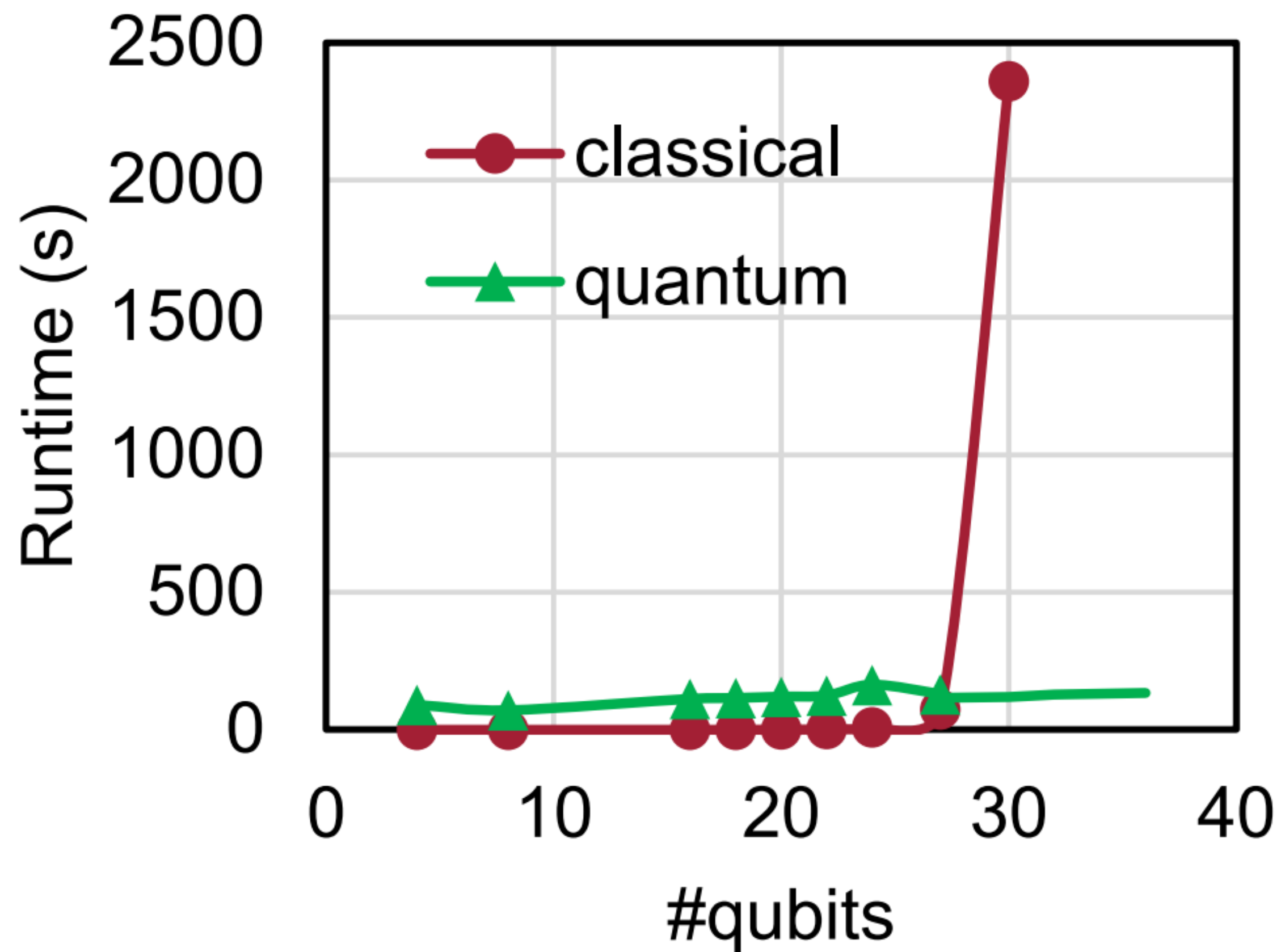
VQE Training Curves

- Gradient pruning can **reduce the gap** between quantum and classical



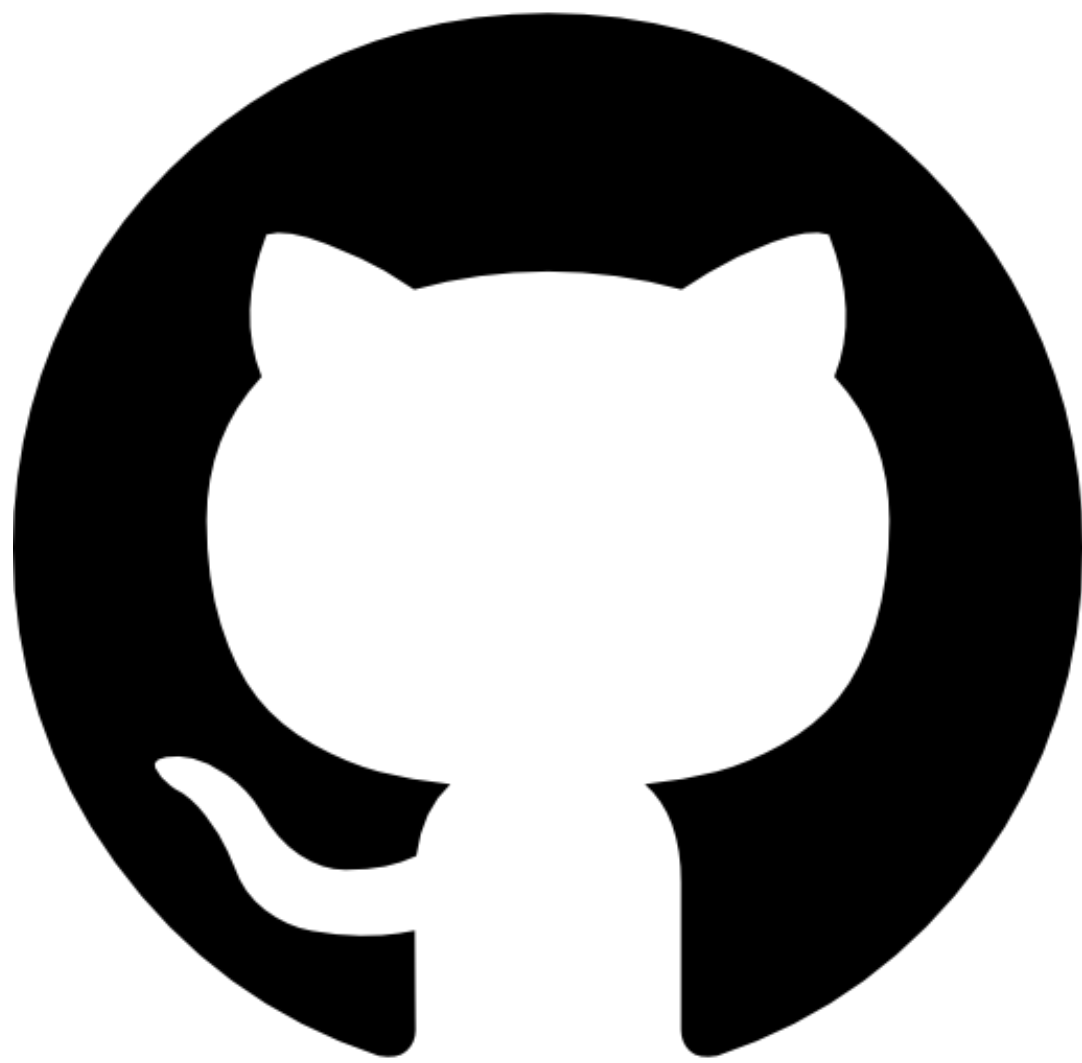
Scalability Improvements

- On-chip Training is scalable



Hands-On Section

2.3 Quantum On-chip Training



TorchQuantum Tutorial Outline

Section 1

TorchQuantum Basic Usage

1.1 Quantum Basics

1.2 TQ operations 

1.3 TQ for State Prep 


1.4 TQ for VQE 

1.4 TQ for QNN 

Section 2

Use TorchQuantum on Gate level

2.1 QuantumNAS: Ansatz
Search and Gate Pruning 

2.2 QuantumNAT: Noise
Injection and Quantization 

2.3 QOC: On-Chip Training 

2.4 Transformer for Quantum
Circuit Reliability Prediction

2.5 QNN Compression 

Section 3

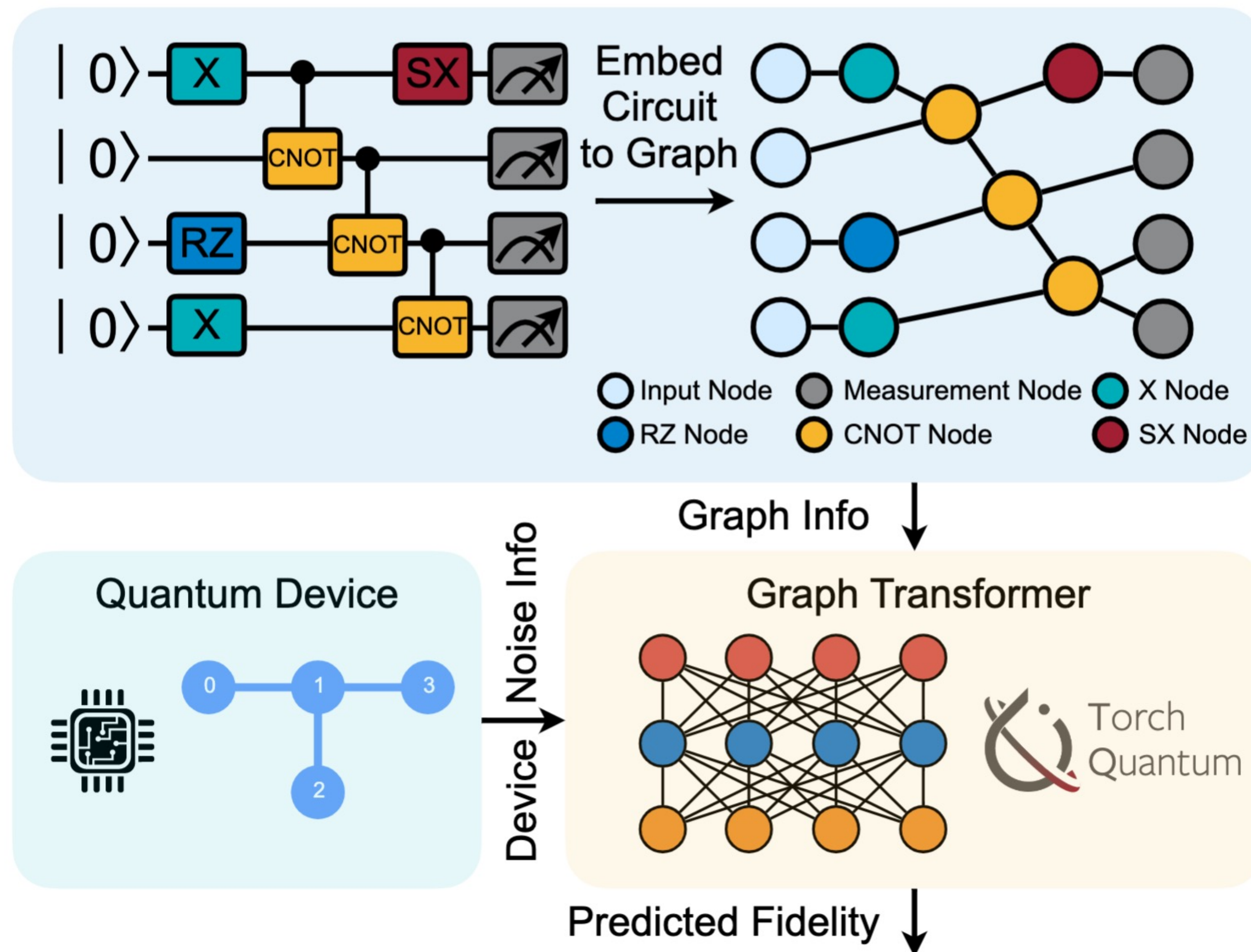
Use TorchQuantum on Pulse level

3.1 Quantum Optimal Control 

3.2 Variational Pulse Learning 

Transformer for Quantum Circuit Reliability Prediction

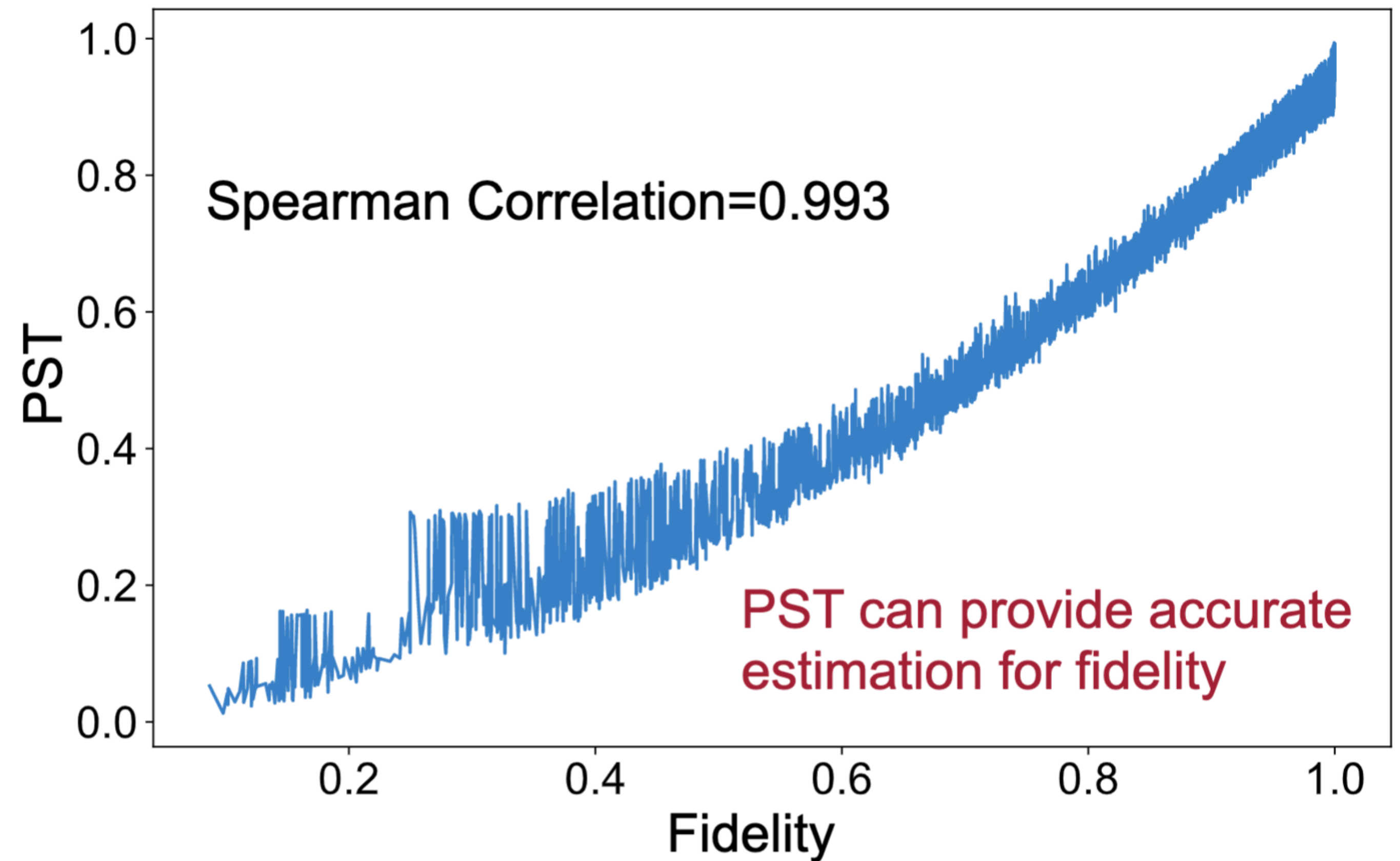
- Use the circuit graph information



Transformer for Quantum Circuit Reliability Prediction

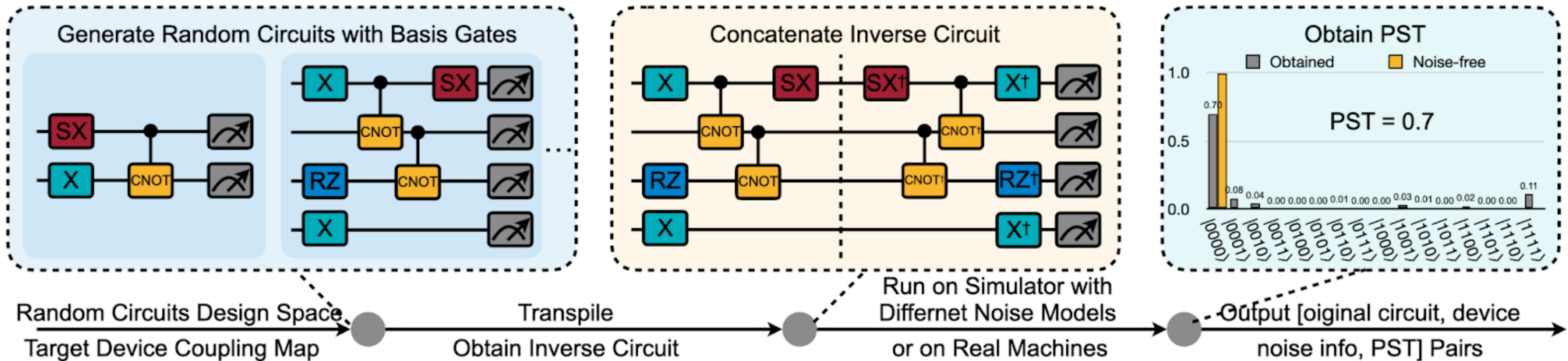
- Use PST as the metrics

$$PST = \frac{\#Trials \text{ with output same as initial state}}{\#Total \text{ trials}}$$



Dataset collection

- Collect dataset on real machine / noisy simulator

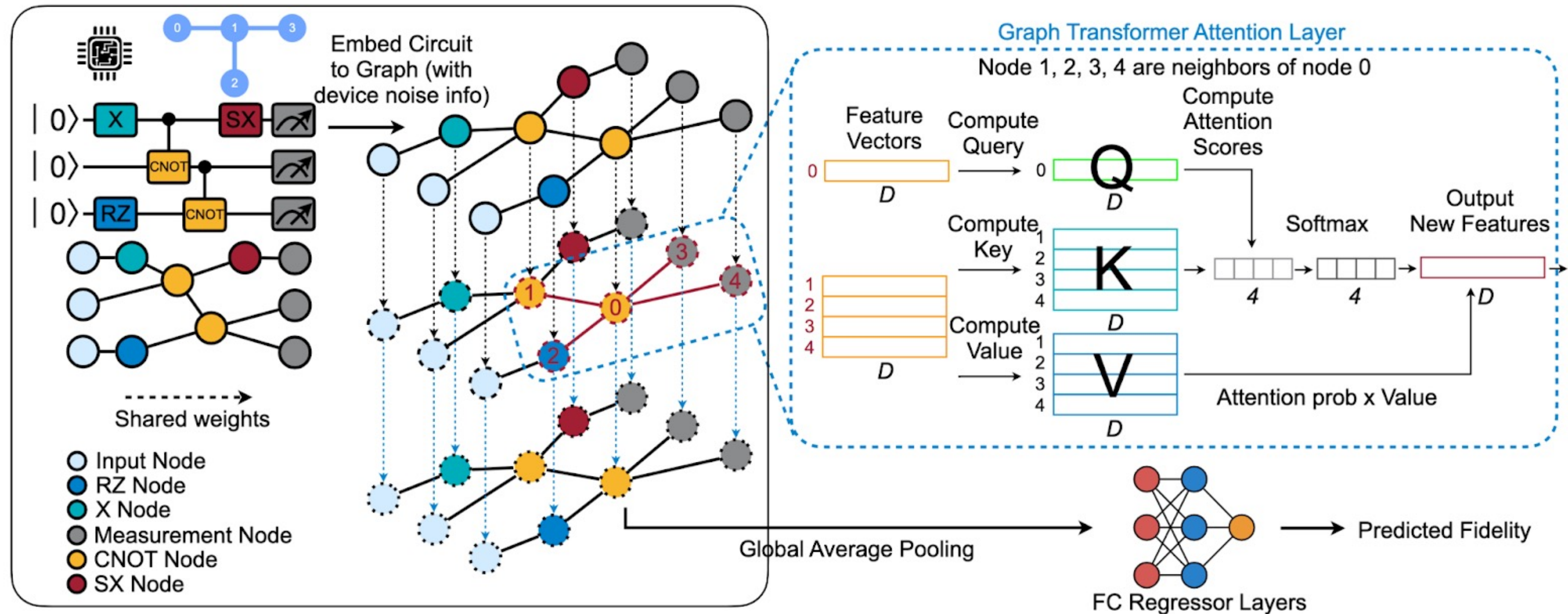


Features on each node

0, 1, 0, 0, 0, 0,	0, 1, 0, 0, 0, 0, 0, 0, 0, 0, 0,	140.3, 200.2,	120.5, 230.6,	0.004,	0.03,	0.05,	11
One-Hot Node Type	One-Hot Gate Qubit	First Qubit T1, T2	Second Qubit T1, T2	Gate Error Rate	Readout Error 0 - 1	Readout Error 1 - 0	Gate Index

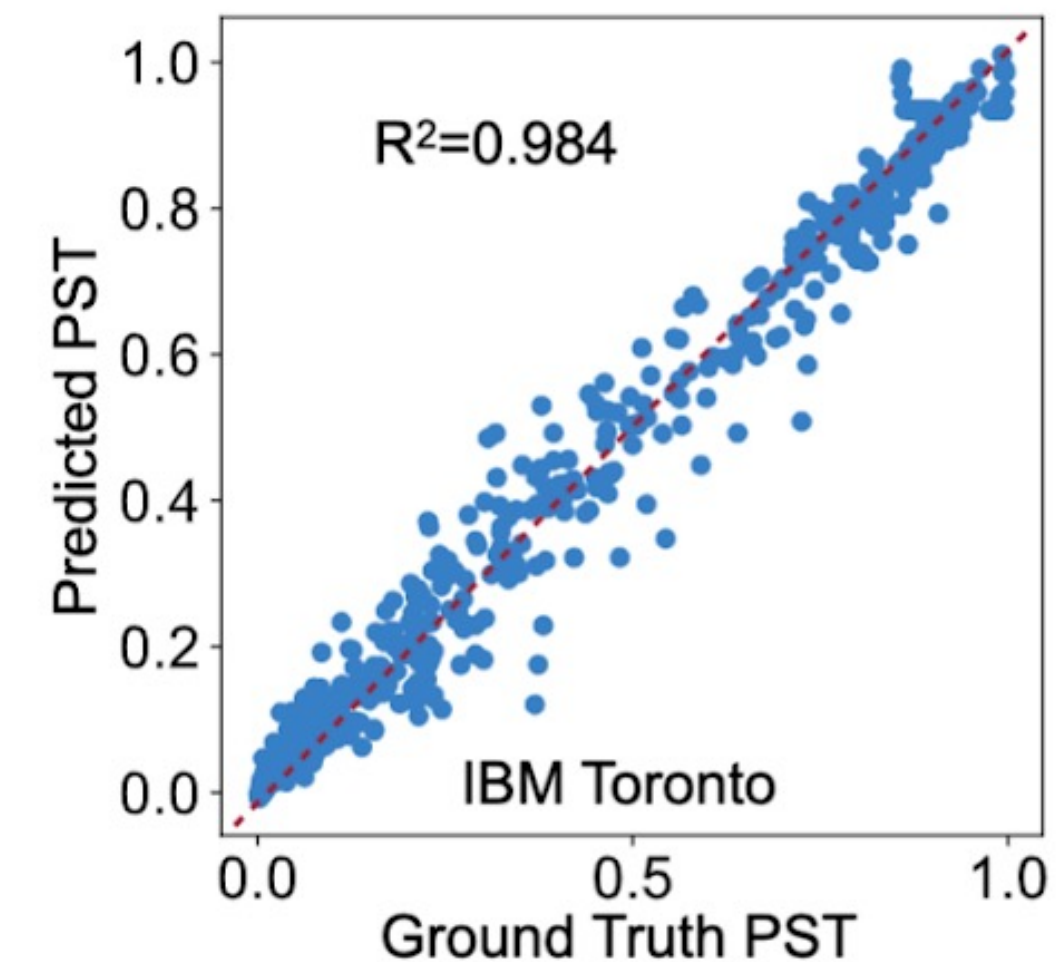
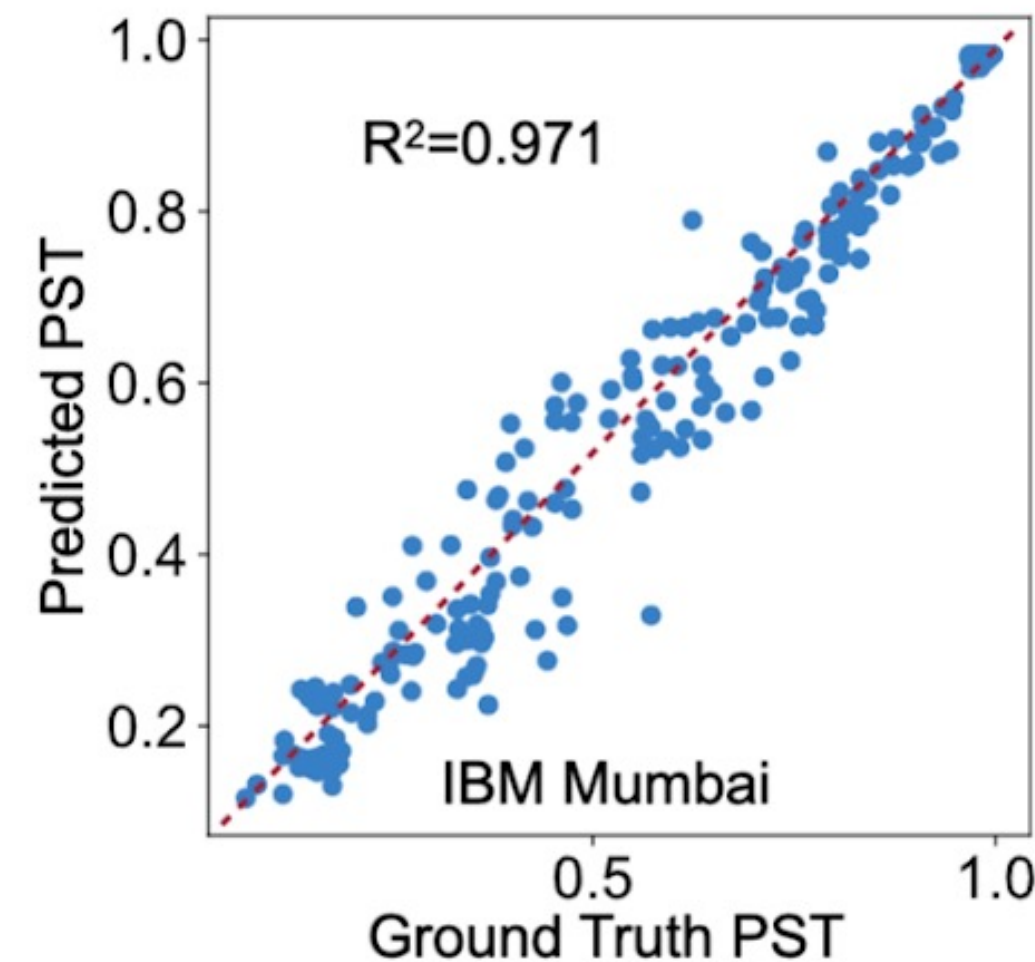
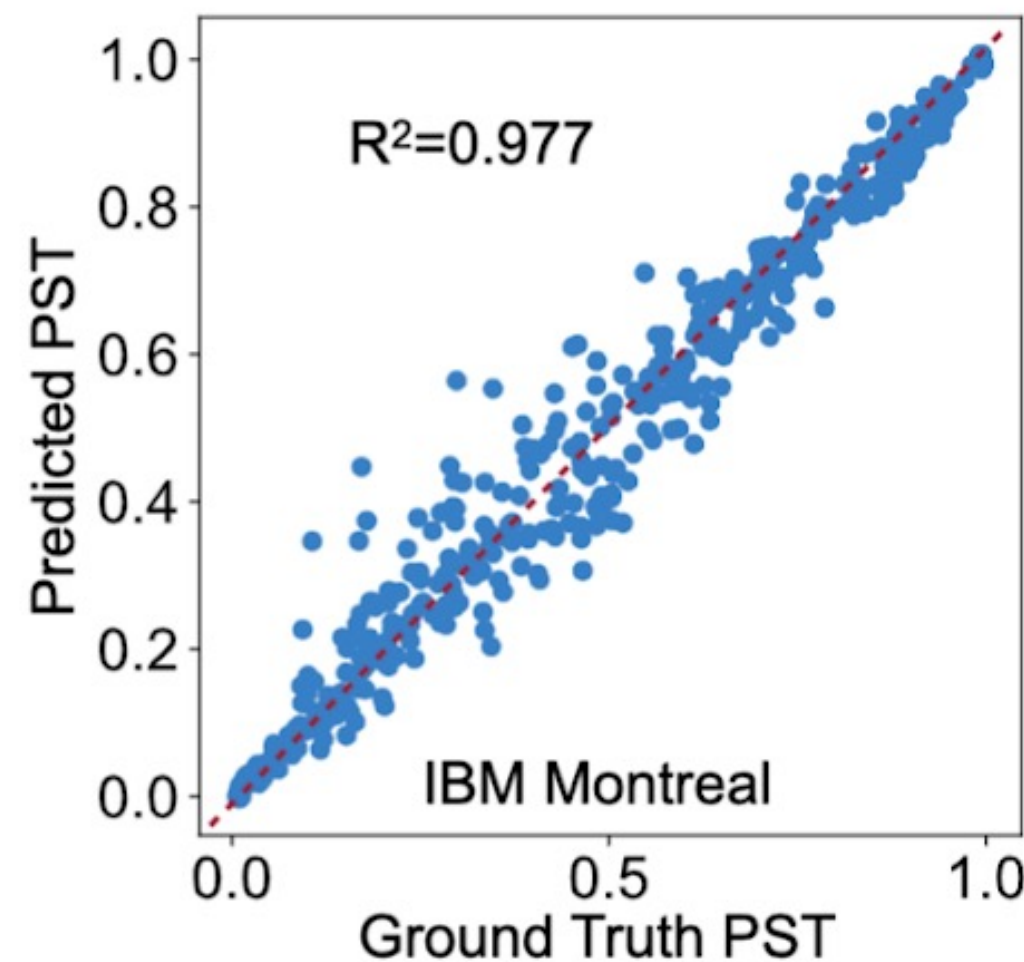
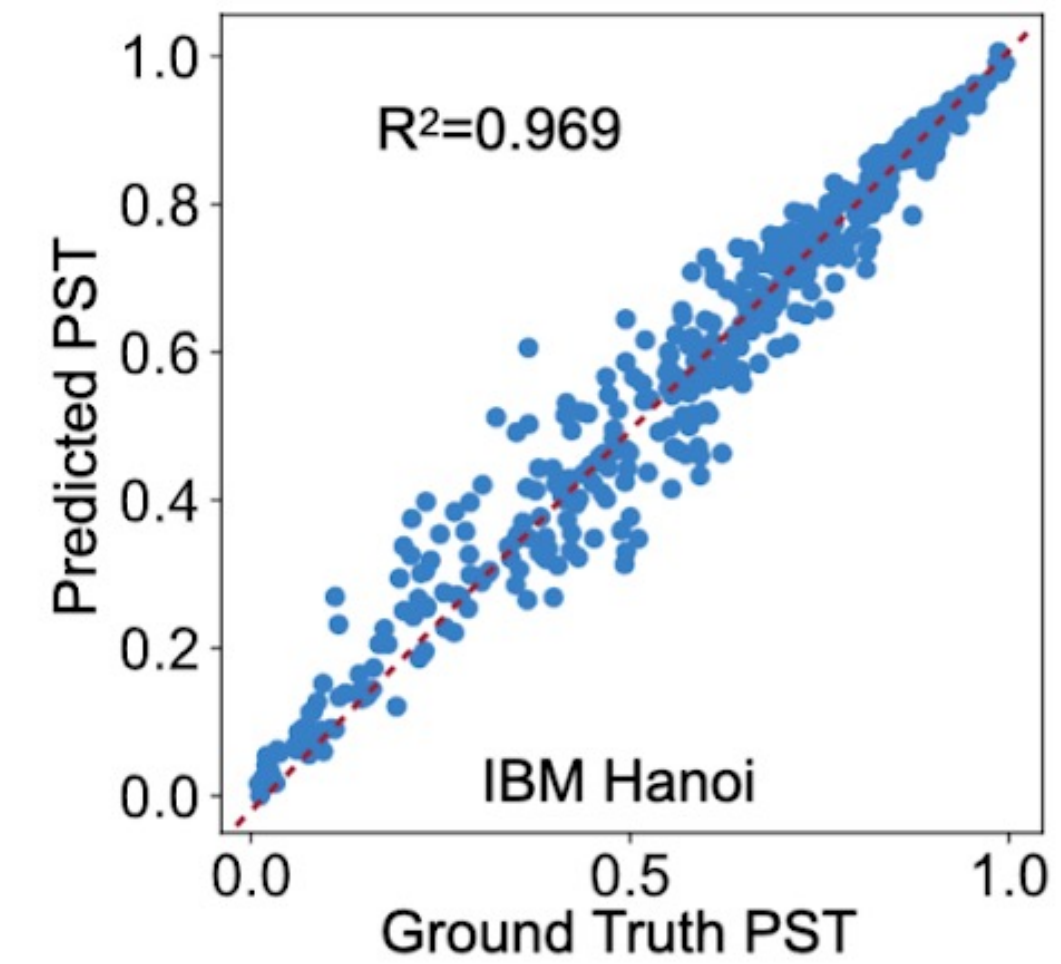
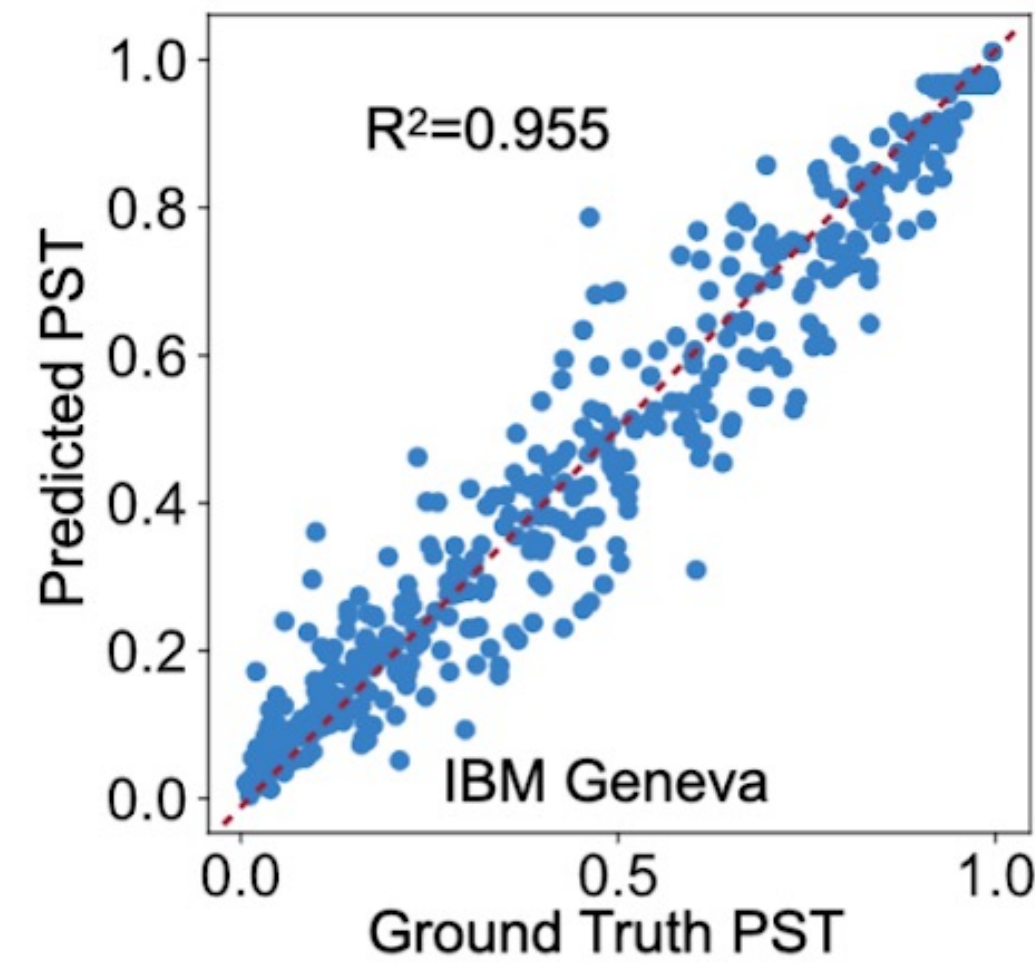
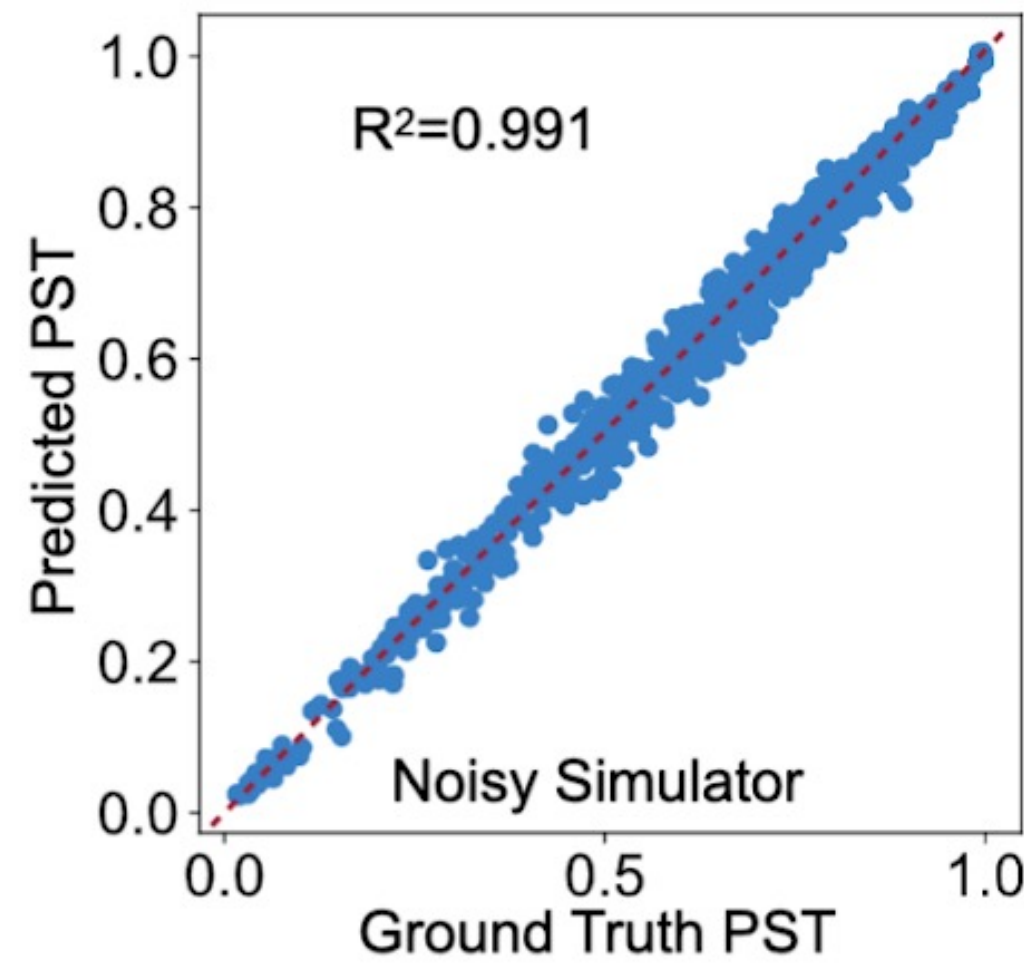
Graph Transformer

