TorchQuantum: A Fast Library for Quantum Computing in PyTorch

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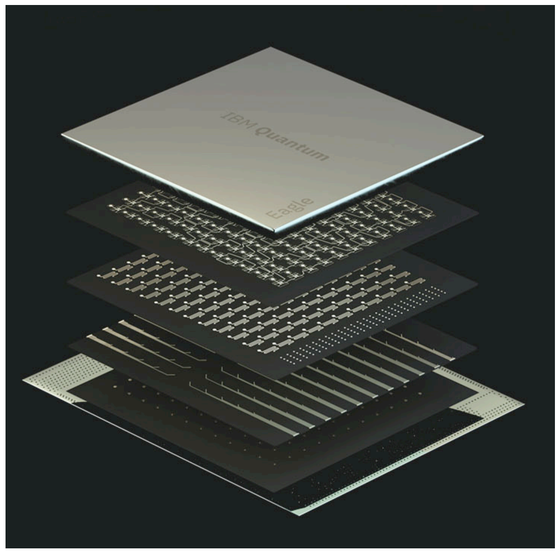
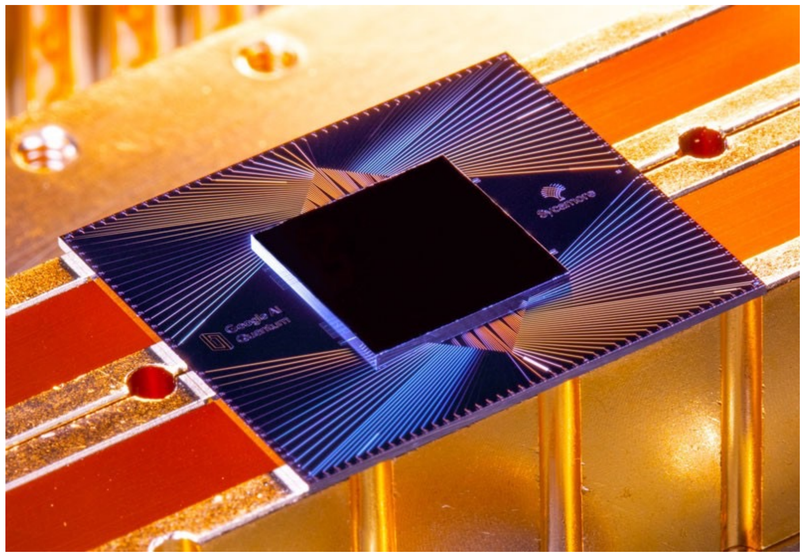
[1]MIT, [2]Notre Dame, [3]Purdue, [4]Yale, [5]GMU, [6]UChicago

Quantum Computing

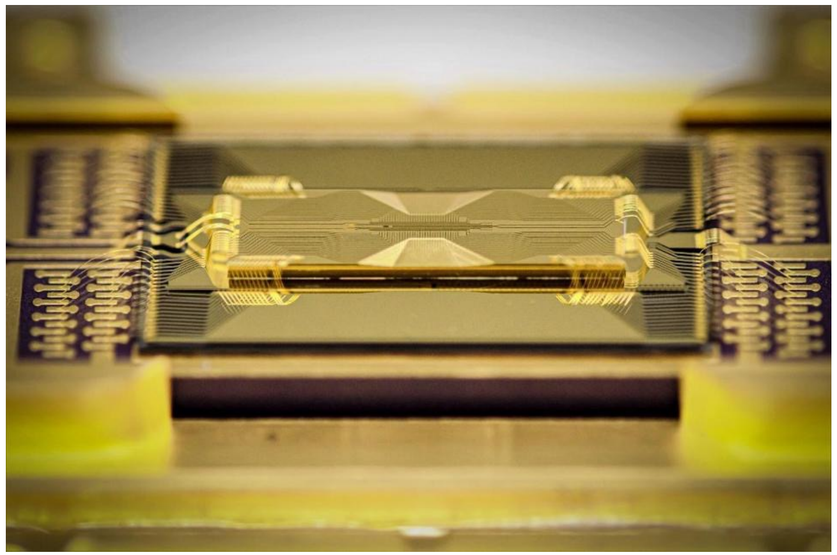
- Fast progress of quantum devices
- Different technologies
  - Superconducting, trapped ion, neutral atom, photonics, etc.



IBM
433 Qubit



Google
53 Qubits



IonQ
32+ Qubits

Torch Quantum

Materials at: https://torchquantum.org

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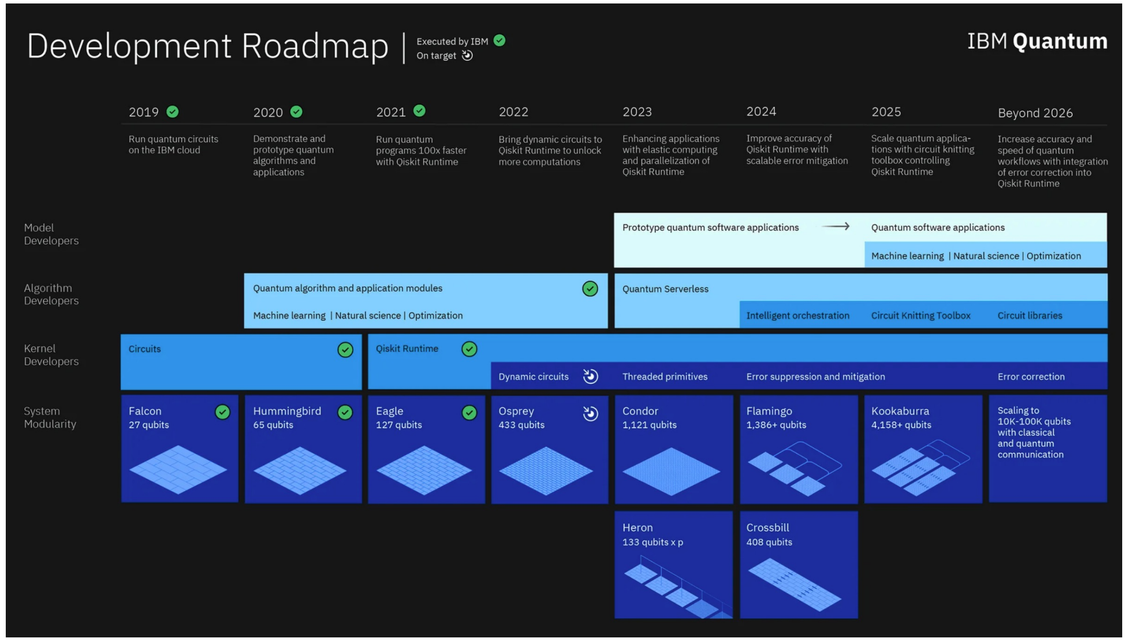
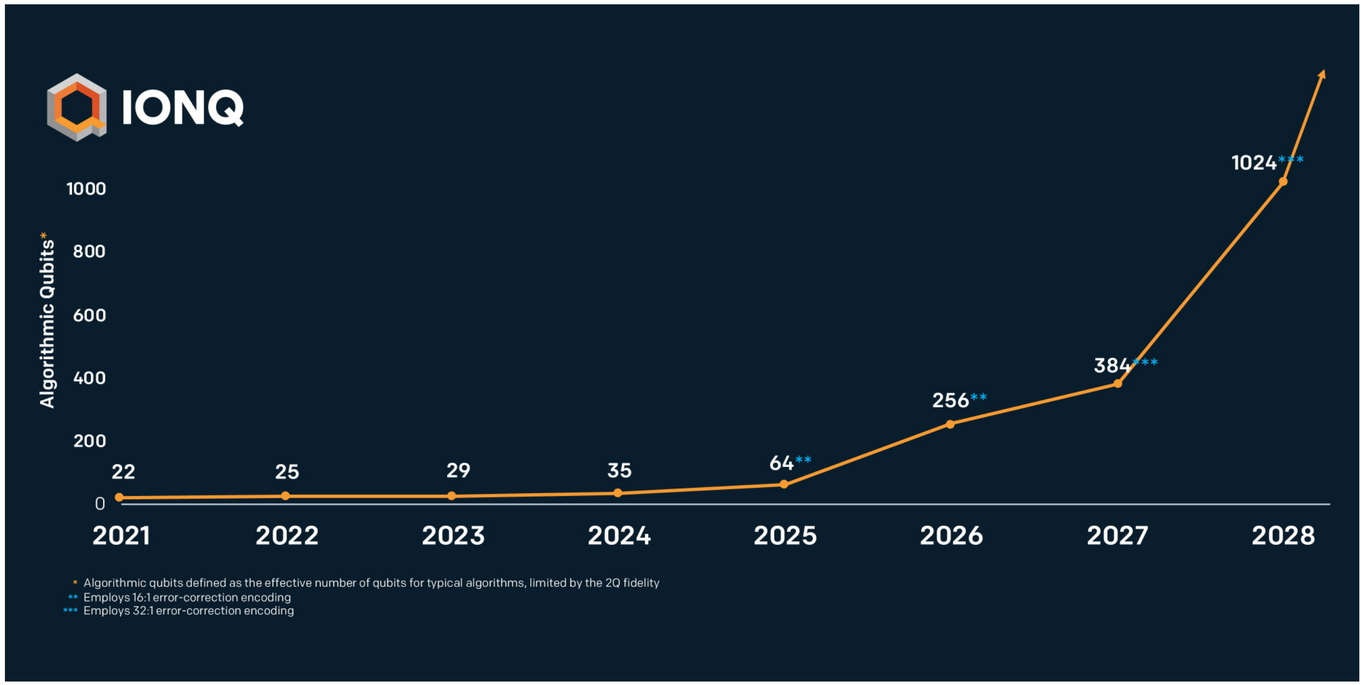
Quantum Computing

- 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

Torch Quantum

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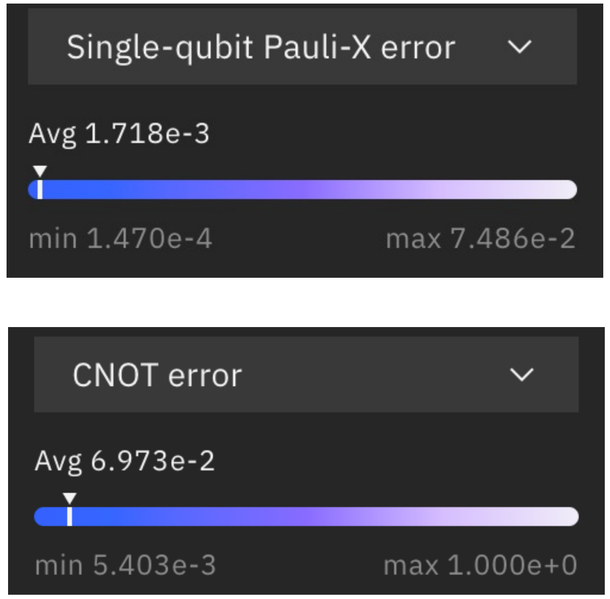
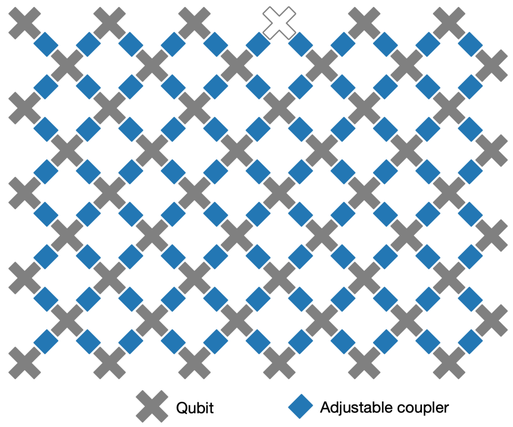
Quantum Computing in NISQ Era

- 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



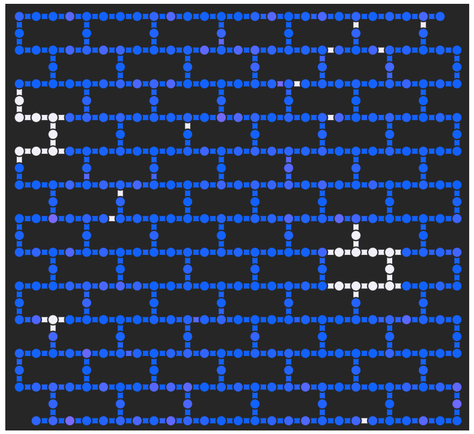
IBMQ Gate Error Rate

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



Google Sycamore 53Q

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

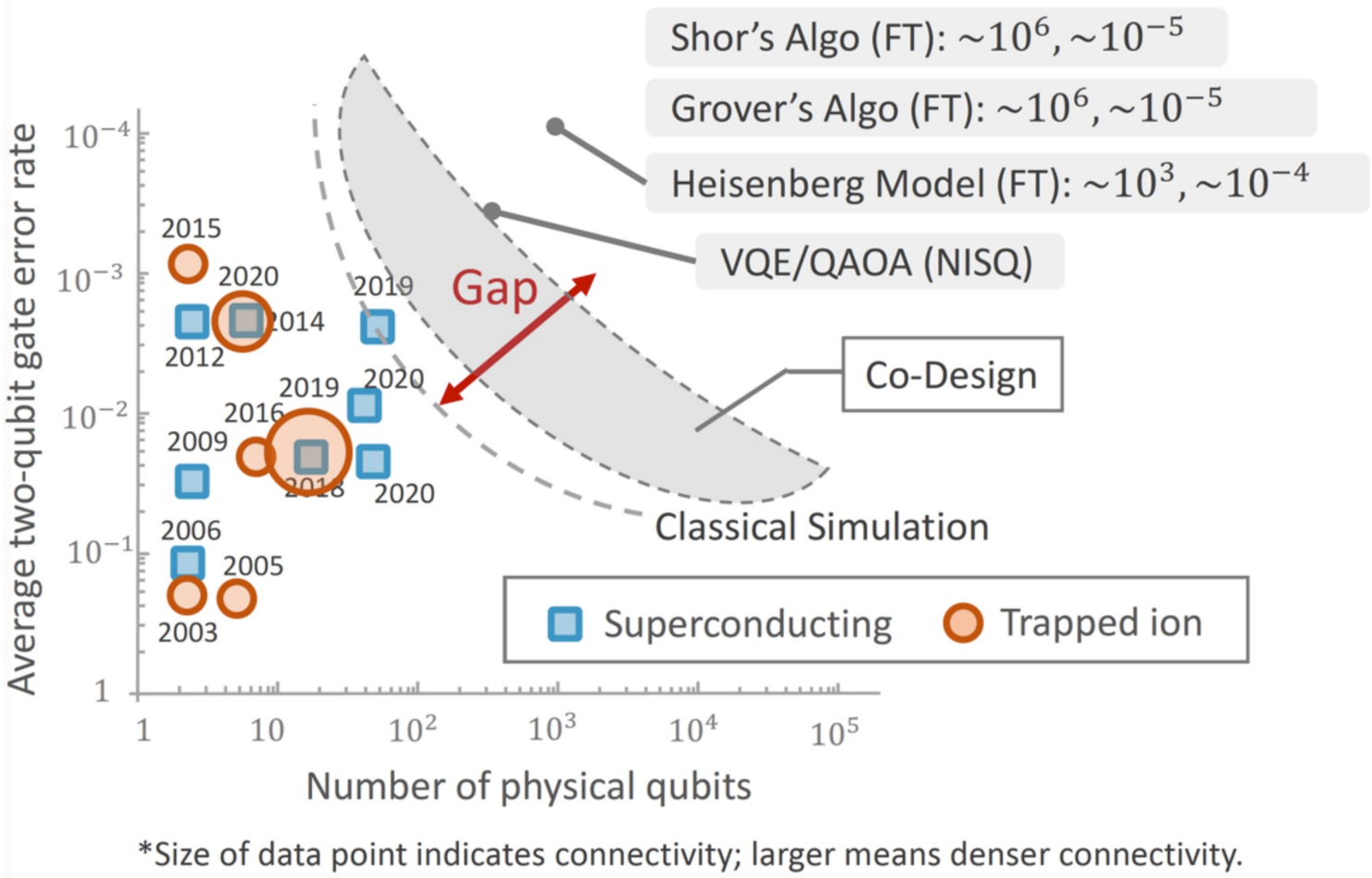


IBM Washington 433Q

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**



*Size of data point indicates connectivity; larger means denser connectivity.

Fred Chong, https://indico.fnal.gov/event/47147/attachments/138920/174186/Chong-JTFI-2021.pdf18.pdf

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Good Infrastructure is Critical

- To enable ML-assisted hardware-aware quantum algorithm design
- Need a simulation framework on classical computer
  - Fast speed
  - Convenience: PyTorch native
  - Portable between different frameworks with common Quantum IR
  - 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
  - **Density matrix and state vector** simulators
  - **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, OpenQASM
  - And so on…

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TorchQuantum Tutorial Outline

Section 1

Quantum Basics and TorchQuantum Usage

1.1 Introduction to Quantum Computing (Prof. Yongshan Ding)

1.2 TorchQuantum API and examples (Hanrui Wang)

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2.3 Various VQA Gradient Estimation Methods (Dantong Li)

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3.1 Intro to Pulse Level Quantum Control (Zhiding Liang)

3.2 Variational Pulse Learning & Optimal Control (Jinglei Cheng)

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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)`
  - Three 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)`
  - Three 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.QuantumDevice stores the statevectors
    - `q_dev = tq.QuantumDevice(n_wires=5)`
  - Three ways of applying quantum gates: method 3:
    - `q_dev.h()`
    - `q_dev.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),
```

TQ for Density Matrix simulation

- Performing matrix-vector multiplication between the gate matrix and statevector
  - The tq.DensityMatrix class stores the denstiy matrix
    - `q_mat = tq.DesityMatrix(n_wires=5)`
  - Applying quantum gates
    - `q_mat.h()`
    - `q_mat.rx(wires=1, params=0.2 * np.pi)`

```python
class DensityMatrix(nn.Module):

    def __init__(self,n_wires: int,
                 bsz: int = 1):
        """Init function for DensityMatrix class(Density Operator)
        Args:
            n_wires (int): how many qubits for the densityMatrix.
        """
        super().__init__()

        self.n_wires=n_wires
        """
        For example, when n_wires=3
        matrix[001110] denotes the index of |001><110|=|index1><index2|
        Set Initial value the density matrix of the pure state |00...00>
        """
        _matrix = torch.zeros(2 ** (2*self.n_wires), dtype=C_DTYPE)
        _matrix[0] = 1 + 0j
        _matrix = torch.reshape(_matrix, [2]*(2*self.n_wires))
        self.register_buffer('matrix', _matrix)


        repeat_times = [bsz] + [1] * len(self.matrix.shape)
        self._matrix = self.matrix.repeat(*repeat_times)
        self.register_buffer('matrix', self._matrix)

        """
        Whether or not calculate by states
        """
        self._calc_by_states=True
```

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Dynamic computation graph

- Performing matrix-vector multiplication between the gate matrix and statevector
  - The tq.QuantumDevice class stores the statevectors
    - `q_dev = tq.QuantumDevice(n_wires=5)`
    - `q_dev.h(wires=1)`
    - `print(q_dev)`
    - `q_dev.sx(wires=3)`
    - `print(q_dev)`

Batch Mode Tensorized Processing

- Performing matrix-vector multiplication between the gate matrix and statevector
  - The tq.QuantumDevice class stores the statevectors
    - `q_dev = tq.QuantumDevice(n_wires=5, bsz=64)`

GPU Support

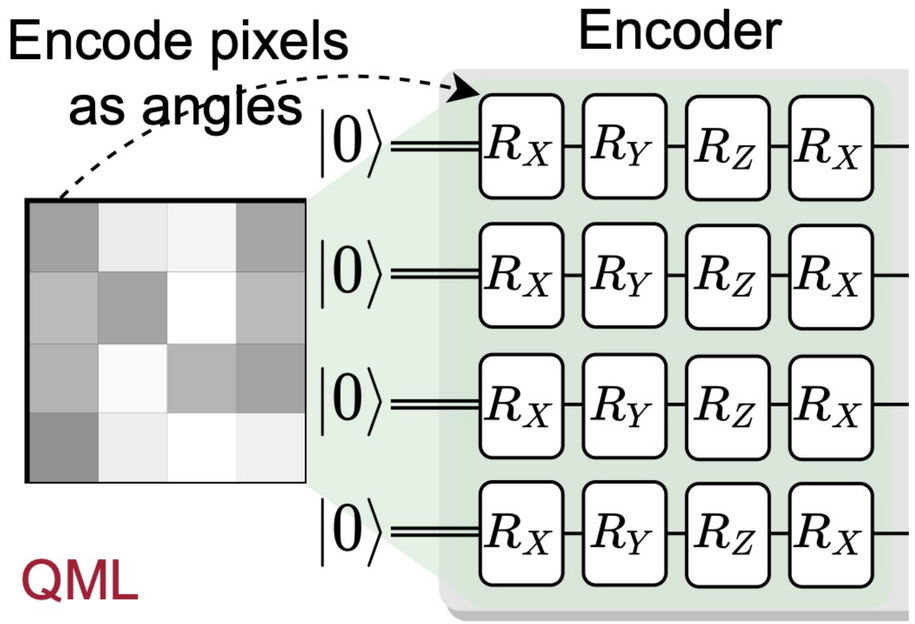
- Performing matrix-vector multiplication between the gate matrix and statevector
  - The tq.QuantumDevice class stores the statevectors
    - `q_dev = tq.QuantumDevice(n_wires=5, bsz=64)`
    - `q_dev.to(torch.device('cuda'))`
  - Leverage the fast GPU support

Automatic Gradient Computation

- Performing matrix-vector multiplication between the gate matrix and statevector
  - The tq.QuantumDevice class stores the statevectors
    - `q_dev = tq.QuantumDevice(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



Measurement

- Measure the state on the default Z basis
  - `tq.measure(qdev, n_shots=1024)`

- Obtain the expval on a observable by stochastic sampling (doable on simulator and real quantum hardware)
  - `expval_sampling = tq.expval_joint_sampling(qdev, 'ZX', n_shots=1024)`

- Obtain the expval on a observable by analytical computation (only doable on classical simulator)
  - `expval = tq.expval_joint_analytical(qdev, 'ZX')`

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)
```

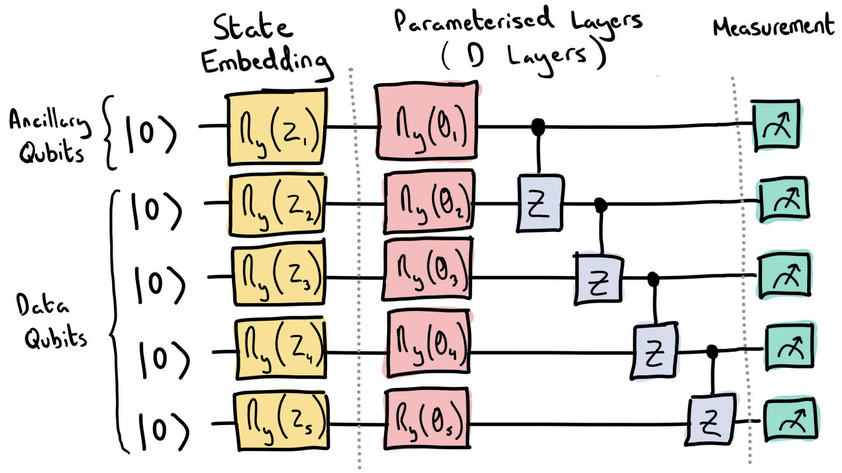
Conversion tq model to other frameworks

- 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')`
- Convert to OpenQASM
  - `qdev = tq.QuantumDevice(n_wires=2, bsz=5, device="cpu", record_op=True)`
  - `from torchquantum.plugins import op_history2qasm`
  - `print(op_history2qasm(qdev.n_wires, qdev.op_history))`

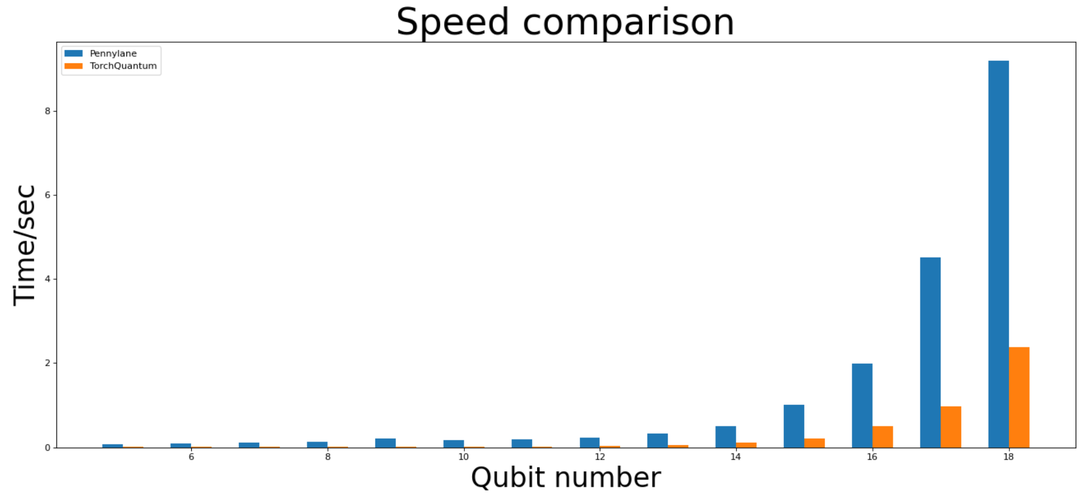
Easy Deployment on Real Quantum Machines

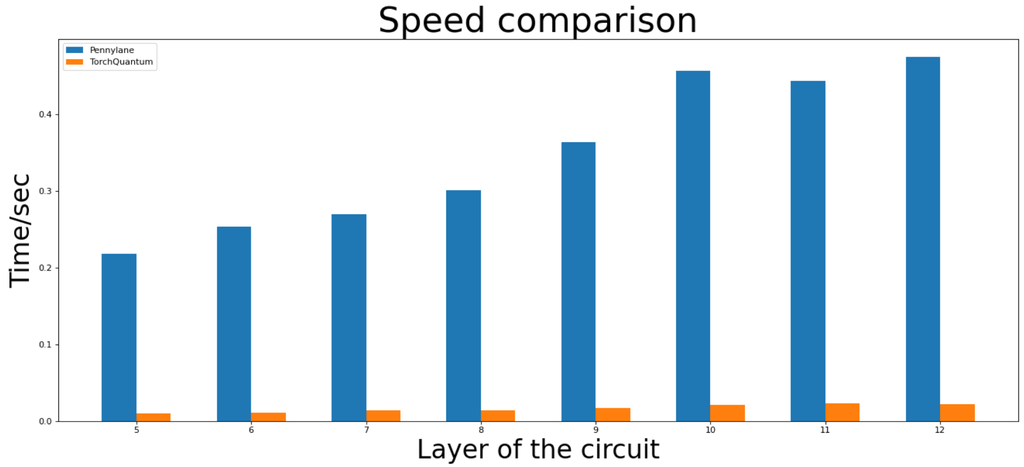
- Convert the tq.QuantumModule to other frameworks such as Qiskit
- `from torchquantum.plugins.qiskit_plugin import tq2qiskit`
- `from torchquantum.plugins.qiskit_processor import QiskitProcessor`
- `processor = QiskitProcessor(use_real_qc=False, max_jobs=1)`
- `circ = tq2qiskit(q_dev, model)`
- `circ.measure_all()`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

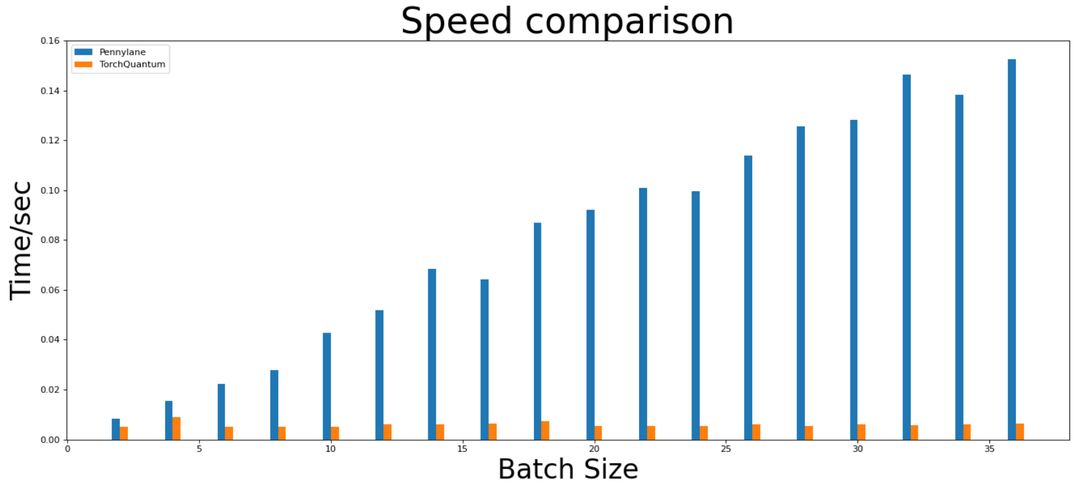
Compare the Speed of TQ and Pennylane



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







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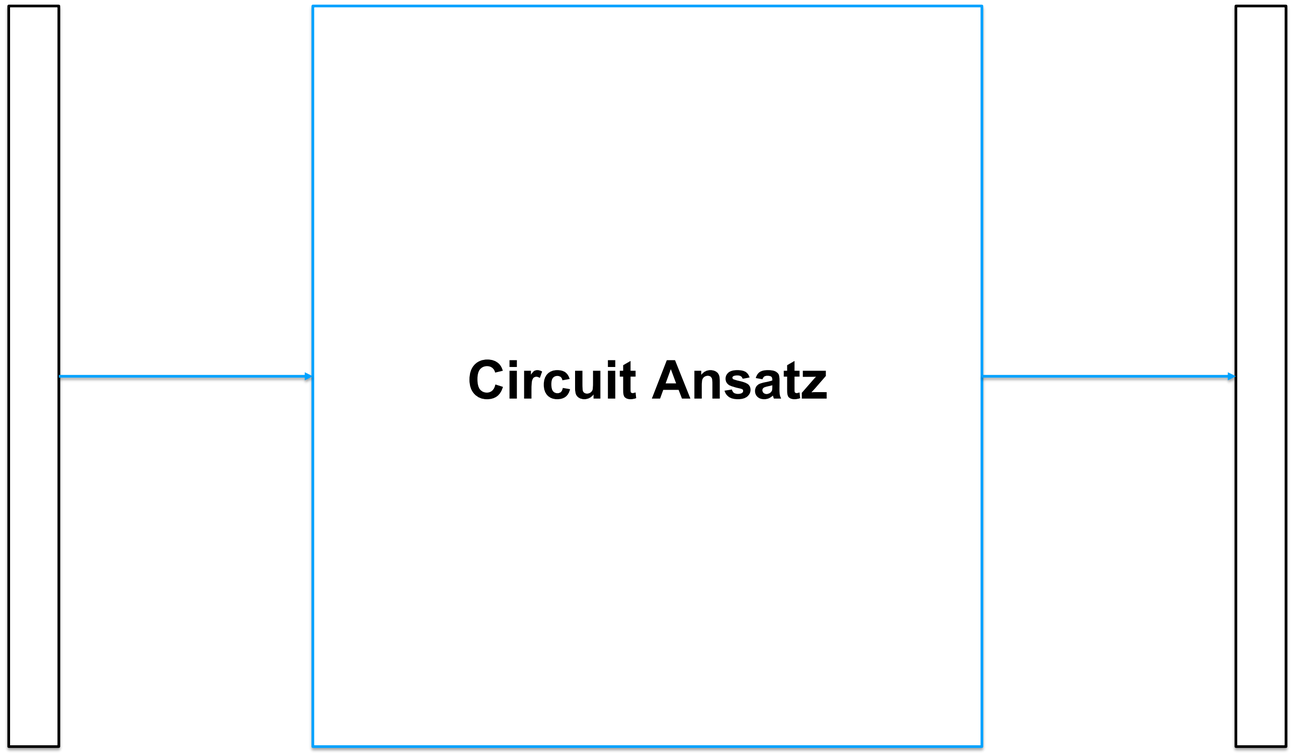
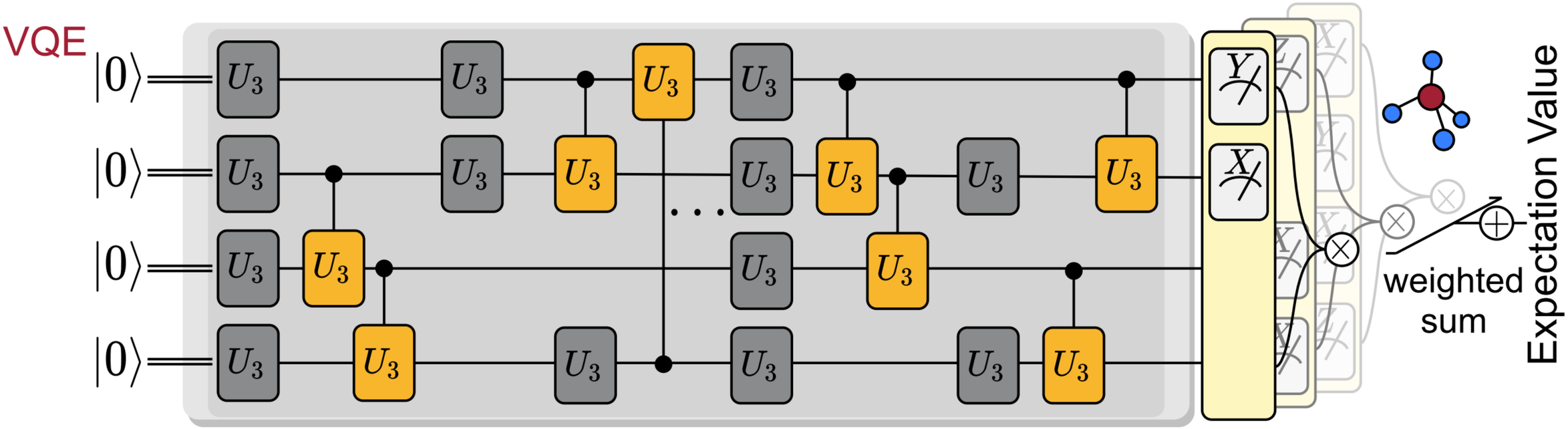
State Preparation with Parameterized Circuit

- Use parameterized circuit to prepare initial quantum states



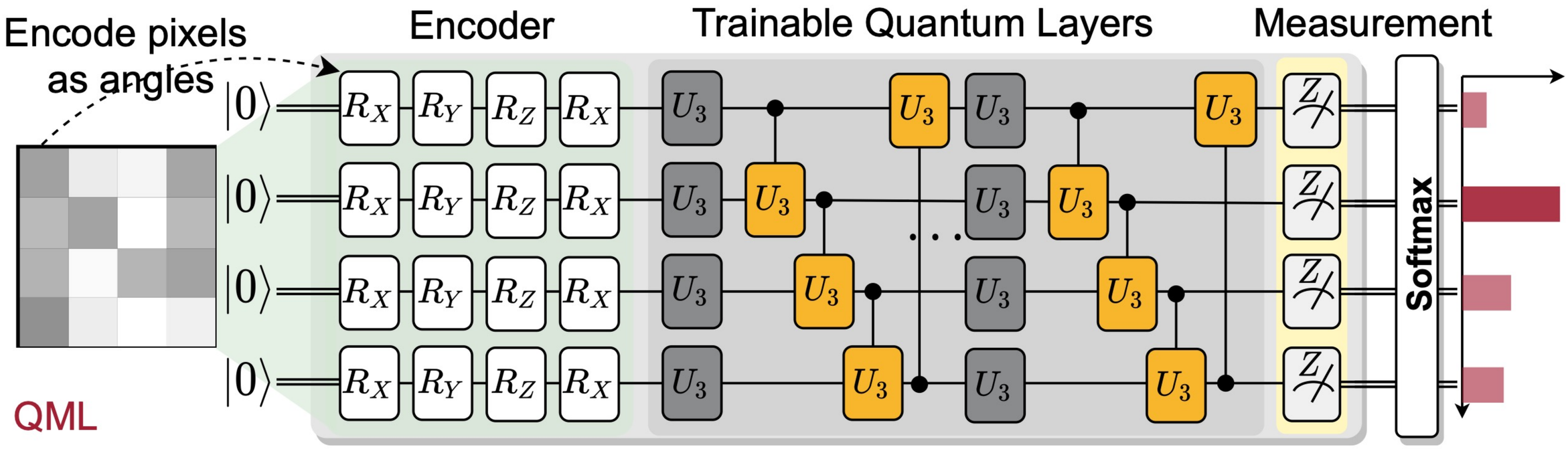
Variational Quantum Eigensolver

- VQE: Finds the ground state energy of molecule Hamiltonian

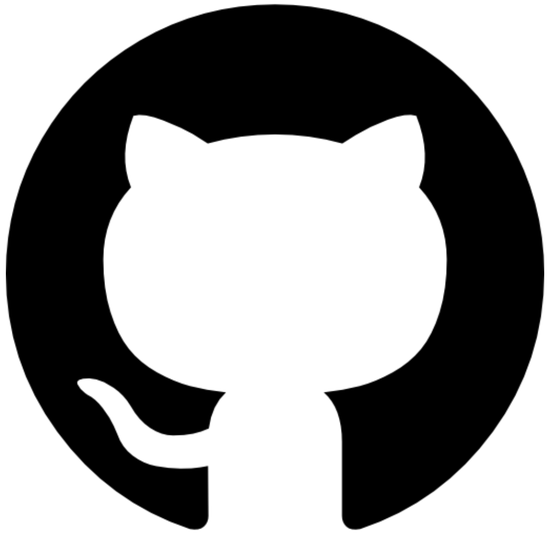


Quantum Neural Networks for MNIST Classification

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



Hands-On Section
2.1 TQ Basic Operations and Examples



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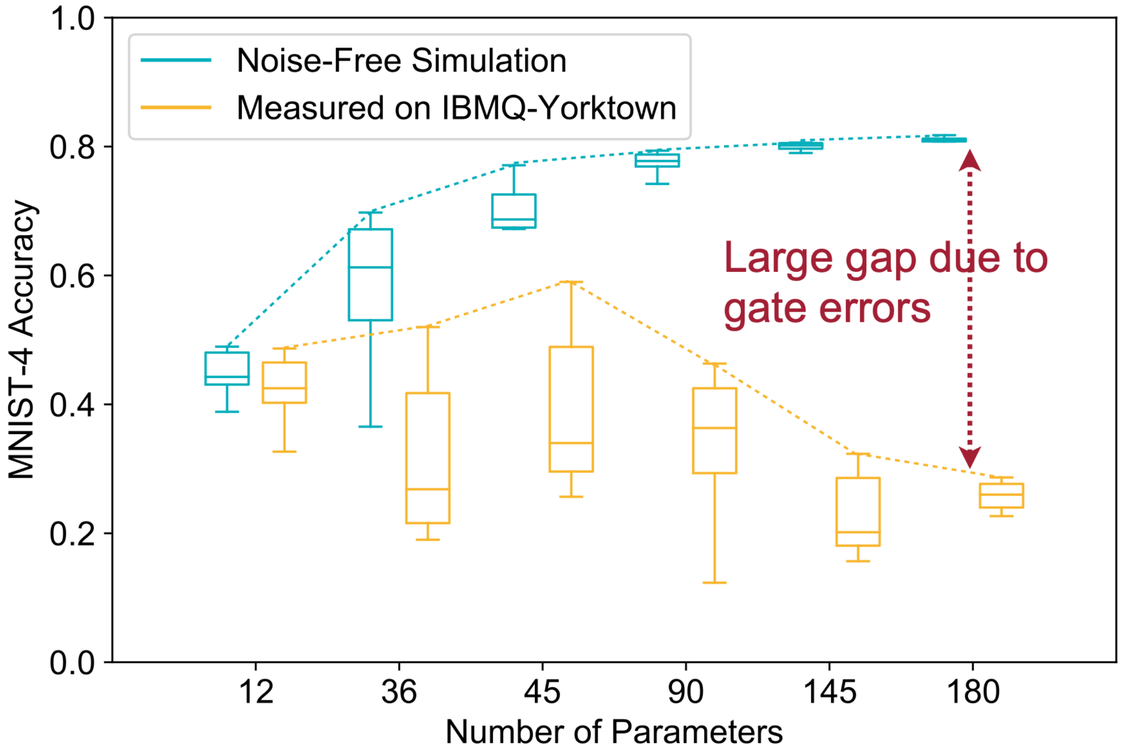
Challenges of PQC — Noise