- Graph Transformer



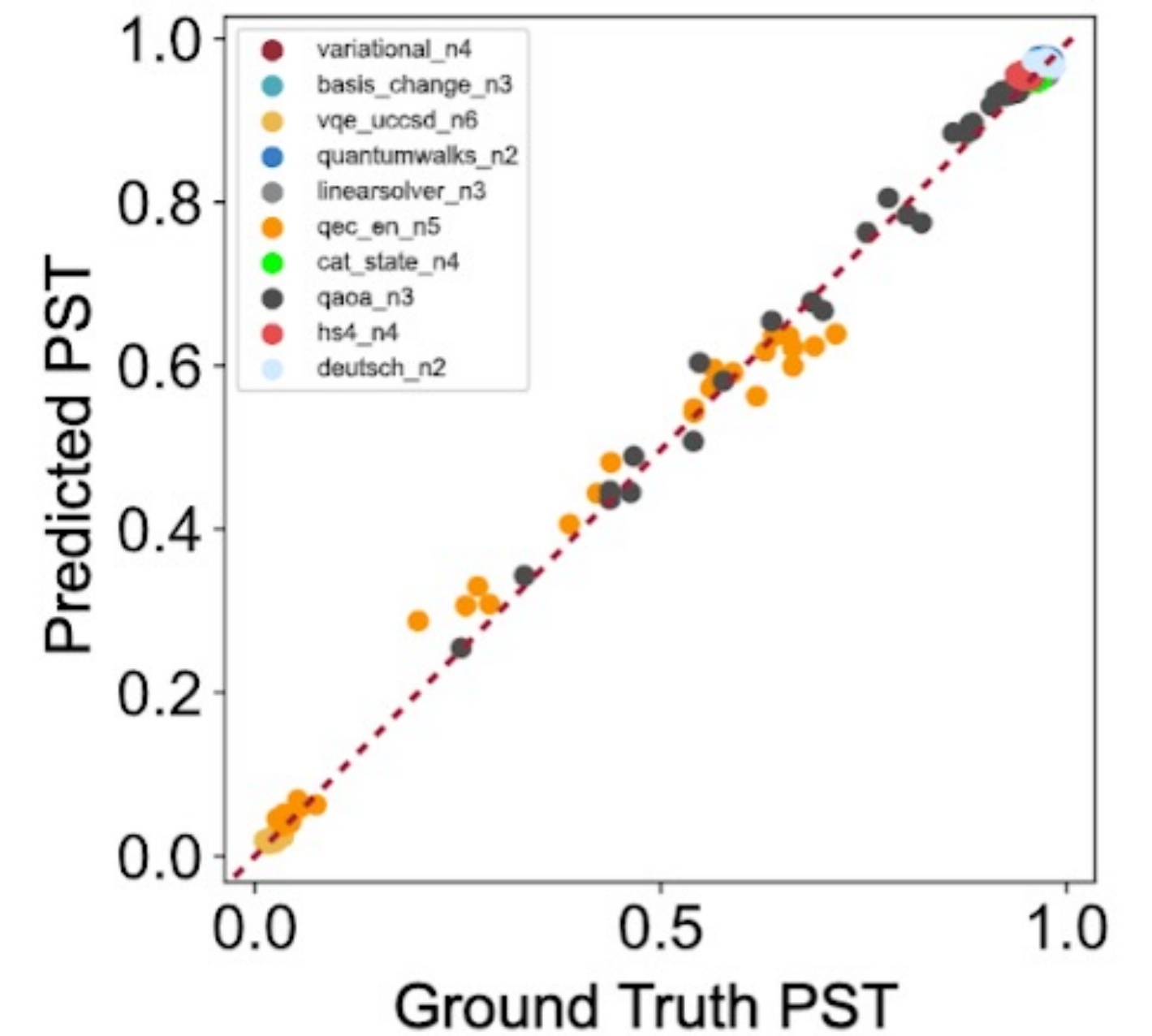
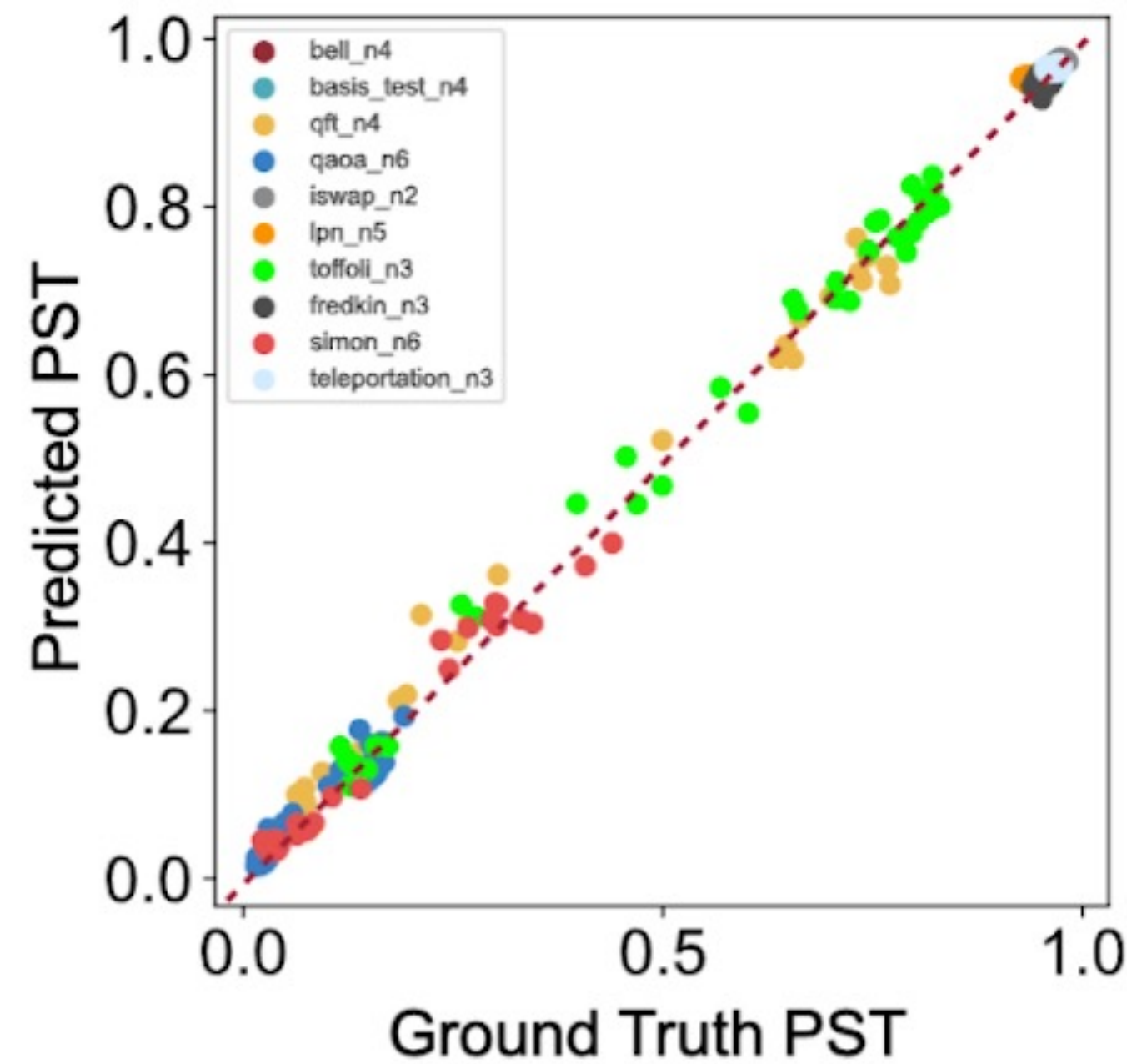
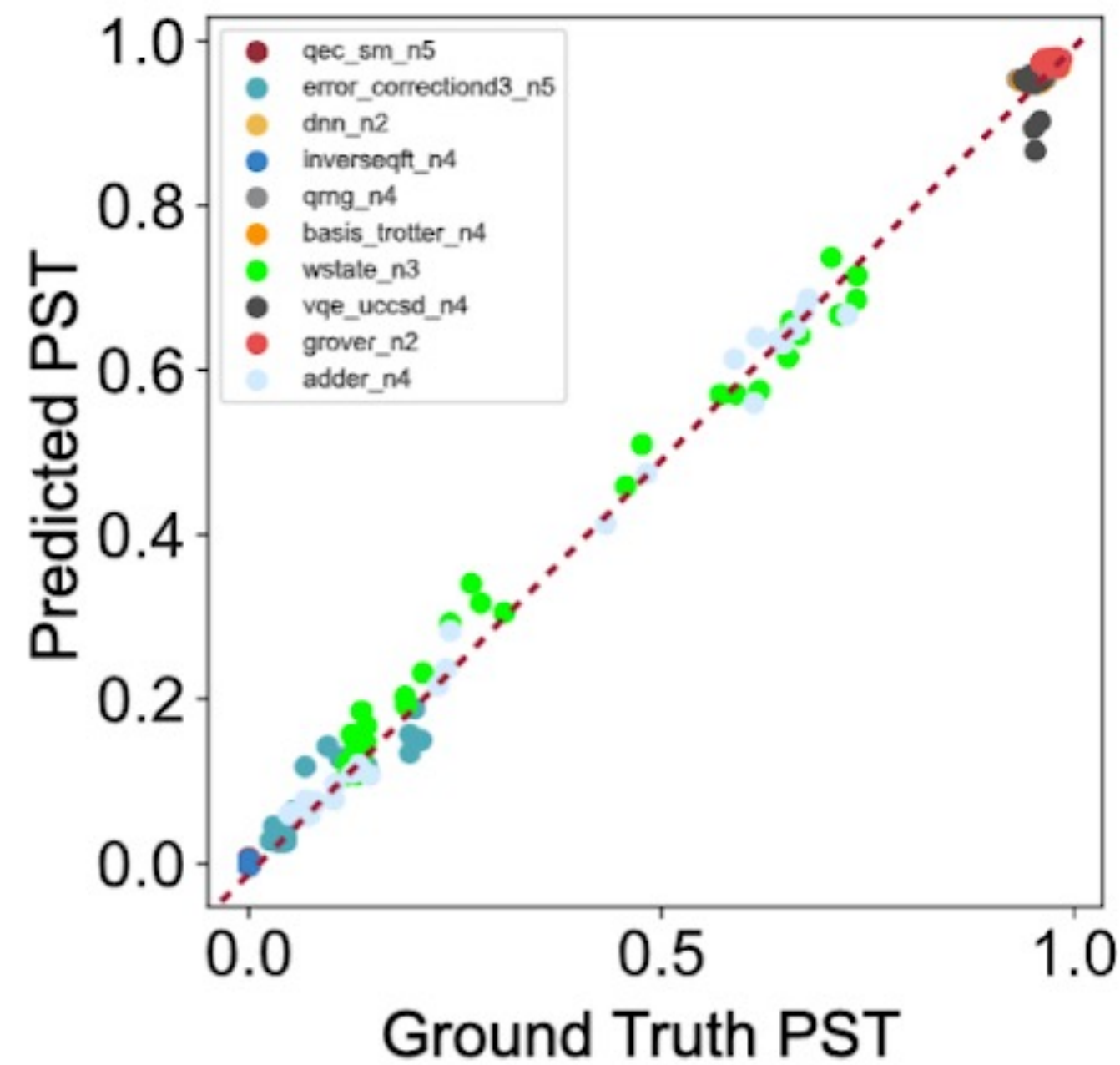
Evaluation

- On random generated circuit



Evaluation

- Circuits from quantum algorithms



More info

- Checkout <https://qmlsys.mit.edu/#transformer> for paper

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Section 3

Use TorchQuantum on Pulse level

3.1 Quantum Optimal Control 

3.2 Variational Pulse Learning 

How to Compress a Quantum Neural Network?

Quantum Neural Network Compression

<https://arxiv.org/pdf/2207.01578.pdf>

Accepted by IEEE/ACM International Conference on Computer-Aided Design 2022

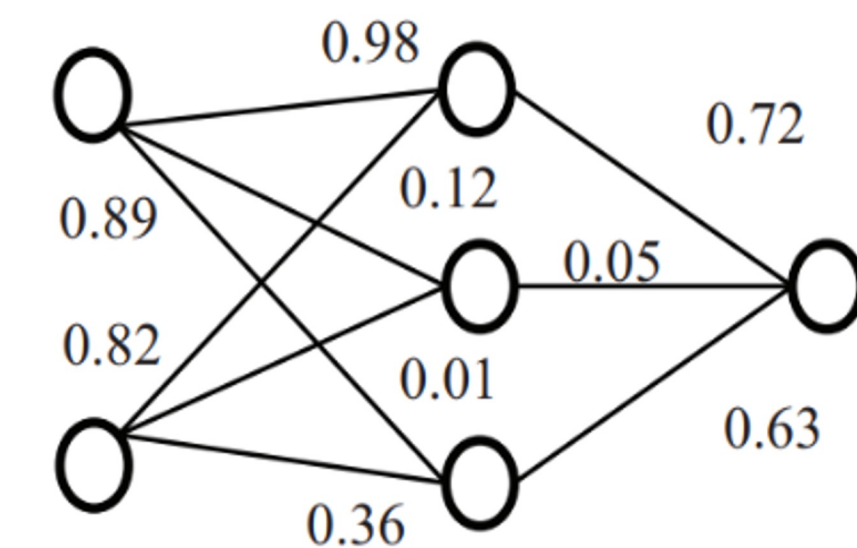
Zhepeng Wang (Presenter), Zhirui Hu, Dr. Weiwen Jiang

Department of Electrical and Computer Engineering

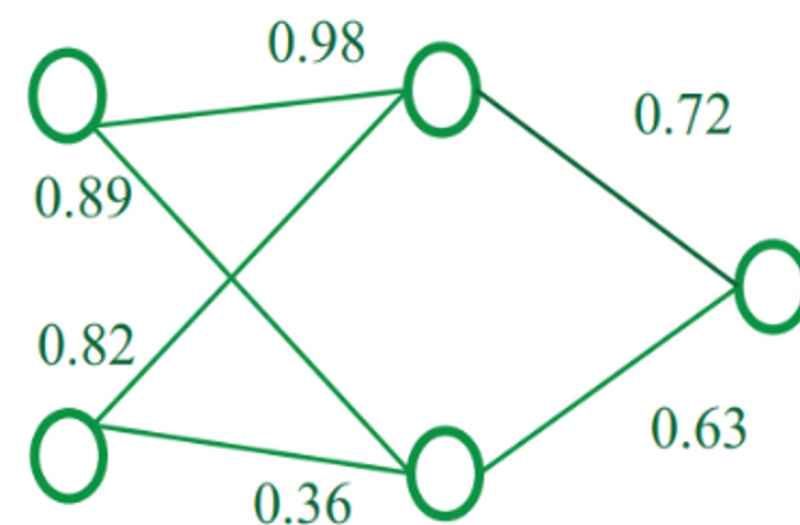
Jqub @ George Mason University

Motivation and Background

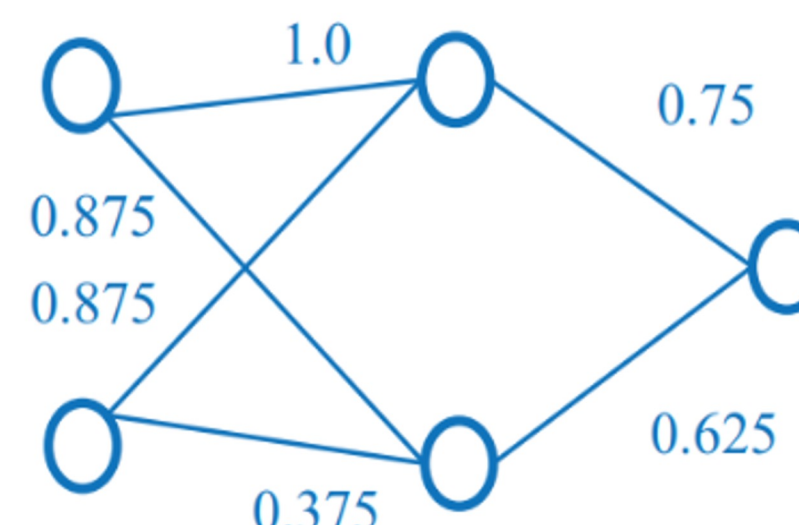
- Pruning and Quantization in Classical ML



(a) Non-Compression Classical NN

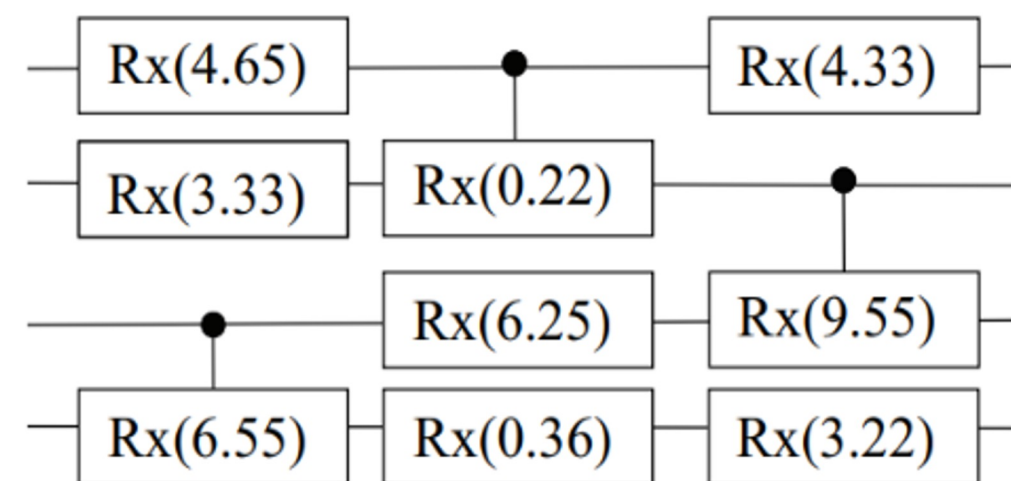


(b) Classical NN with Pruning

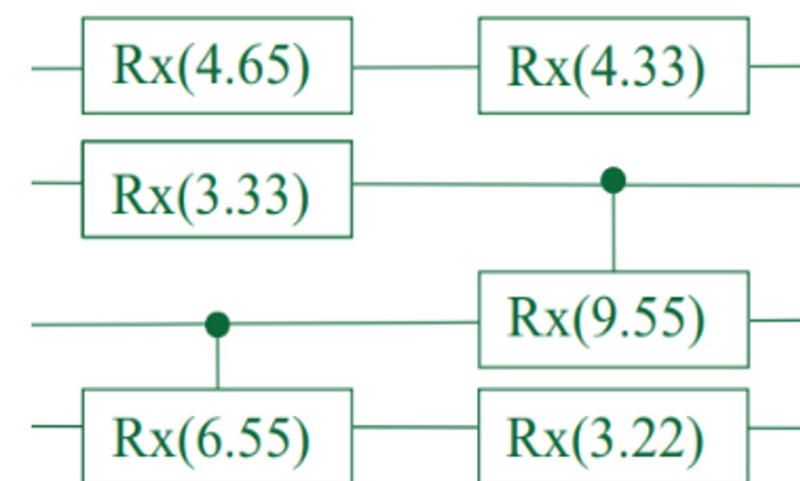


(c) Pruned NN with Quantization

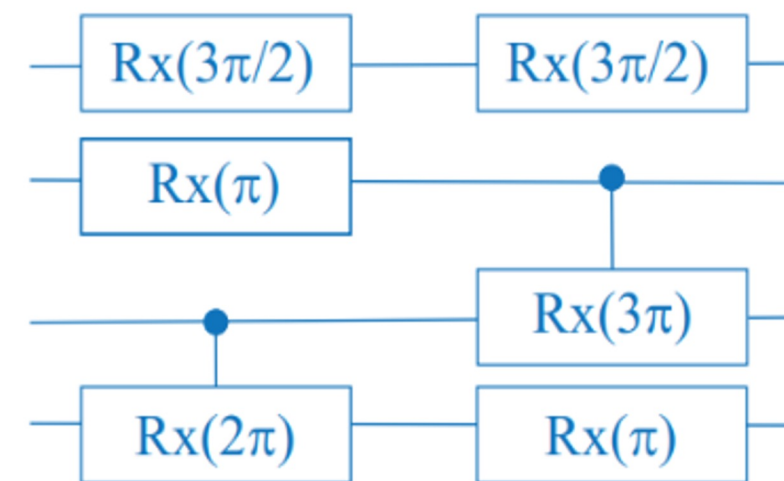
- Pruning and Quantization in Quantum ML



(e) Non-Compression QNN



(f) QNN with Pruning

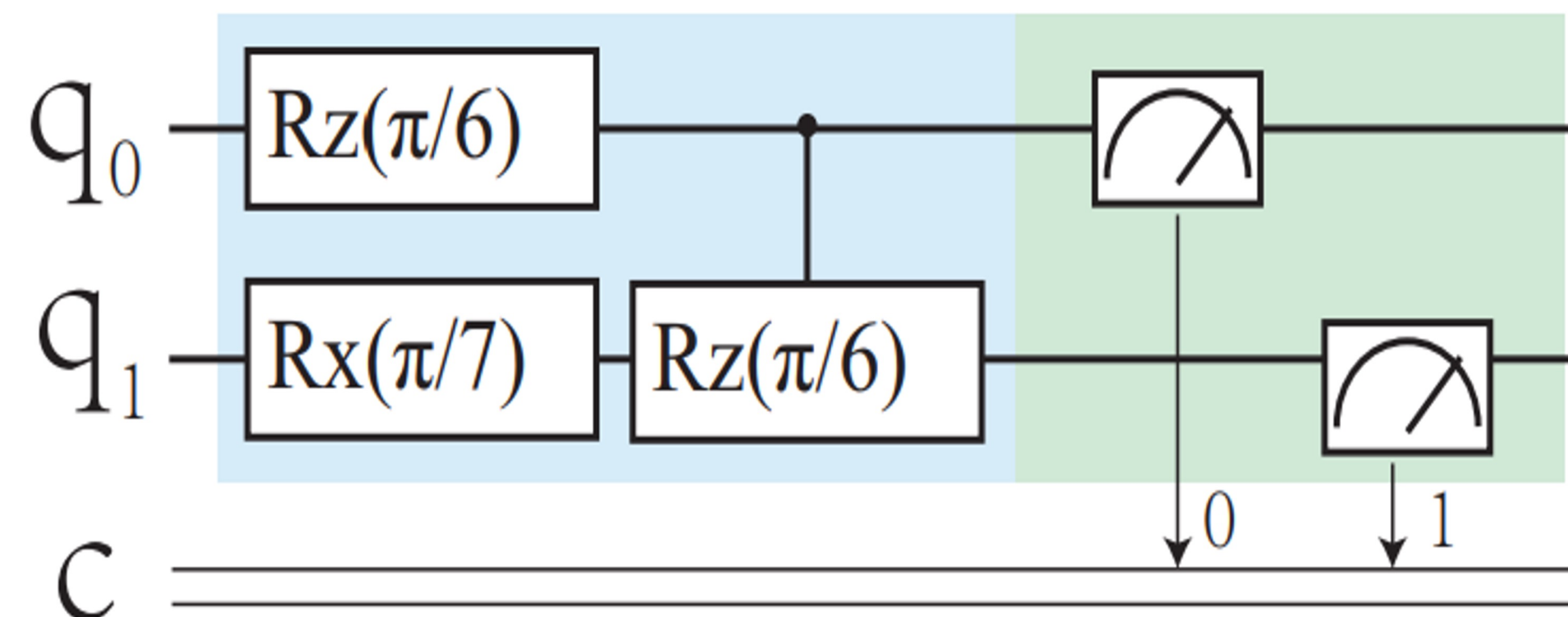


(g) Pruned QNN with Quantization

- Pruning:** Not only 0 can be pruned, but also 2π , 4π , etc.
- Quantization:** Different quantization level may have different cost

Motivation and Background

- Quantum Neural Network Compression Should be Compilation Aware



Compilation

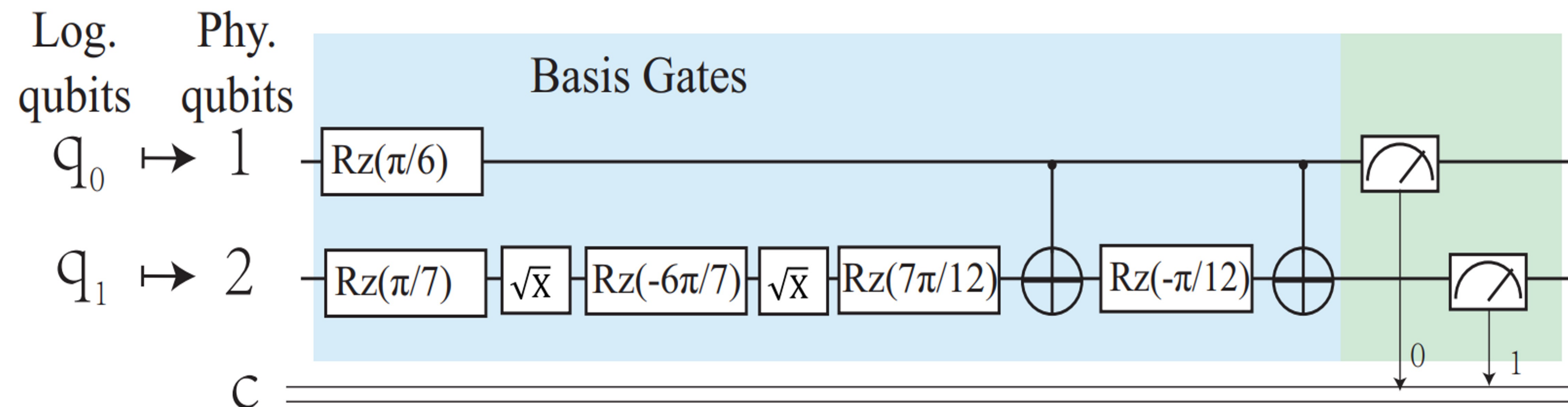


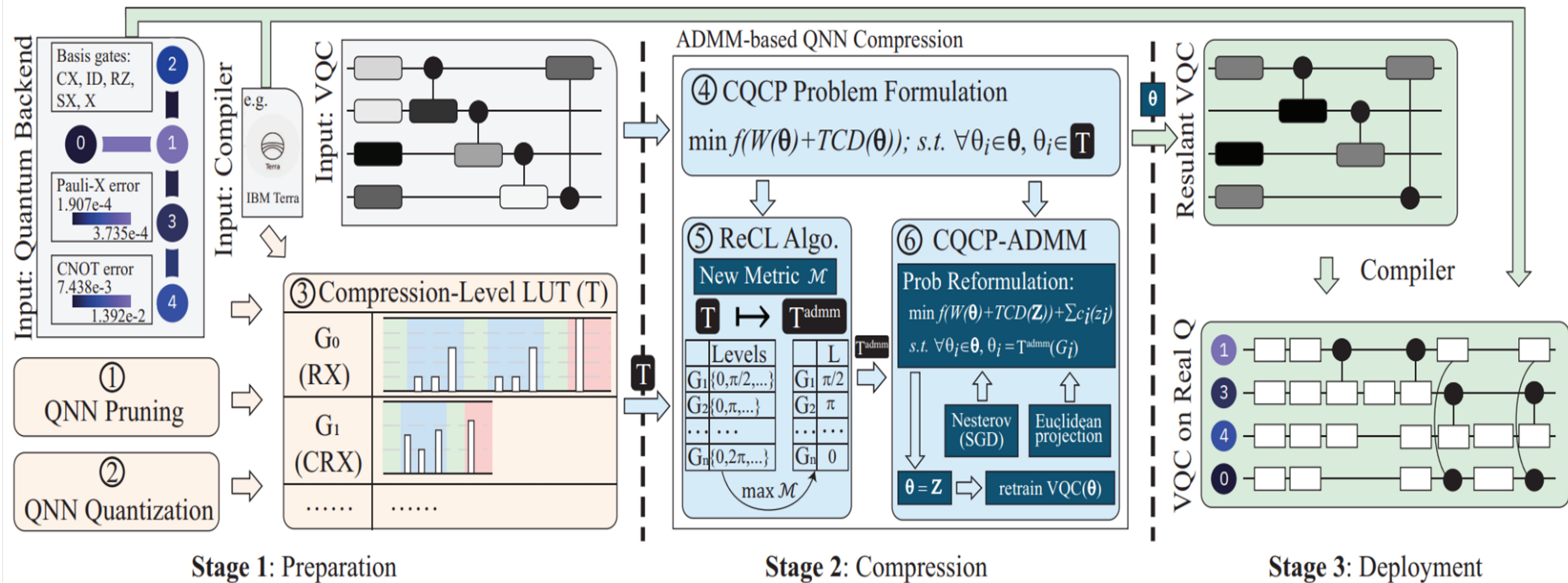
Table 1: circuit depth of compiled quantum gates on IBM quantum processors; parameters are in the range of $[0, 4\pi]$

Gate	0	π	2π	3π	4π	$\pi/2$	$3\pi/2$	$5\pi/2$	$7\pi/2$	others
RX	0	1	0	1	0	1	3	1	3	5
RY	0	2	0	2	0	3	3	3	3	4
CRX	0	8	5	9	0	11	11	11	11	11
CRY	0	8	6	8	0	10	10	10	10	10

CompVQC

- General Overview

Three stages: 1. Preparation; 2. Compression; 3. Deployment

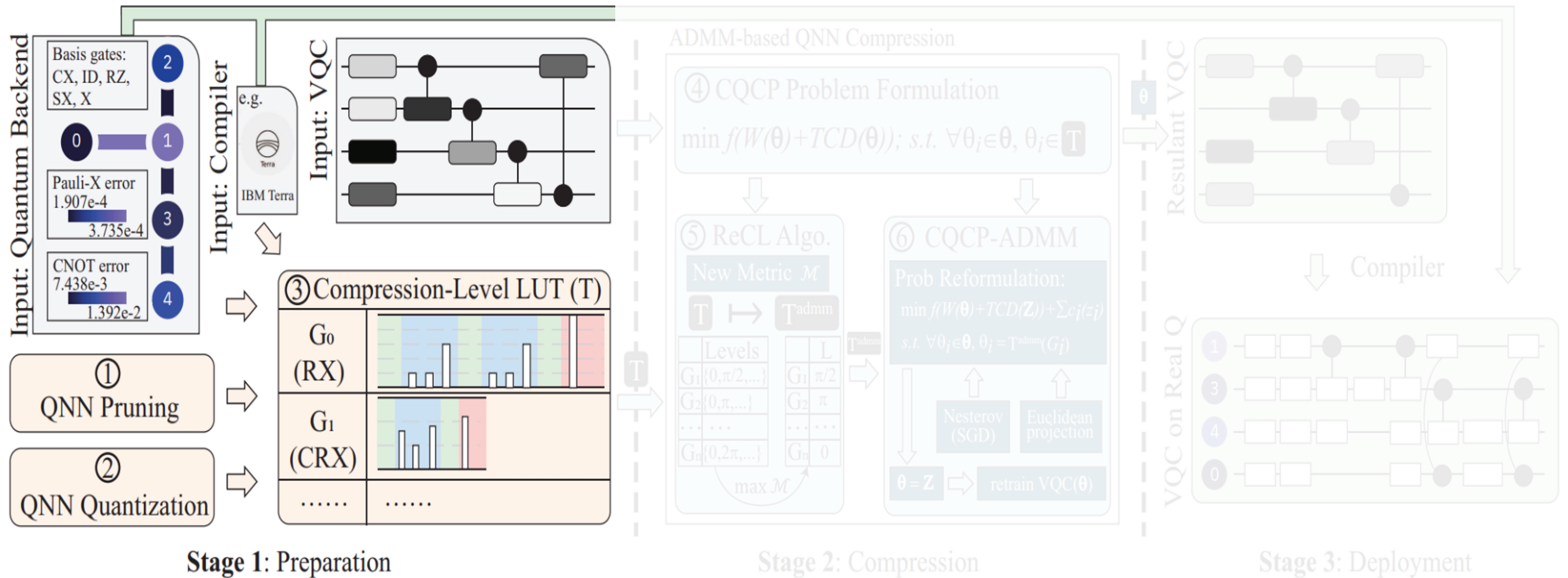


CompVQC

- LUT Construction and Training a Quantum Model
- Reconstruct LUT for ADMM
- Compression based on ADMM
- Deployment

CompVQC

- LUT Construction and Training a Quantum Model



CompVQC

- LUT Construction and Training a Quantum Model

- **Compression-Level Lookup Table (LUT)**

A combination of pruning/quantization level called as “compression level”.