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



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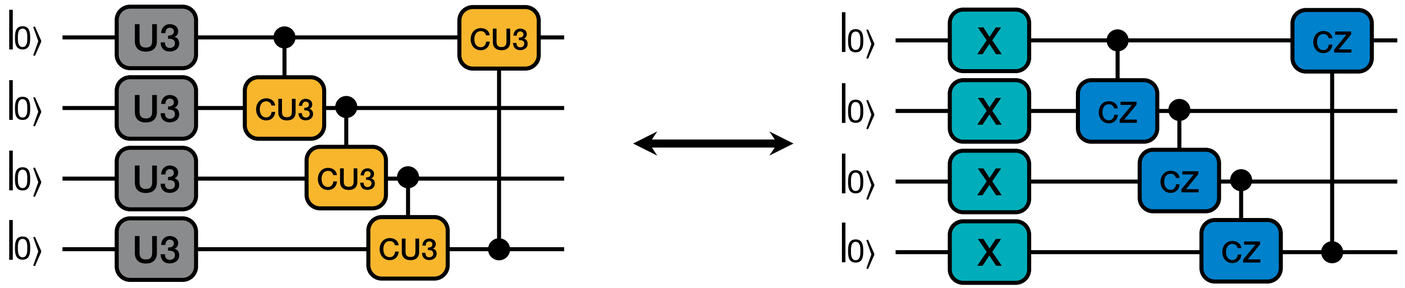
Challenges of PQC — Large Design Space

- Large design space for circuit architecture
  - Type of gates



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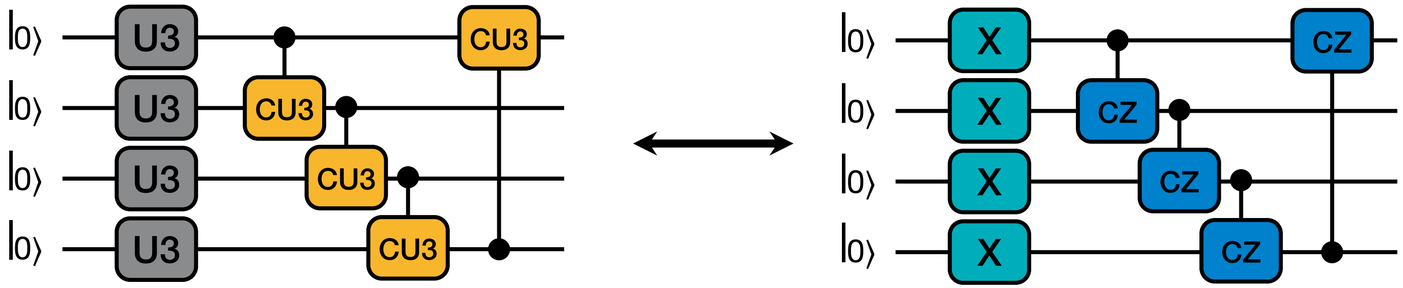

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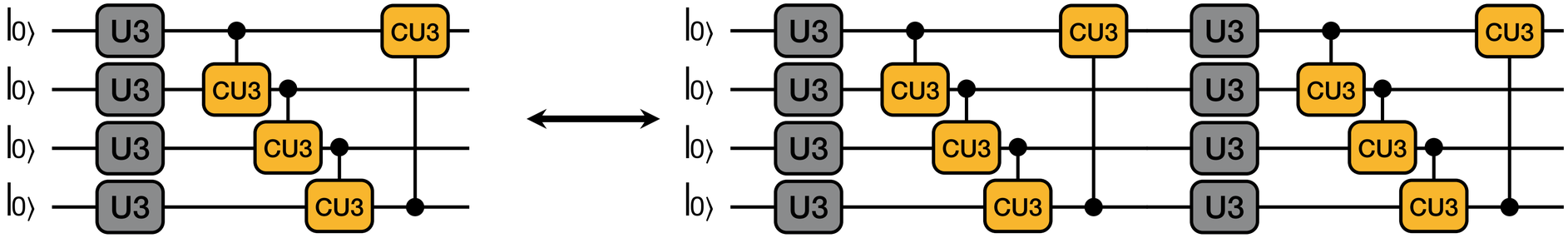

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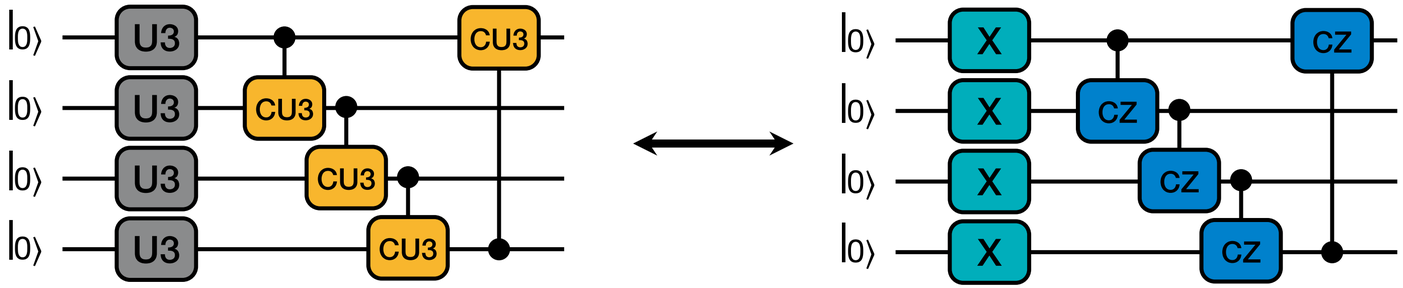
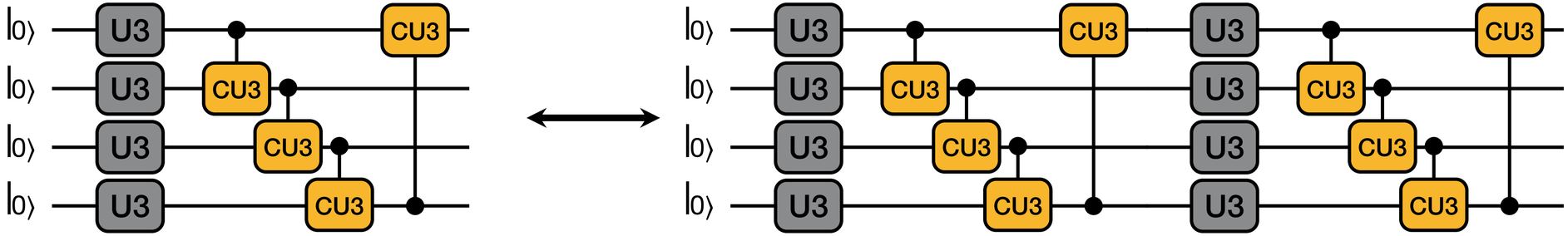
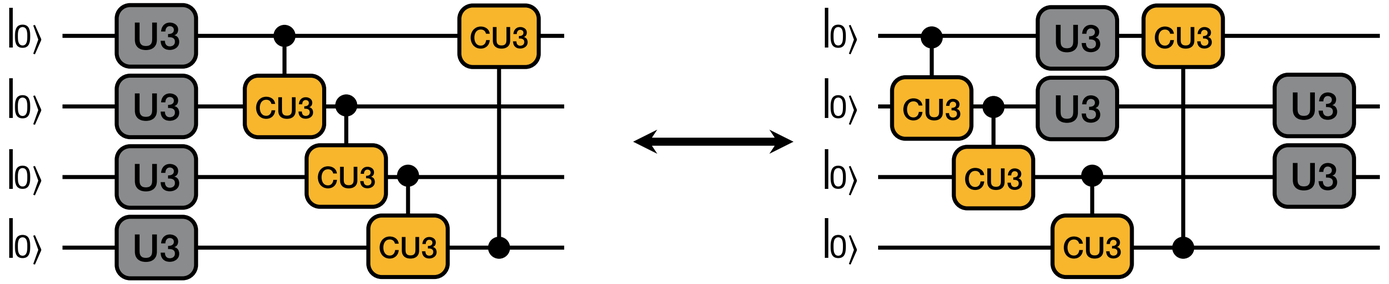


  - Number of gates



  - Position of gates



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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

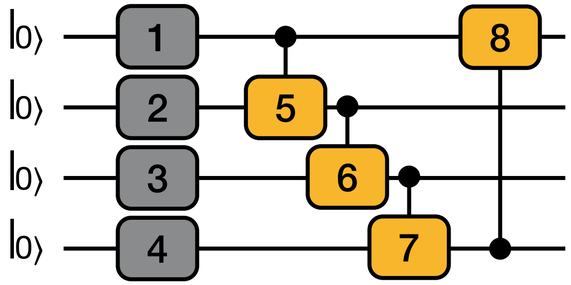
SuperCircuit & SubCircuit

- 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

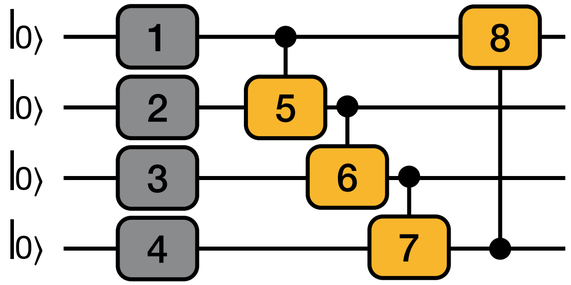
- SuperCircuit: the circuit with the **largest** number of gates in the design space
  - Example: SuperCircuit in U3+CU3 space



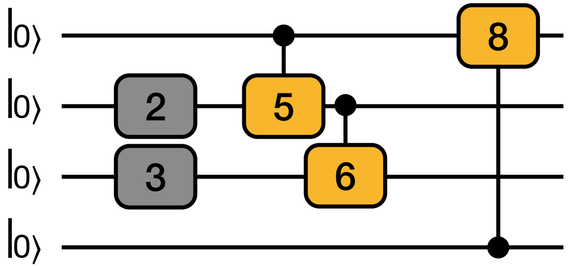
SuperCircuit & SubCircuit

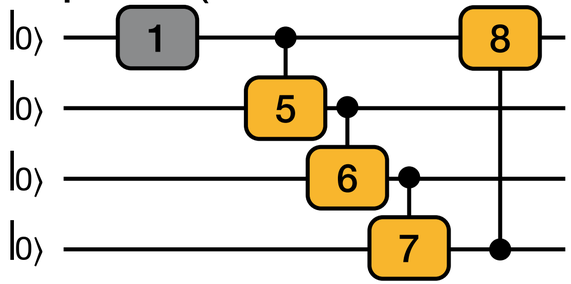
- Firstly construct a design space. For example, a design space of maximum 4 U3 in the first layer and 4 CU3 gates in the second layer

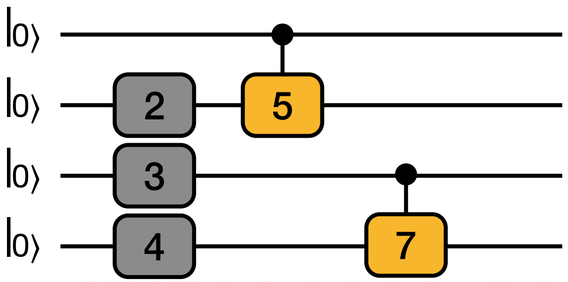
- SuperCircuit: the circuit with the **largest** number of gates in the design space
  - Example: SuperCircuit in U3+CU3 space



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







Torch Quantum

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SuperCircuit Construction

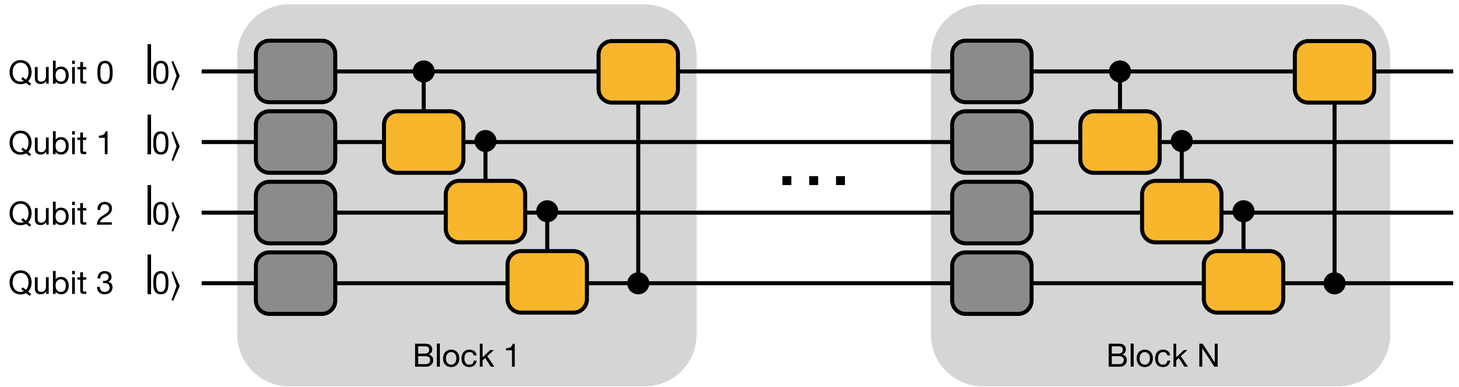
- Why use a SuperCircuit?
  - Enables **efficient** search of architecture candidates without training each
  - SubCircuit inherits parameters from SuperCircuit
  - With **inherited** parameters, we find some good SubCircuits, we find that they are **also good SubCircuits** with parameters **trained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

Train SuperCircuit for Multiple Steps

- In one SuperCircuit Training step: Sample and Train



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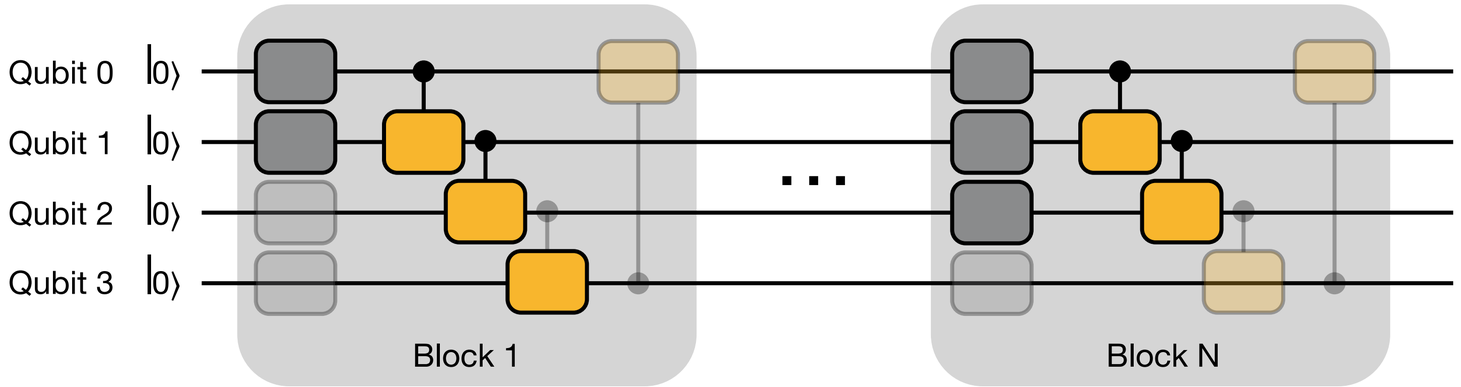

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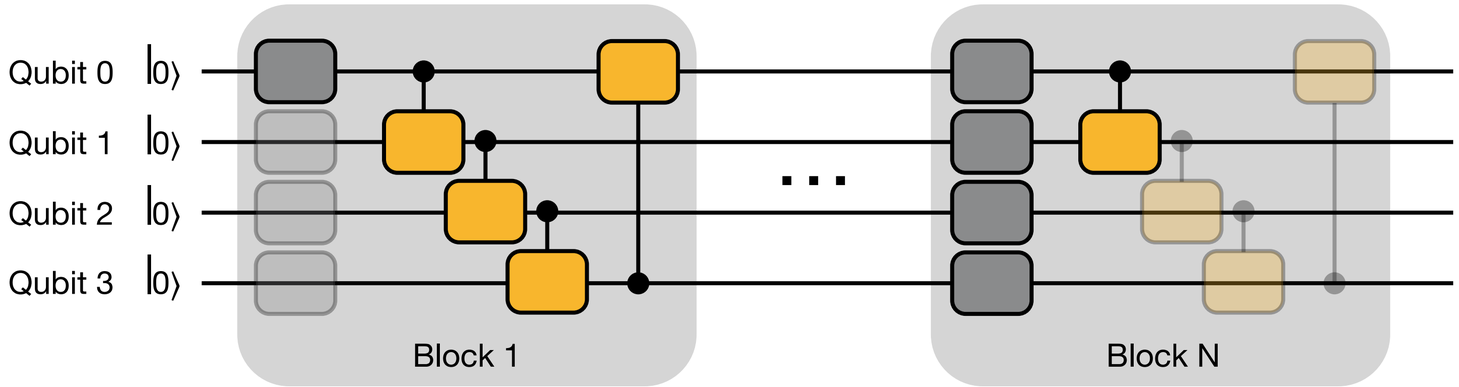

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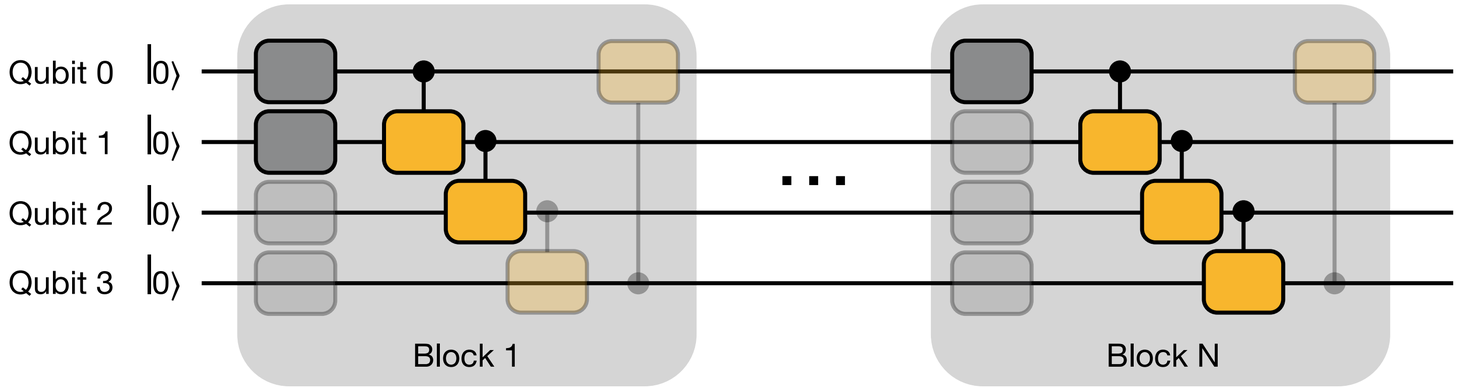

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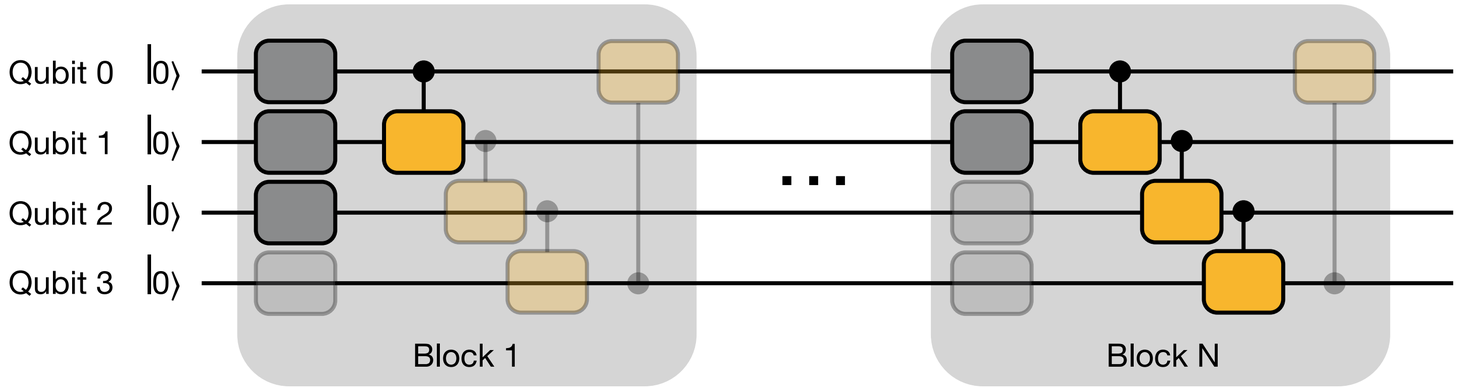

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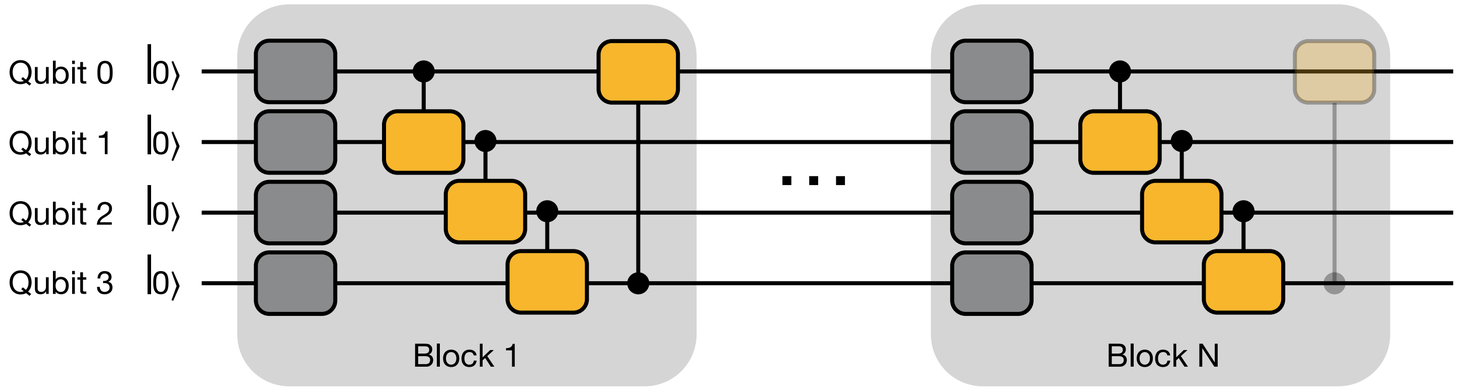

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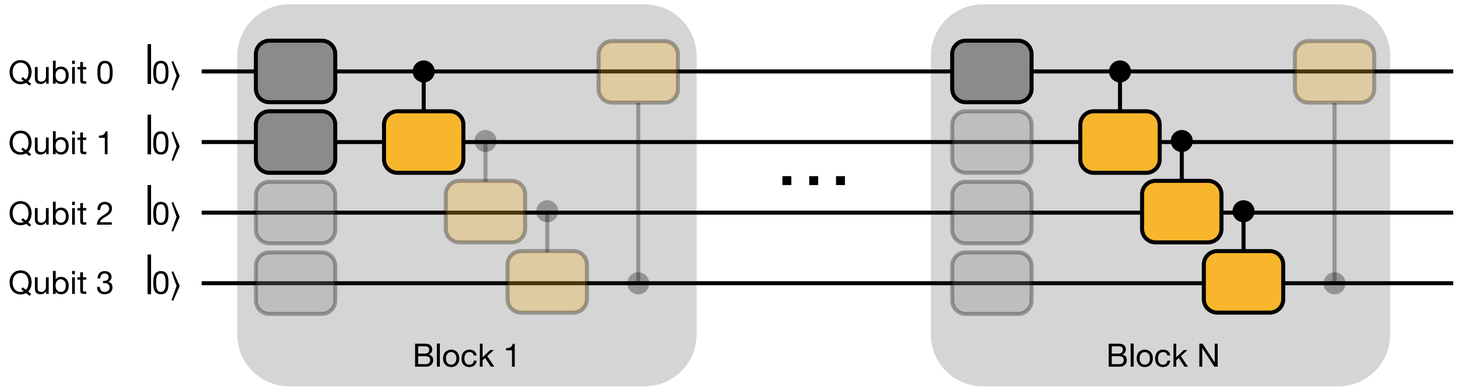

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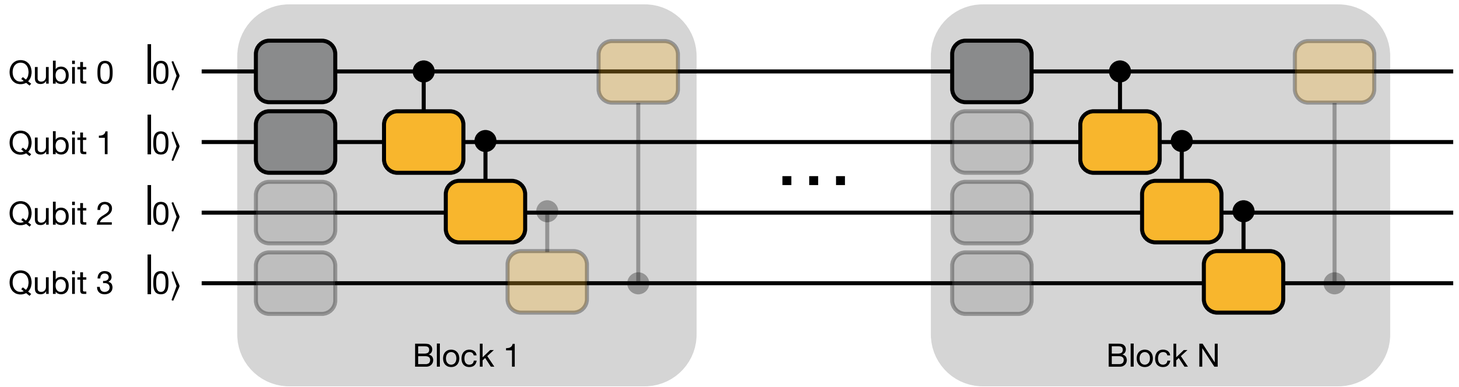
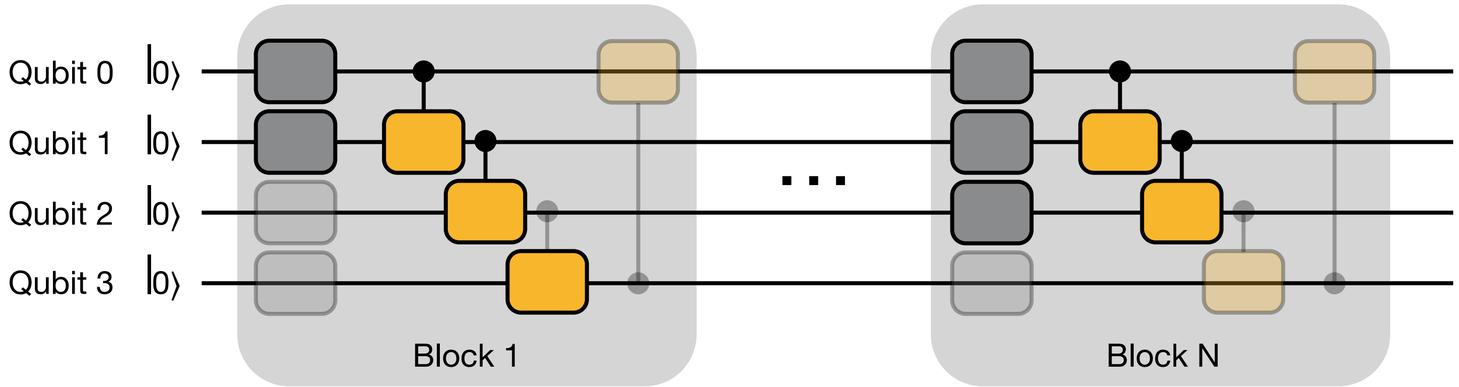


Train SuperCircuit for Multiple Steps

- In one SuperCircuit Training step: Sample and Train



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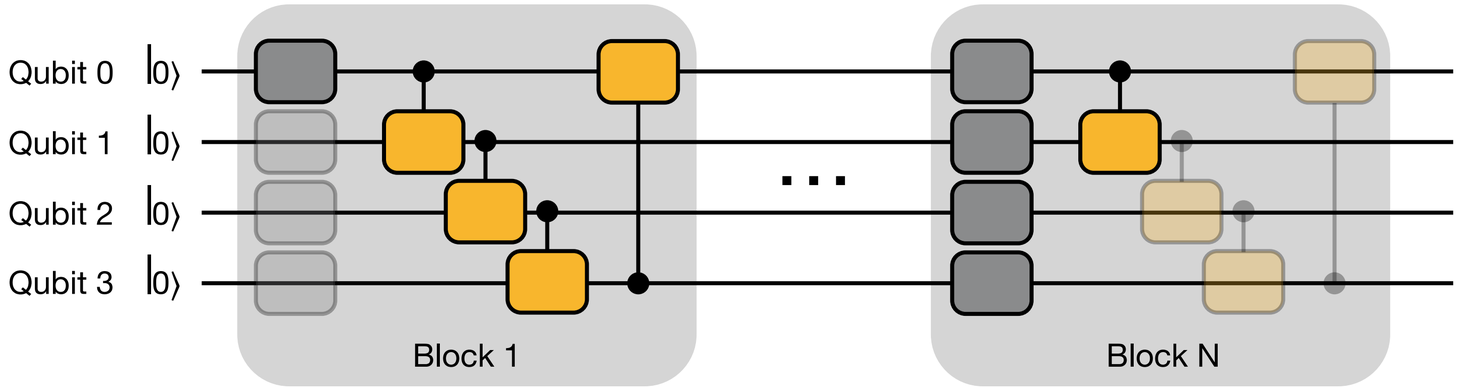

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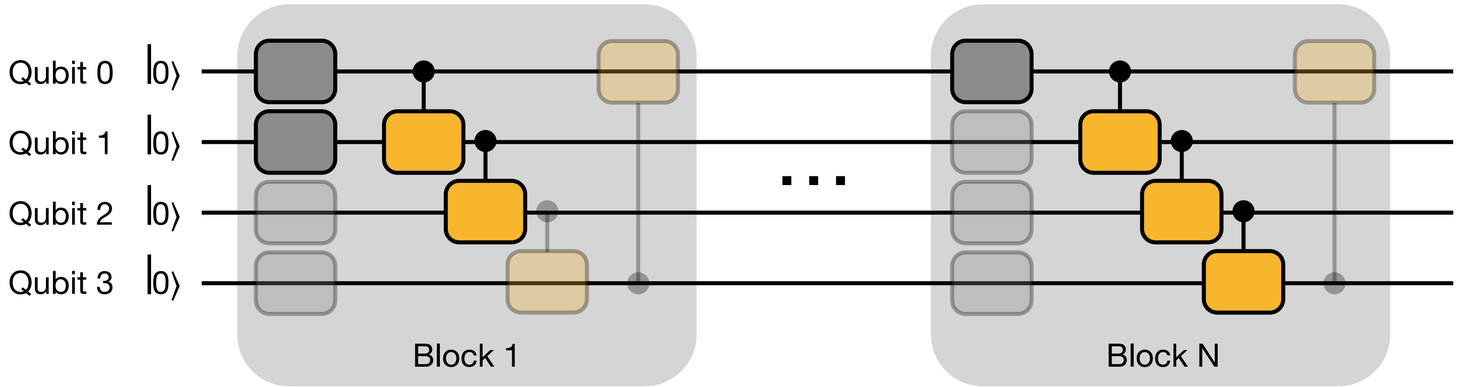

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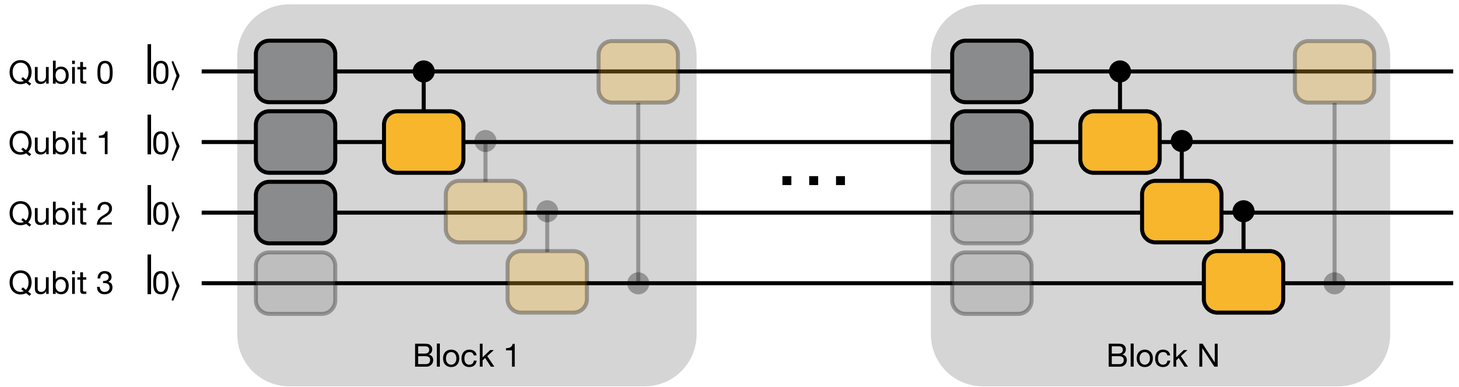

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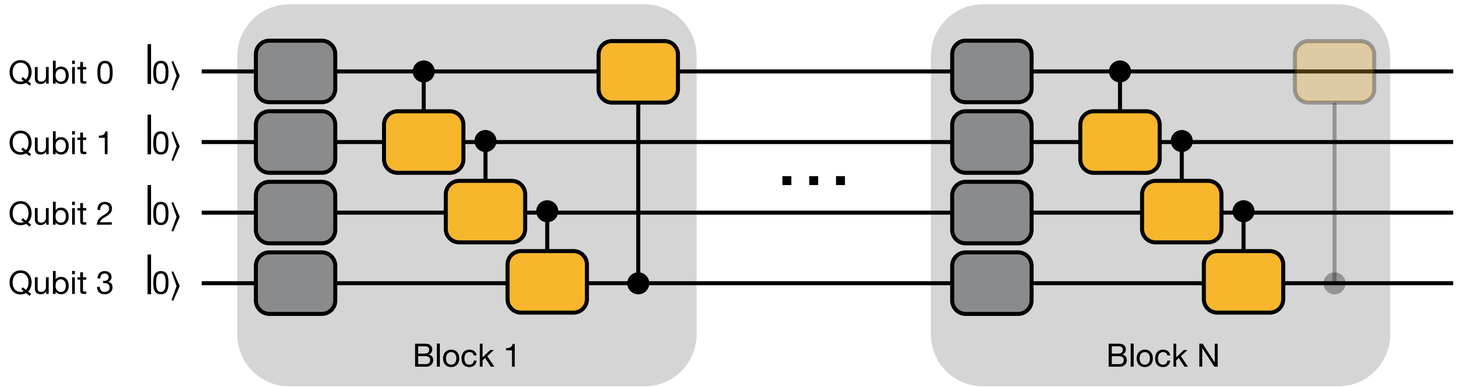

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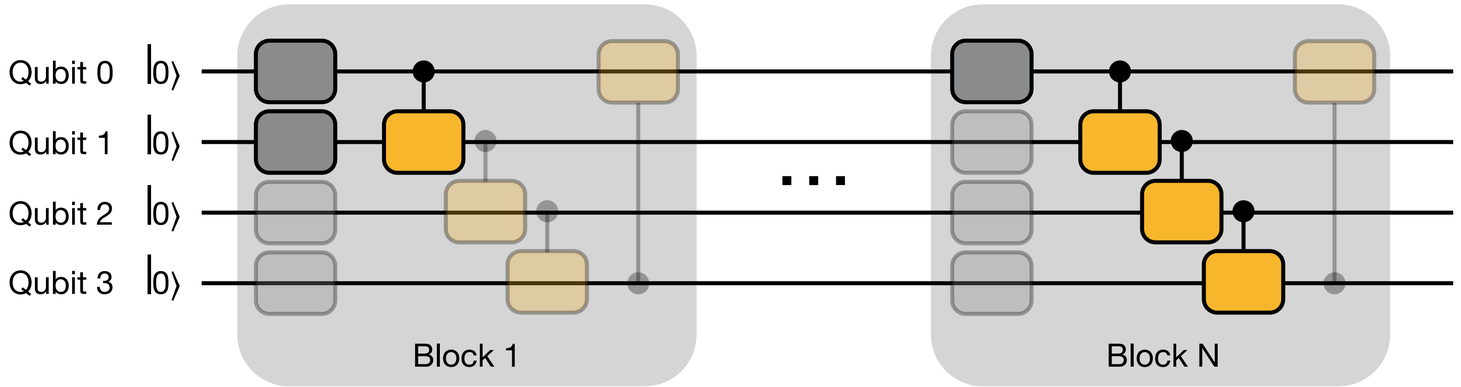

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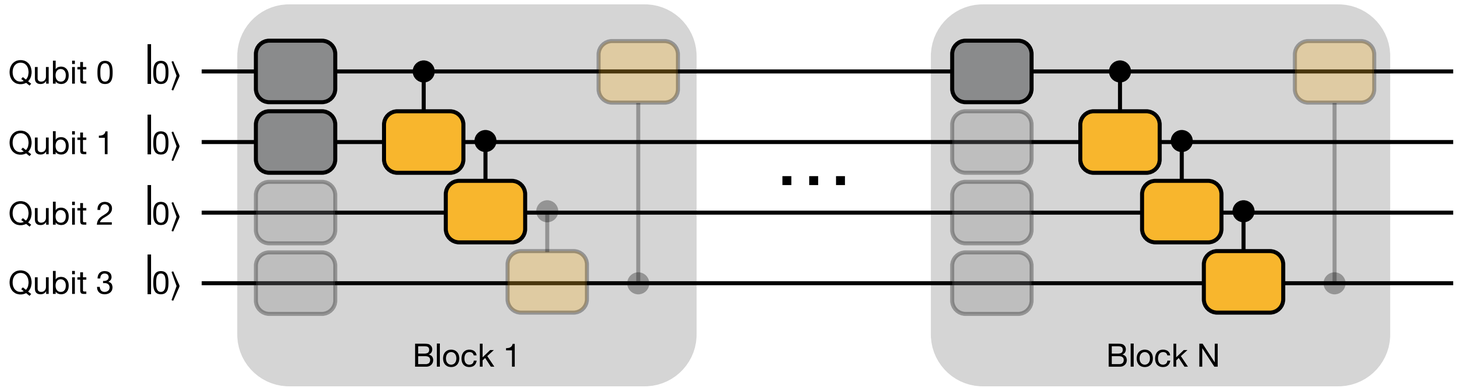