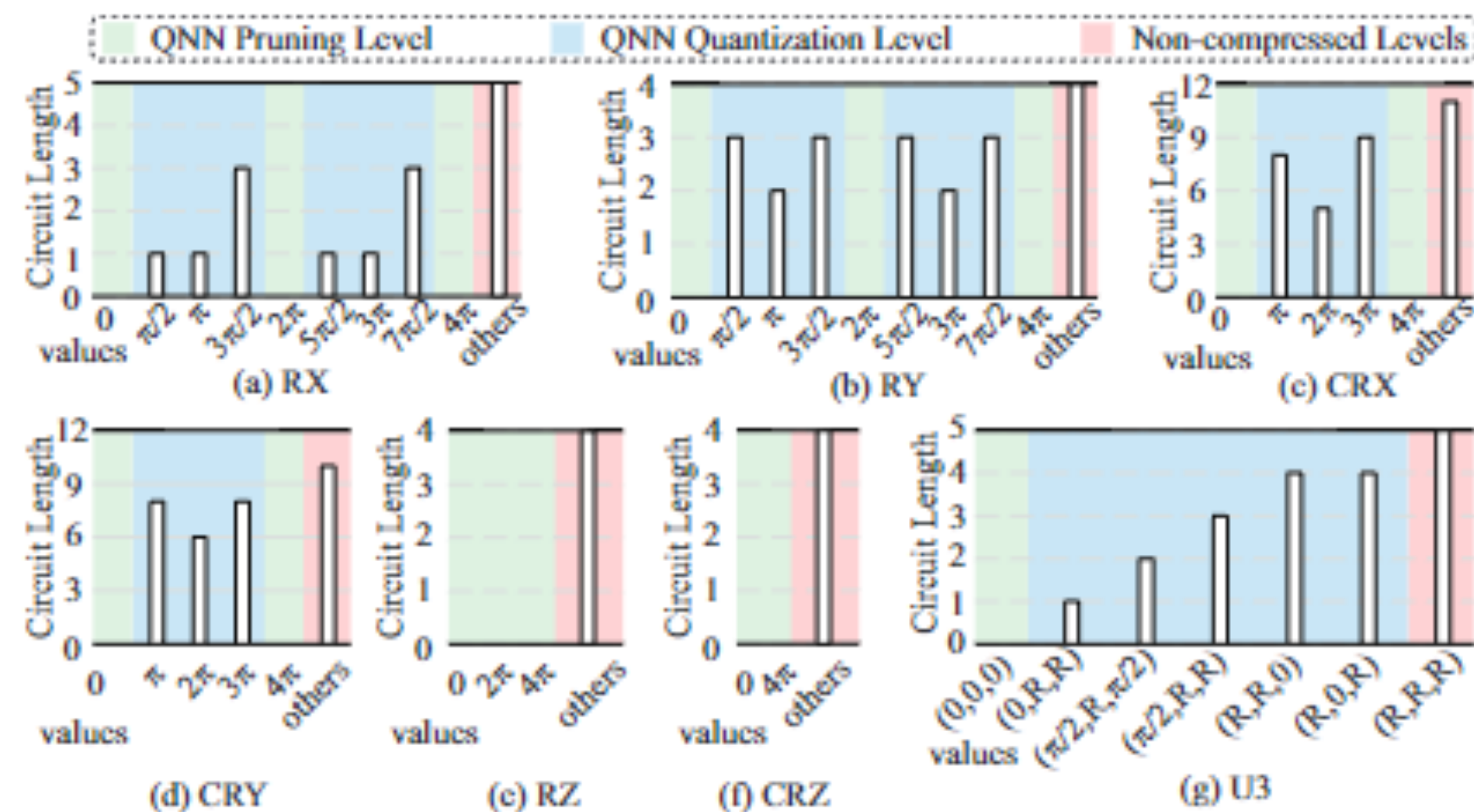


Table 1: circuit depth of compiled quantum gates on IBM quantum processors; parameters are in the range of $[0, 4\pi]$

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RX	0	1	0	1	0	1	3	1	3	5
RY	0	2	0	2	0	3	3	3	3	4
CRX	0	8	5	9	0	11	11	11	11	11
CRY	0	8	6	8	0	10	10	10	10	10

- **VQC Pre-Training**

A VQC model is pre-trained for compression and the training process is implemented with **Torch Quantum**.

Hands-On Tutorial (1) : LUT Construction

- **Input**

- Fixing points list
- Logical Gates List to be used
- Quantum Backend

- **Do**

- Get the compiler for the backend
- Get the compiled circuit length of each Logical Gate at each special fixing points

- **Output**

- Compression-Level Lookup Table (LUT)

```
#Input
test_fixing_points = [math.pi*4, math.pi*2, math.pi, math.pi*3, math.pi/2,
                      math.pi/2*5, math.pi/2*7, math.pi/2*3, math.pi/6]
logical_gates = ['rx', 'ry', 'rz', 'crx', 'cry', 'crz']
backend = FakeValencia()

#api
df = LUT_construction(test_fixing_points, logical_gates, backend)
```

fixing_points	rx	ry	rz	crx	cry	crz
12.57	0	0	0	0	0	0
6.28	0	0	0	5	6	4
3.14	1	2	1	8	8	4
9.42	1	2	1	9	8	4
1.57	1	3	1	11	10	4
7.85	1	3	1	11	10	4
11.00	3	3	1	11	10	4
4.71	3	3	1	11	10	4
0.52	5	4	1	11	10	4

Hands-On Tutorial (1)

LUT Construction



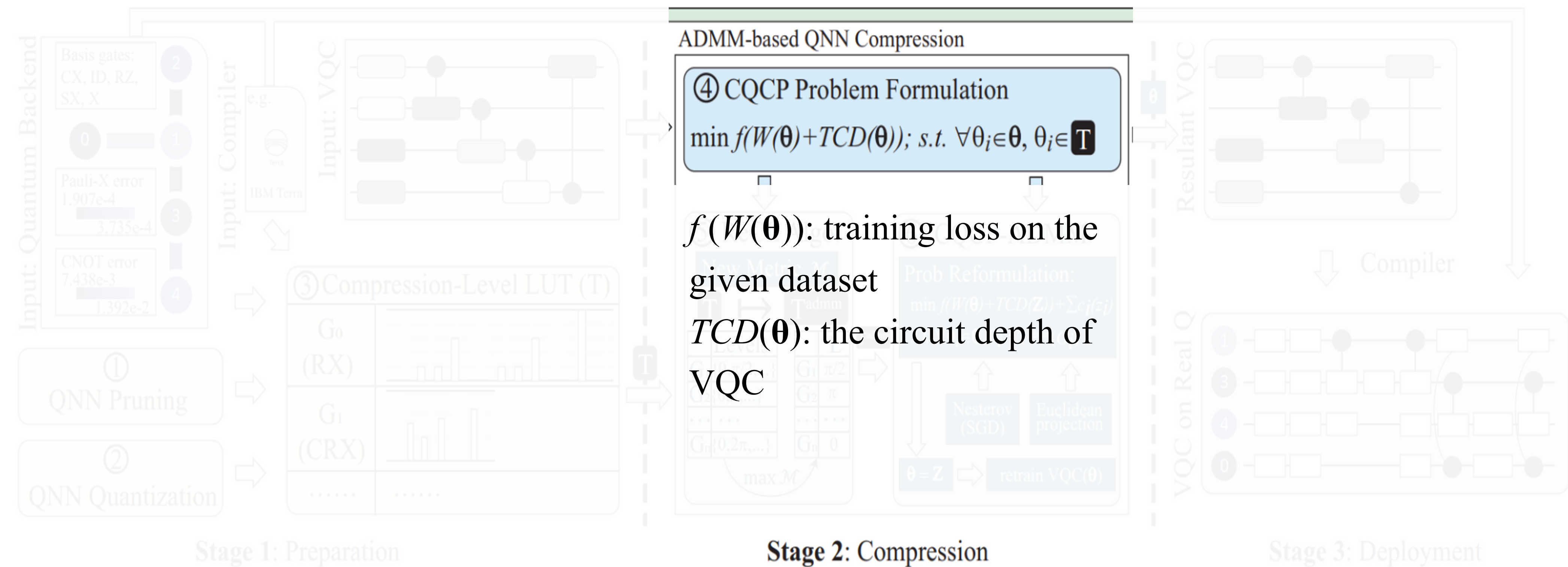
CompVQC

- LUT Construction and Training a Quantum Model
- **Reconstruct LUT for ADMM**
- Compression based on ADMM
- Deployment

CompVQC

- Problem Definition

Given VQC $W(\theta)$, LUT T , quantum compiler C , the problem is to determine trainable parameters θ , such that:



CompVQC

- Reconstruction LUT for ADMM

Process is conducted by traversing all quantum gates in VQC and **select the compression target with highest metric.**

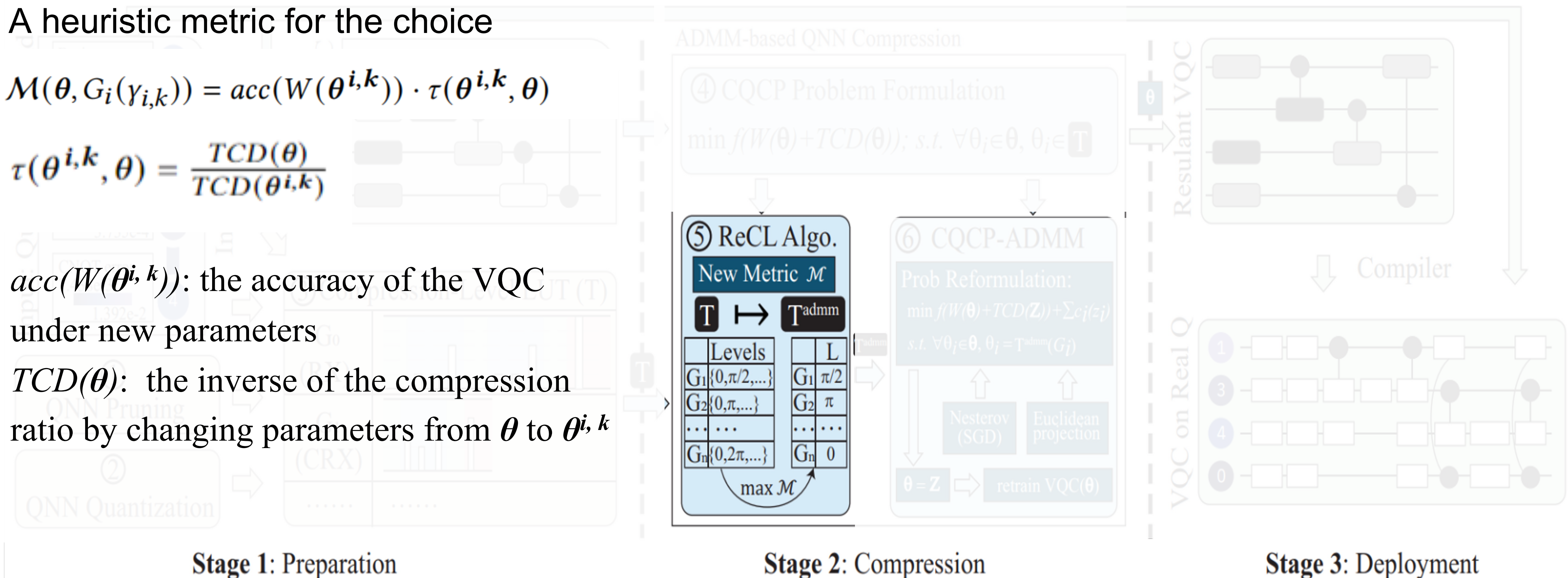
A heuristic metric for the choice

$$\mathcal{M}(\theta, G_i(\gamma_{i,k})) = \text{acc}(W(\theta^{i,k})) \cdot \tau(\theta^{i,k}, \theta)$$

$$\tau(\theta^{i,k}, \theta) = \frac{TCD(\theta)}{TCD(\theta^{i,k})}$$

$\text{acc}(W(\theta^{i,k}))$: the accuracy of the VQC under new parameters

$TCD(\theta)$: the inverse of the compression ratio by changing parameters from θ to $\theta^{i,k}$



Hands-On Tutorial (2) : Reconstruct LUT for ADMM

- **Input**

- A trained model
- Original LUT
- The metrics function of accuracy and length

```
#input
model = torch.load('model.pth')
lut = pd.read_csv('lut.csv')
def metrics_func(acc, depth):
    return acc+1.0/depth
backend = FakeValencia()
```

- **For each parameter, Do**

- Replace it with points at compression level in original LUT while fixing other parameters
- Calculate the metrics of each new model
- Select the point with the highest metric as the compression level for ADMM

```
#api
new_lut = LUT_reconstruction(model, lut, backend, metrics_func)
```

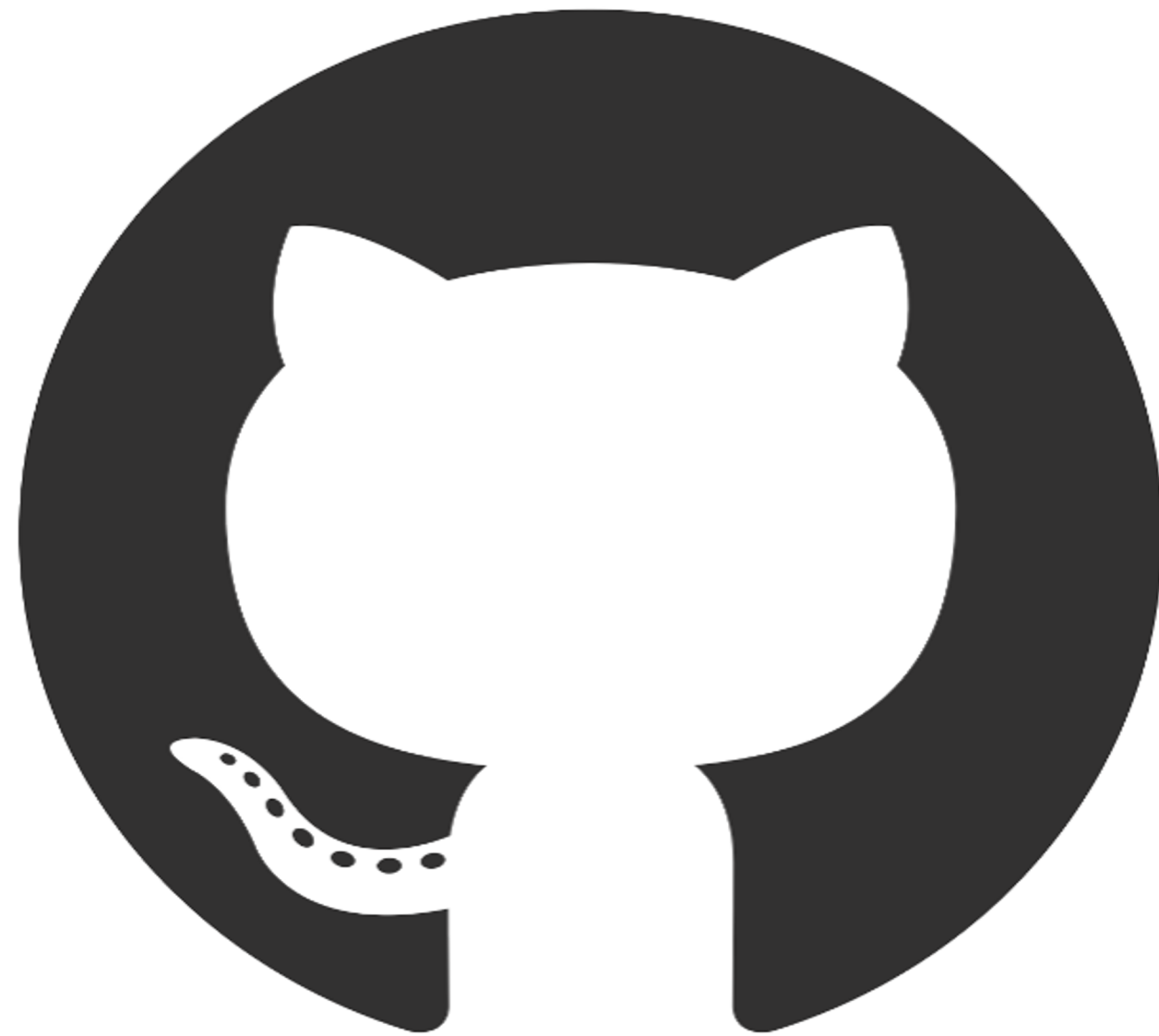
- **Output**

- A new LUT for ADMM

```
[ 1.57  6.28 11.    6.28  4.71  1.57  3.14  9.42  6.28 12.57 12.57  9.42
 7.85 12.57  9.42  1.57 11.    9.42]
```


Hands-On Tutorial (2)

Reconstruct LUT for ADMM



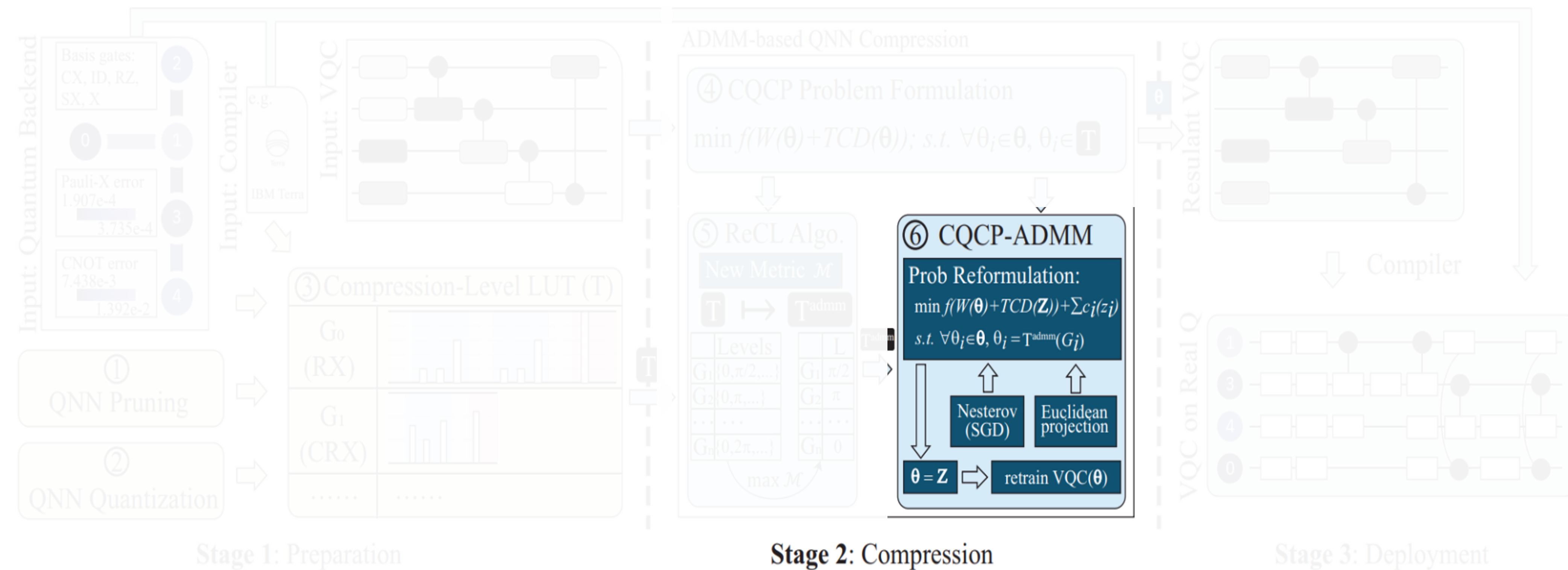
CompVQC

- LUT Construction and Training a Quantum Model
- Reconstruct LUT for ADMM
- **Compression based on ADMM**
- Deployment

CompVQC

- Compression based on ADMM

Each parameter can either be compressed to the target value in \mathbf{T}^{admm} or not compressed.



CompVQC

- Compression based on ADMM

Given reconstructed compression-level LUT T^{admm} , the CQCP is formulated as:

$$\begin{aligned} \min_{\{\theta_i\}} \quad & f(W(\theta)) + TCD(Z) + \sum_{\forall z_i \in Z} c_i(Z_i), \\ \text{s.t.} \quad & \forall \theta_i \in \theta, \quad \theta_i = T^{admm}(G_i). \end{aligned}$$

Z : a set of auxiliary variables for subproblem decomposition and $z_i \in \mathbf{Z}$ is corresponding to $\theta_i \in \theta$

$f(W(\theta)) + TCD(Z)$: the objective function in the original CQCP problem(Previously seen).

$$c_i(Z_i) = \begin{cases} 0 & \text{if } \theta_i \in T^{s,r}(G_i), T^{s,r} = T^{admm} \odot \text{mask}^r \\ +\infty & \text{if otherwise.} \end{cases}$$

$c_i(Z_i)$: An indicator function to serve as a penalty term

mask^r : variable to indicate whether the parameters will be compressed at iteration r .

Hands-On Tutorial (3) : Compression based on ADMM

- **Input**

- A trained model
- A new LUT for ADMM

- **Do**

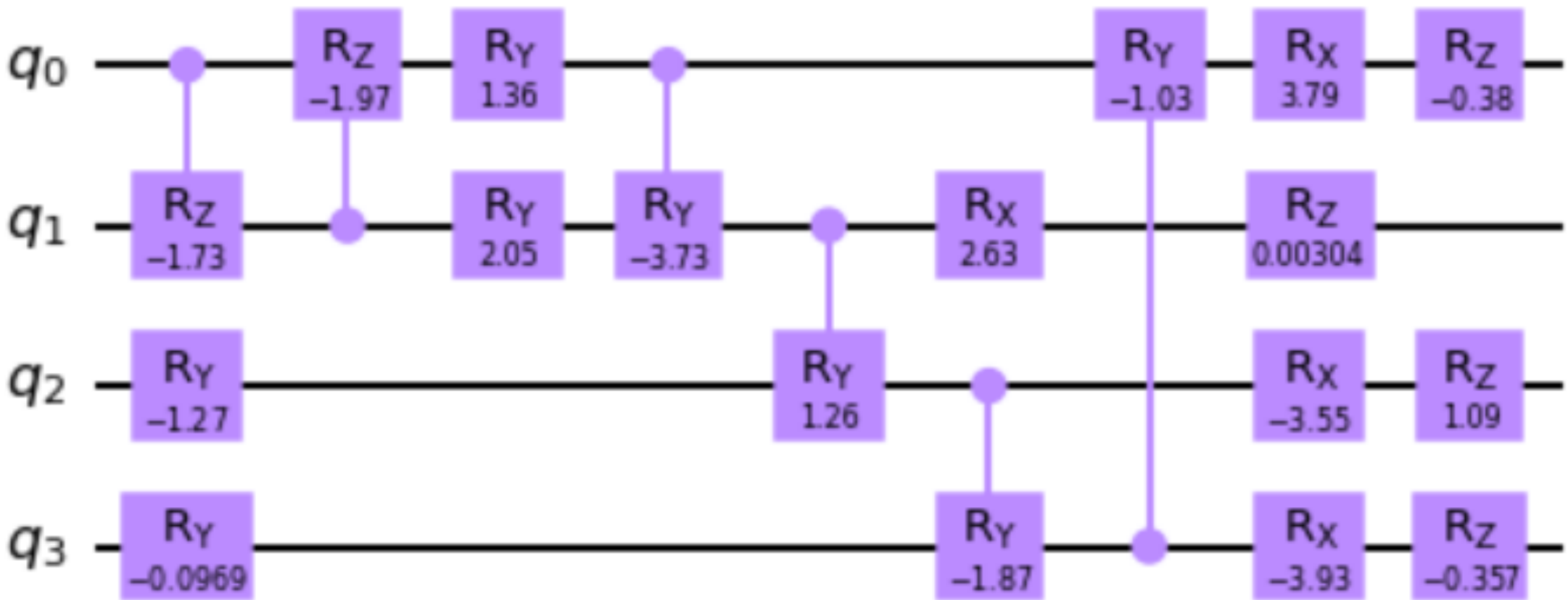
- Compress a model with ADMM
- Fine-tune the compressed model

- **Output**

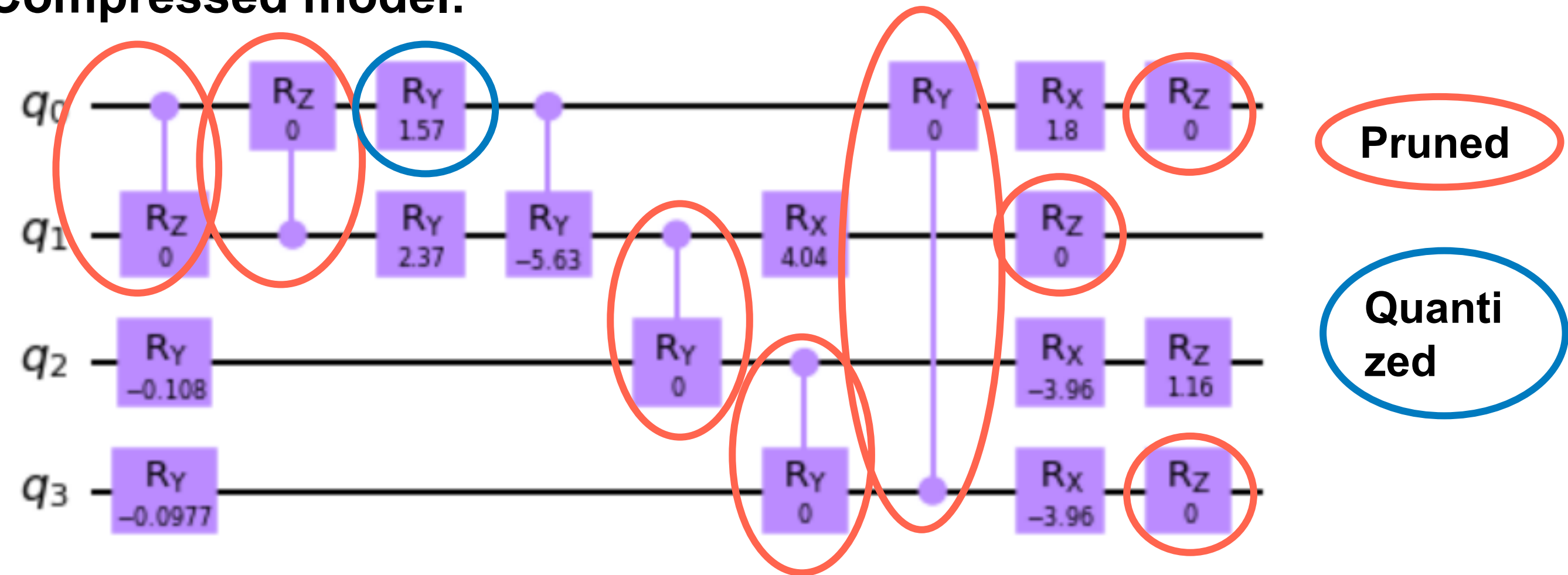
- A compressed model

	Circuit Length	Accuracy
Original model	51	95.6%
Compressed	21	96.60%

- **Original model:**

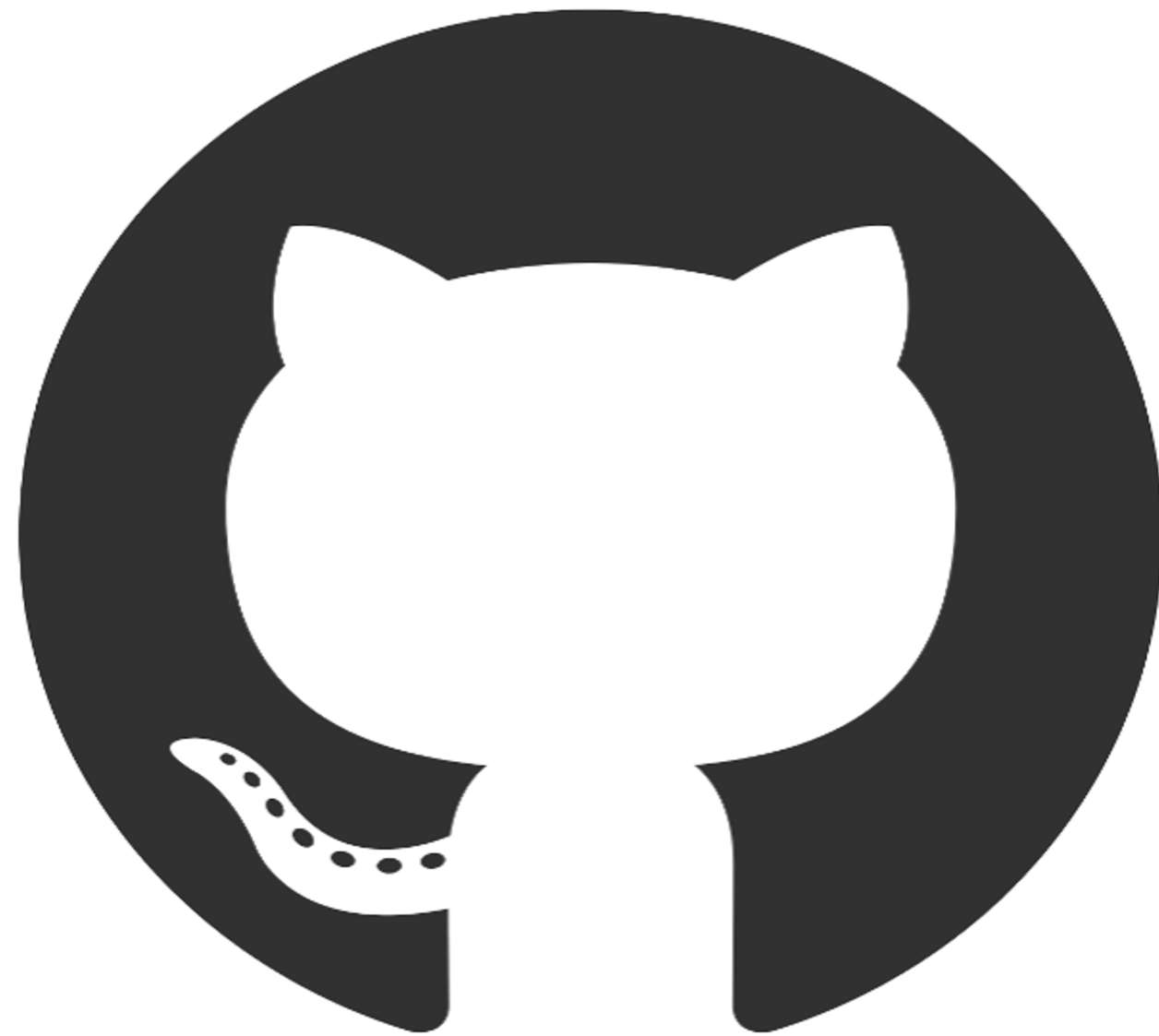


- **Compressed model:**



Hands-On Tutorial (3)

Compression based on ADMM

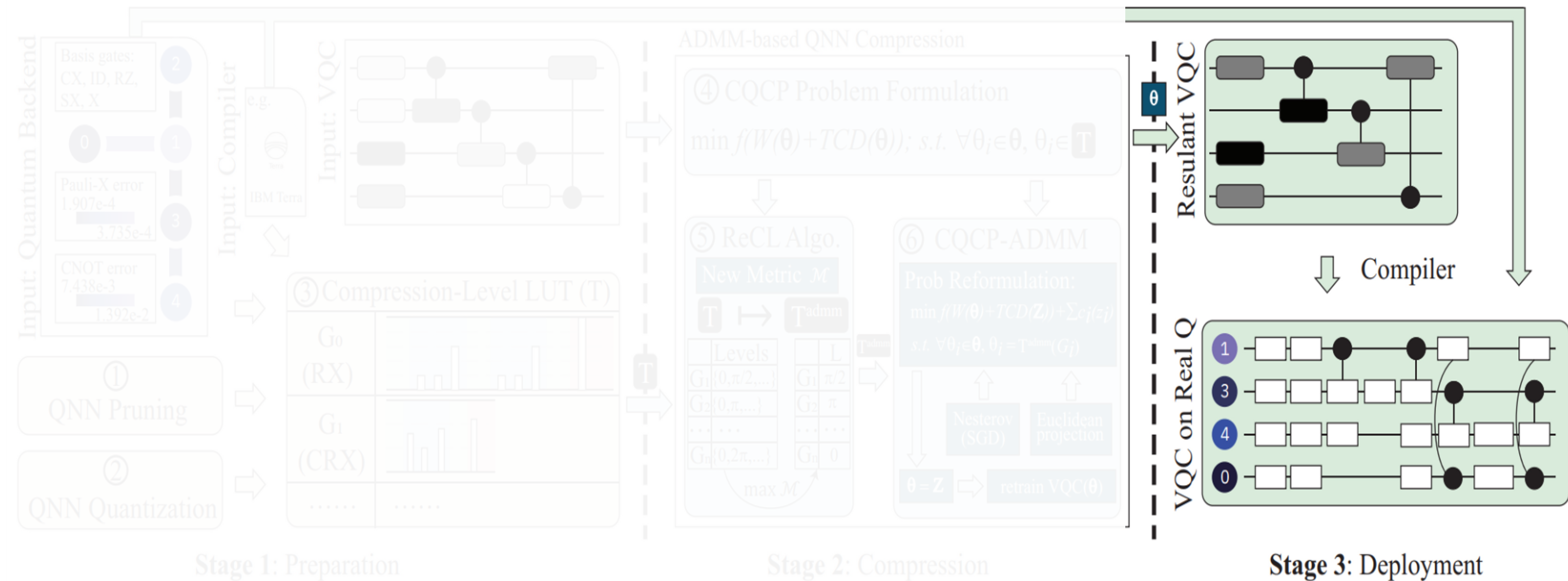


CompVQC

- LUT Construction and Training a Quantum Model
- Reconstruct LUT for ADMM
- Compression based on ADMM
- Deployment

CompVQC

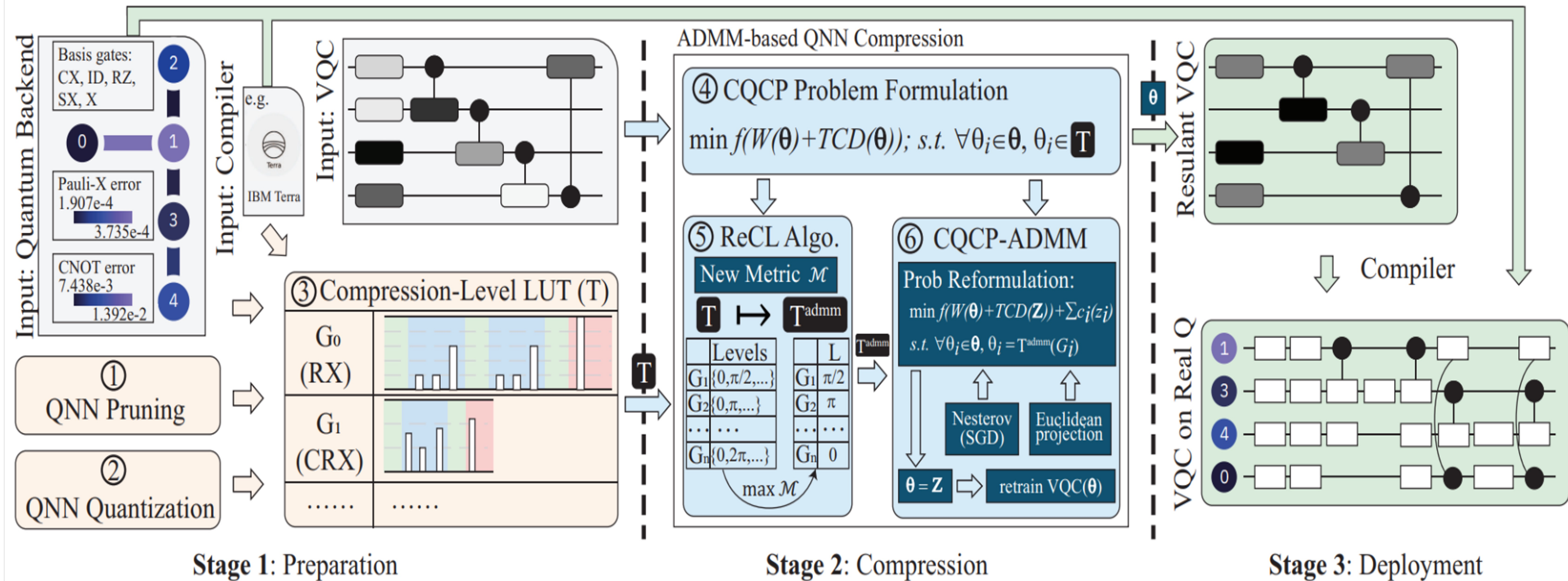
- Deployment



CompVQC

- General Overview

Three stages: 1. Preparation; 2. Compression; 3. Deployment



Experimental Results

- Simulation Results on ML Dataset
CompVQC can maintain high accuracy with **<1% accuracy loss**. And the reduction of circuit length is up to **2.5X**.