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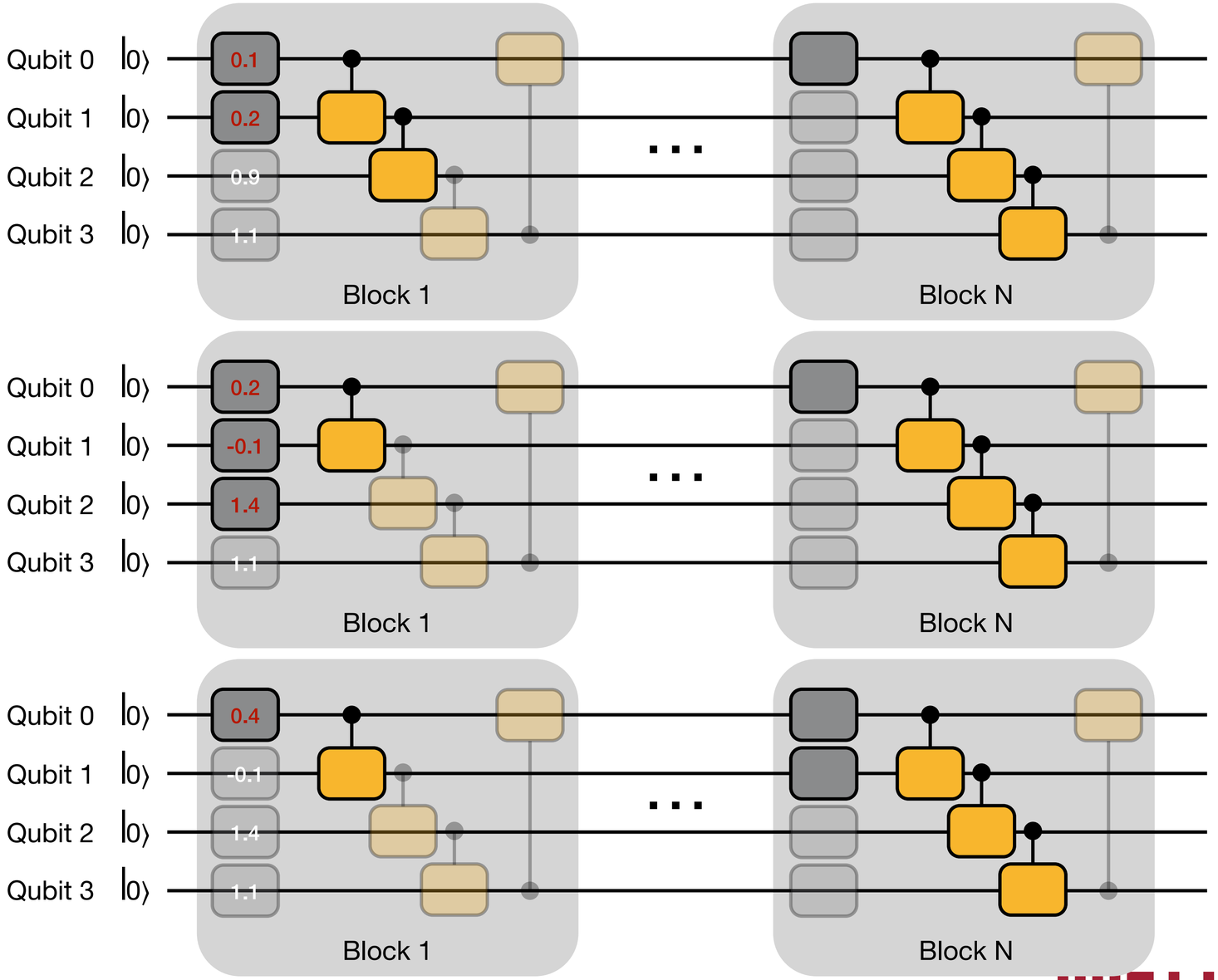

Torch Quantum

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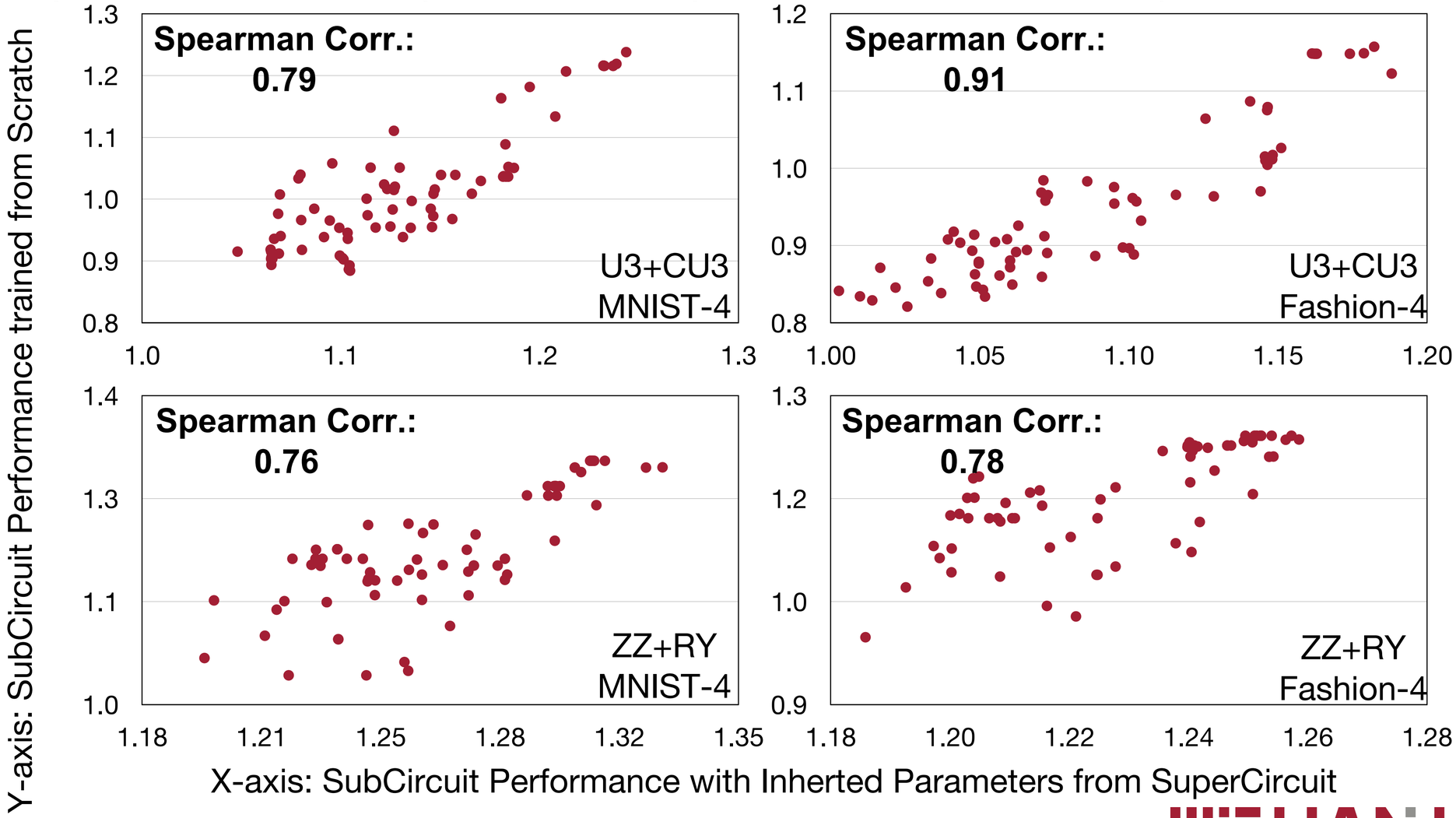
How Reliable is the SuperCircuit?

- Inherited parameters from SuperCircuit can provide accurate relative performance



Torch Quantum

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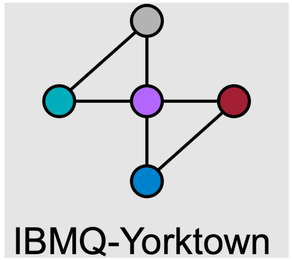
QuantumNAS

- 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



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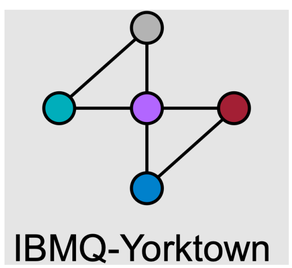
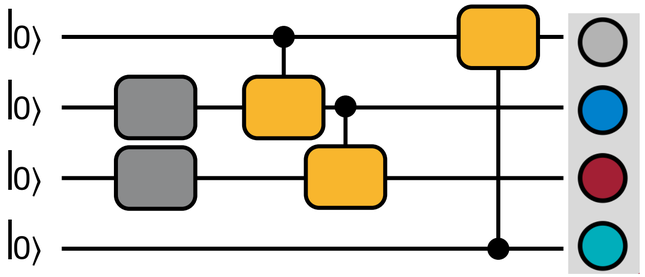
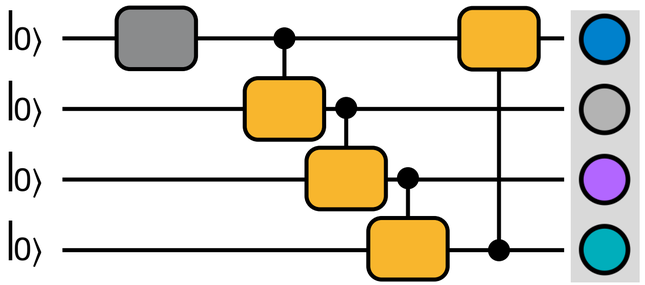
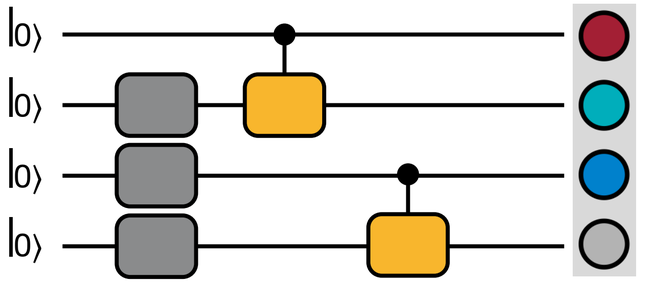








Evolutionary Search Engine
Mutation
Crossover

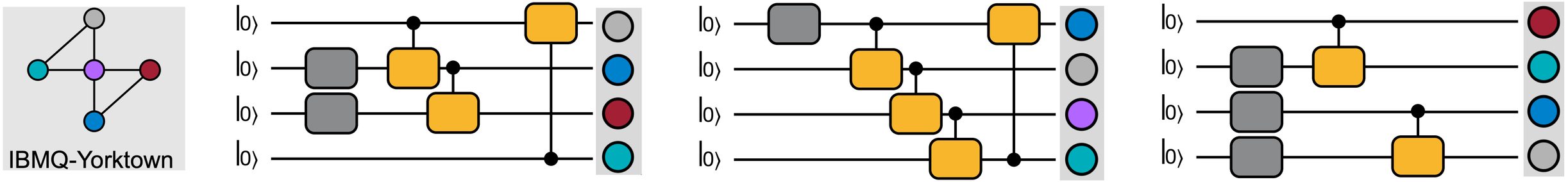
SubCircuit and Qubit Mapping pairs

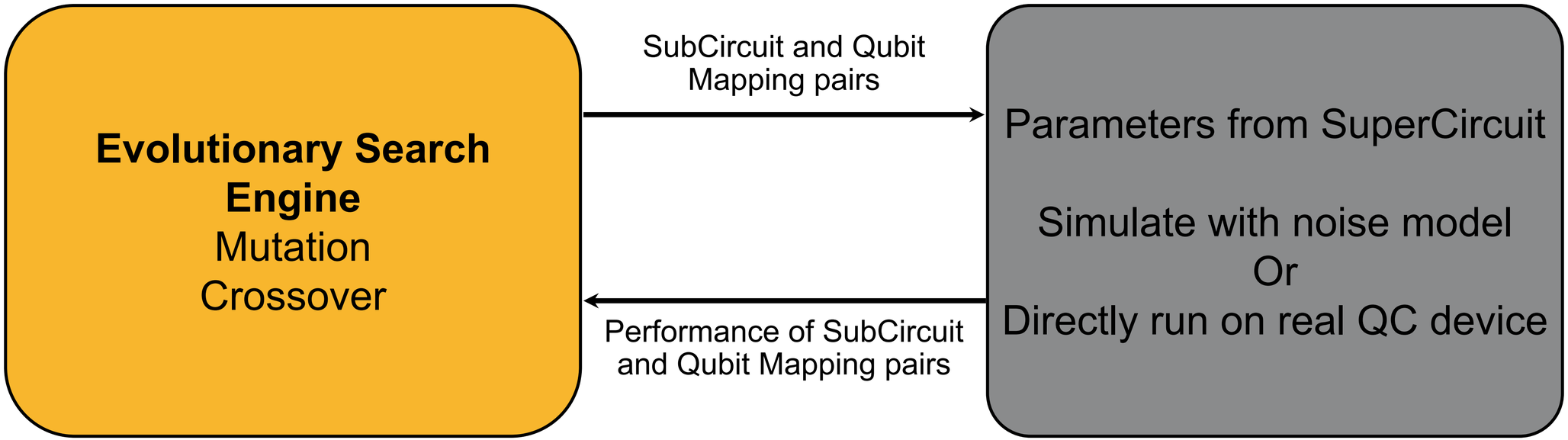
Parameters from SuperCircuit

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





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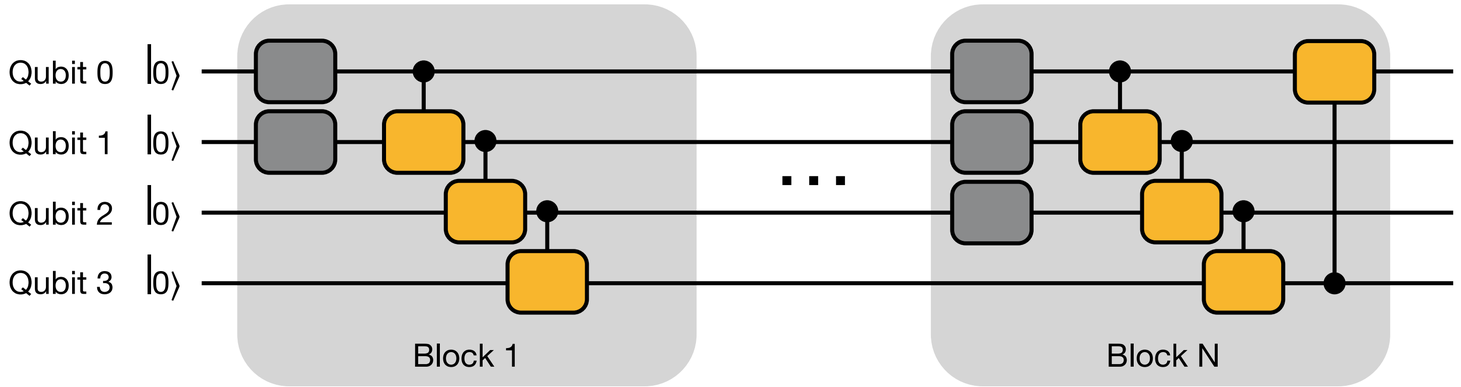
Iterative Pruning

- 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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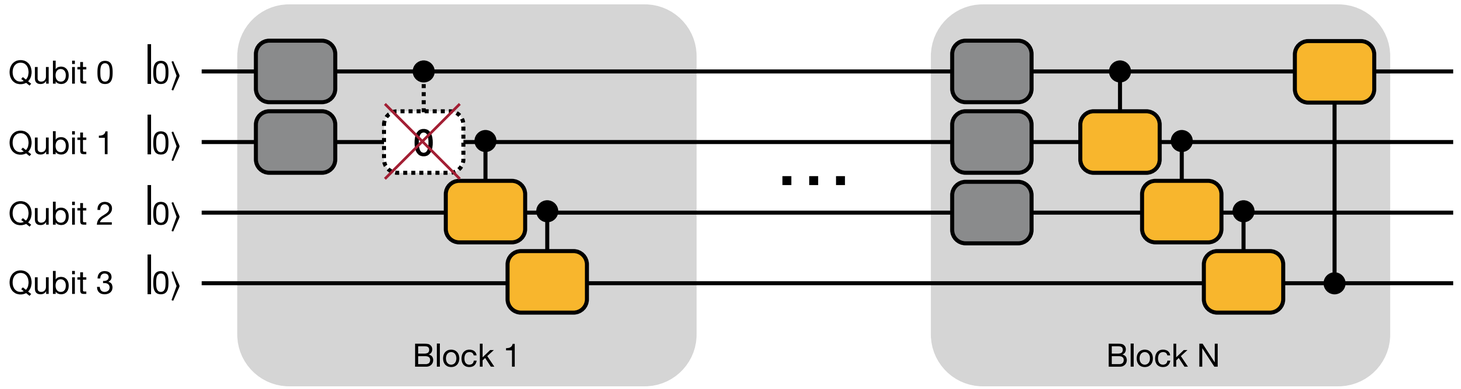

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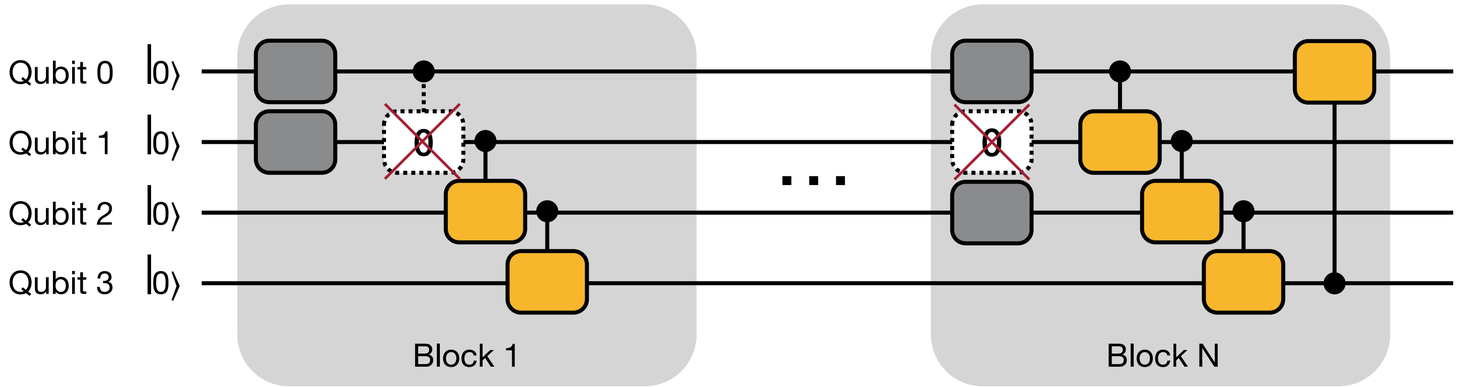

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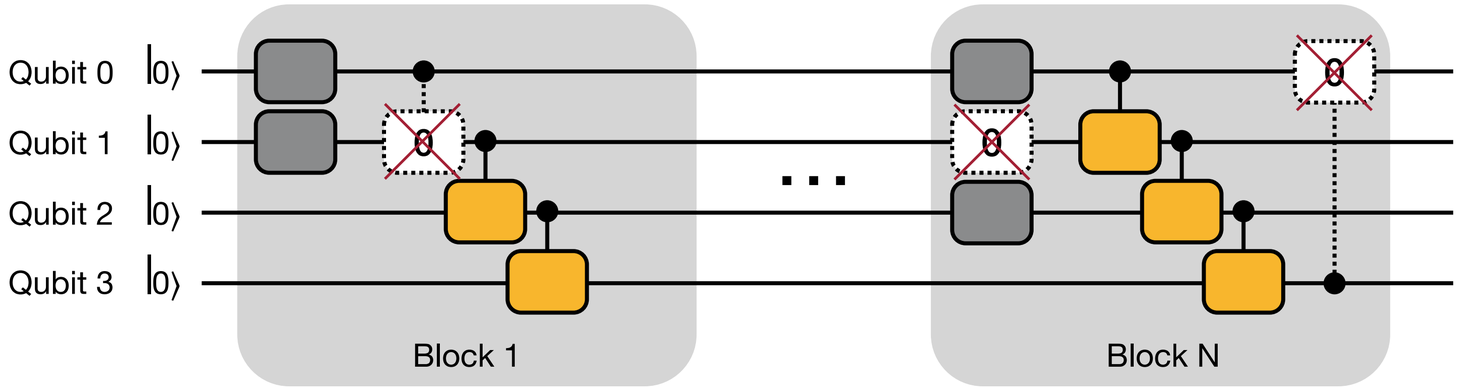

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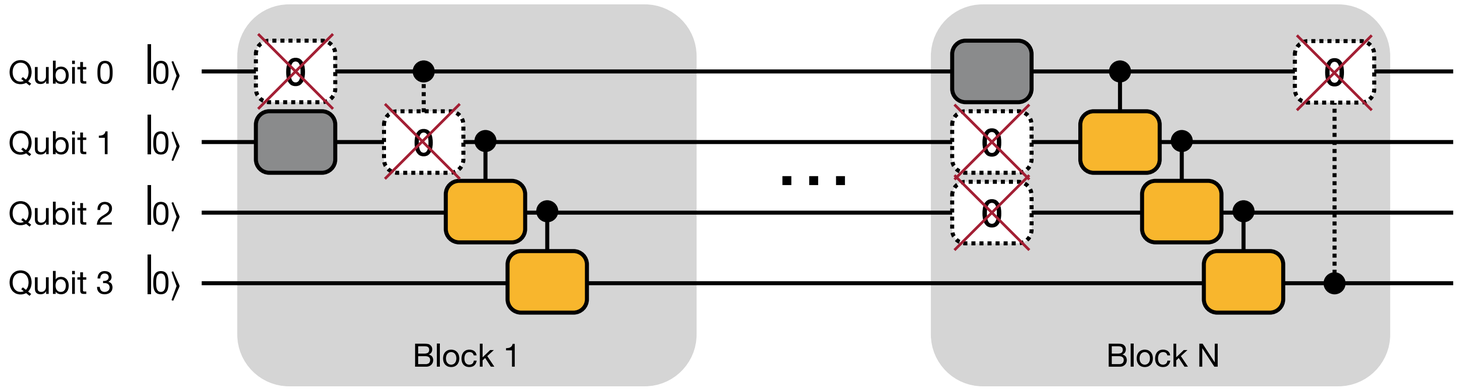
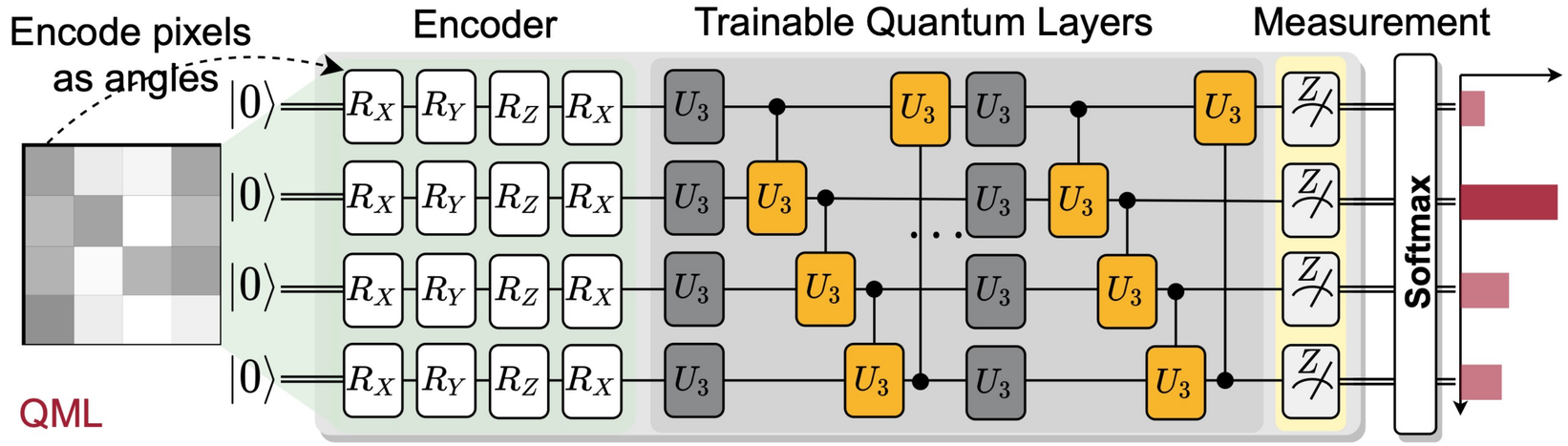


Evaluation Setups: Benchmarks and Devices

- 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

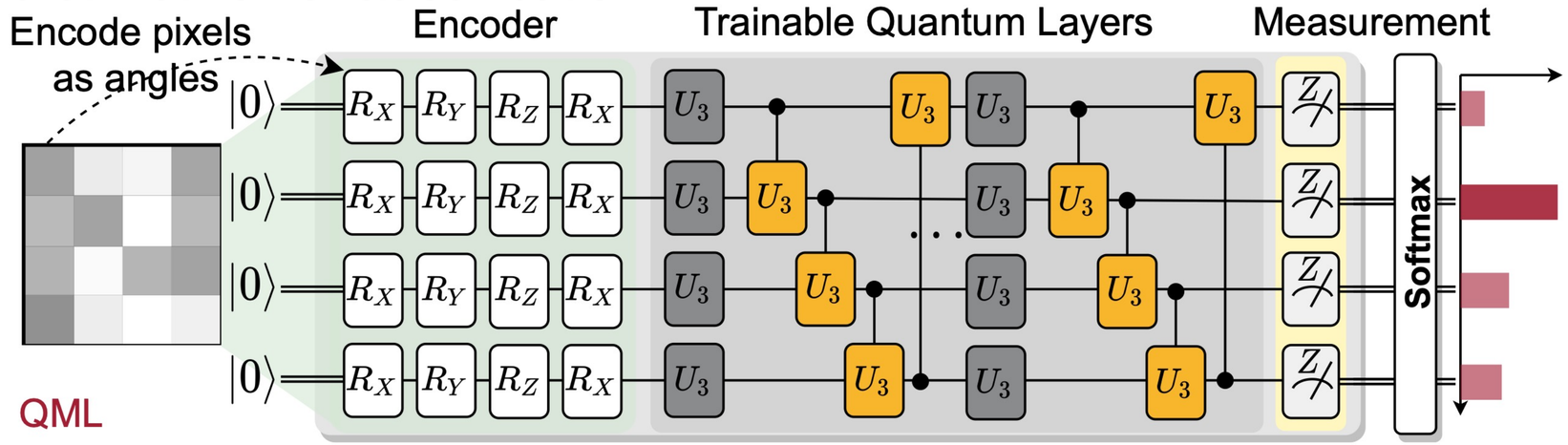
Benchmarks: QNN and VQE

- Quantum Neural Networks: classification

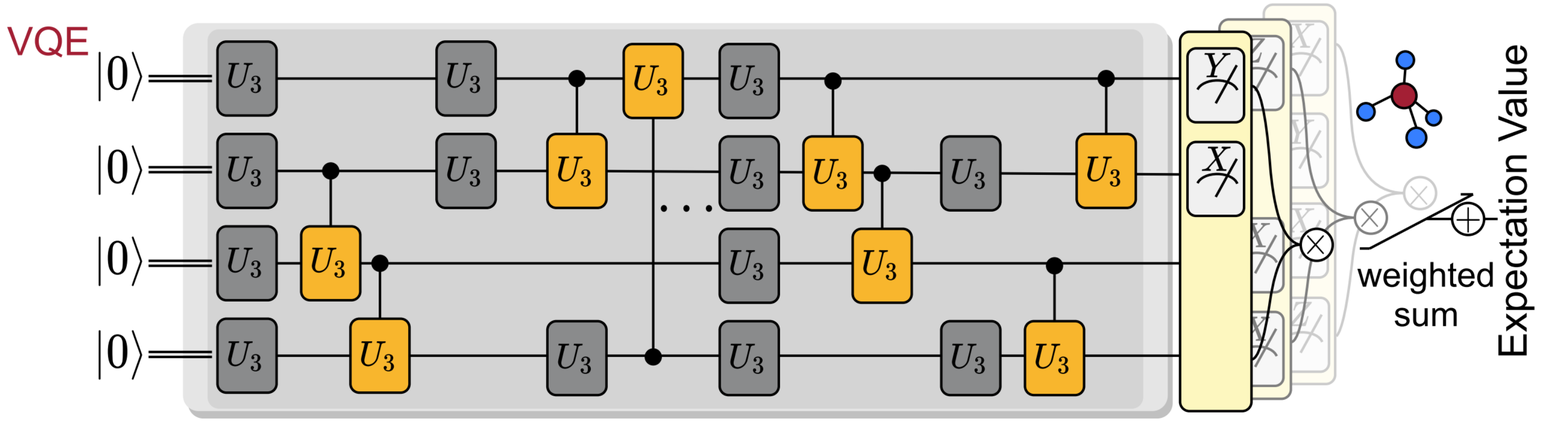


Benchmarks: QNN and VQE

- Quantum Neural Networks: classification



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



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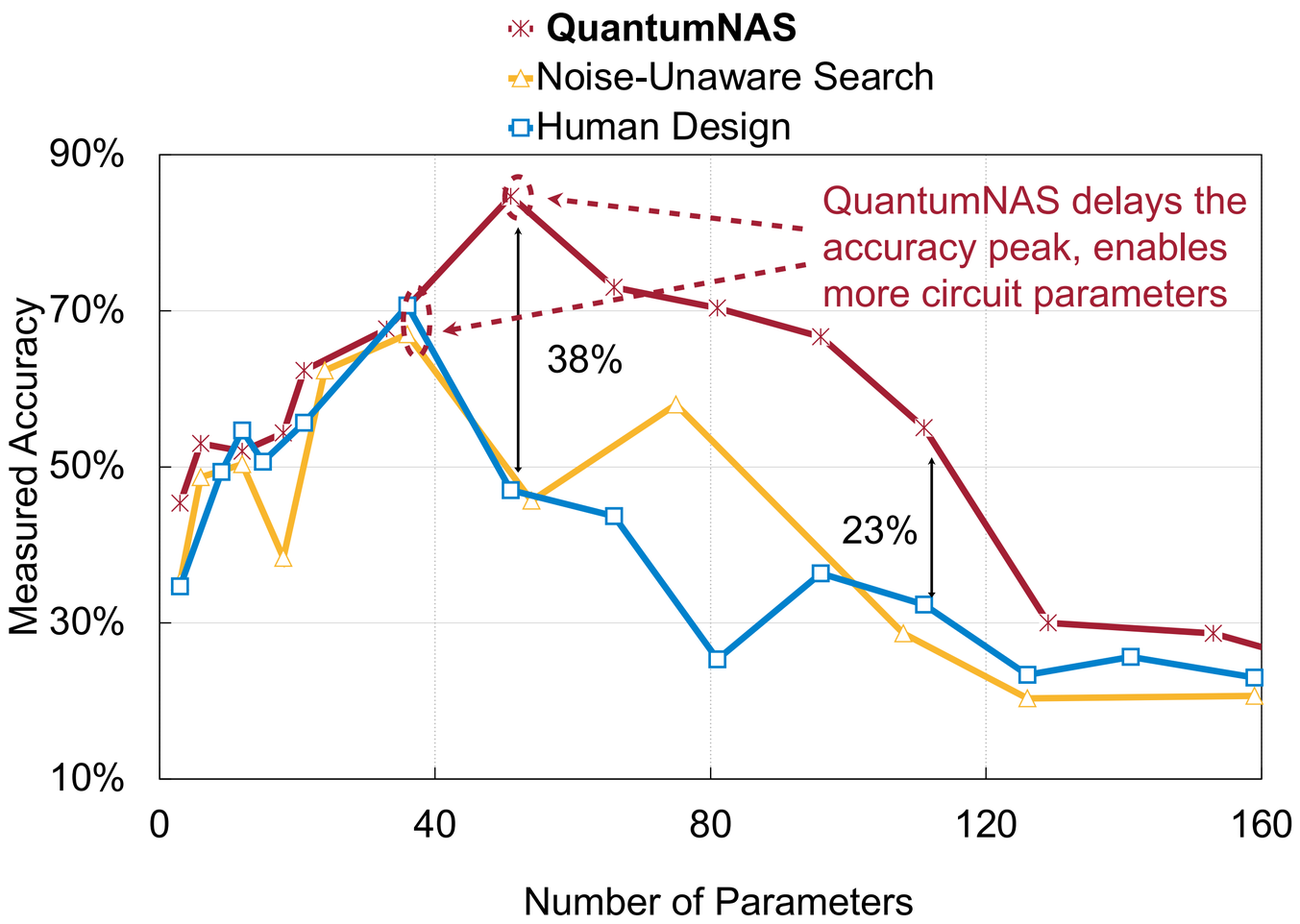
QML Results

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



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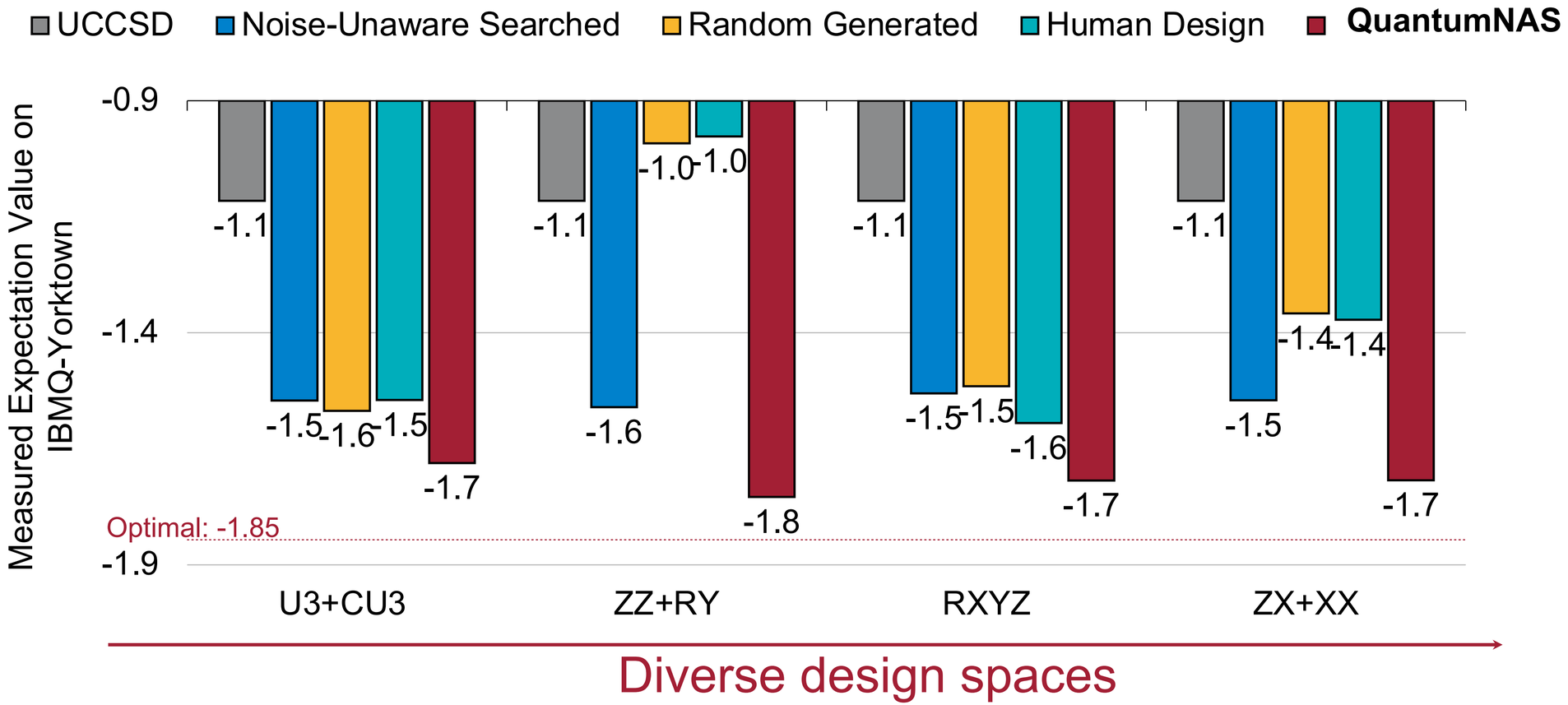
Consistent Improvements on Diverse Design Spaces

- H2 in different design spaces on IBMQ-Yorktown



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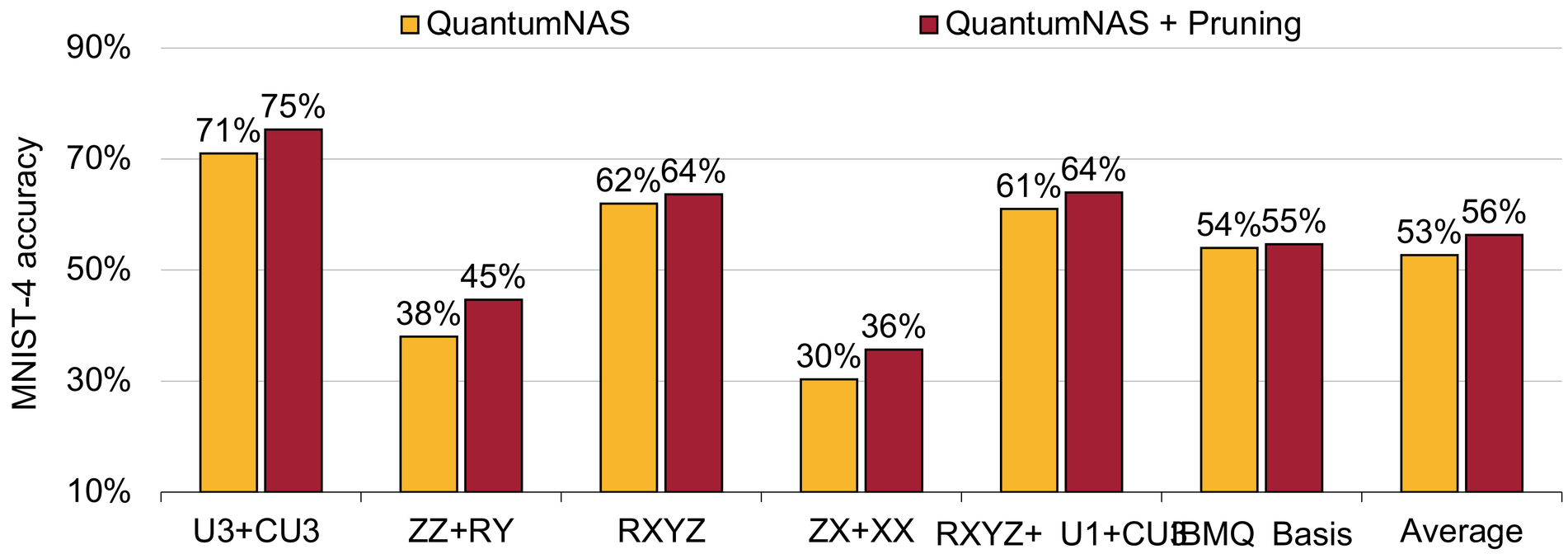
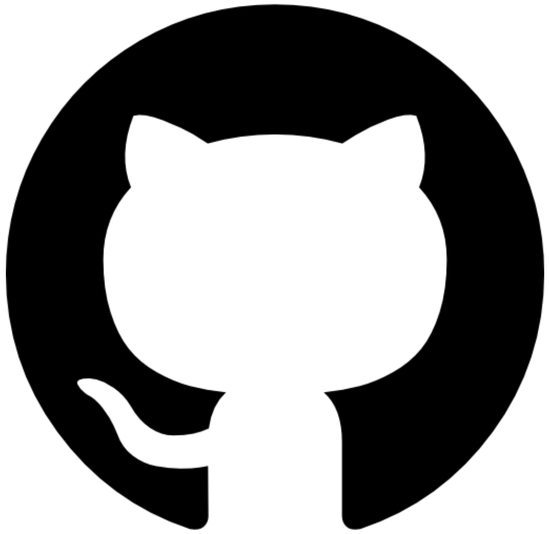
Effective of Quantum Gate Pruning