Table 2: Comparison among different methods on the accuracy performance and the TCD of the VQC

Compression Method	MNIST-2		Fashion-MNIST-2	
	Acc. (vs. Baseline)	TCD (Speedup)	Acc. (vs. Baseline)	TCD (Speedup)
Vanilla VQC	82.74%(0)	121(0)	87.58%(0)	92(0)
Zero-Only-Pruning	80.58%(-2.16%)	70(1.73×)	86.92%(-0.67%)	63(1.46×)
CompVQC-Pruning	81.83%(-0.91%)	74(1.64 ×)	87.41%(-0.17%)	47(1.96×)
CompVQC-Quant	80.99%(-1.75%)	108(1.10×)	86.25%(-1.33%)	74(1.24×)
CompVQC	81.83%(-0.91%)	47(2.57×)	87.58%(-0.00%)	47(1.96×)

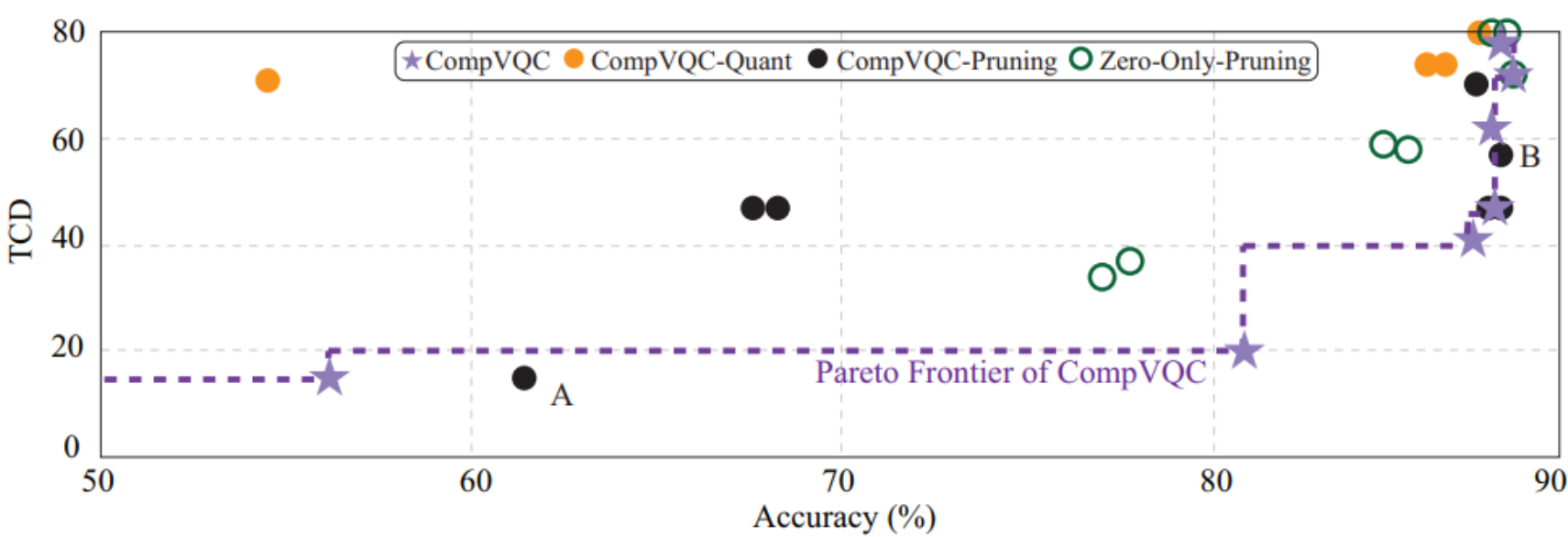


Figure 5: Main results: The Accuracy-Circuit Depth Tradeoff on Fashion-MNIST2

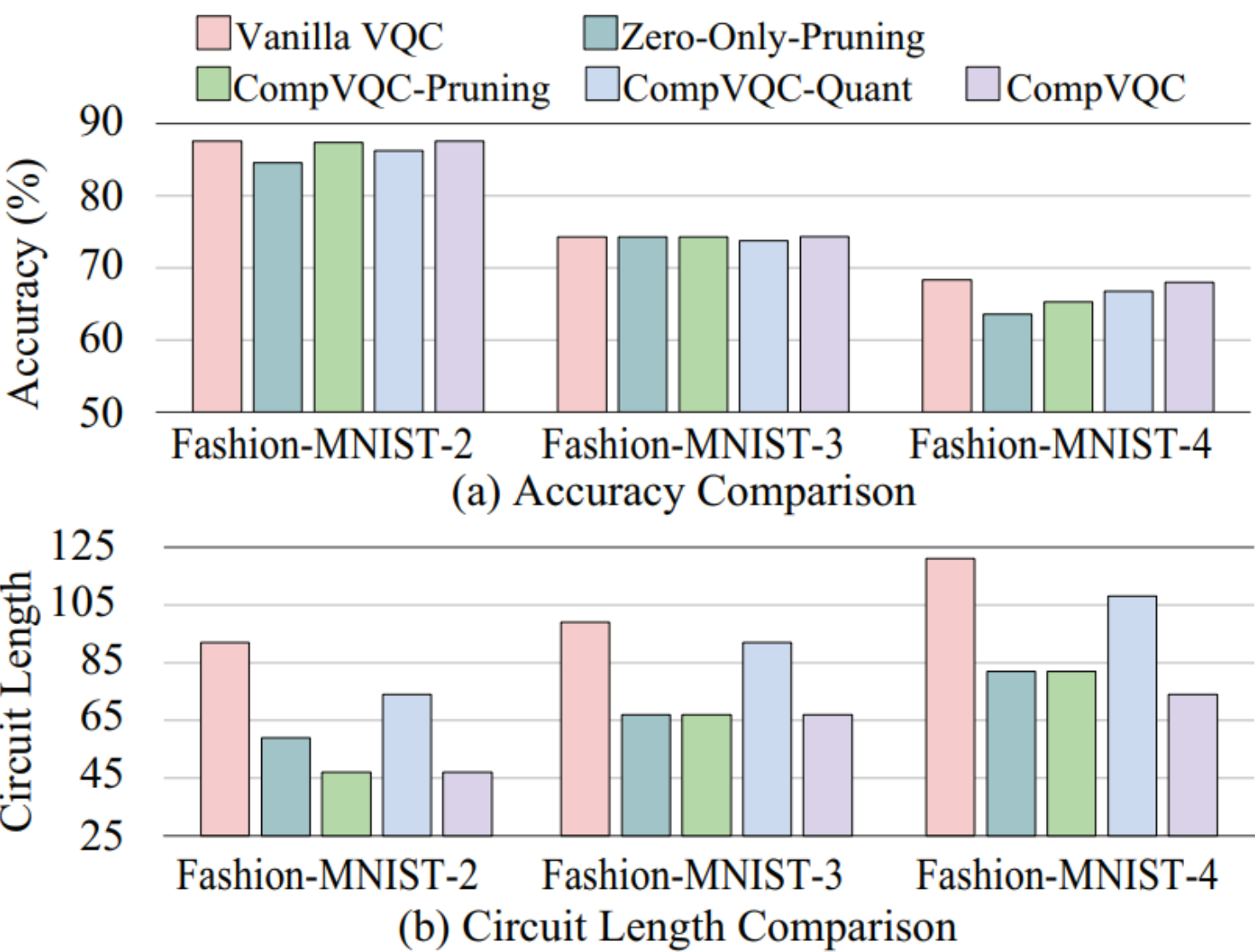


Figure 6: Main Results: CompVQC Scalability on Fashion-MNIST with 2-4 class

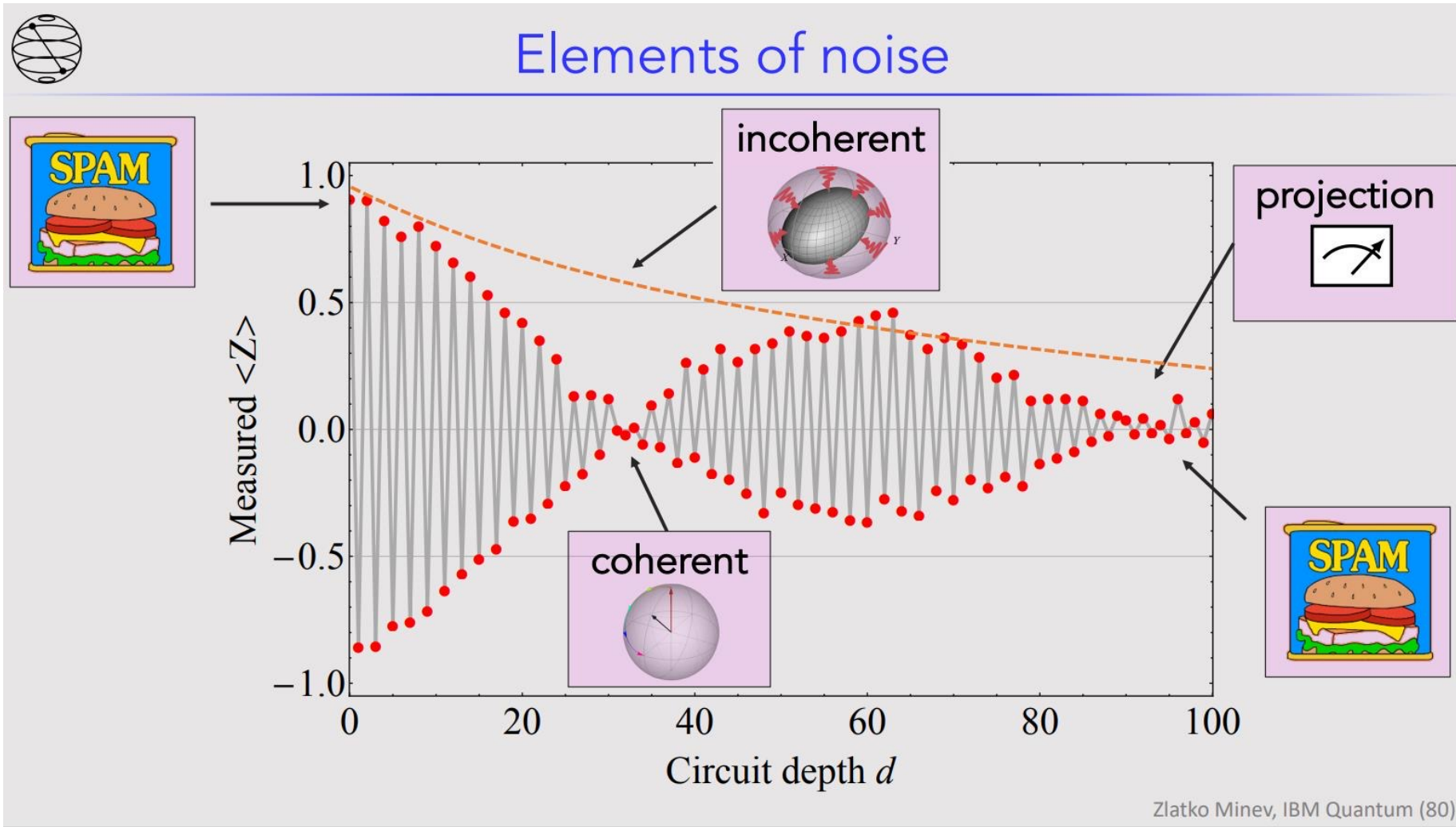
Experimental Results

- Results on Multiple IBM Quantum Computers

CompVQC can reduce circuit length by 2x while the accuracy is also higher in a noisy environment

Datasets		Syn-Dataset-4		Syn-Dataset-16	
Compression Method		Acc.	TCD	Acc.	TCD
		(vs. Baseline)	(Speedup)	(vs. Baseline)	(Speedup)
Qiskit Aer	Vanilla VQC	94%(0)	23(0)	96%(0)	51(0)
	Comp-VQC	99%(5%)	11(2.09×)	98%(2%)	23(2.22×)
IBM Q	Vanilla VQC	79%(-15%)	23(1.00×)	86%(-10%)	51(1.00×)
	Comp-VQC	99%(5%)	11(2.09×)	98%(2%)	23(2.22×)

Acc.(vs. Baseline)	ibm_lagos	ibm_perth	ibm_jakarta
Vanilla VQC(TCD=23)	79%(0)	86%(0)	92%(0)
CompVQC(TCD=11)	99%(20%)	98%(12%)	100%(8%)



Circuit compression can make the QNN model more robust to the noise

TorchQuantum Tutorial Outline

Section 1

TorchQuantum Basic Usage

1.1 Quantum Basics

1.2 TQ operations 

1.3 TQ for State Prep 


1.4 TQ for VQE 

1.4 TQ for QNN 

Section 2

Use TorchQuantum on Gate level

2.1 QuantumNAS: Ansatz
Search and Gate Pruning 

2.2 QuantumNAT: Noise
Injection and Quantization 

2.3 QOC: On-Chip Training 

2.4 Transformer for Quantum
Circuit Reliability Prediction

2.5 QNN Compression 

Section 3

Use TorchQuantum on Pulse level

3.1 Quantum Optimal Control 

3.2 Variational Pulse Learning 

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Section 3

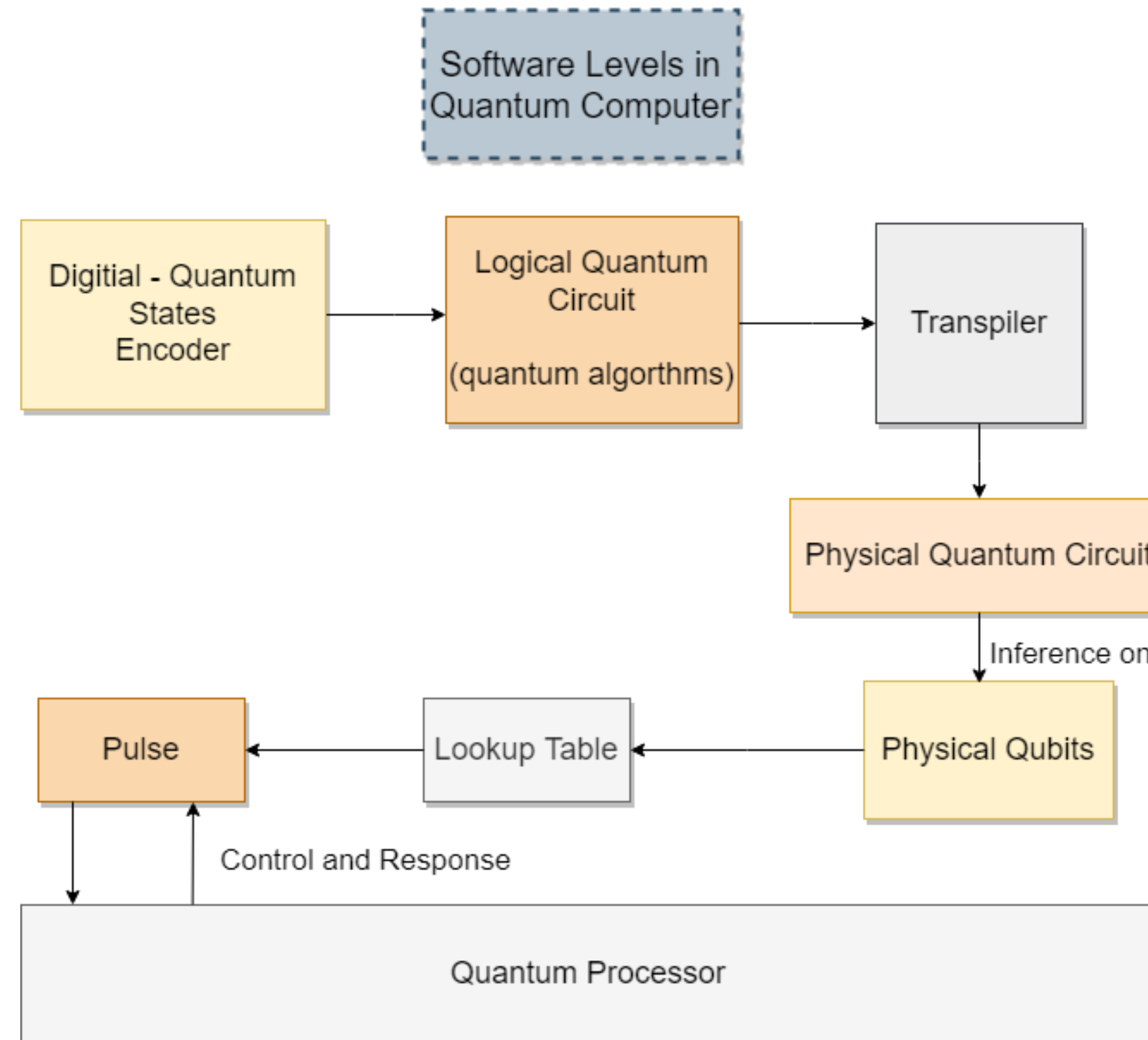
Use TorchQuantum on Pulse level

3.1 Quantum Optimal Control 

3.2 Variational Pulse Learning 

Brief Overview of Workflow

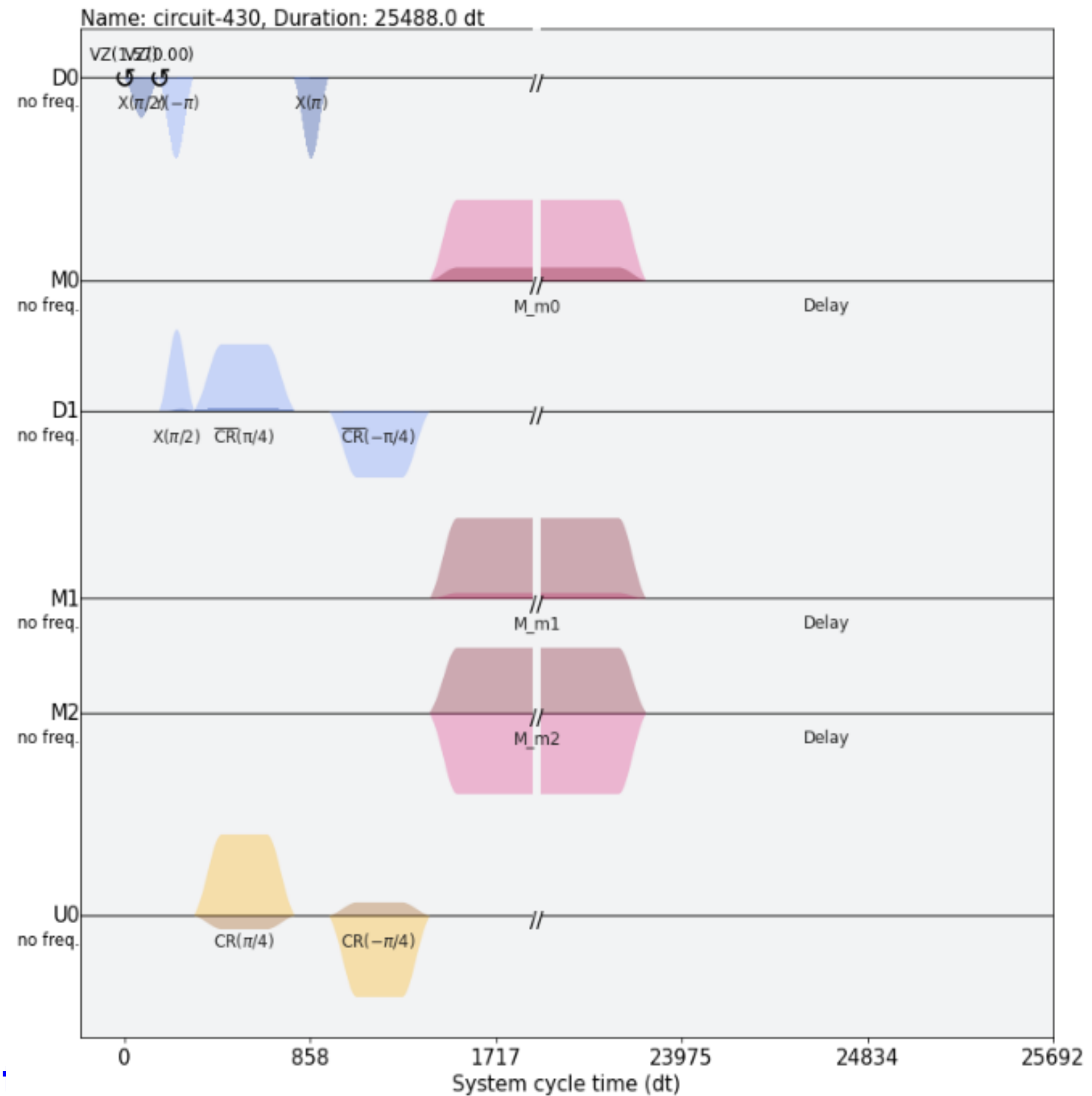
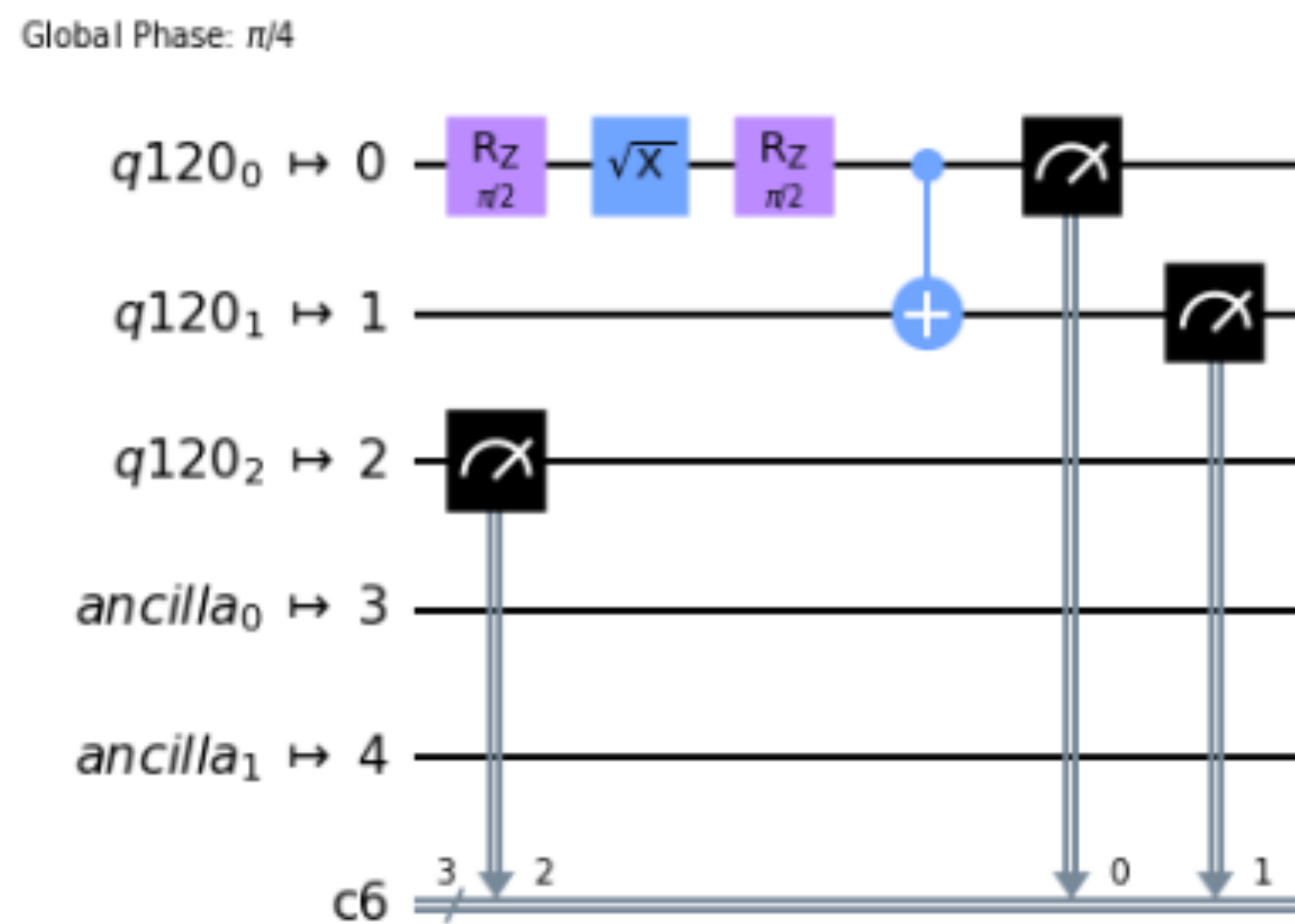
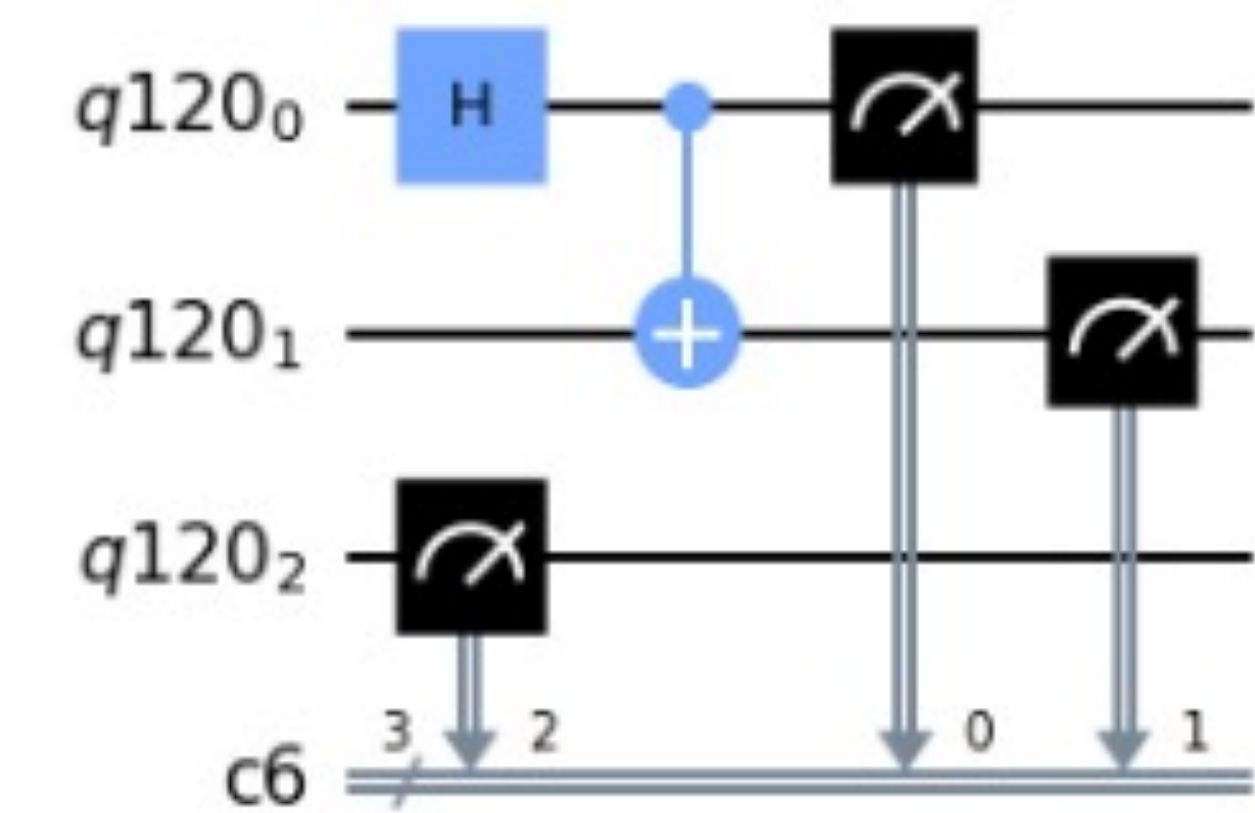
- When we want to execute a quantum program on a quantum computer, we need to compile it first:



Materials at: <https://torchquantum.org>

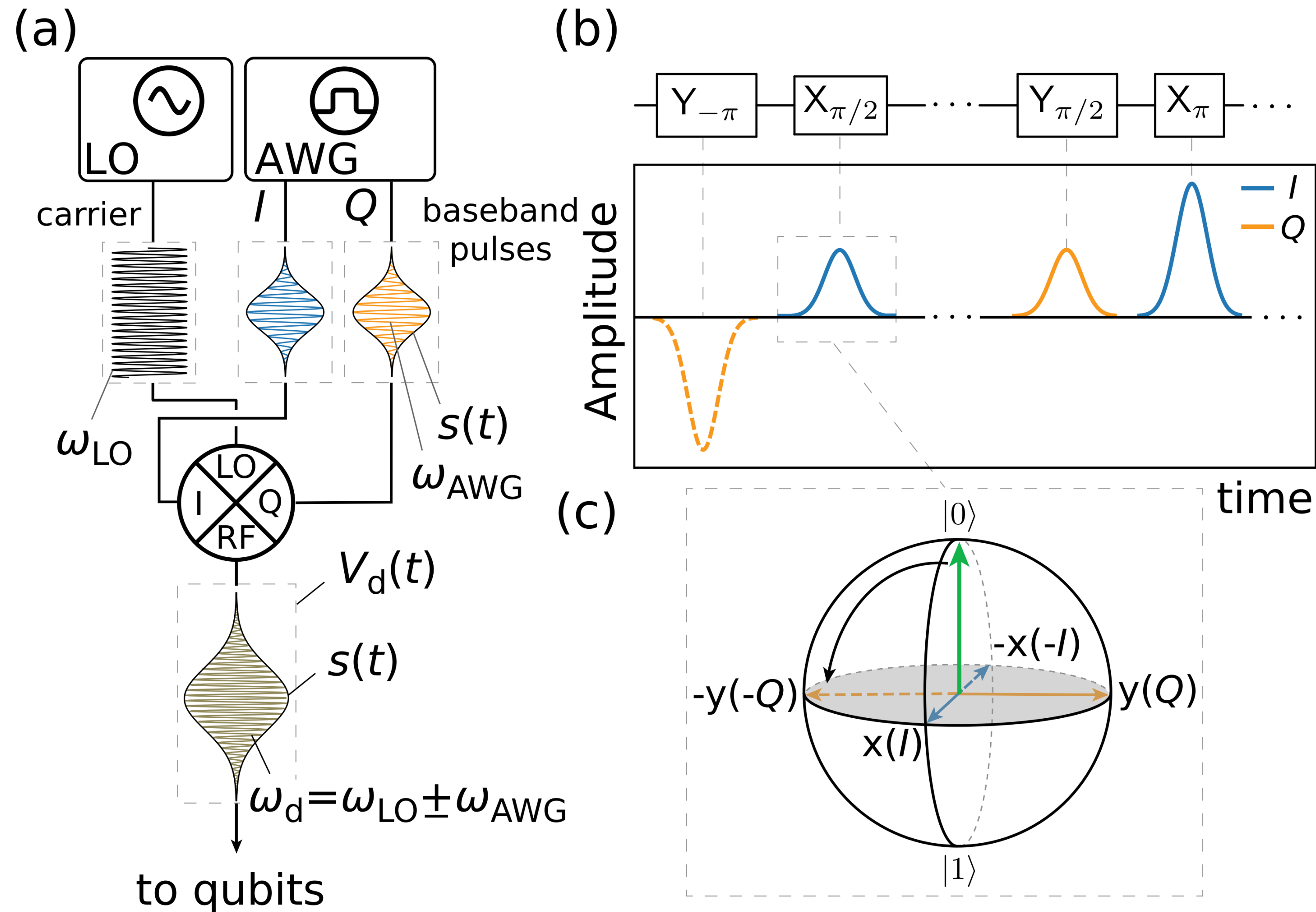
Pulse-Based and Gate-Based

- Gate- and Pulse-level are two different abstraction layers.



Pulse-Based and Gate-Based

- The microwave is used to control the quantum bits.



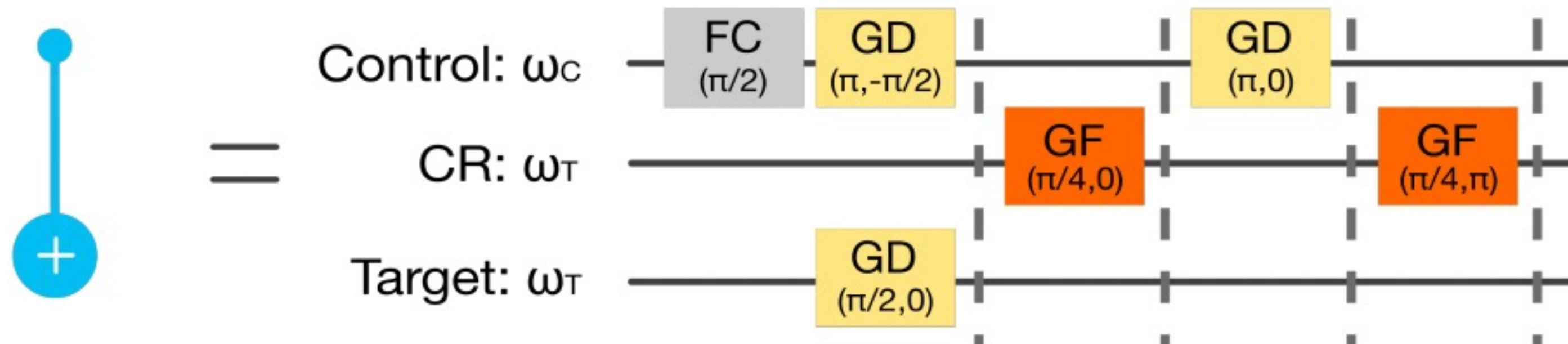
Gate-based Compilation

- Each gate corresponds to a pulse. One-by-one concatenation of all pulses realize the function of many gates.

$$U1_{(\lambda)} = \omega_q \text{ --- FC }_{(-\lambda)} \text{ ---}$$

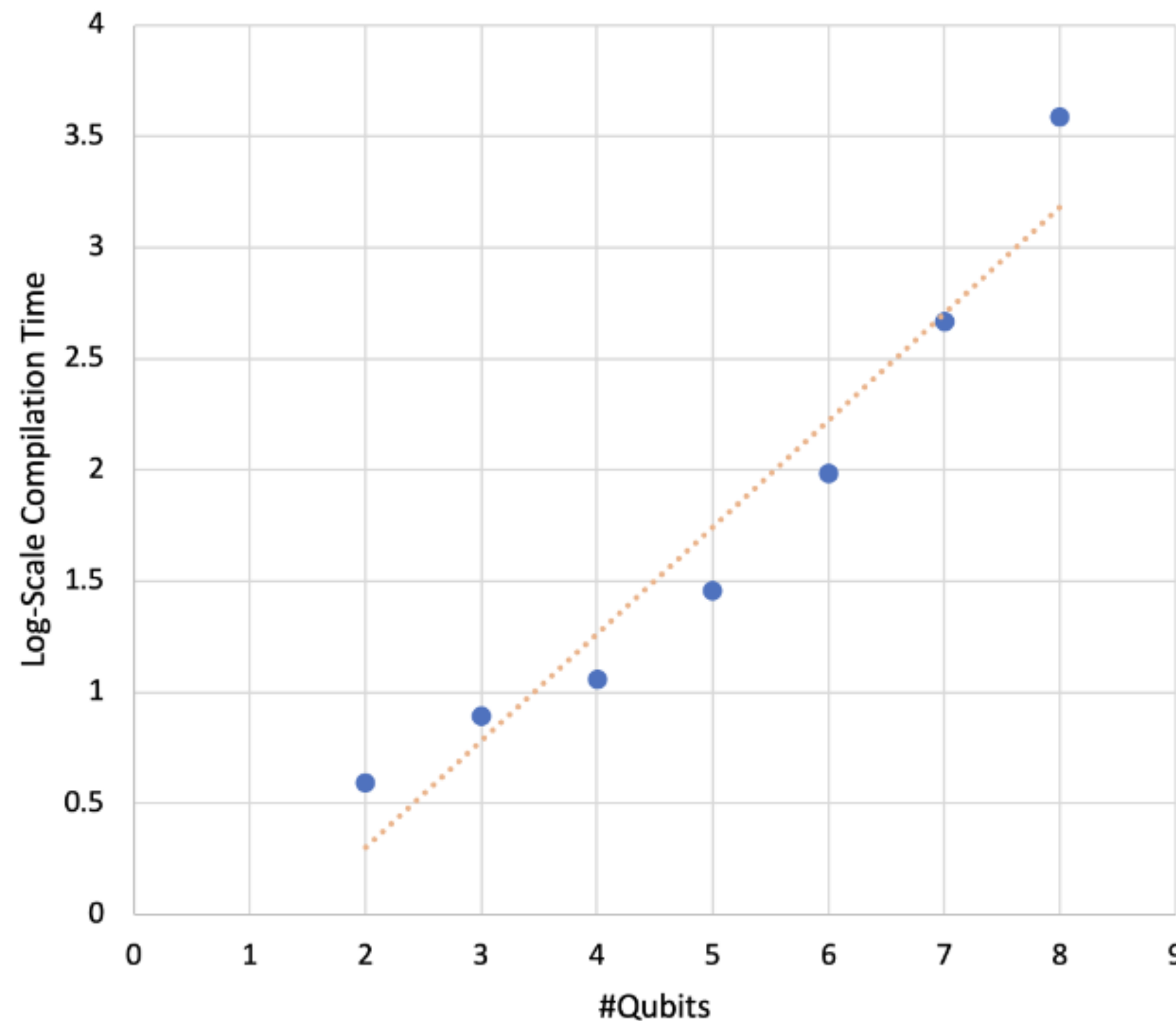
$$U2_{(\phi, \lambda)} = \omega_q \text{ --- FC }_{(-\lambda)} \text{ --- GD }_{(\pi/2, \pi/2)} \text{ --- FC }_{(-\phi)} \text{ ---}$$

$$U3_{(\theta, \phi, \lambda)} = \omega_q \text{ --- FC }_{(-\lambda)} \text{ --- GD }_{(\pi/2, 0)} \text{ --- FC }_{(-\theta)} \text{ --- GD }_{(\pi/2, \pi)} \text{ --- FC }_{(-\phi)} \text{ ---}$$



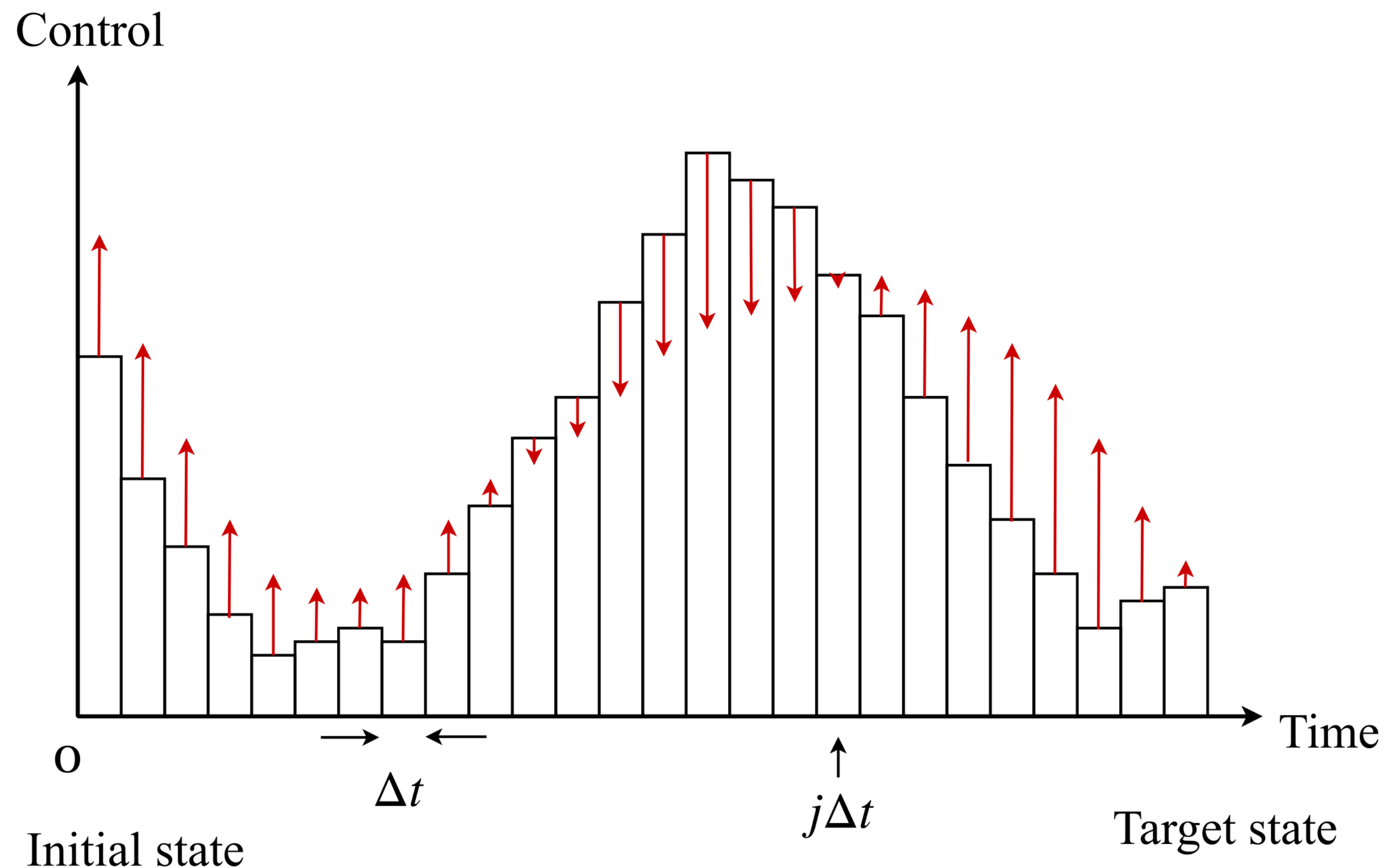
Quantum Optimal Control(QOC)

- QOC is commonly used to generate pulses (from target unitary matrices to pulses)
- QOC is computationally expensive



Quantum Optimal Control (QOC)

- As shown in the figure, the control pulse is divided into multiple time slots. The amplitude of each time slot will be adjusted through optimization.



Accqoc: Group-based Pre-compilation

- Instead of dealing with single gate, we generate pulses from groups of gates.

Algorithm 1 Bit Dividing

Require: qasm files, bit constraint(bc)

Ensure: large-groups

```
1: Initialize large-groups
2: for qasm in all qasm files do
3:   DAG = ToDAG(qasm)
4:   for node in DAG.topological-order: do
5:     if node can be grouped with both predecessor then
6:       Merge the groups the two predecessors are in
7:     else if node can be grouped with one predecessor
       then
8:       Group the node with the predecessor
9:       Update large-groups
10:    else if node can be group with no predecessor then
11:      Put the node in a new group
12:      Update large-groups
13:    end if
14:  end for
15: end for
16: return large-groups
```

Algorithm 2 Layer Dividing

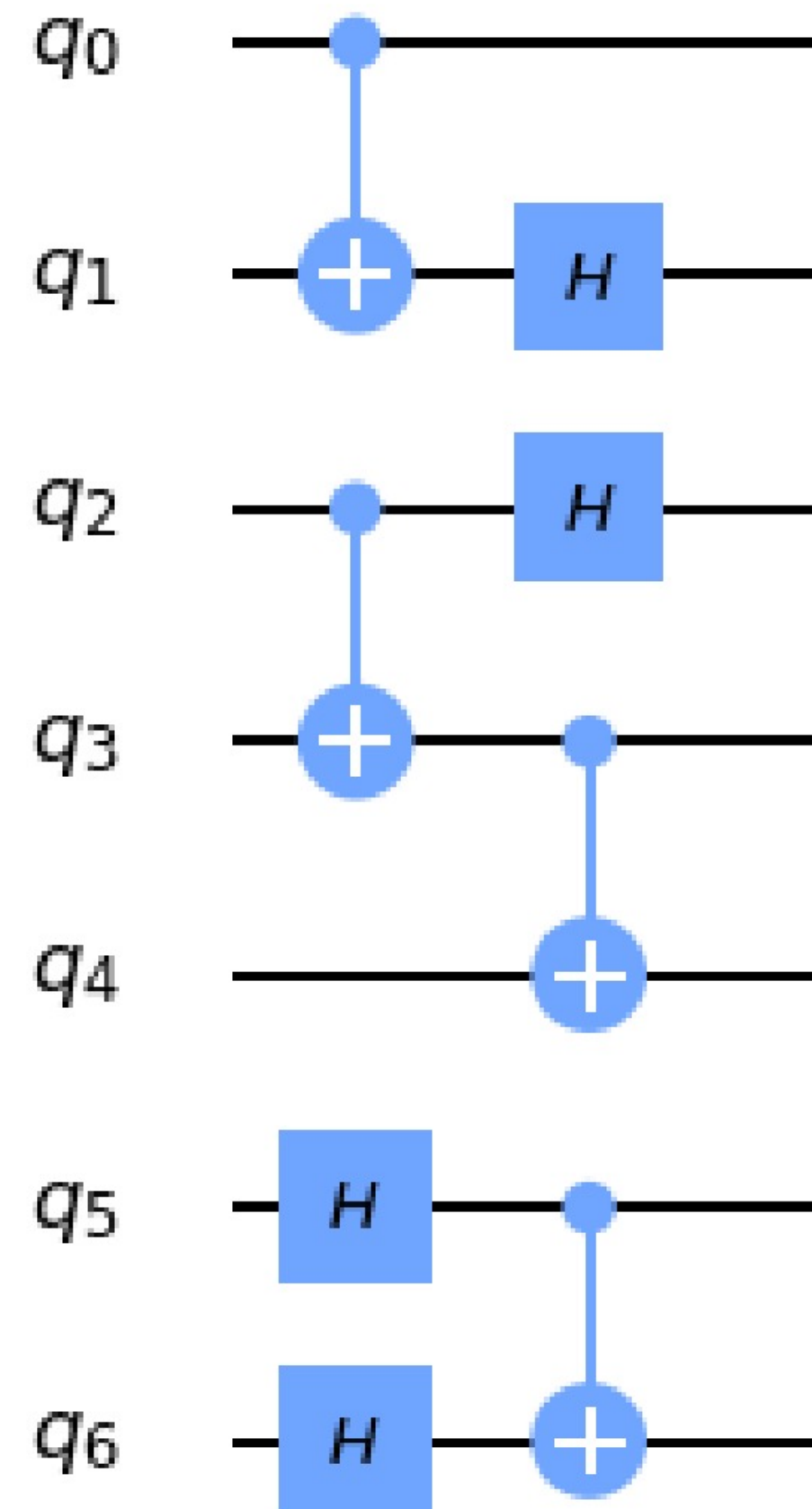
Require: large-groups, layer constraint(lc)

Ensure: group list

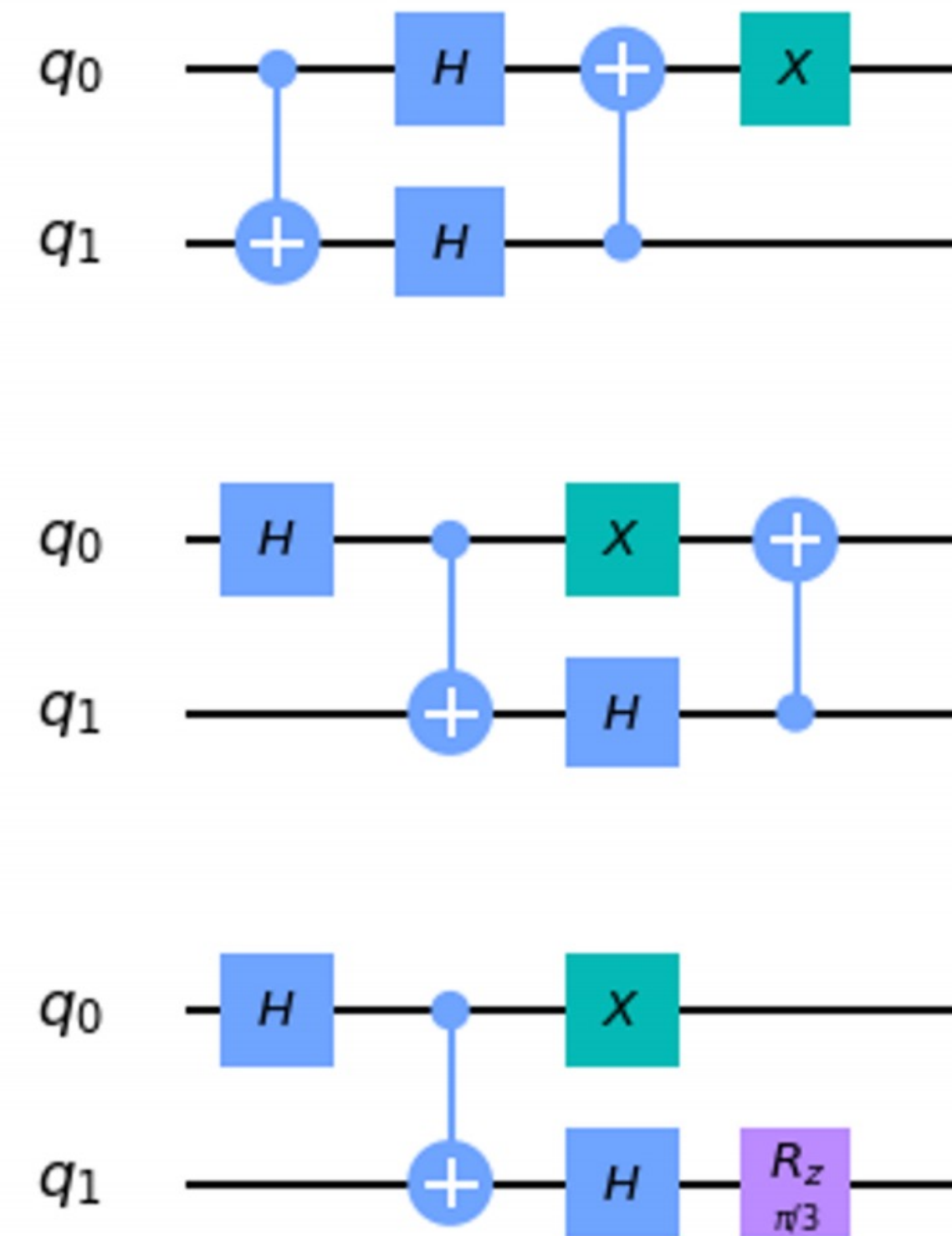
```
1: Initialize group-list
2: for node in DAG.topological-order: do
3:   Depth[node] = max(Depth[node's predecessor(s)]) + 1
4: end for
5: for subgroup in large-groups: do
6:   startDepth = depth of shallowest node
7:   layer = 0
8:   Initialize temp-group
9:   for node in subgroup: do
10:    diff = depth[node] - start
11:    if diff mod lc  $\leq$  layer then
12:      Append node to temp-group
13:    else
14:      Append temp-group to group-list
15:      Clear temp-group
16:      Append node to temp-group
17:      layer += 1
18:    end if
19:  end for
20: end for
21: return group-list
```

Accqoc: Group-based Pre-compilation

- We limit the size of the groups that QOC takes. (Key Insight)



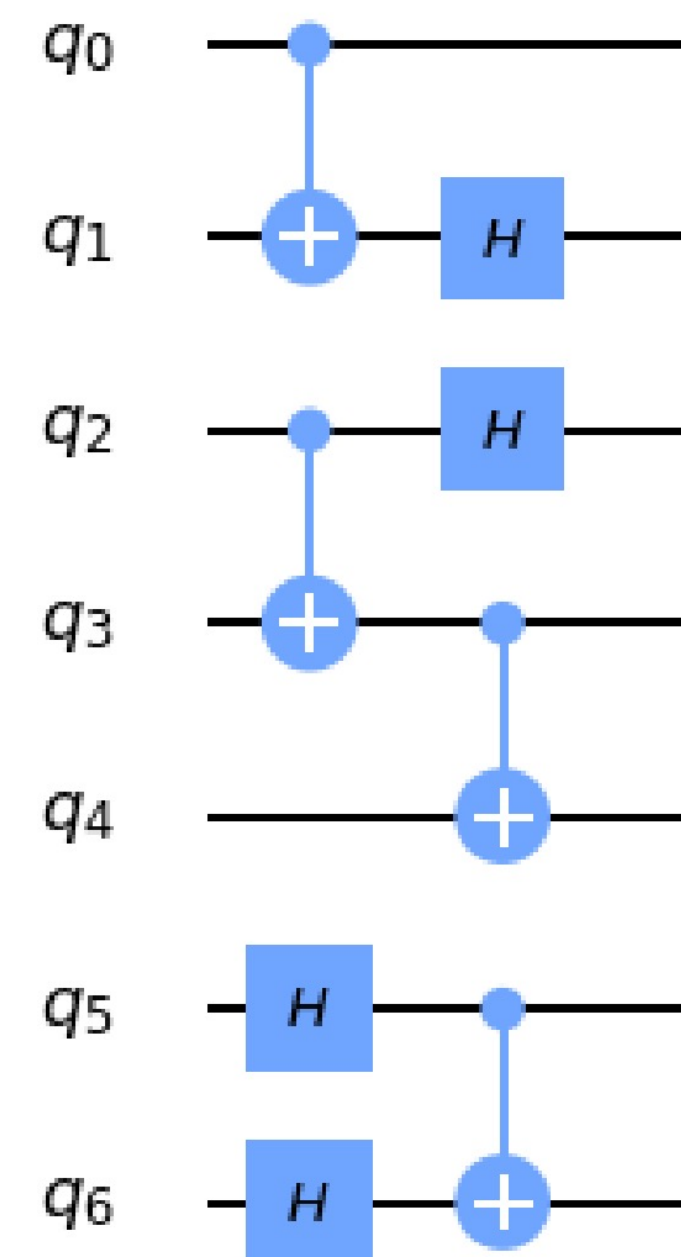
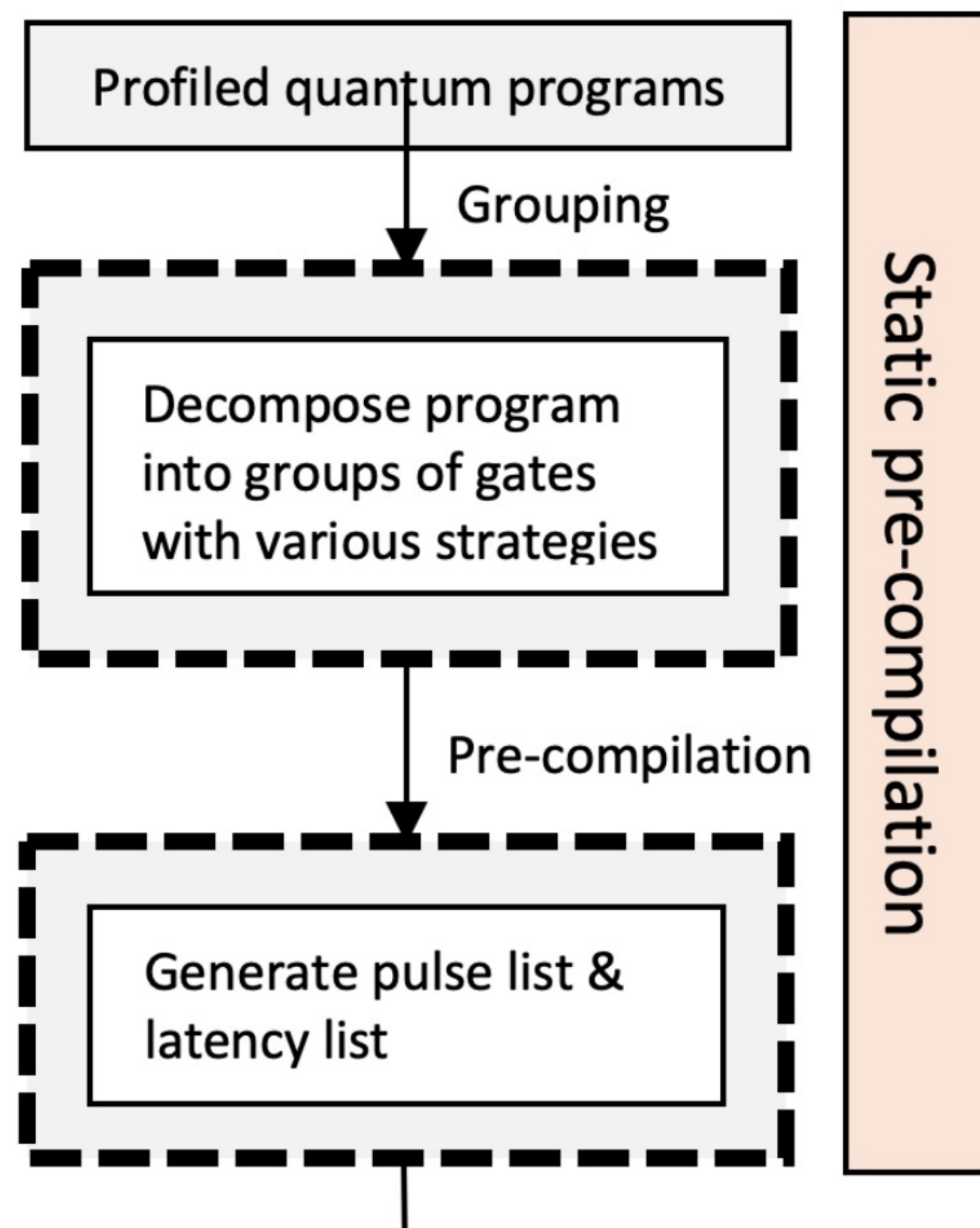
(c) Group with many qubits



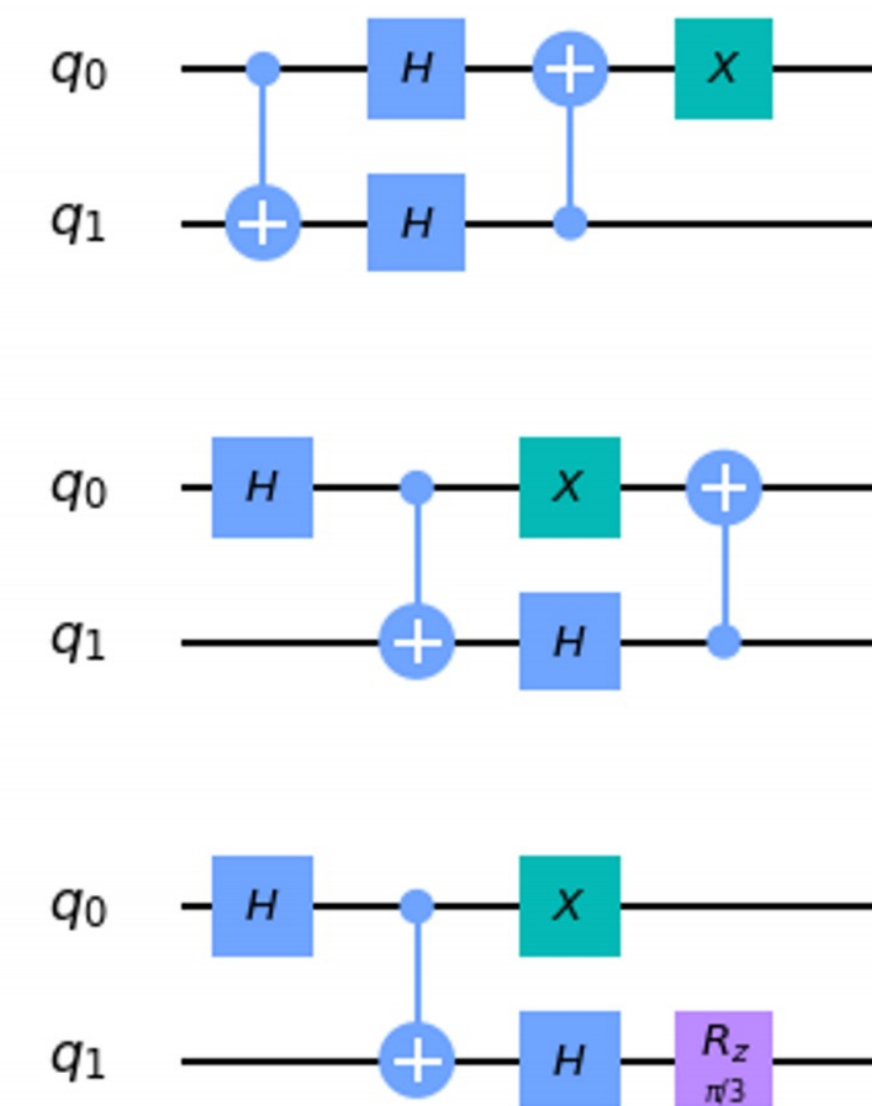
(d) Typical group in our paper

Build the Library

- Pulses of these groups will be generated through QOC. And we get a library that stores group-pulse pairs.



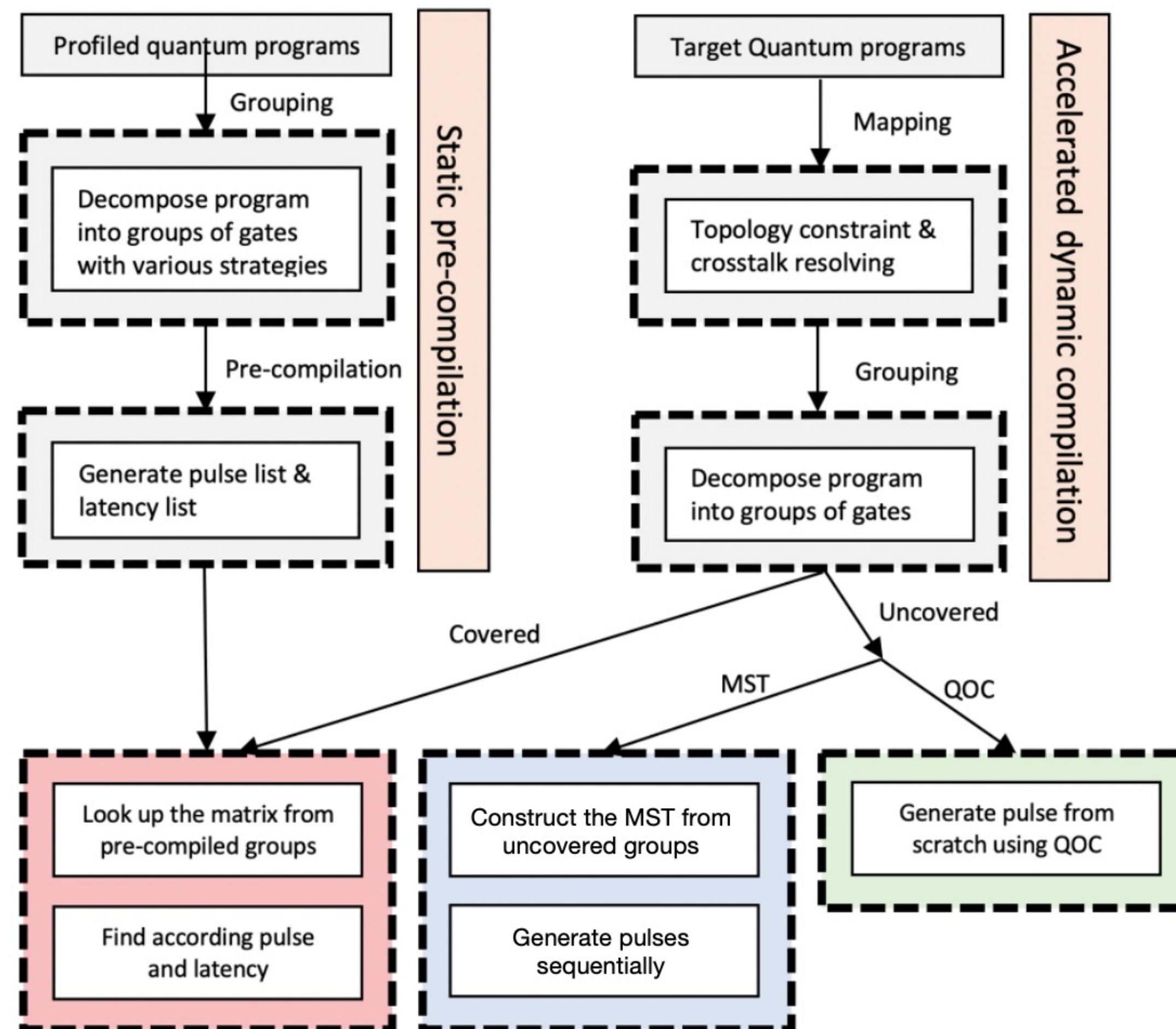
(c) Group with many qubits



(d) Typical group in our paper

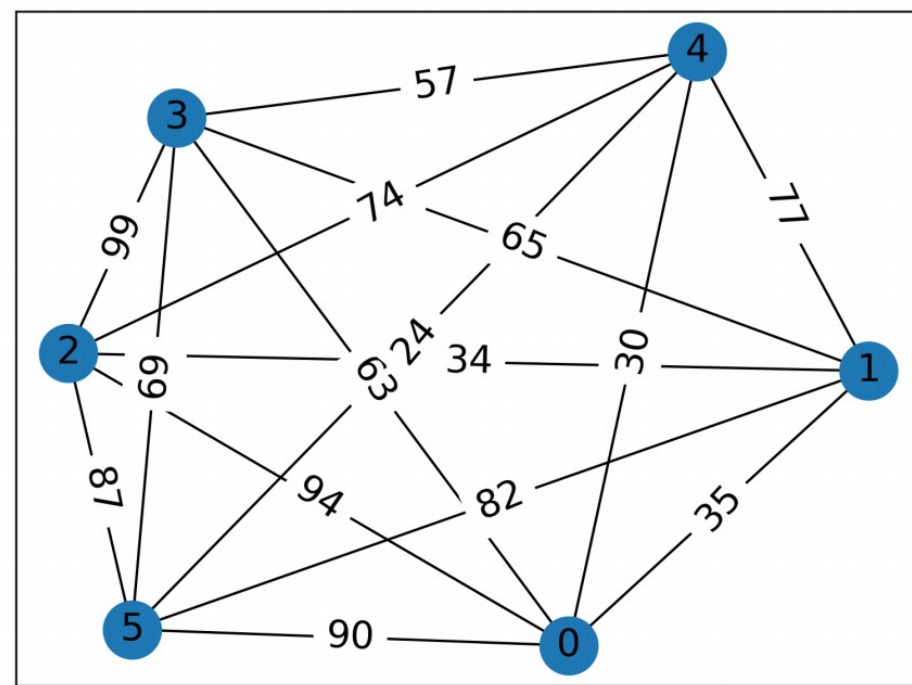
Utilize the Library

- For groups that are covered by library, the pulse could be directly looked up.
- For uncovered groups, we could generate the pulses using pulses of very similar groups