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



Hands-On Section
3.1 QuantumNAS



Torch Quantum

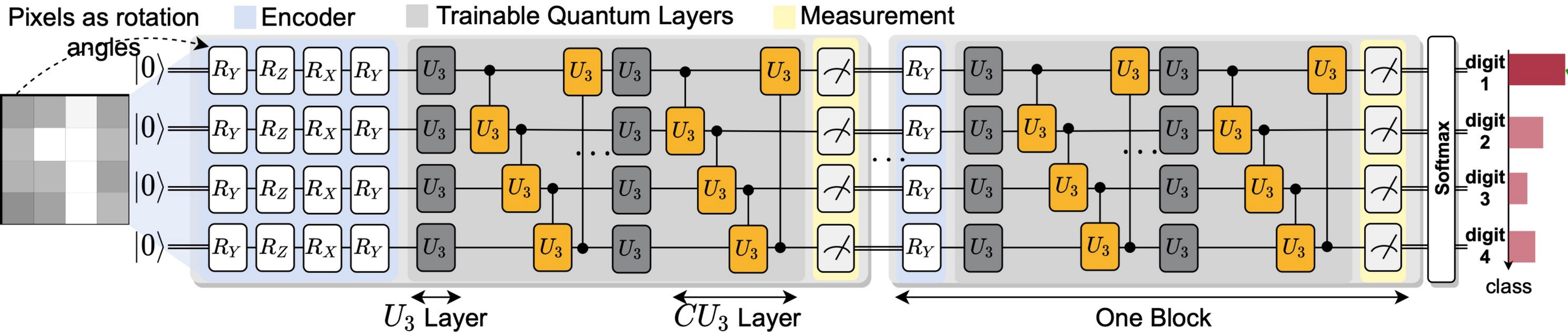
Materials at: https

QuantumNAS vs. QuantumNAT

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

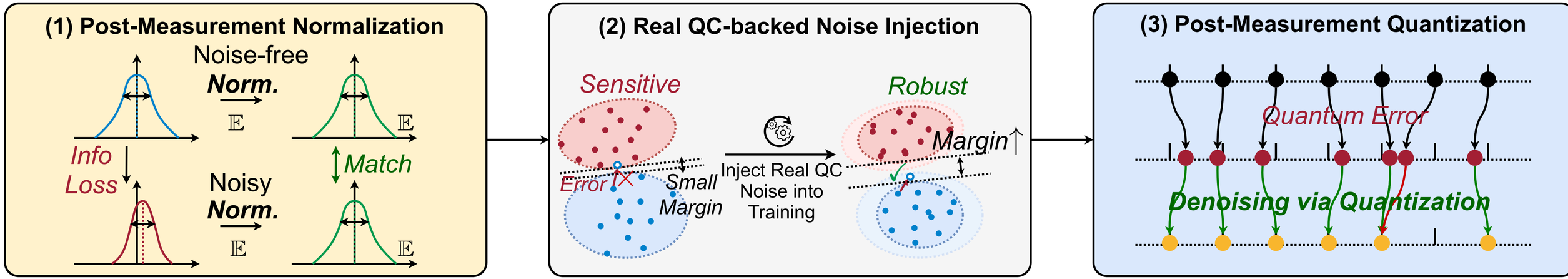
PQC Circuit in QuantumNAT

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

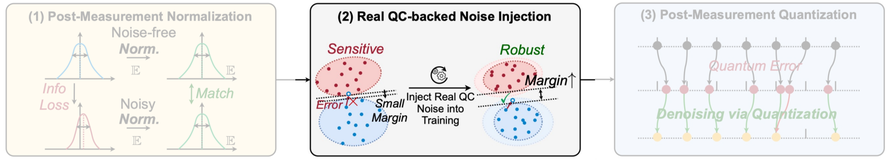


Three Techniques in QuantumNAT

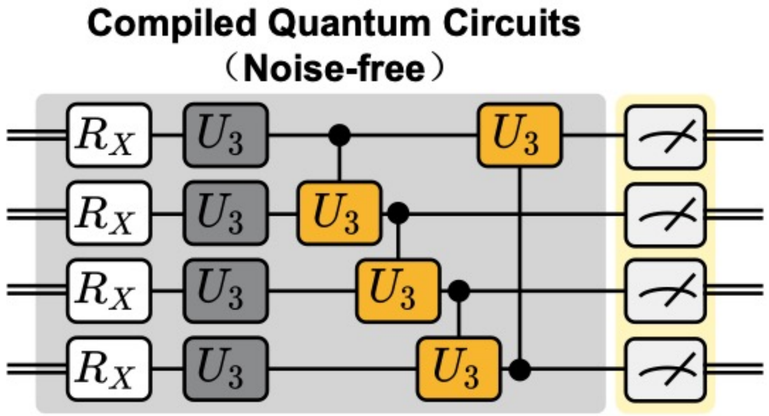
- QuantumNAT:
  - Normalization: mitigate noise impact
  - Noise injection: make the parameters aware of noise
  - Quantization: mitigate noise impact



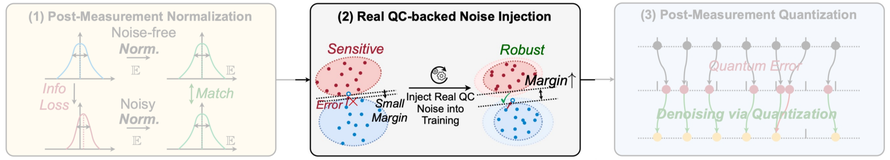
Noise Injection



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



Noise Injection



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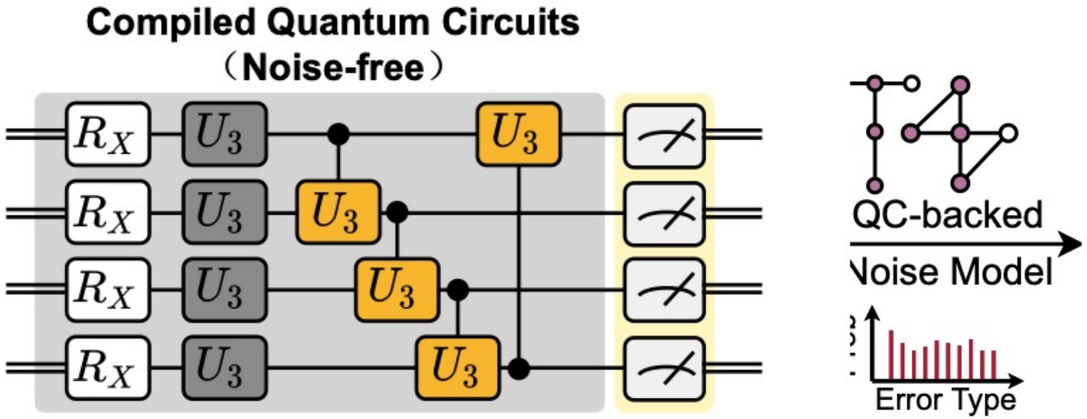

Pauli error: SX gate: {X: 0.00096, Y: 0.00096, Z: 0.00096, None: 0.99712}

Readout Error Matrix:

0.984, 0.016

0.022, 0.978

Materials at: https://torchquantum.org

Torch Quantum

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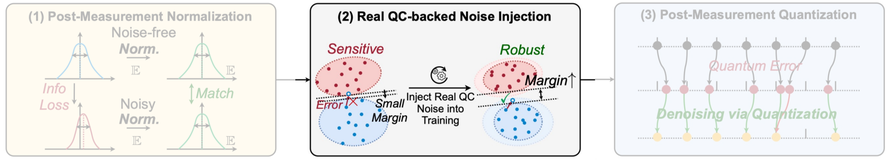
Noise Injection



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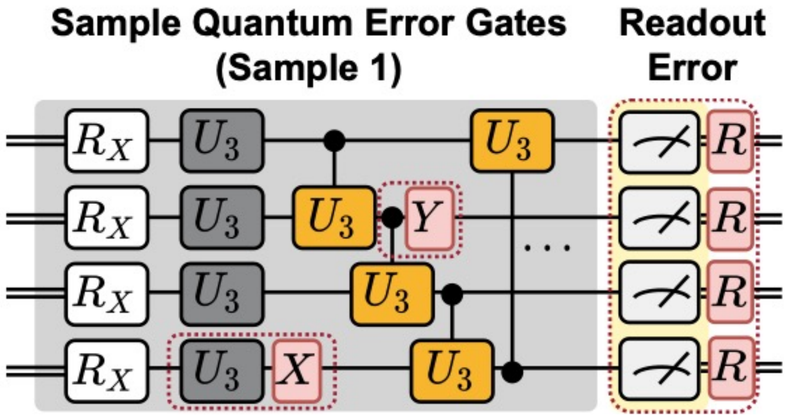

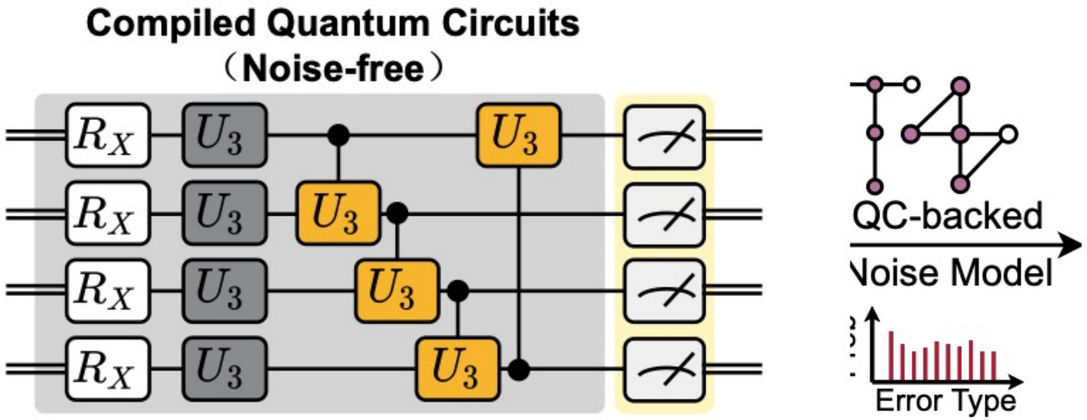

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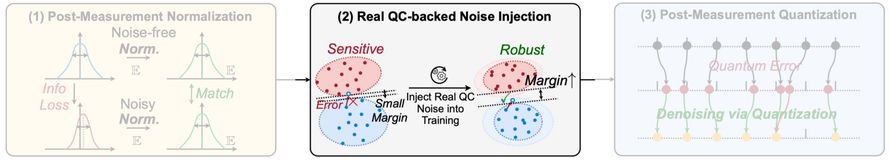
Noise Injection



- Inject noise during training on classical simulator
  - Pauli error
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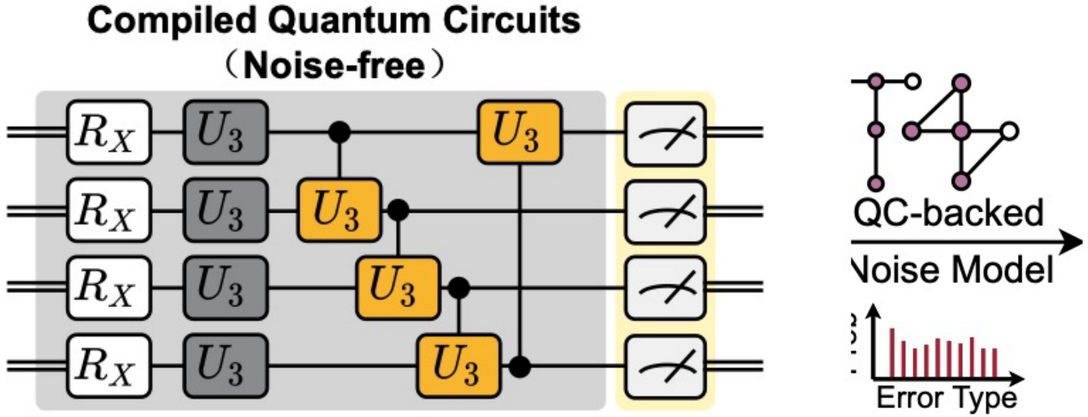

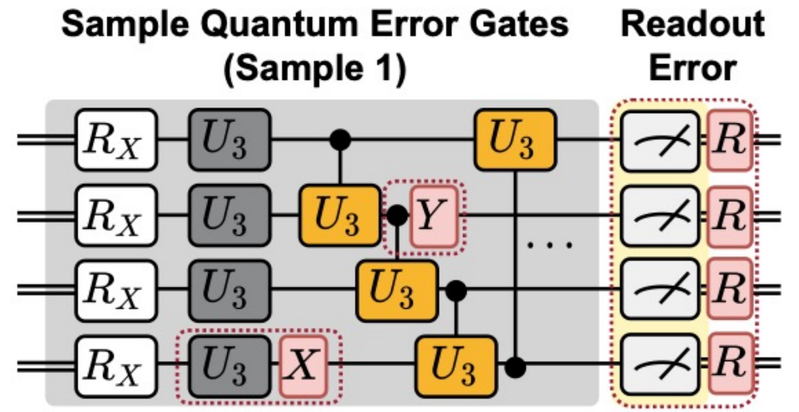

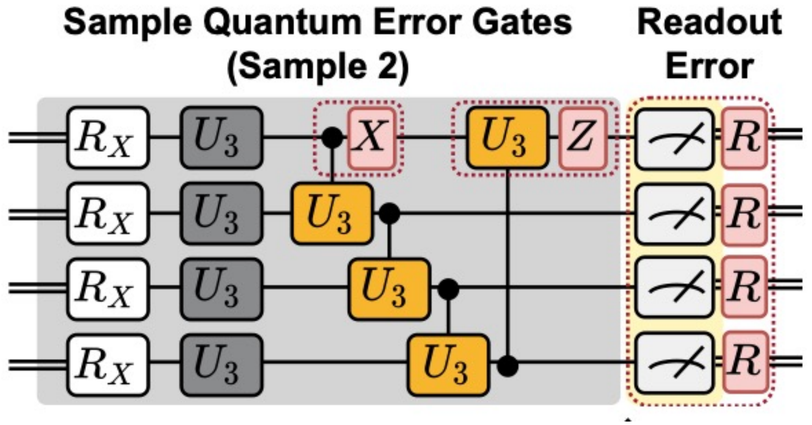

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Readout Error Matrix: 0.984, 0.016
0.022, 0.978

Materials at: https://torchquantum.org

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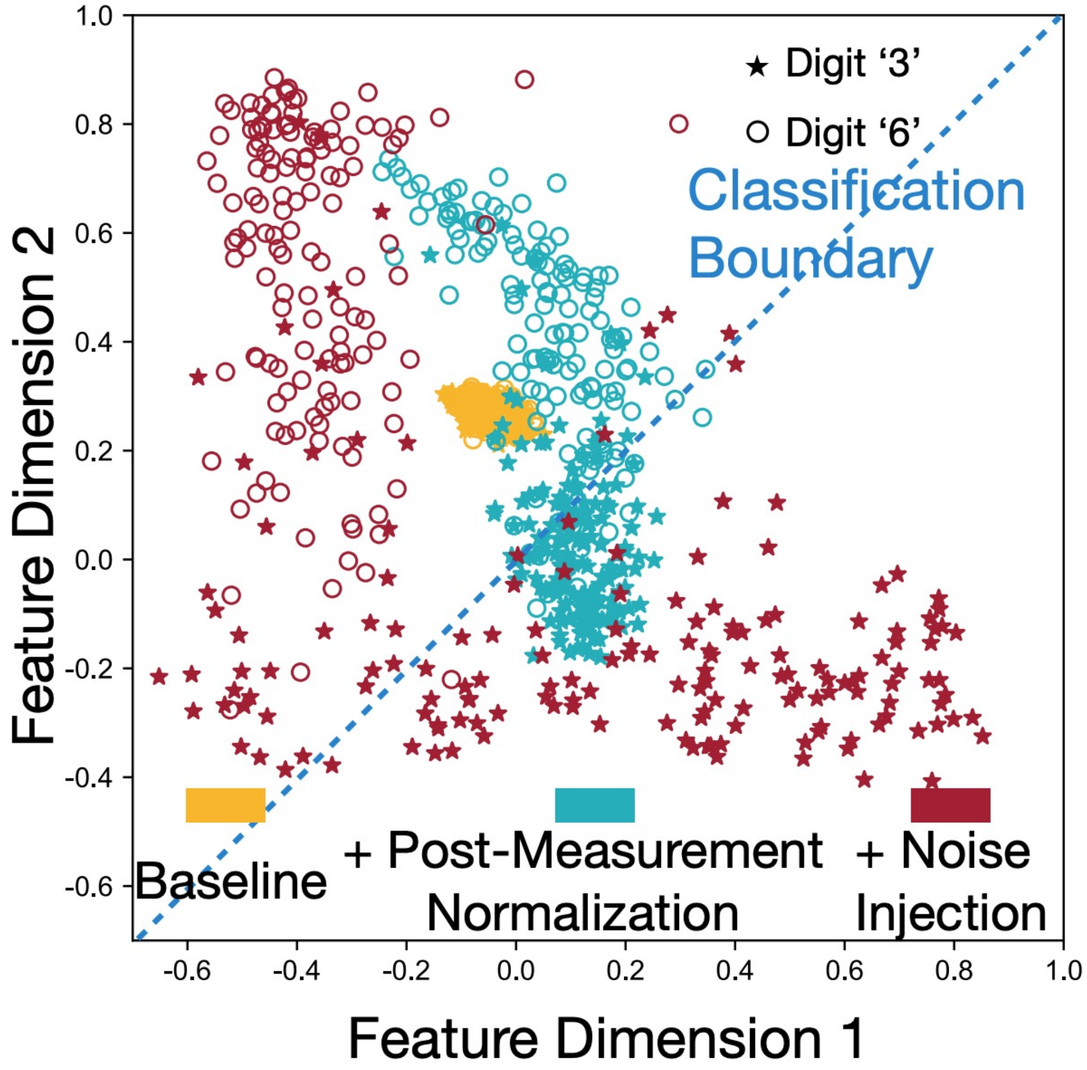
Visualization