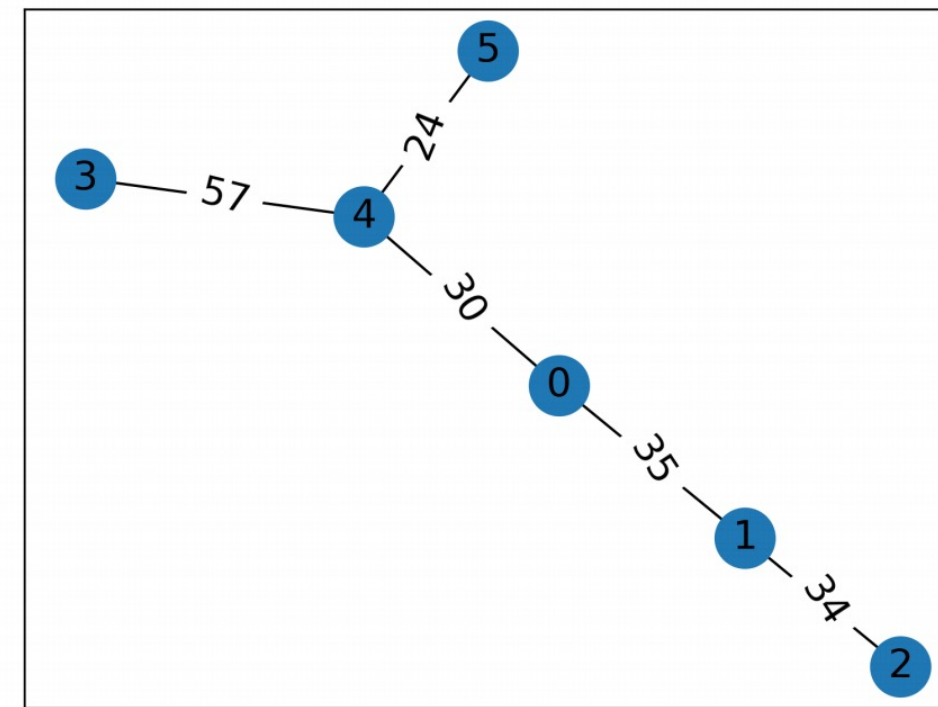


Use MST to Accelerate QOC

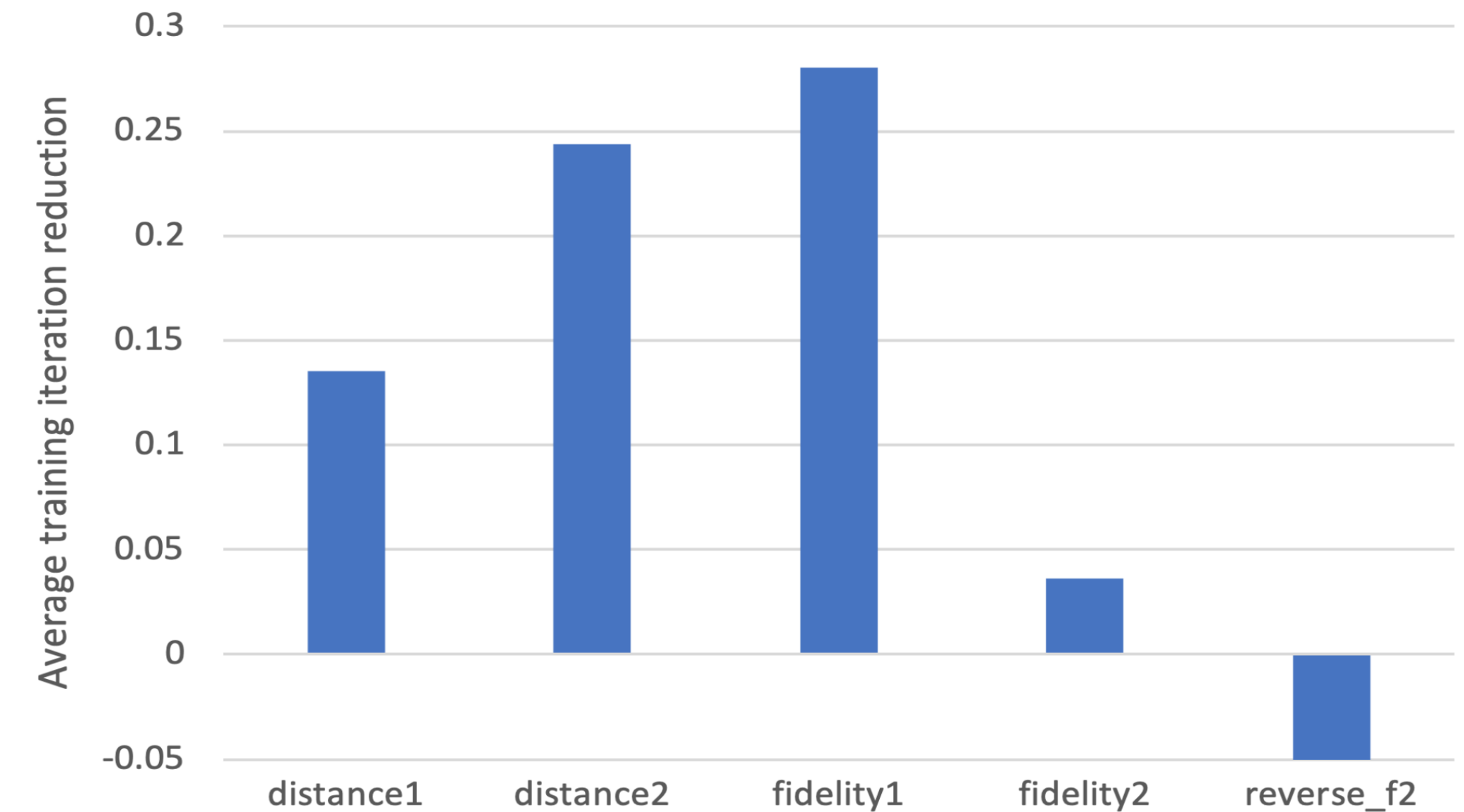
- We need to define similarity and find the corresponding Minimum spanning tree.



(a) A 6-node SG



(b) Minimum spanning tree

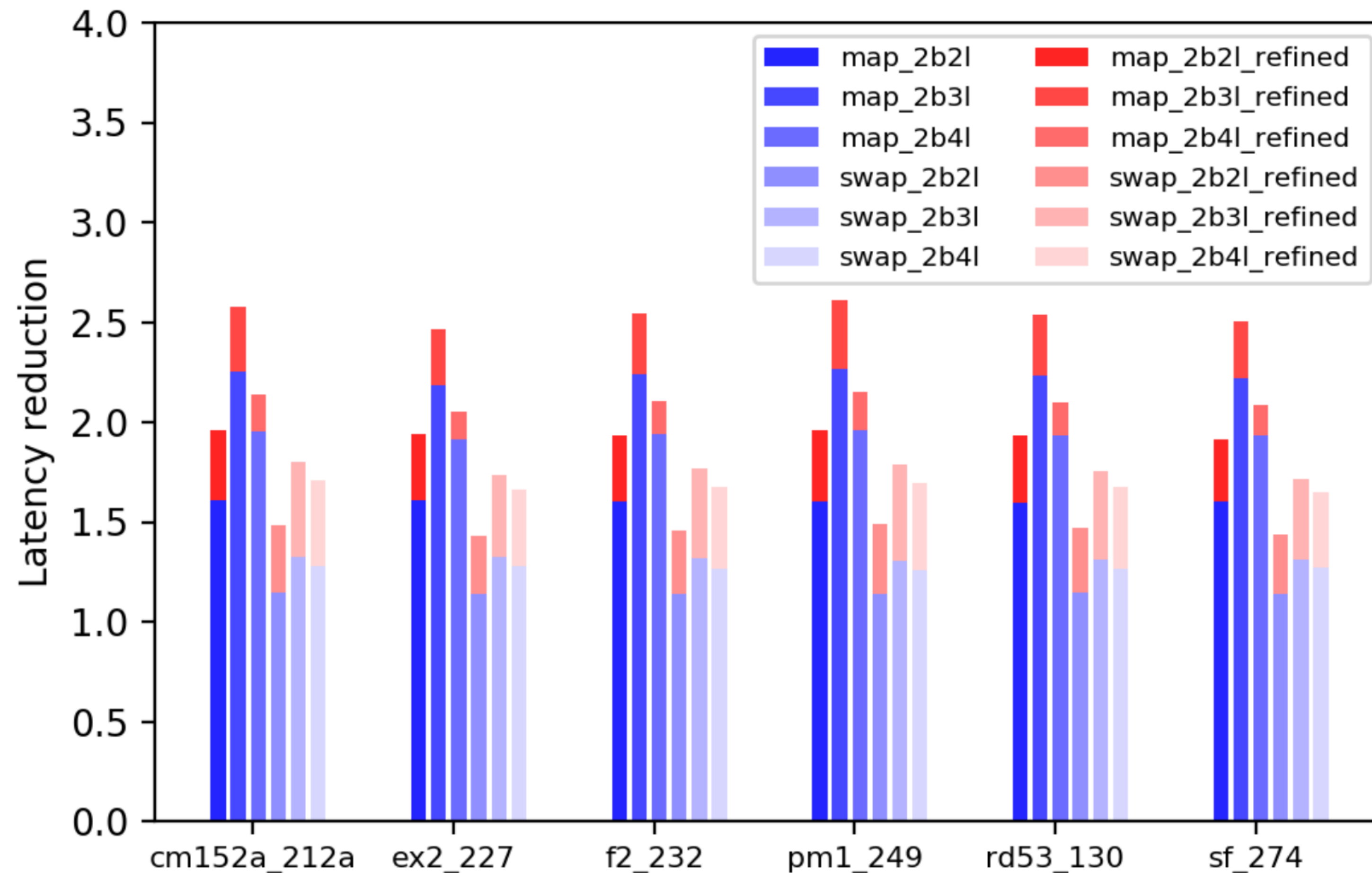


$$d_1(\mathbf{A}, \mathbf{B}) = \sum_{i=1}^n \sum_{j=1}^n |a_{ij} - b_{ij}| \quad d_2(\mathbf{A}, \mathbf{B}) = \sqrt{\sum_{i=1}^n \sum_{j=1}^n (a_{ij} - b_{ij})^2}$$

$$d_3(\mathbf{A}, \mathbf{B}) = \text{Tr}(\mathbf{A}^* \mathbf{B}) \quad d_4(\mathbf{A}, \mathbf{B}) = F(\mathbf{A}, \mathbf{B}) = \left(\text{tr} \sqrt{\sqrt{\mathbf{A}} \mathbf{B} \sqrt{\mathbf{A}}} \right)^2$$

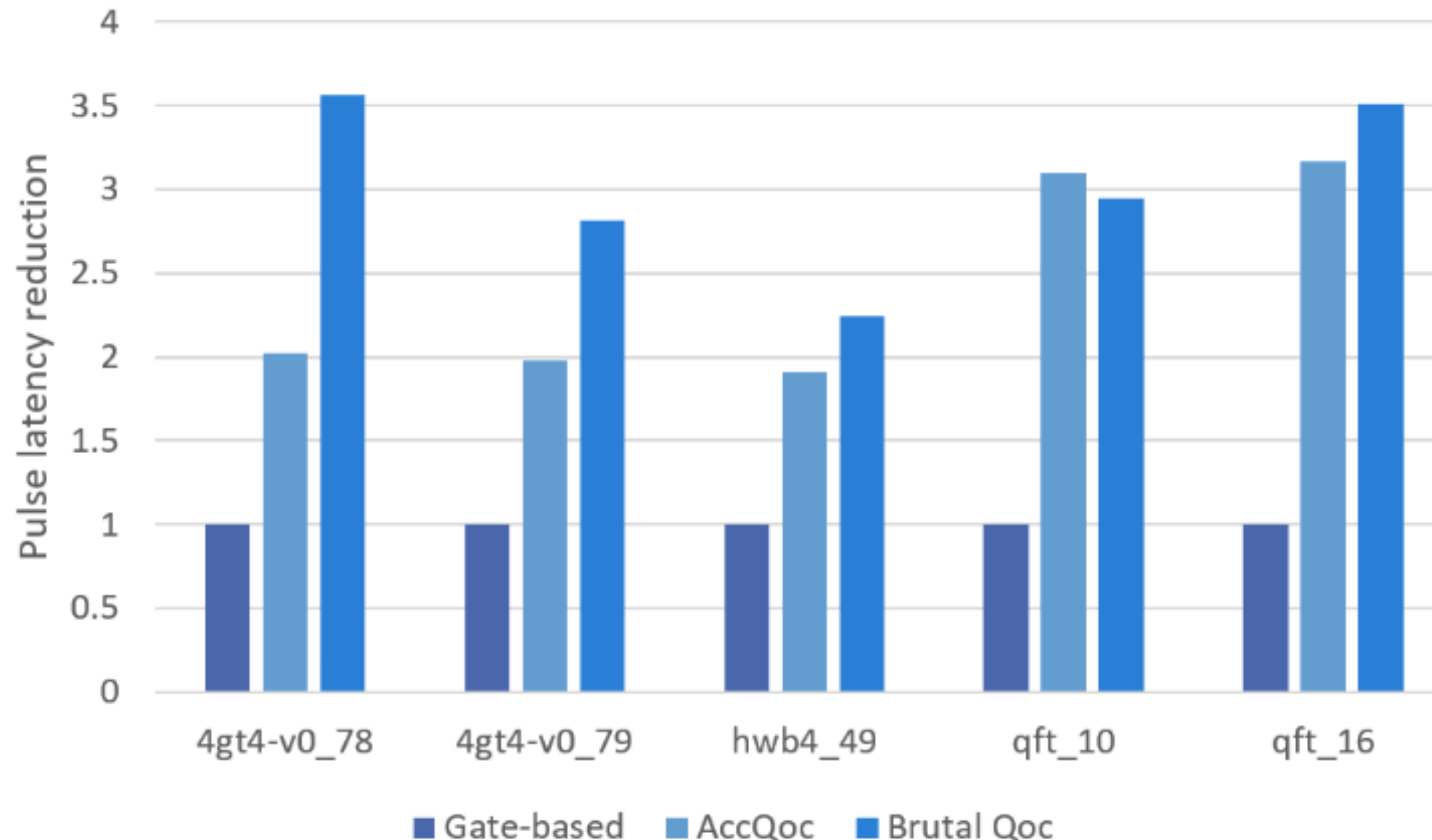
Latency Reduction over Gate-based

- This figure shows the latency reduction compared with gate-based compilation. We show that the latency is reduced for various grouping strategy.



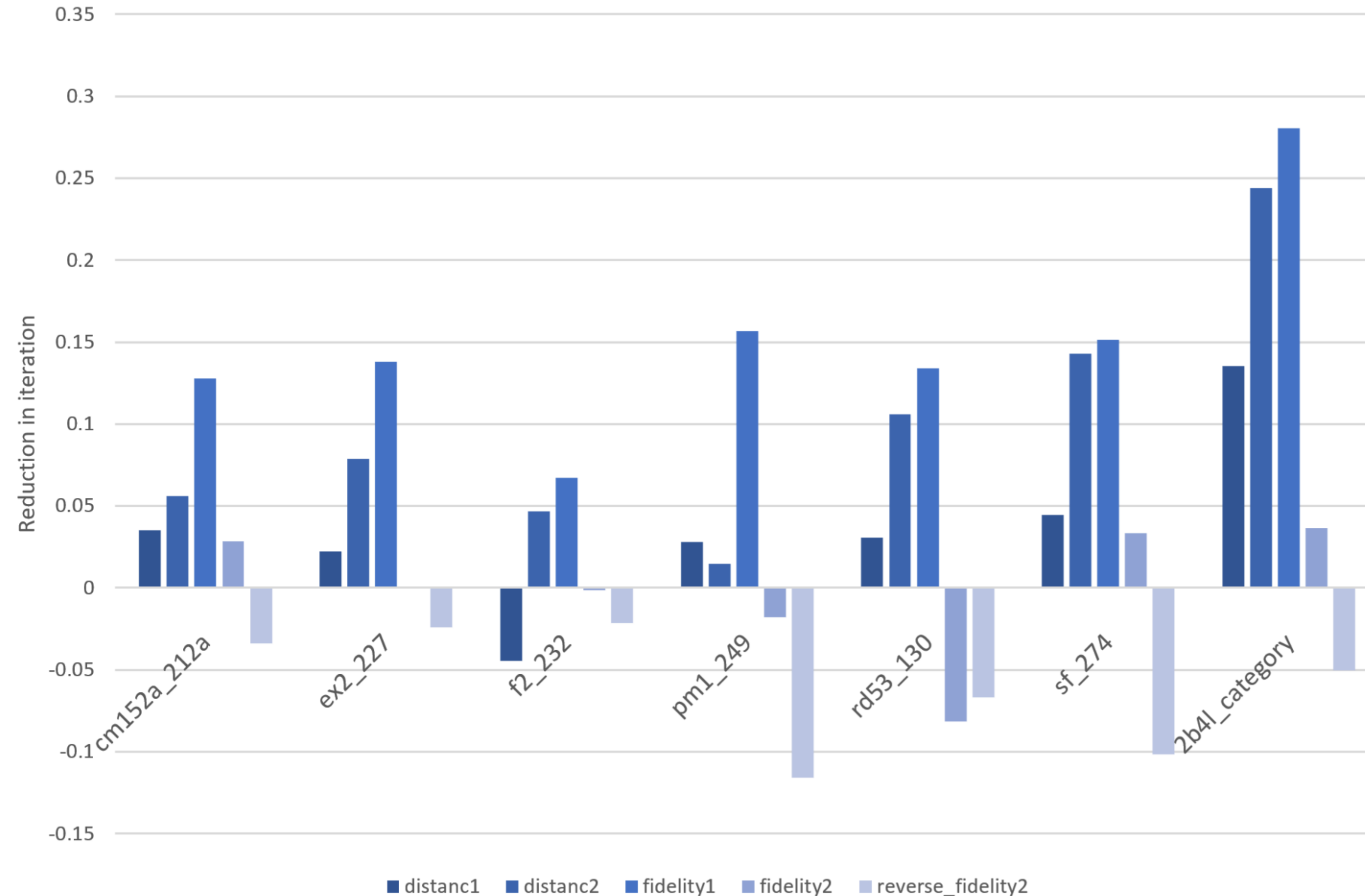
Latency Reduction V.S. Brute-force

- This figure shows the latency reduction compared with brute-force compilation. Brute-force QOC means that we give QOC a very large group of gates to reach maximum latency reduction.



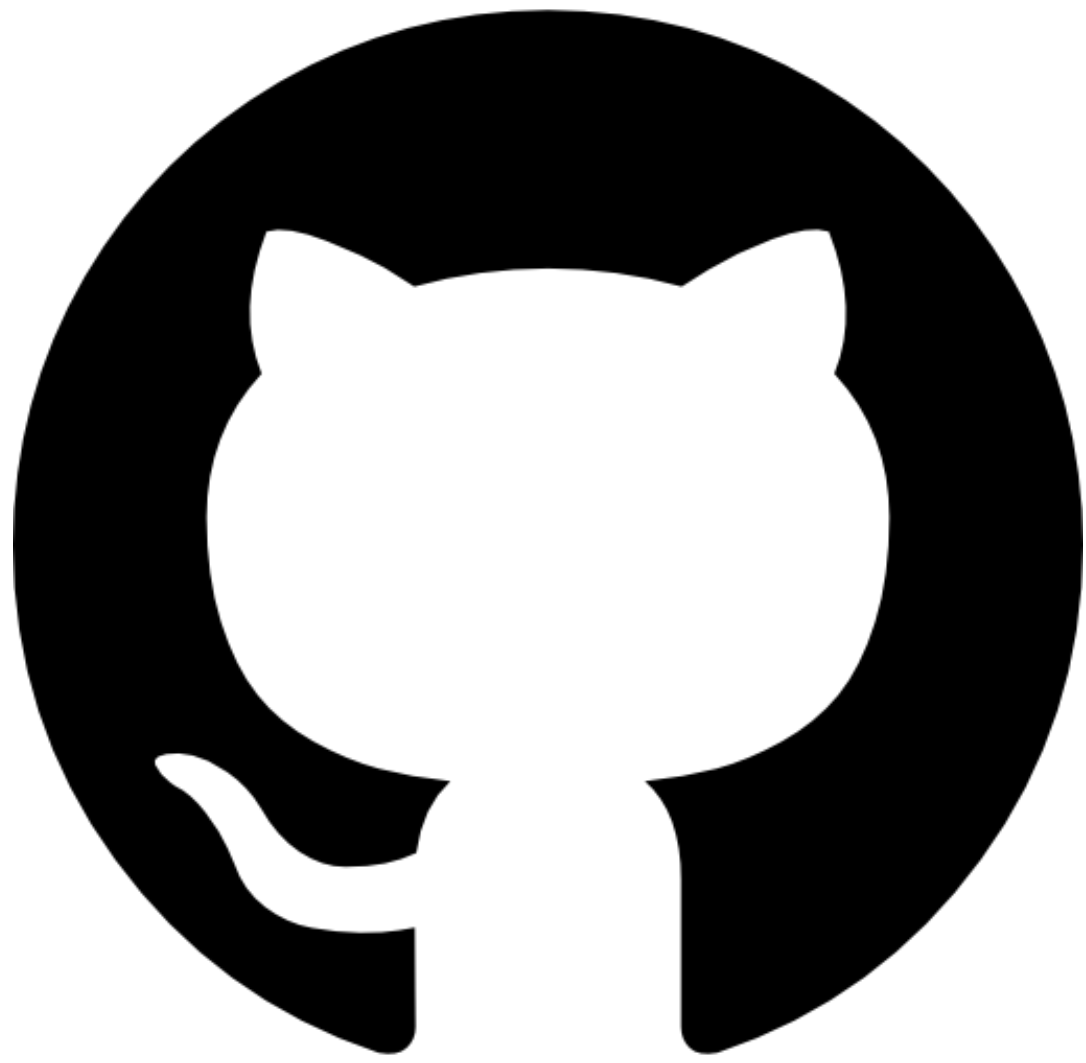
Reduction of Training Iteration

- We see reduction of training iteration when we adopt the idea of similarity.



Hands-On Section

3.1 Quantum Optimal Control



TorchQuantum Tutorial Outline

Section 1

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1.1 Quantum Basics

1.2 TQ operations 

1.3 TQ for State Prep 


1.4 TQ for VQE 

1.4 TQ for QNN 

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Use TorchQuantum on Gate level

2.1 QuantumNAS: Ansatz
Search and Gate Pruning 

2.2 QuantumNAT: Noise
Injection and Quantization 

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2.4 Transformer for Quantum
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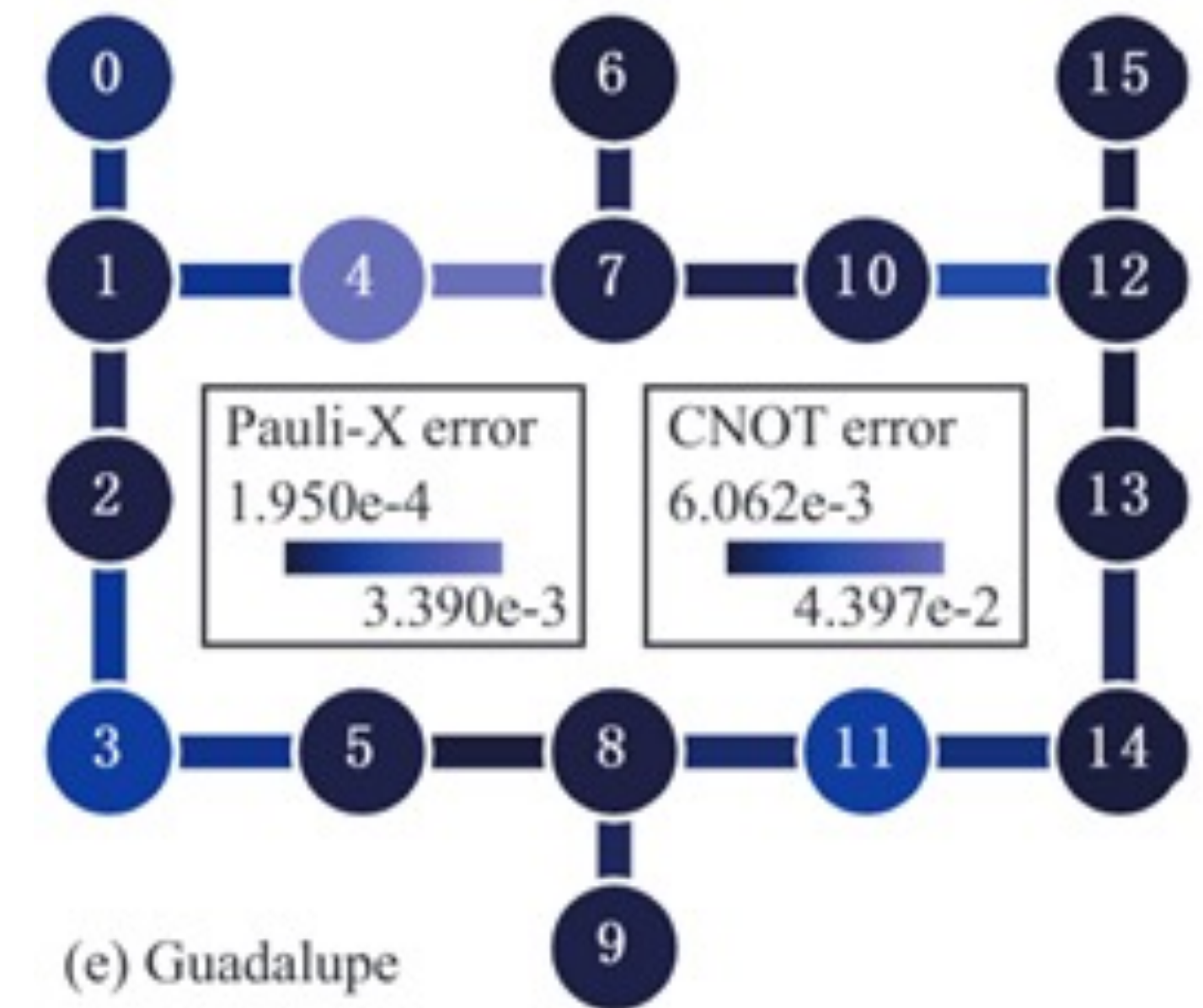
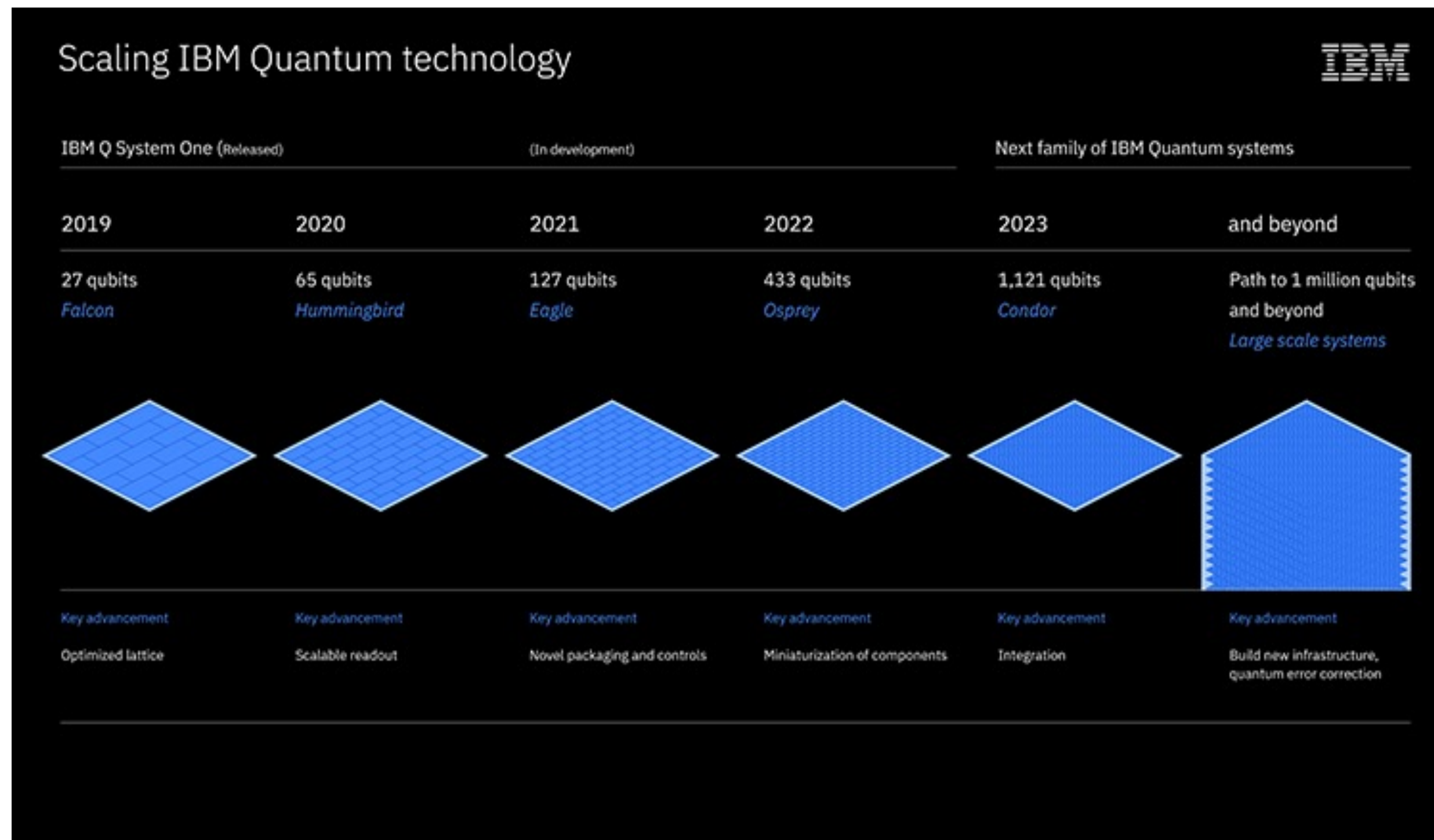
Use TorchQuantum on Pulse level

3.1 Quantum Optimal Control 

3.2 Variational Pulse Learning 

Variational Quantum Pulse Learning (VQP)

- Coherence time is limited in NISQ machines, which means we cannot perform a huge quantum circuit with enough depth and width in NISQ machines.
- Noise and compilation overhead seriously affect the performance of a quantum program.

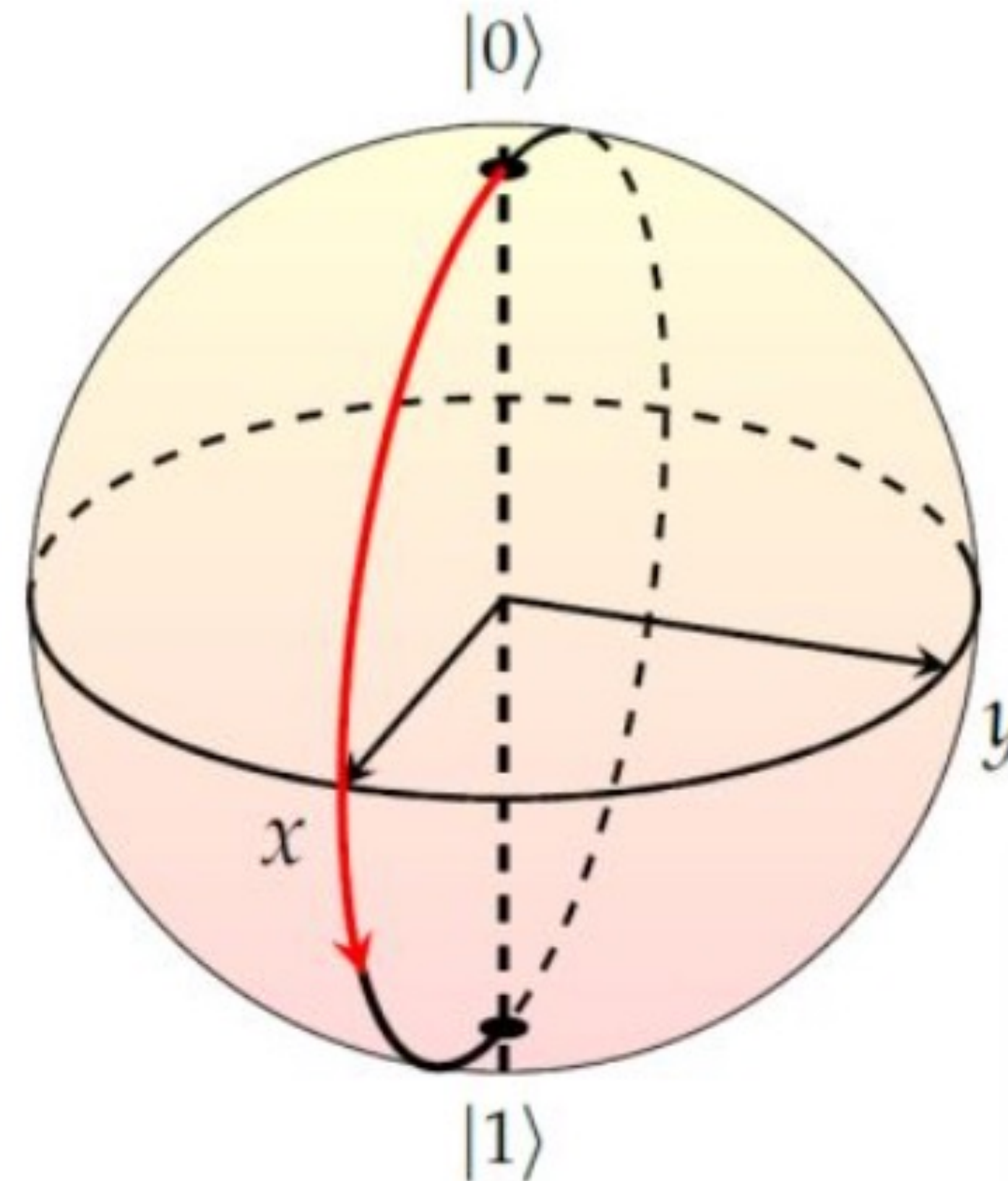
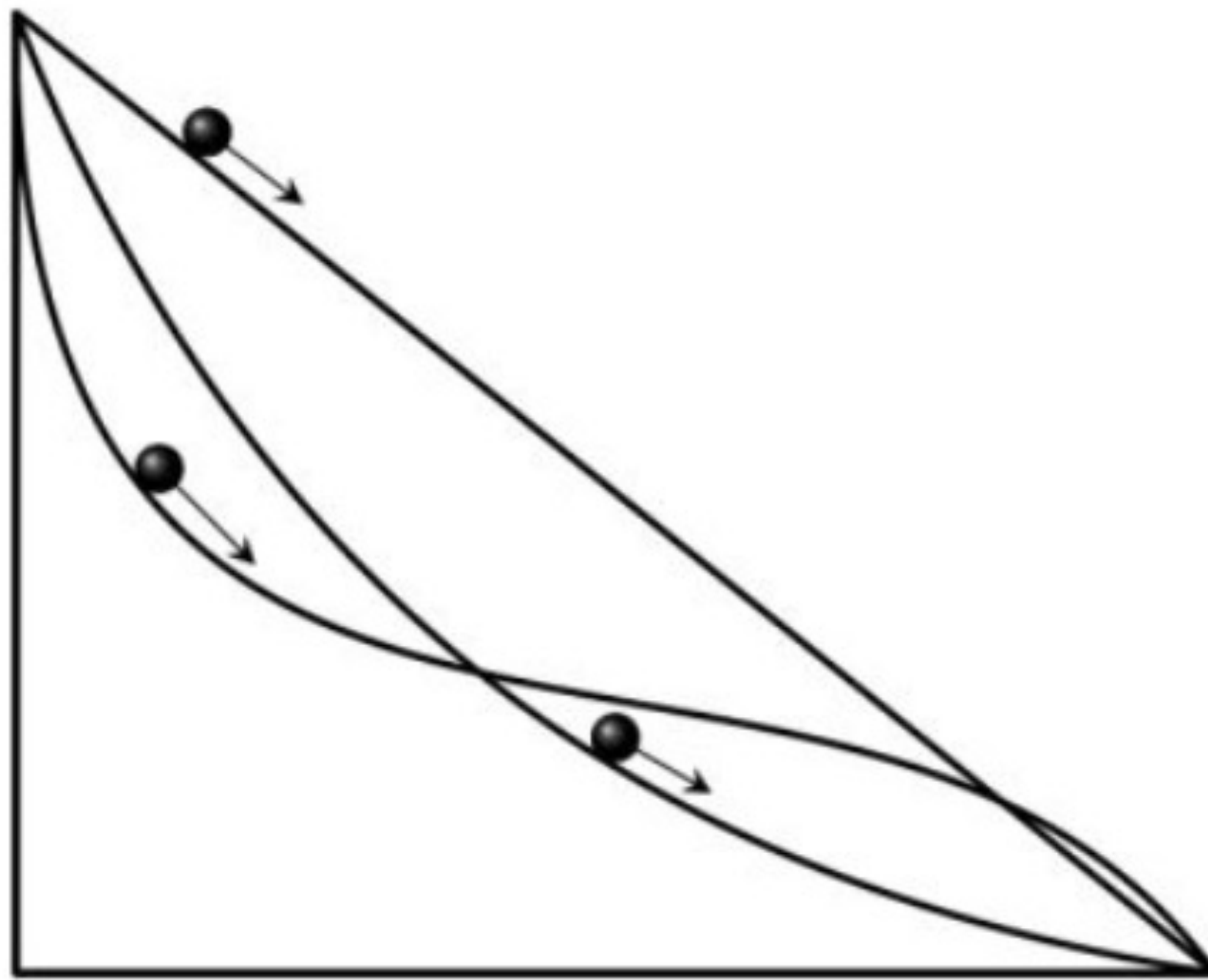


Error rate on a bit in CMOS Device
error rate is about 10^{-15}

But error rate on a quantum bit
reaches 10^{-4} to 10^{-2}

Motivation and Challenges

- QOC is limited to few qubits since it is computationally expensive.
- Most works demonstrate QOC on quantum simulators, however, it is hard to be evaluated on NISQ machines.



Attempt on Quantum Neural Network

- Can we find an intermediate-level approach between the gate level operations and quantum optimal control?
- Can we achieve benefits by doing so?

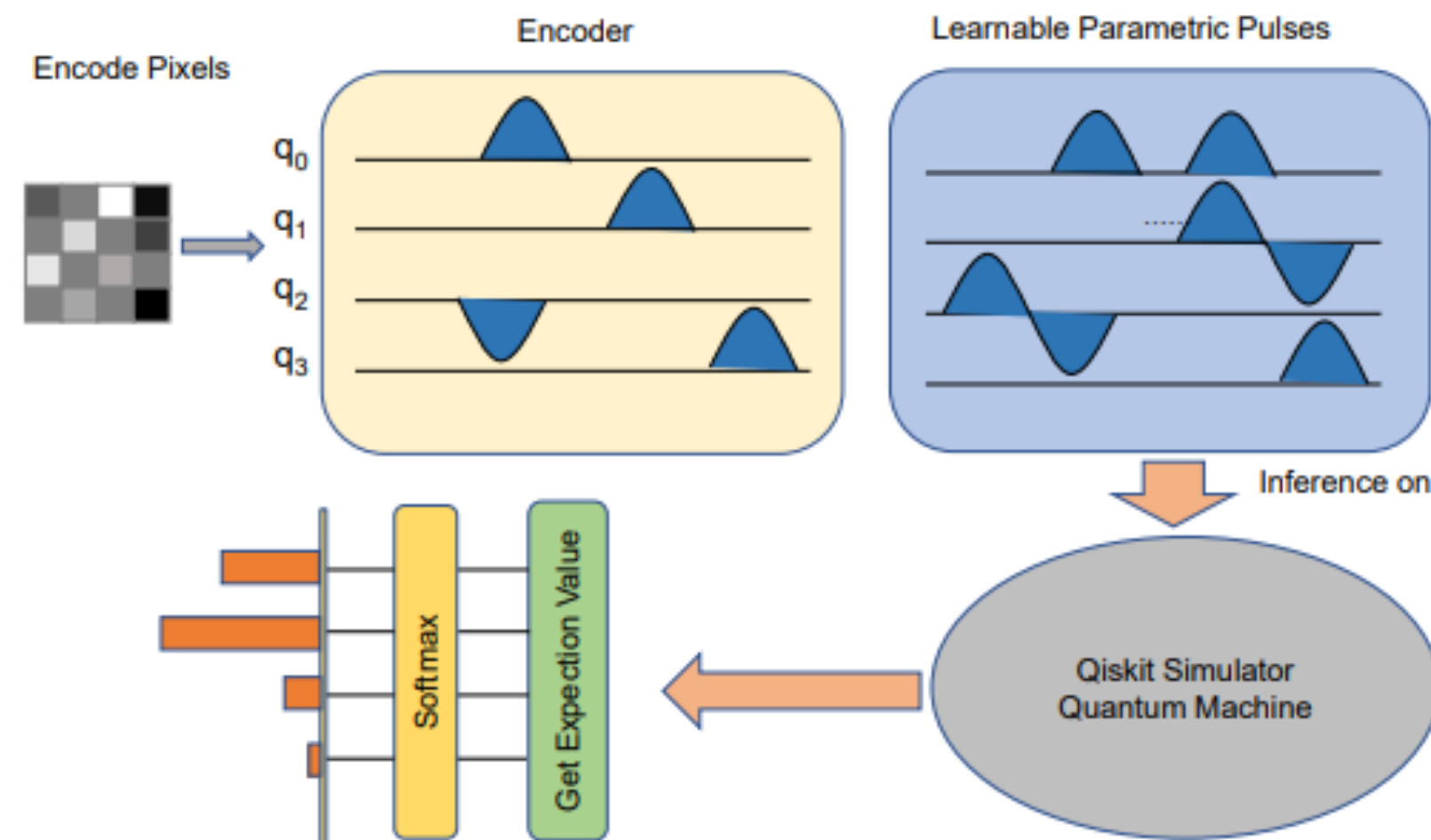


Fig. 1: Conceptual illustration of VQP for QML tasks.

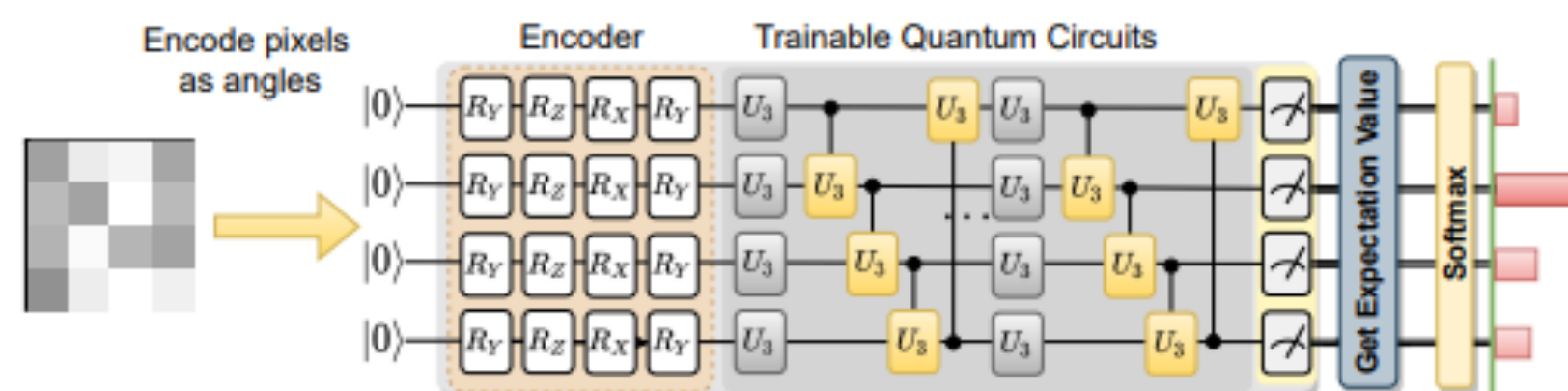
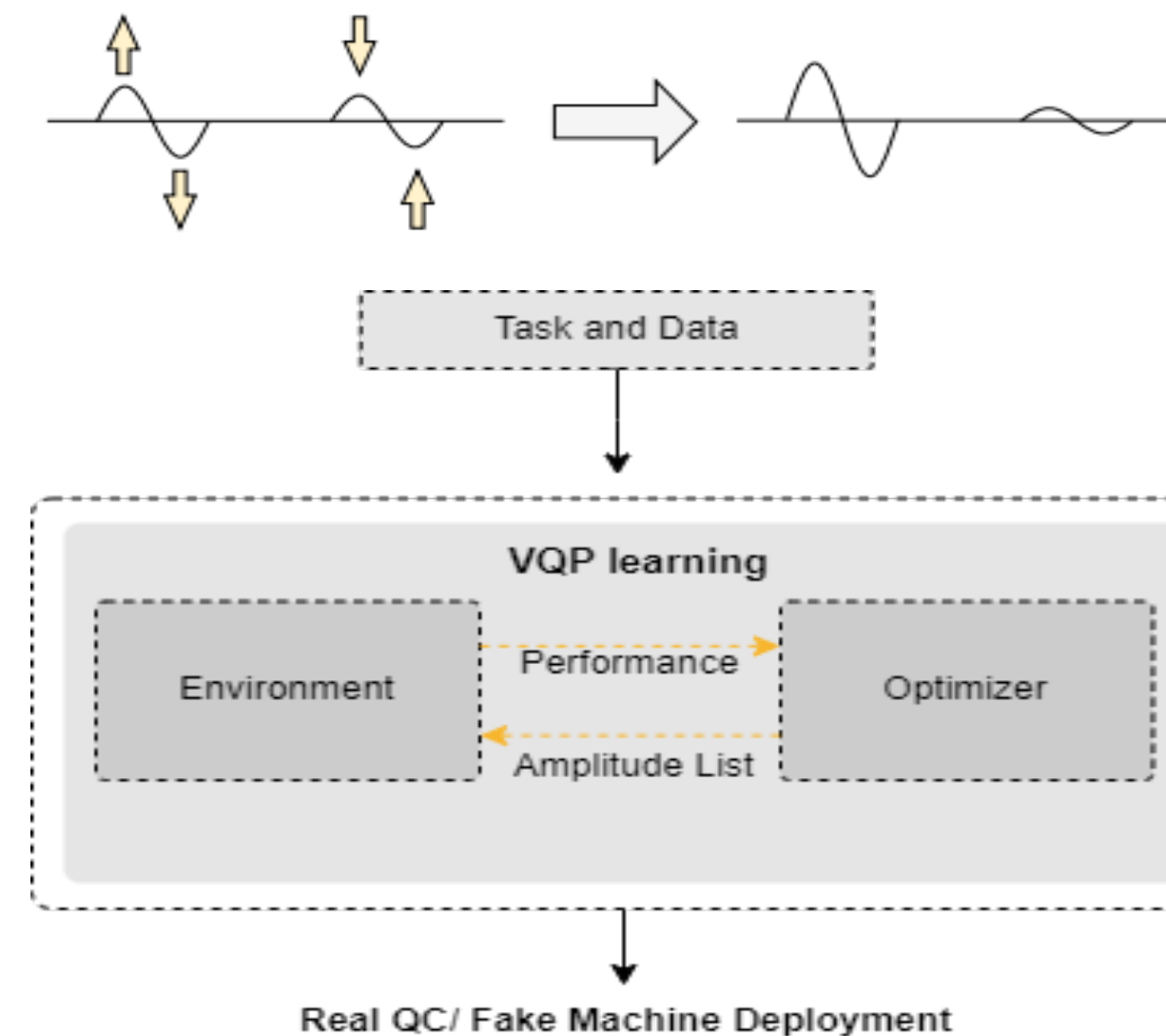
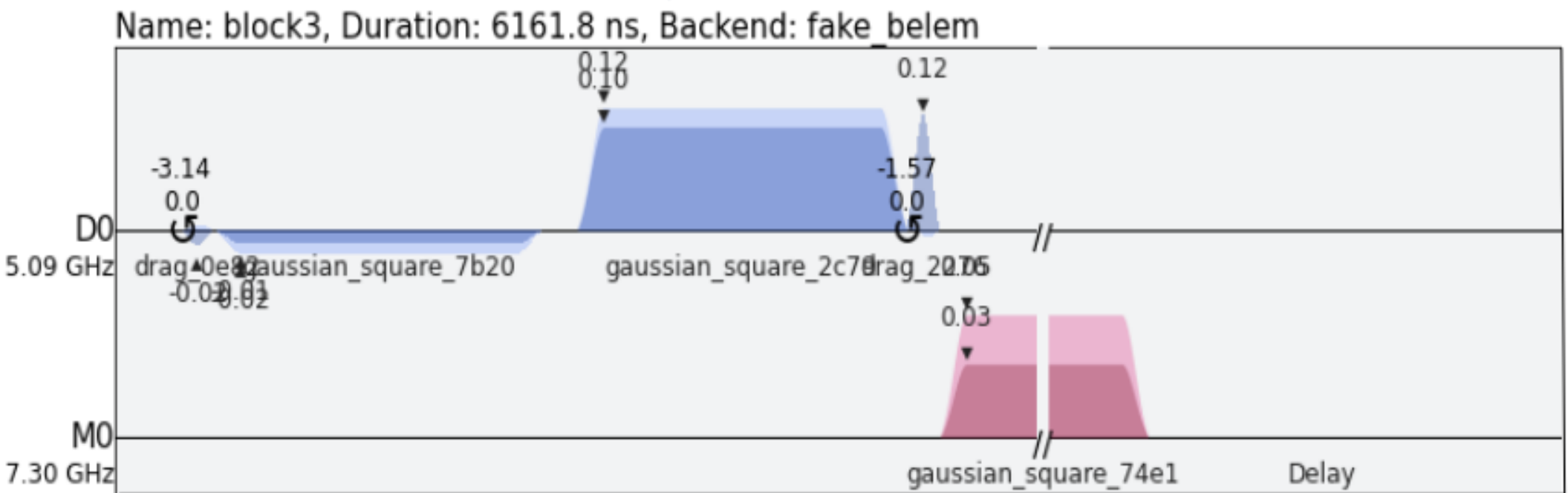
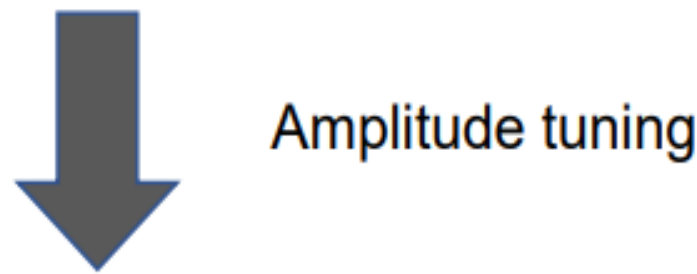
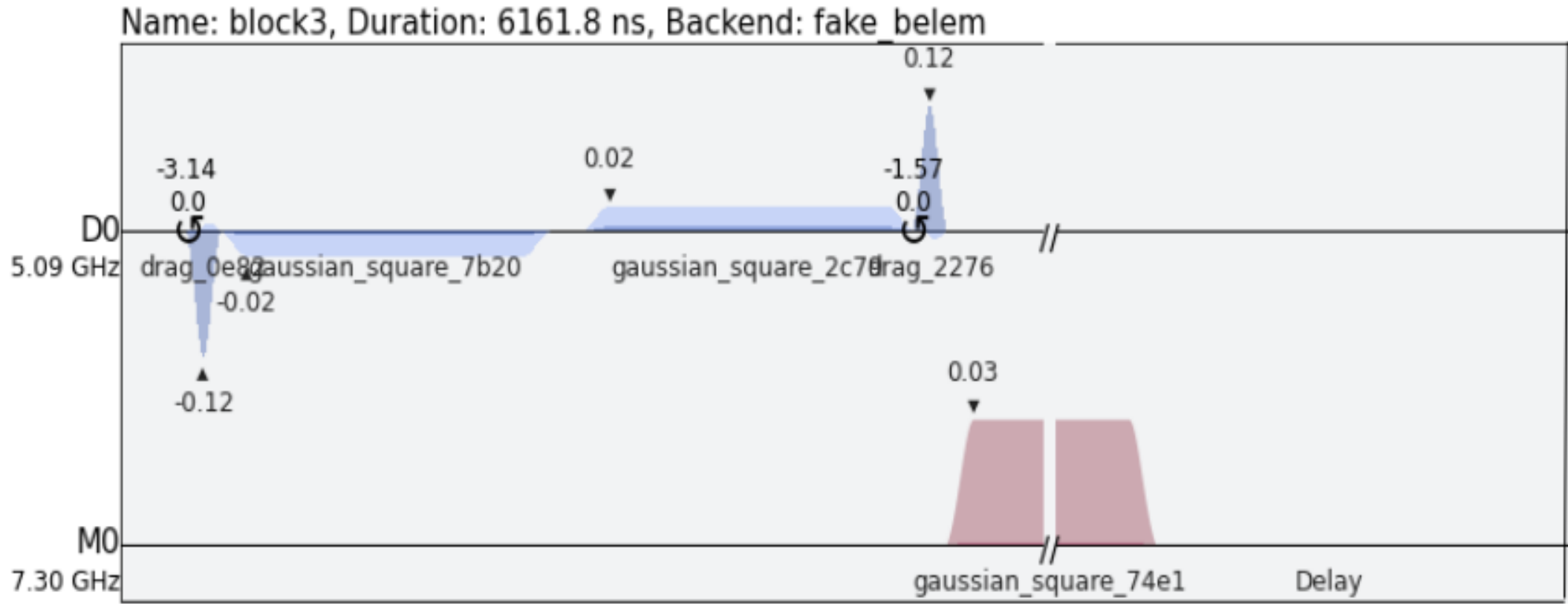


Fig. 2: An example QNN that uses VQC for QML tasks.



Why Variational Quantum Pulse Learning ?

- VQC with more gates has similar performance in terms of accuracy



$$H = \sum_{i=0}^1 (U_i(t) + D_i(t)) \sigma_i^X + \sum_{i=0}^1 2\pi\nu_i(1 - \sigma_i^Z)/2 + \omega_B a_B a_B^\dagger + \sum_{i=0}^1 g_i \sigma_i^X (a_B + a_B^\dagger) \quad (1)$$

$$D_i(t) = \text{Re}(d_i(t)e^{i\omega_{d_i}t})$$

$$U_i(t) = \text{Re}[u_i(t)e^{i(\omega_{d_i} - \omega_{d_j})t}] \quad (2)$$

Model	# of Gates	Accuracy
VQC_base	9	0.62
VQP	9	0.71
VQC*	12	0.68

Optimization Framework

Algorithm 1: Variational Pulse BO Learning

Data: ρ, χ, M, D

// ρ is the amplitude list, χ is the search bound, D consists of x_i and y_i , M is the Gaussian Process Regression model.

$D \leftarrow \text{InitPulses}(\rho, \chi);$

for $i \leftarrow |D|$ **to** N_{total} **do**

 // iterative optimization

$p(y|x, D) \leftarrow \text{FitModel}(M, D);$

 // Acquisition function actively searches for the next optimized amplitudes.

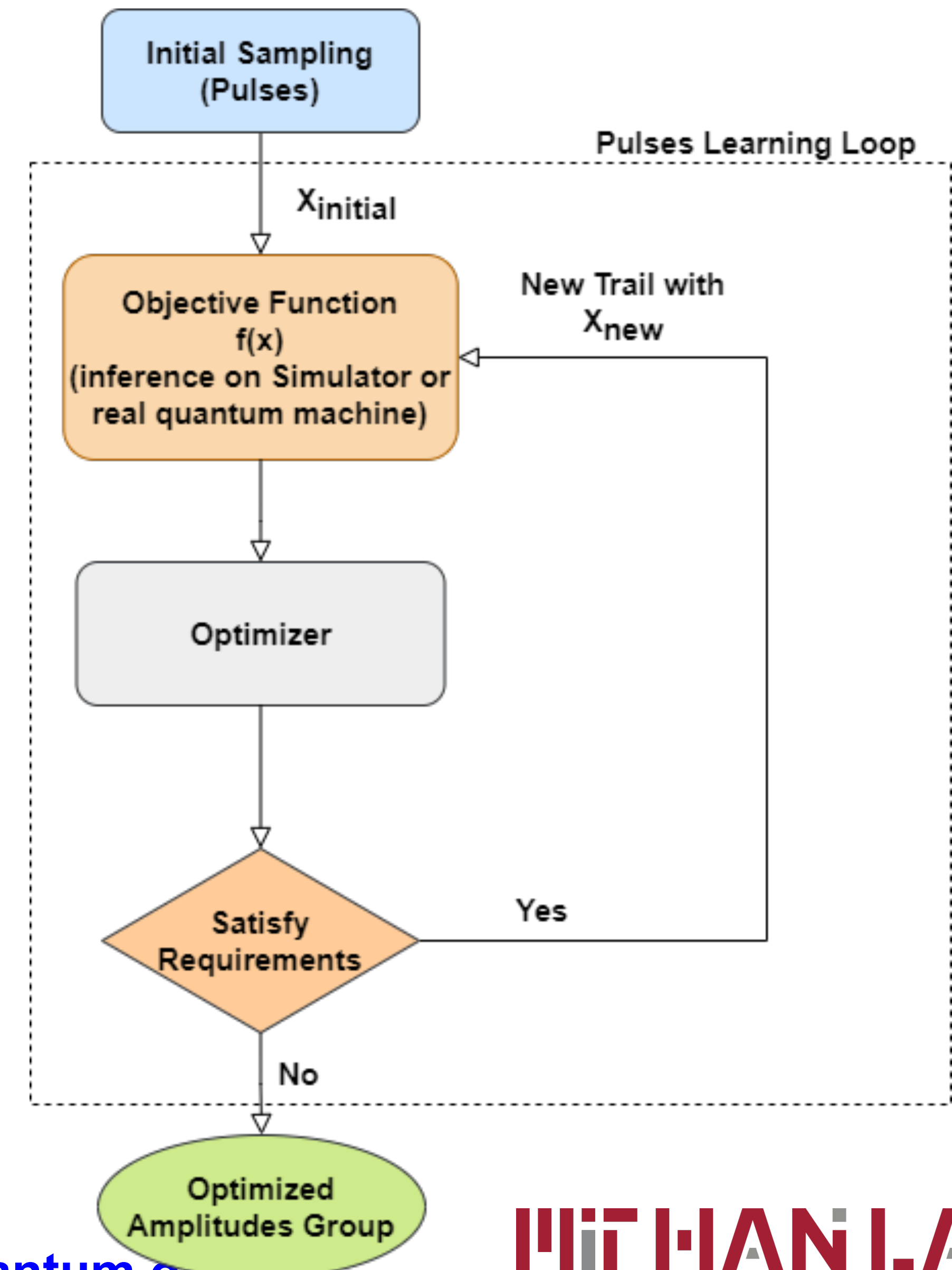
$x_i \leftarrow \text{argmin}_{x \in \chi} S(x, p(y|x, D));$

 // Calculate corresponding error rate by processing in quantum machine.

$y_i \leftarrow f(x_i);$

$D \leftarrow D \cup (x_i, y_i);$

end



Experiment Result

Model	Accuracy	
	Noise simulator (Belem)	ibmq_jakarta
VQC learning 20	0.57	0.58
VQP learning 20	0.6	0.69
VQC learning 100	0.61	0.59
VQP learning 100	0.63	0.64
VQC learning MNIST 20	0.6	0.56
VQP learning MNIST 20	0.66	0.62
VQC learning MNIST 100	0.57	0.62
VQP learning MNIST 100	0.61	0.71

Achieves higher accuracy under same condition

Model	# of Gates	Accuracy
VQC_base	9	0.62
VQP	9	0.71
VQC*	12	0.68

VQC with more gates has similar performance in terms of accuracy

Benefits Observed from VQP

Form of CX gate	Noise simulator (Quito)	Time Duration	
		Noise simulator (Belem)	Noise simulator (Jakarta)
CRX(π) gate	26832.0dt	32016.0dt	26832.0dt
CX gate	25136.0dt	27728.0dt	25136.0dt

Advantage in specific gate

Model	# of Gate	Time Duration	
		ibmq_jakarta	Noise simulator (Belem)
VQP	9	40816.0dt	45168.0dt
VQC*	12	58896.0dt	58768.0dt
VQP_transpiled	11	32368.0dt	32816.0dt
VQC*_transpiled	17	53008.0dt	46192.0dt

Advantage in general circuit

Challenge for Pulse Learning

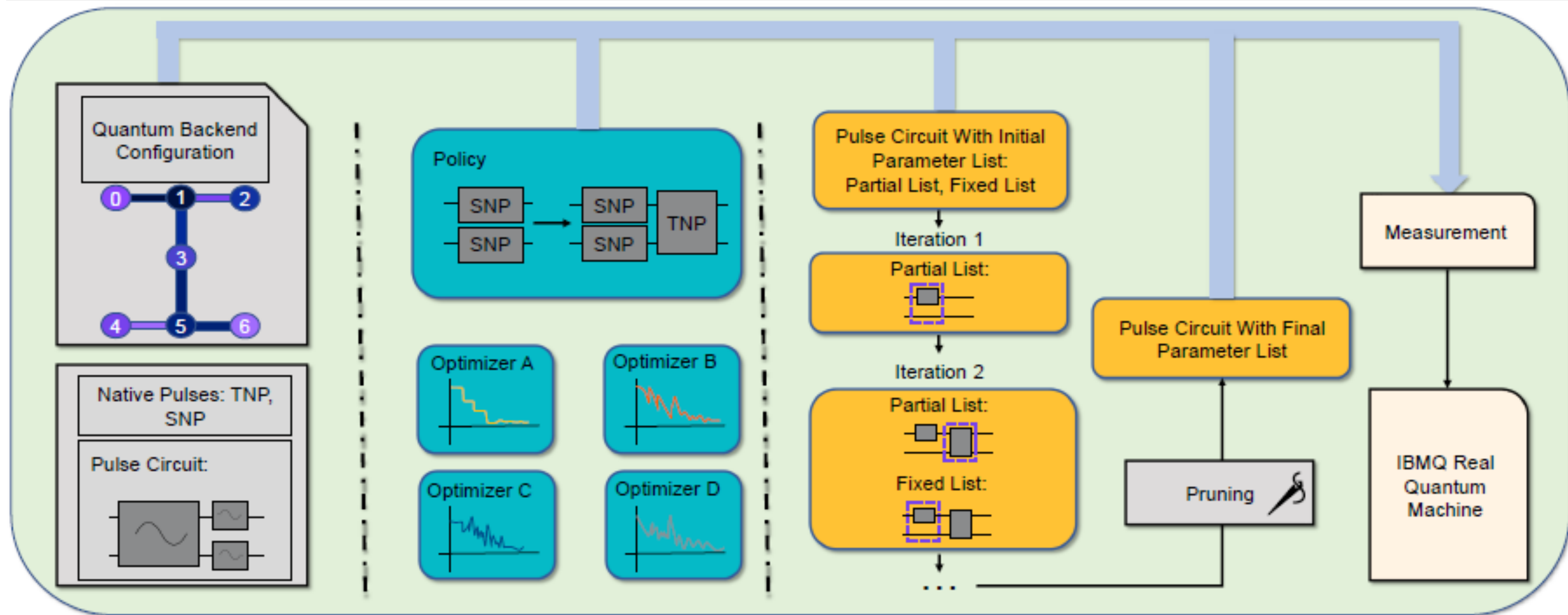
- Non-gradient-based optimizer has randomness when parameter in high dimensional space.
- Qiskit pulse simulator is not efficient, e.g., need around 3 mins to finish a 9-gate circuit.

Model	# of Gates	Accuracy
VQC_base	9	0.62
VQP	9	0.71
VQC*	12	0.68

Model	# of Gates	Accuracy
VQP	9	0.71
VQC with gradient	9	0.73
VQC* with gradient	12	0.77

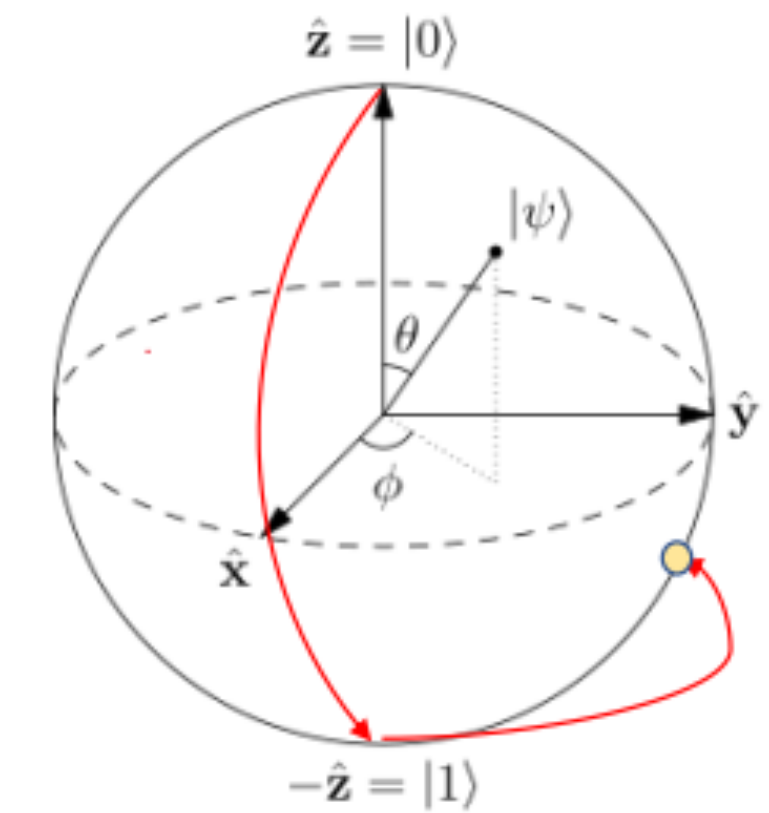
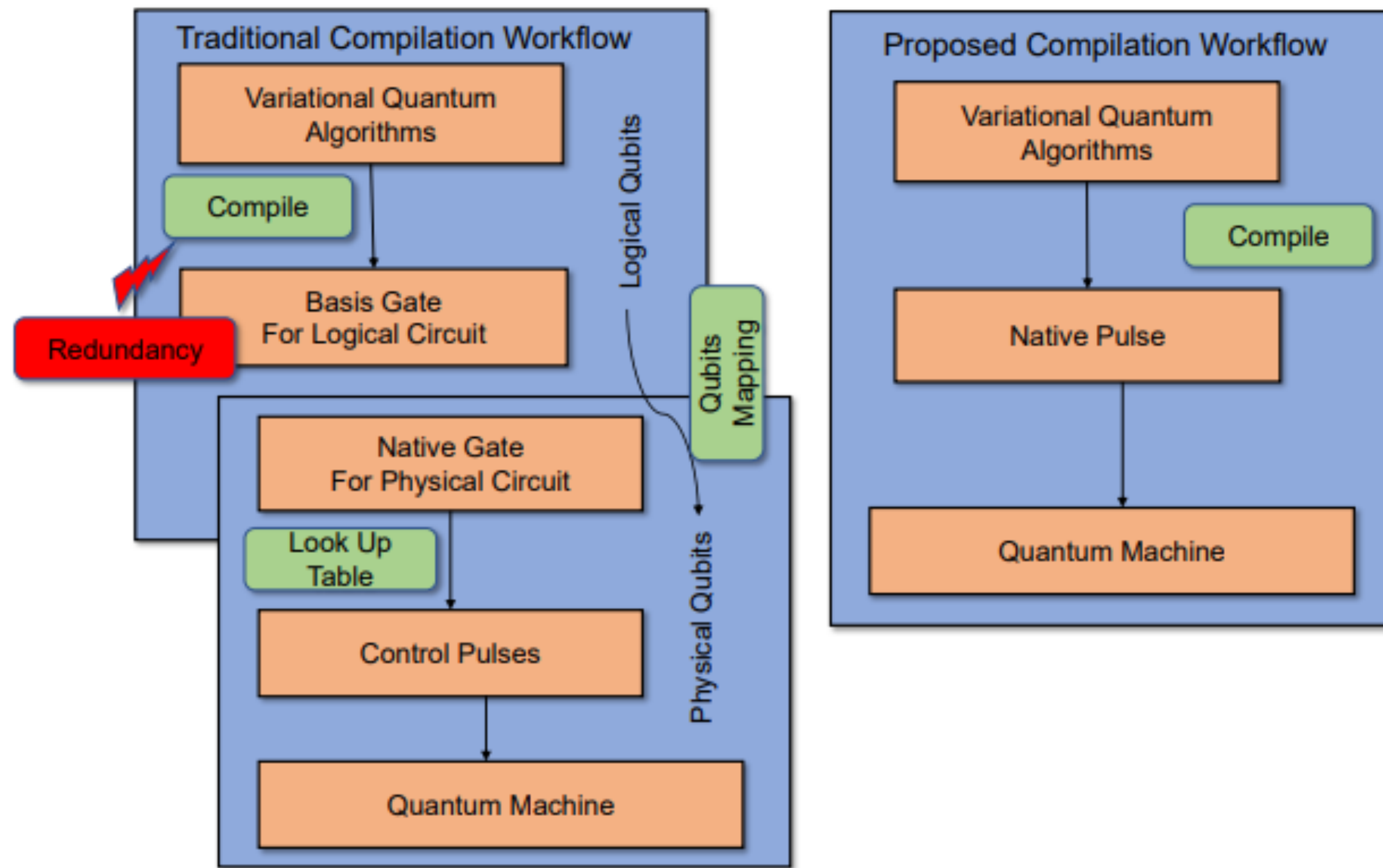
Pulse Ansatz on VQAs

- Can we find a hardware efficient ansatz at the pulse level?
- What is a good pulse ansatz?

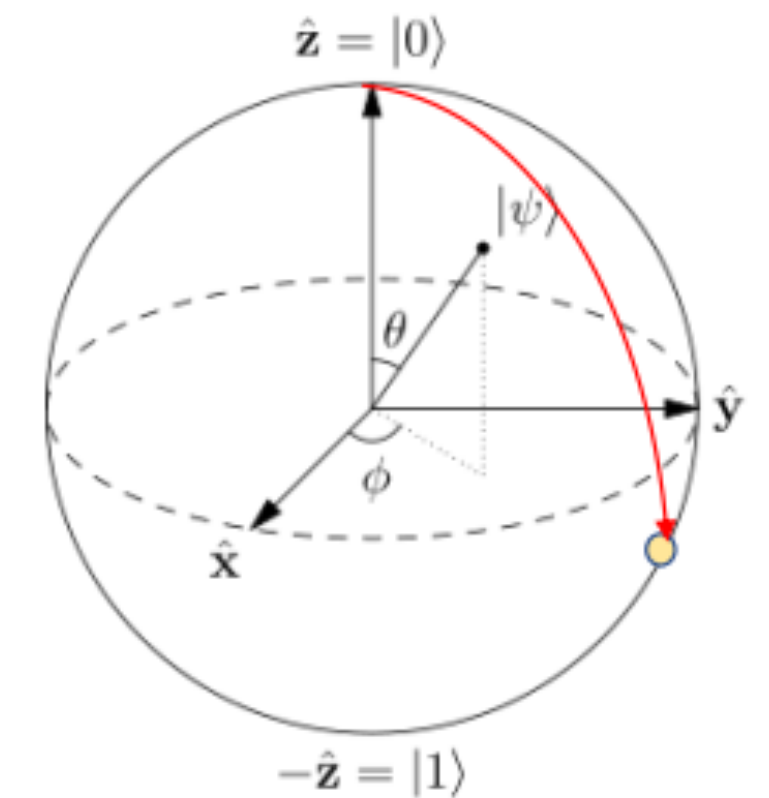


Benefits of Pulse Ansatz

- Source of Advantages:
- Enable flexible and efficient compilation workflow on pulse-level.



a)



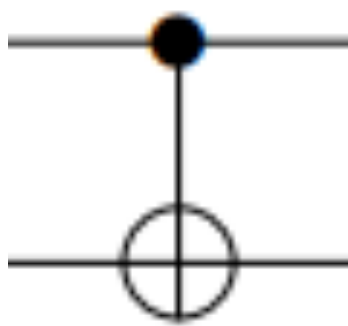
b)

Benefits of Pulse Ansatz

- Source of Advantages:
- Two-qubit pulse is tunable, whereas two-qubit gates have few flexibility.

COMPARISON OF TRAINABILITY FOR DIFFERENT PULSE CIRCUITS AND GATE CIRCUITS ON IBMQ_JAKARTA.

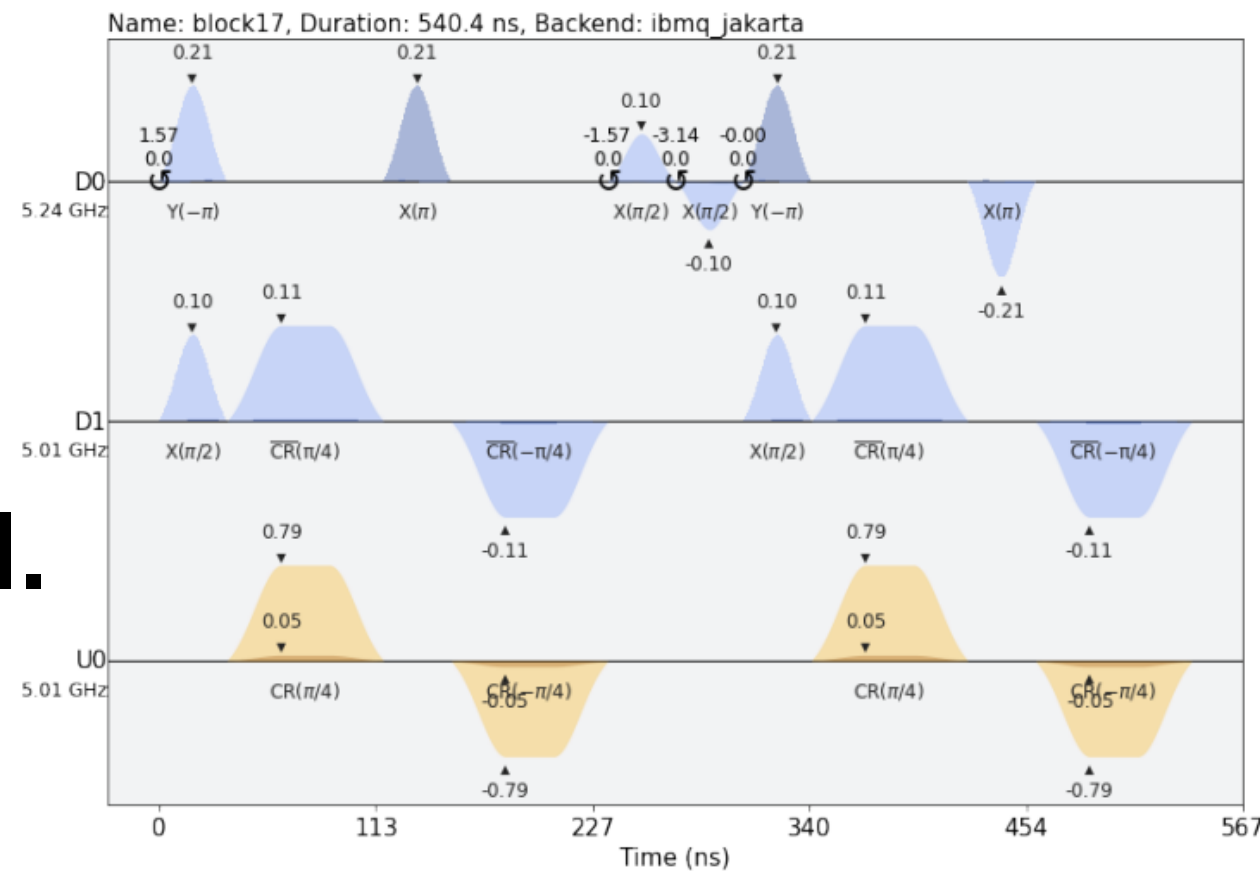
Operations	Circuit Level	Molecule Bond Length	Reference Energy	VQE (H_2) Result	Duration(on ibmq_jakarta)
SNP	Pulse Circuit	0.1Å	2.710H	4.380H	71.1ns
TNP	Pulse Circuit	0.1Å	2.710H	2.927H	163.6ns
SNP	Pulse Circuit	0.75Å	-1.137H	-0.549H	71.1ns
TNP	Pulse Circuit	0.75Å	-1.137H	-1.032H	163.6ns
TNP + SNP	Pulse Circuit	0.75Å	-1.137H	-1.036H	234.7ns
Two Gate Ansatz	Gate Circuit	0.75Å	-1.137H	-0.534H	341.3ns



✗ Nothing can do with two qubits gate

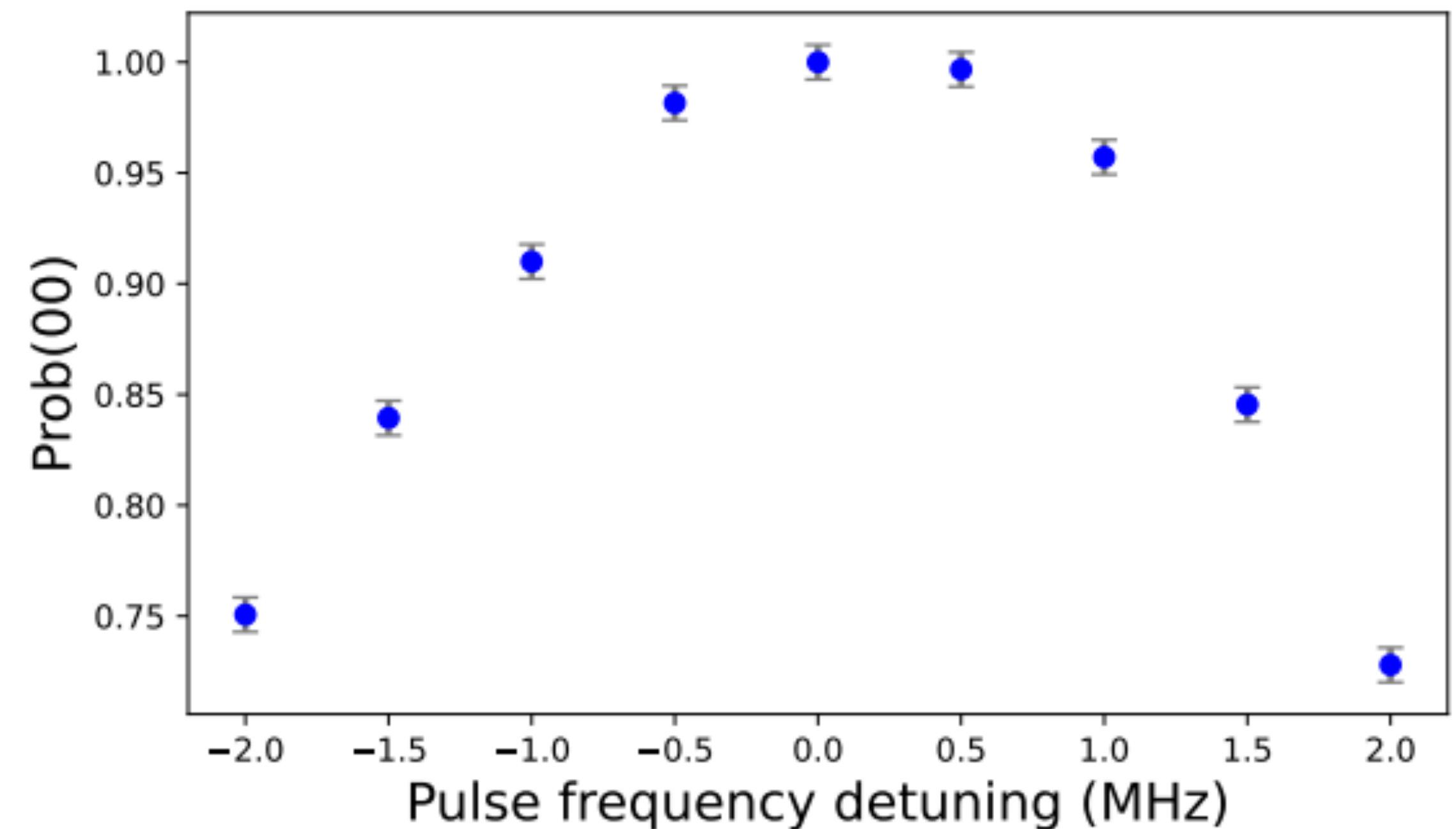
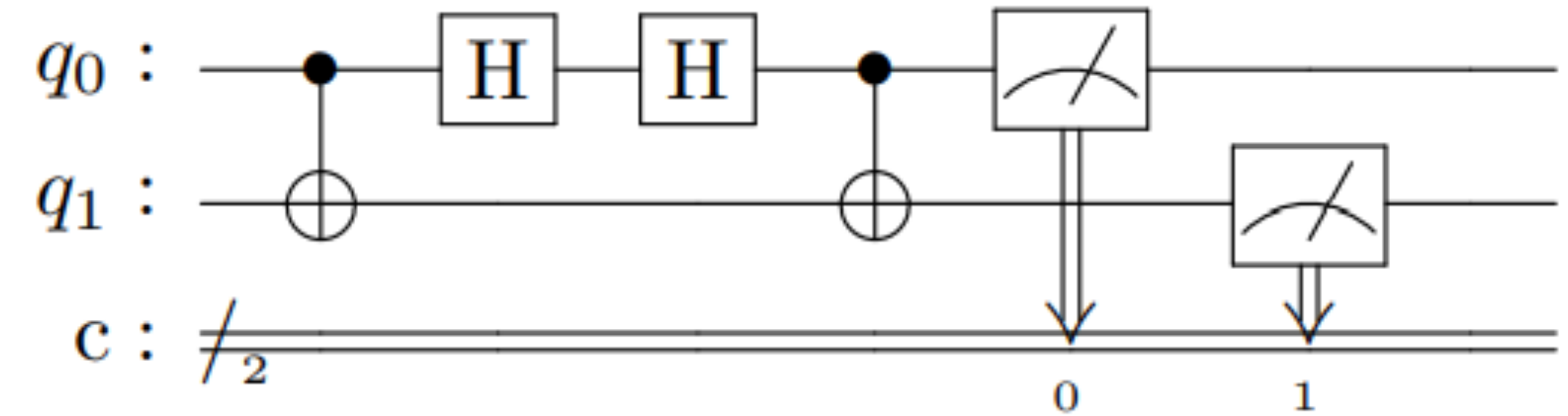


✓ Parameters are tunable on control channel.



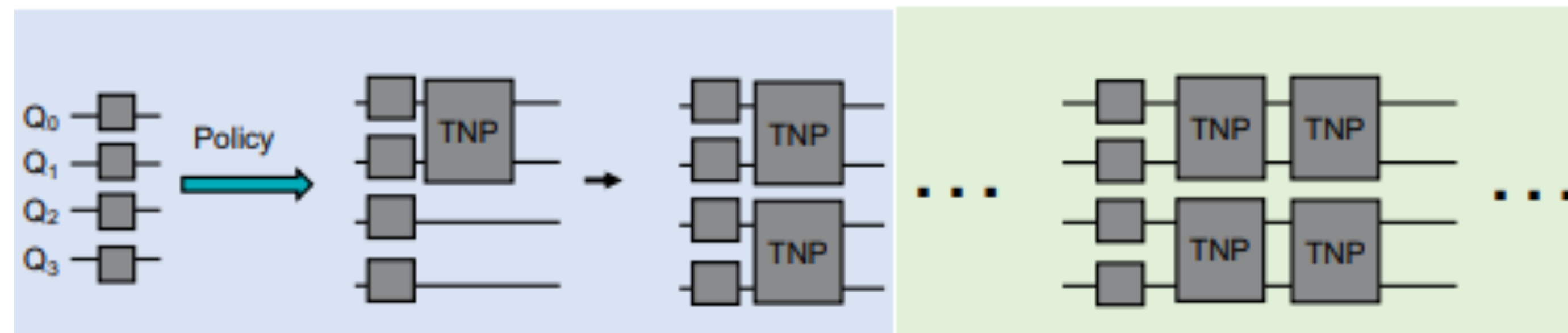
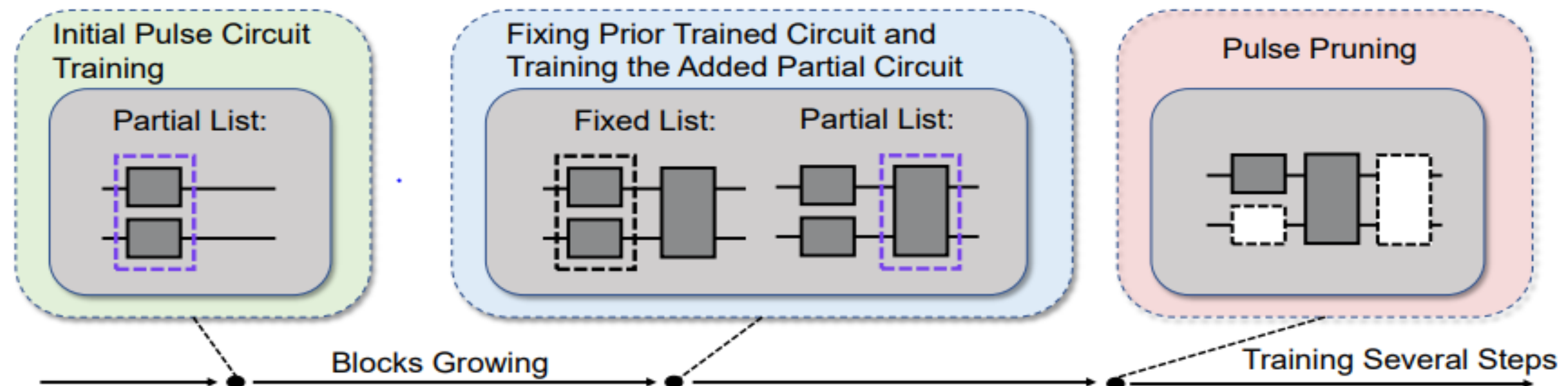
Benefits of Pulse Ansatz

- Source of Advantages:
- Capability to tune frequency on pulse-level



Framework and Evaluation

- Progressive learning fix the problem that non gradient optimizer cannot hold high dimensional parameters, and progressive approaching to target point is also fit the quantum speed limit (QSL) theory.

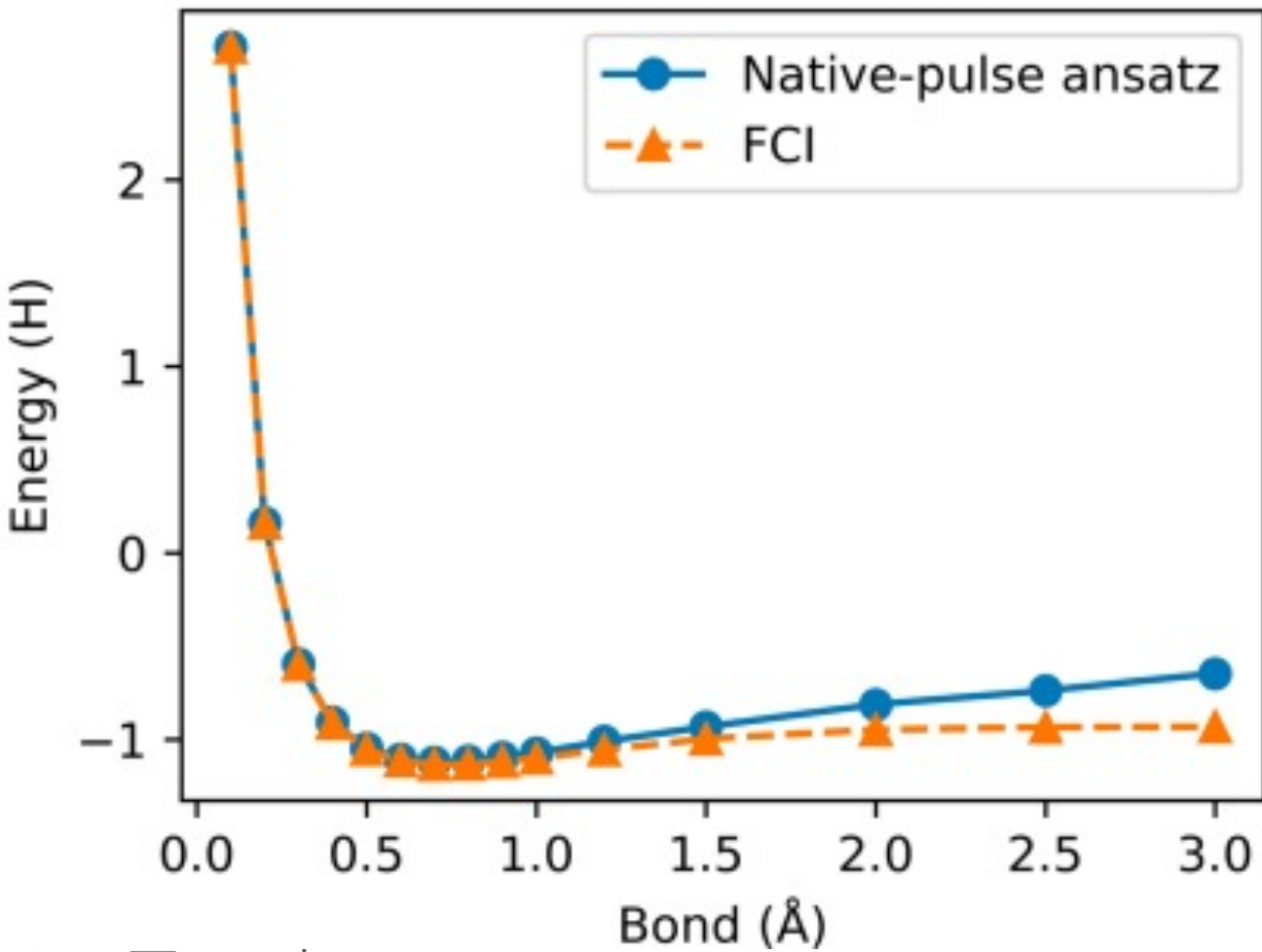


Framework and Evaluation

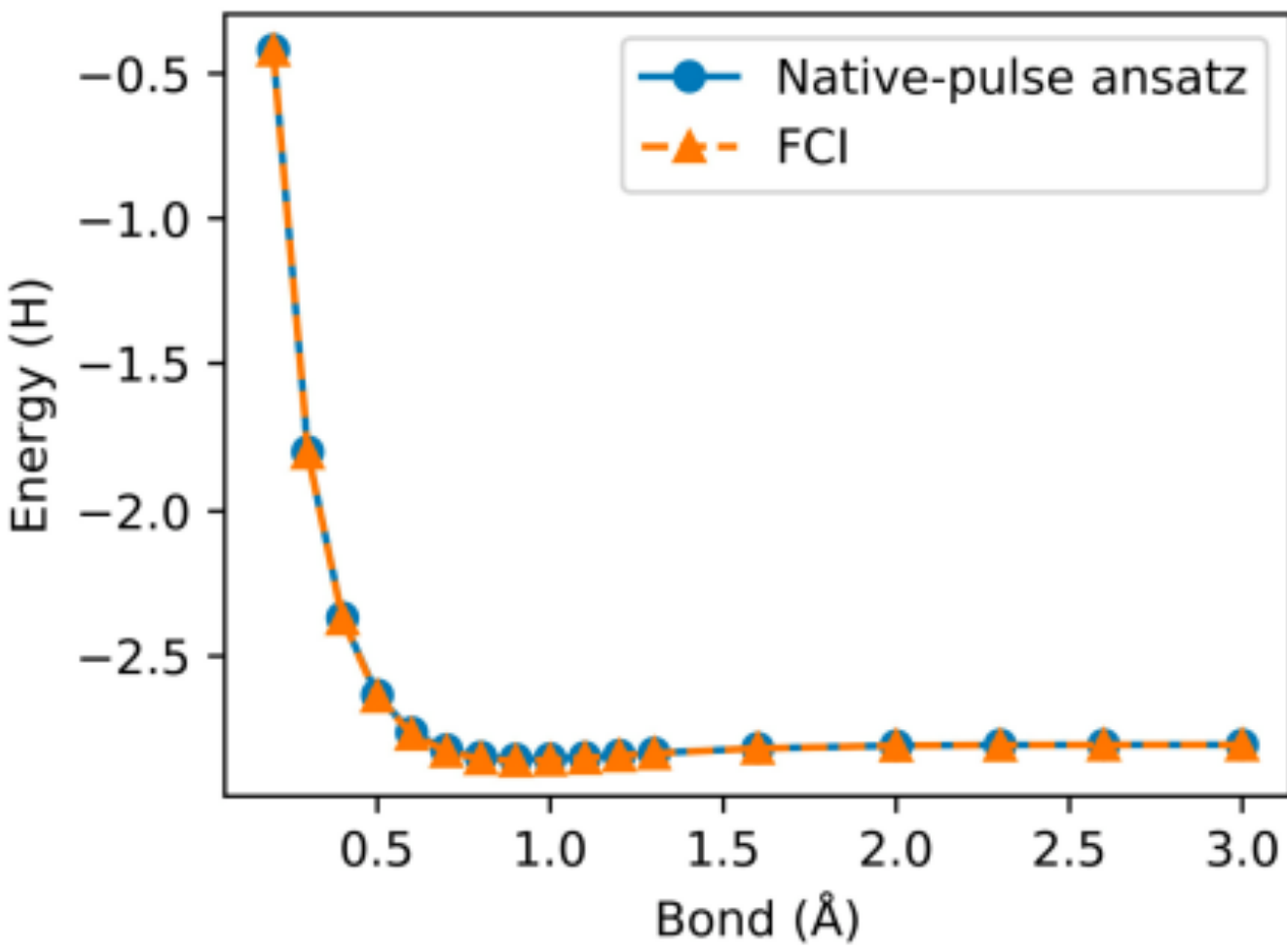
COMPARISON OF DURATION, PULSE COUNTS, AND ESTIMATED ENERGY OF GATE ANSATZES AND THE NATIVE-PULSE ANSATZ GENERATED BY PAN ON NISQ MACHINES.

Model	Ansatz Level	Qubits	Duration	Single-Qubit Pulse Count	Multi-Qubit Pulse Count	Molecule	Energy	Reference Energy
Random Genrated Ansatz	Gate Ansatz	2	682.7ns	16	2	H_2	-0.853	-1.137
RealAmplitude Ansatz [2]	Gate Ansatz	2	376.9ns	12	1	H_2	-0.974	-1.137
QuantumNAS [75]	Gate Ansatz	2	682.7ns	16	2	H_2	-1.033	-1.137
PAN	Pulse Ansatz	2	71.1ns	3	0	H_2	-1.100	-1.137
RealAmplitude Ansatz	Gate Ansatz	2	753.8ns	24	2	$HeH+$	-2.691	-2.863
PAN	Pulse Ansatz	2	199.1ns	1	1	$HeH+$	-2.866	-2.863
QuantumNAS	Gate Ansatz	6	7296.0ns	40	12	LiH	-6.914	-7.882
PAN	Pulse Ansatz	4	199.1ns	4	2	LiH	-7.590	-7.882

Simulation results for H2



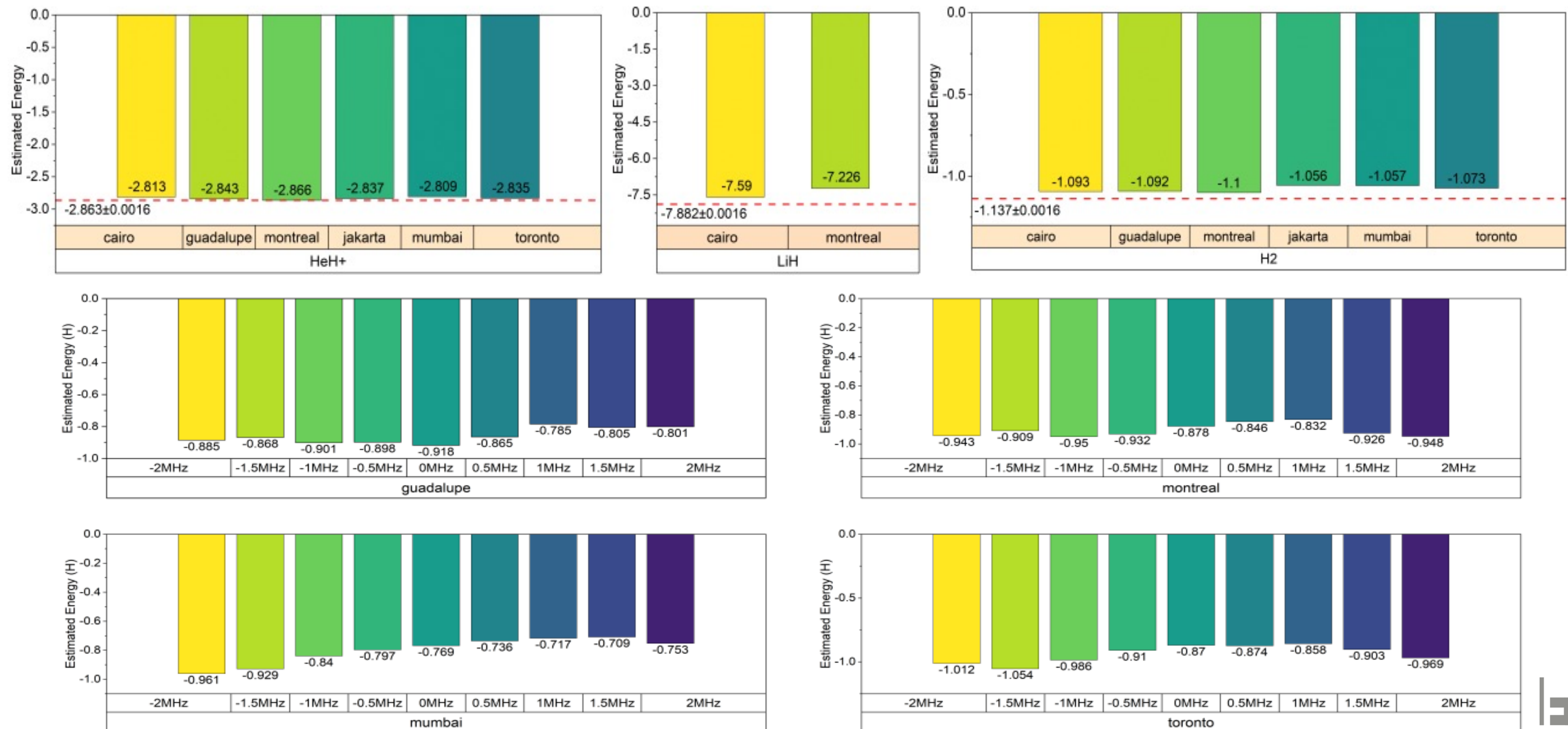
Simulation results for HeH+



97.3% reduction in ansatz duration compared to QuantumNAS.
Reduce duration by **73.6%** compared to RealAmplitude Ansatz while maintaining ansatz performance.

Framework and Evaluation

- **HeH⁺**: average accuracy **99.336%**, with **99.895%** being the highest achievable accuracy. The absolute difference in energy is **0.003H**, close to the requirement of computational chemistry error (**0.0016H**) with only a toy model.

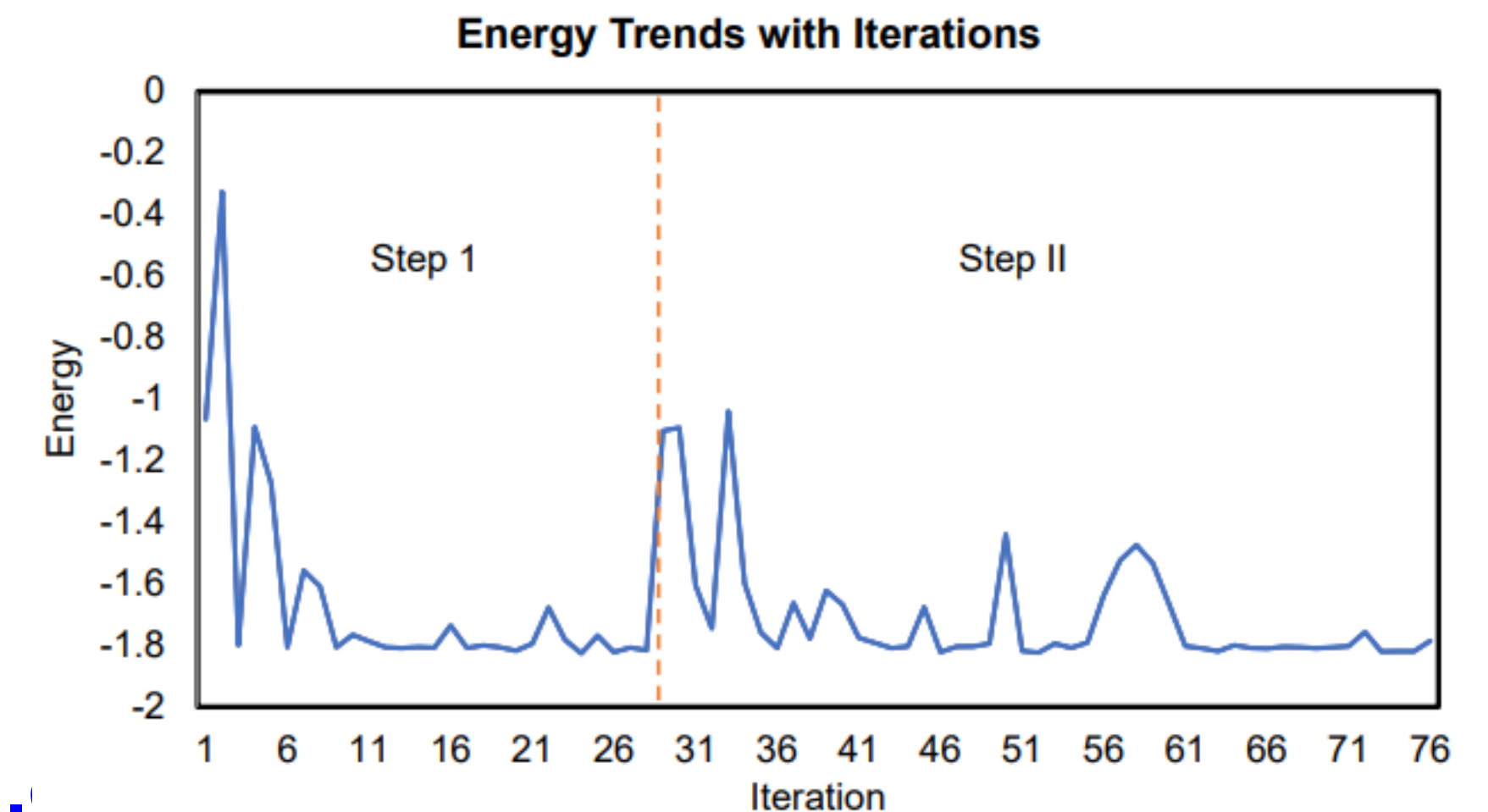


Framework and Evaluation

- Verify the effectiveness of progressive learning scheme.

RESULTS OF ESTIMATED ENERGY FOR MOLECULES IN DIFFERENT STEPS

Model		Cairo	Montreal	Toronto	NISQ machine Avg	Simulator	FCI
H_2	Step I	-1.093 (3.870%)	-1.087 (4.398%)	-1.073 (5.629%)	-1.084 (4.661%)	-1.121 (1.407%)	-1.137
	Step II	-1.107 (2.639%)	-1.110 (2.375%)	-1.073 (5.629%)	-1.097 (3.518%)	-1.123 (1.231%)	-1.137
	Inaccuracy Reduction	31.83%	46.00%	0.000%	24.52%	12.51%	-
HeH^+	Step I	-2.813 (1.746%)	-2.845 (0.663%)	-2.820 (1.485%)	-2.826 (1.292%)	-2.855 (0.279%)	-2.863
	Step II	-2.833 (1.047%)	-2.866 (0.105%)	-2.834 (1.013%)	-2.844 (0.664%)	-2.856 (0.244%)	-2.863
	Inaccuracy Reduction	40.03%	84.16%	31.78%	48.61%	12.54%	-



Hands-On Section

3.2 Quantum Pulse Learning



Summary

Section 1

TorchQuantum Basic Usage

1.1 Quantum Basics

1.2 TQ operations 


1.3 TQ for State Prep 


1.4 TQ for VQE 

1.5 TQ for QNN 

Section 2

Use TorchQuantum on Gate level

2.1 QuantumNAS: Ansatz
Search and Gate Pruning 

2.2 QuantumNAT: Noise
Injection and Quantization 

2.3 QOC: On-Chip Training 

2.4 Transformer for Quantum
Circuit Reliability Prediction

2.5 QNN Compression 

Section 3

Use TorchQuantum on Pulse level

3.1 Quantum Optimal Control 

3.2 Variational Pulse Learning 

Thank you for listening!



qmlsys.mit.edu



<https://github.com/mit-han-lab/torchquantum>