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

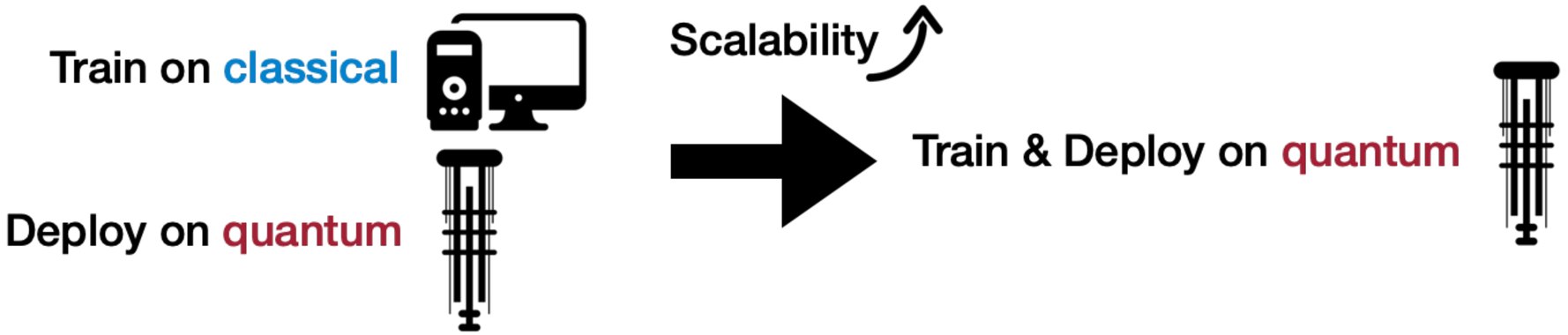


Noise Model in TQ

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

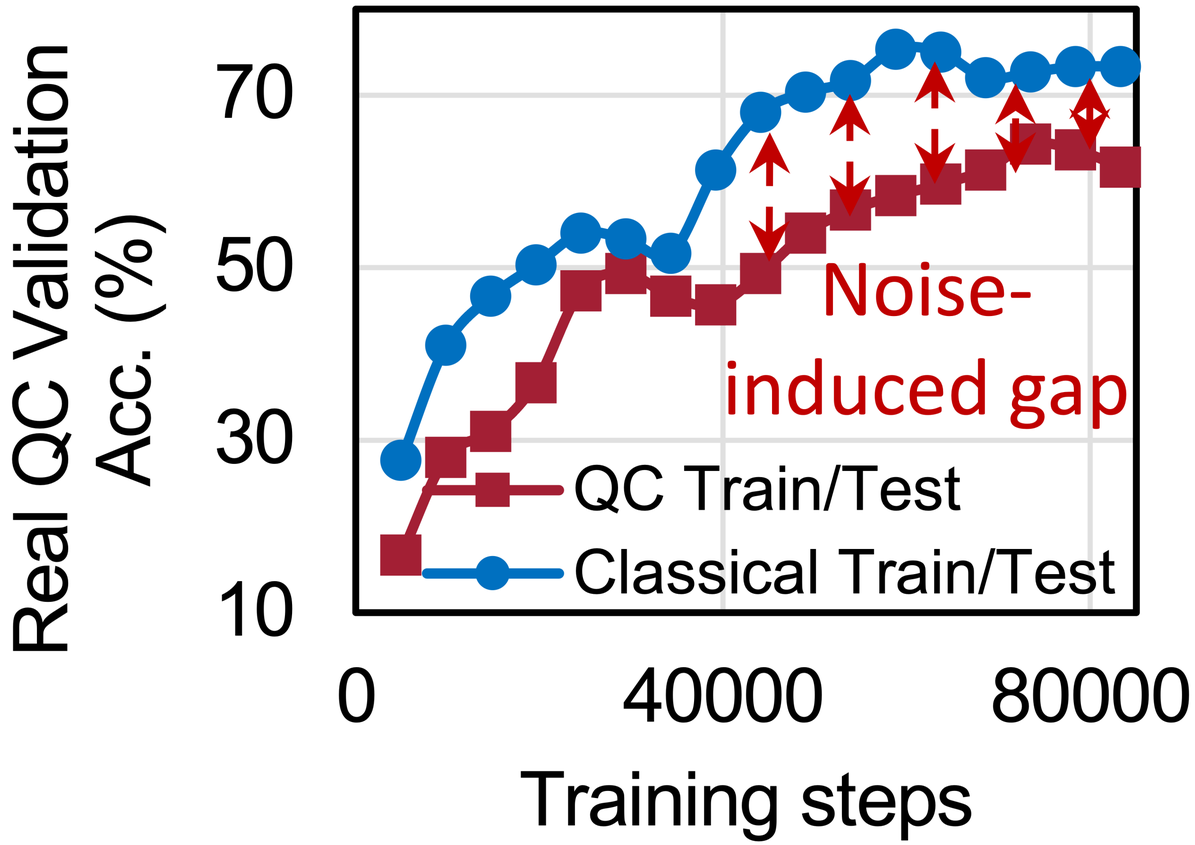
QOC for High Scalability

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



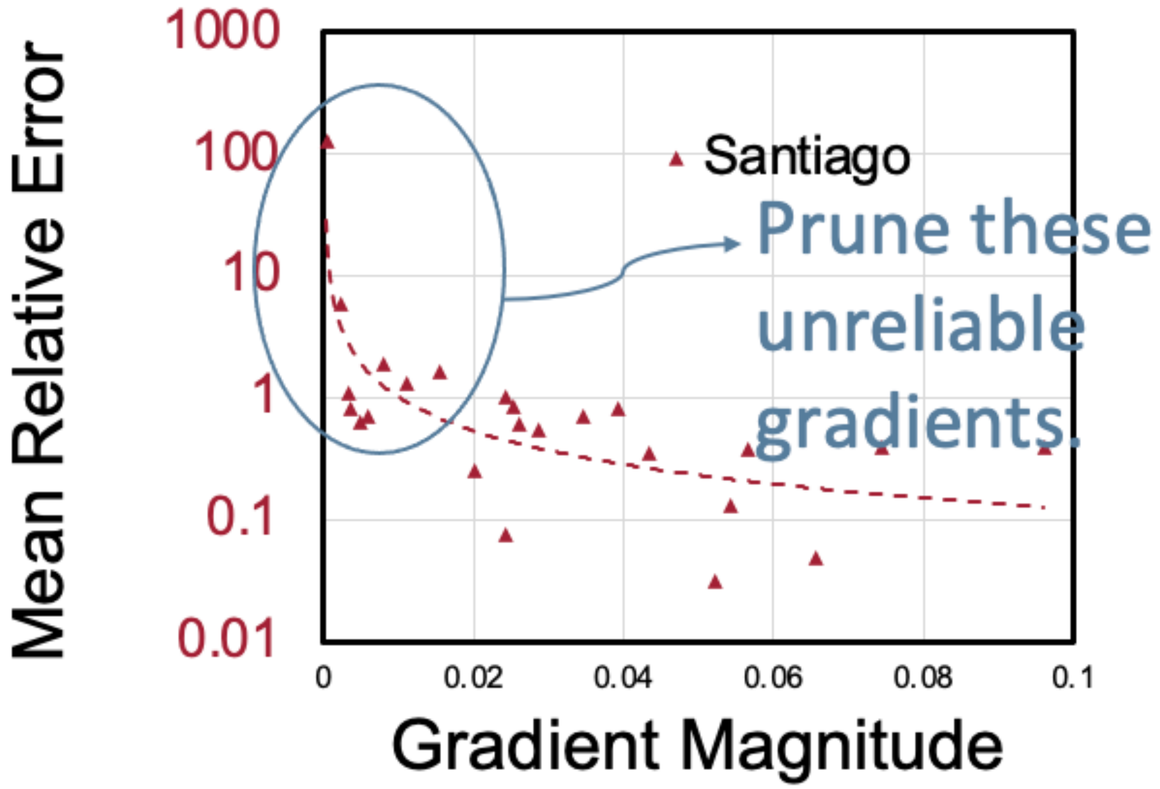
Challenge of On-chip Training: noise

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



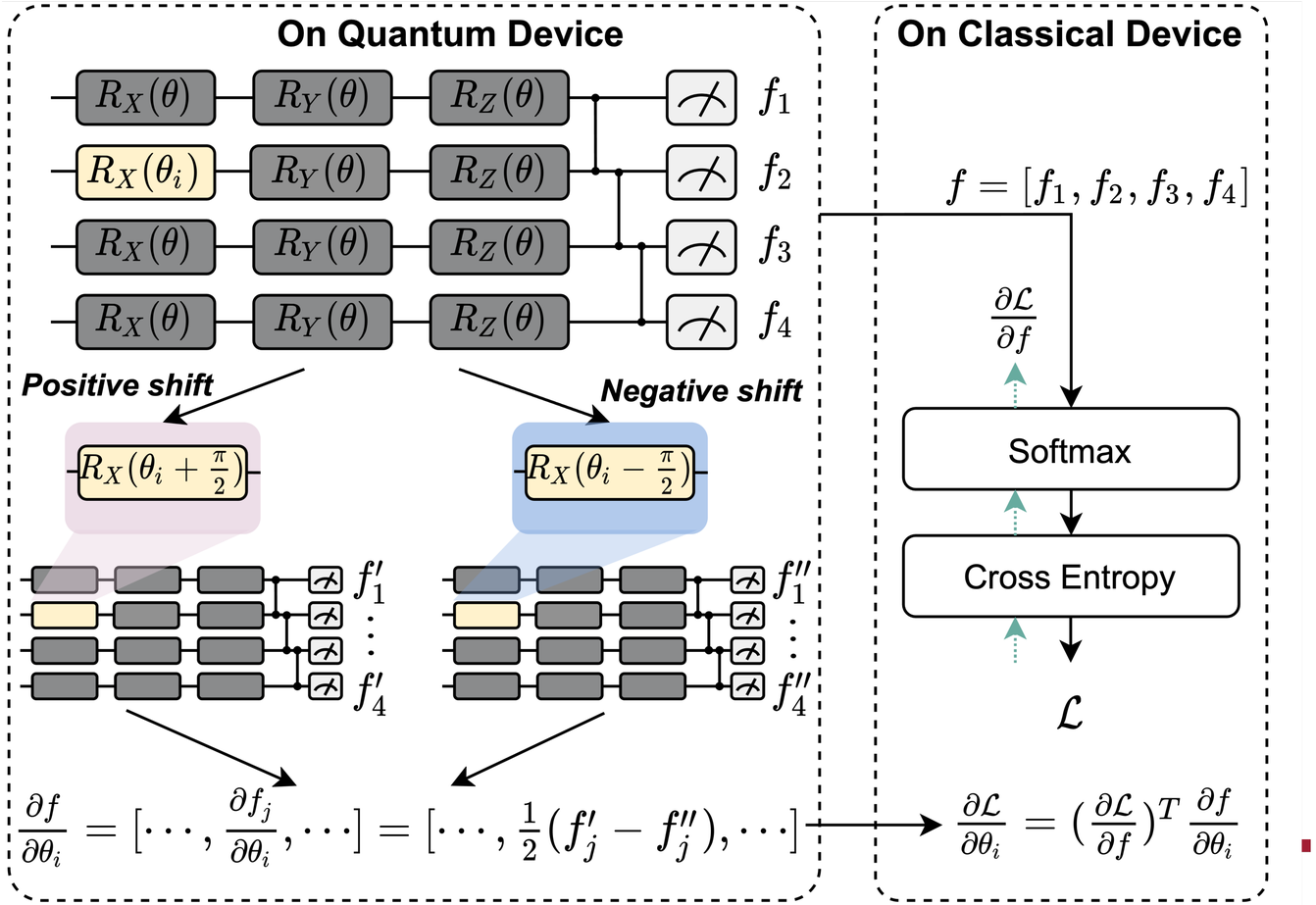
Challenge of On-chip Training: noise

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



Calculate Gradients of PQC

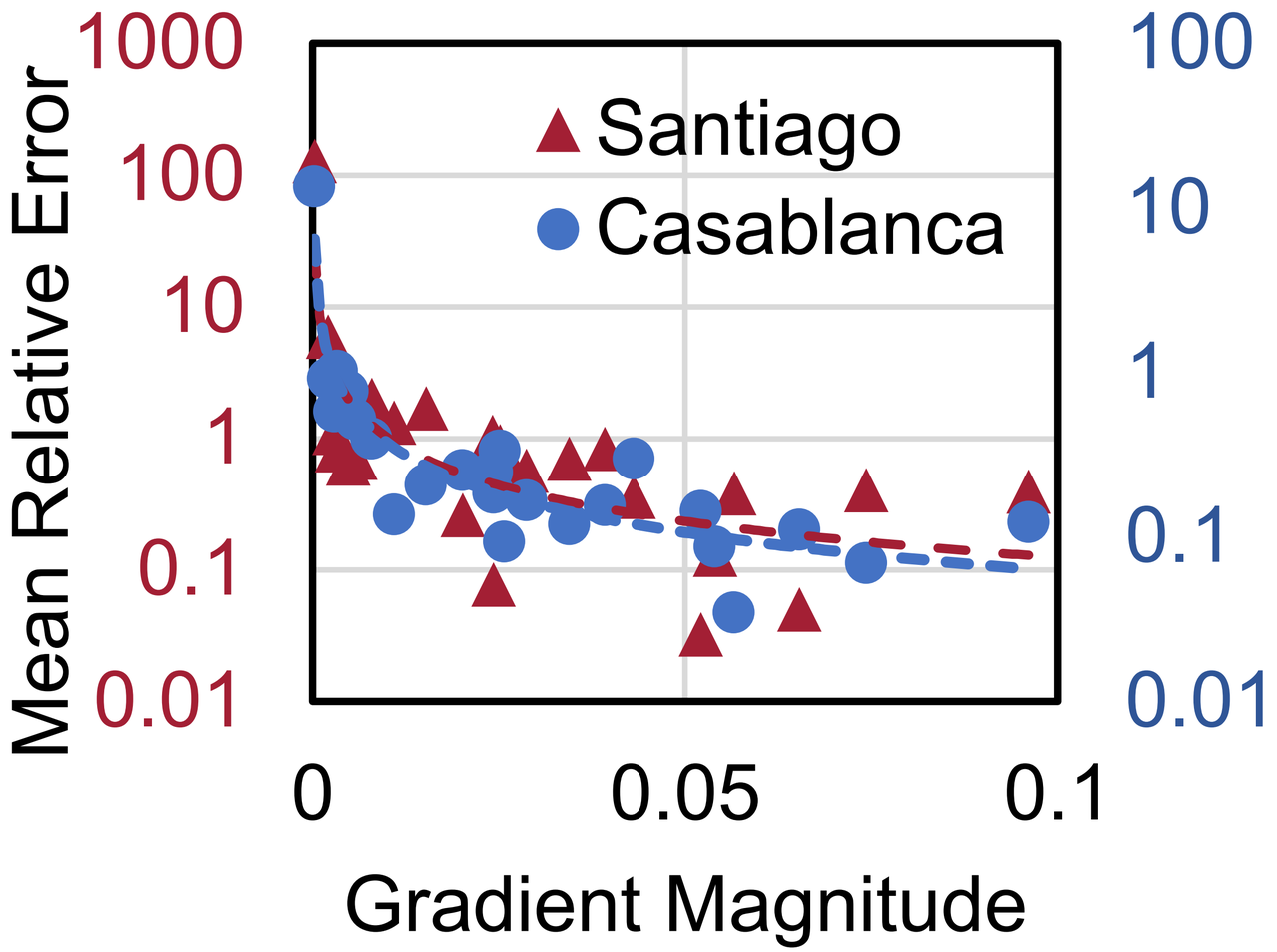
- Only **forward** on quantum device



Torch Quantum

Probabilistic Gradient Pruning

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



Torch Quantum

Materials at: https://torchquantum.org

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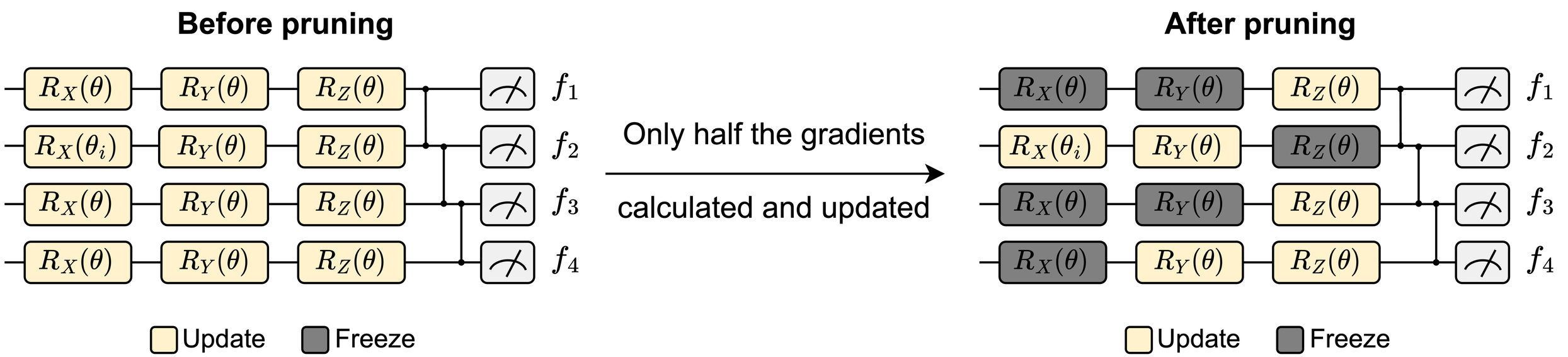
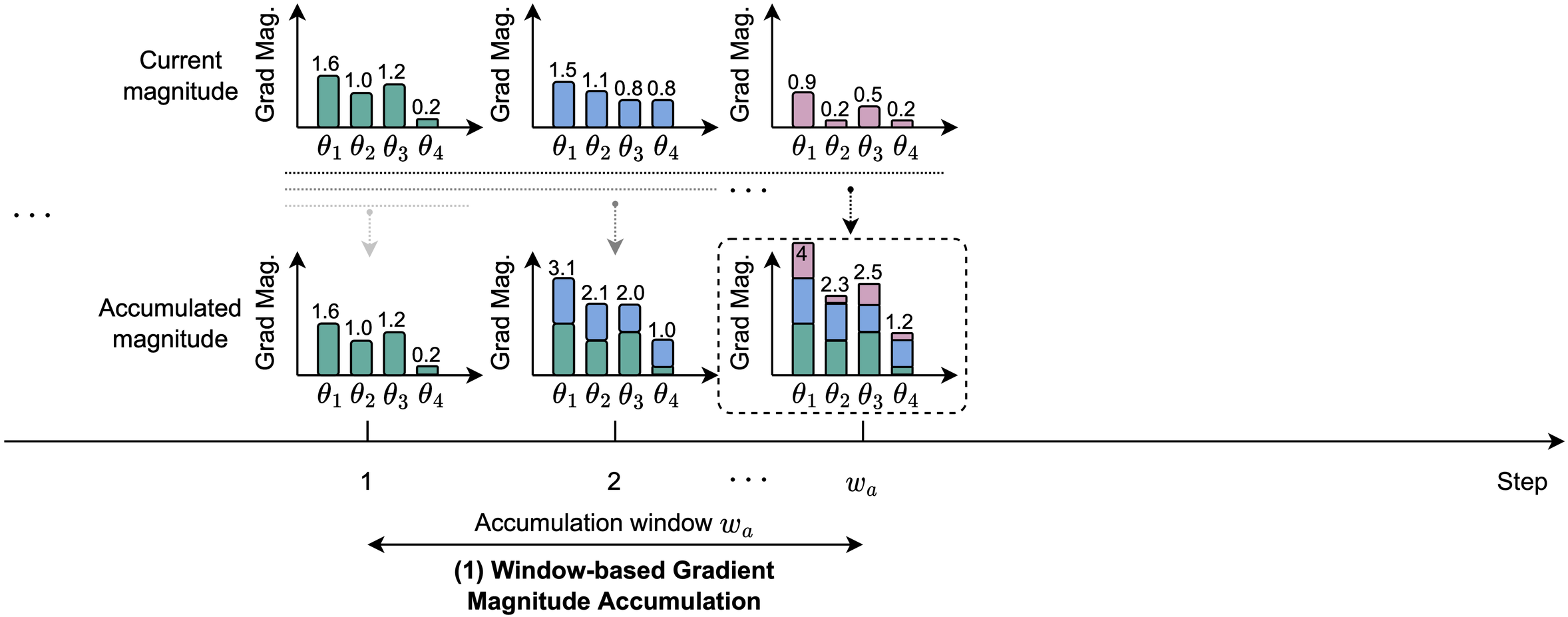
Probabilistic Gradient Pruning



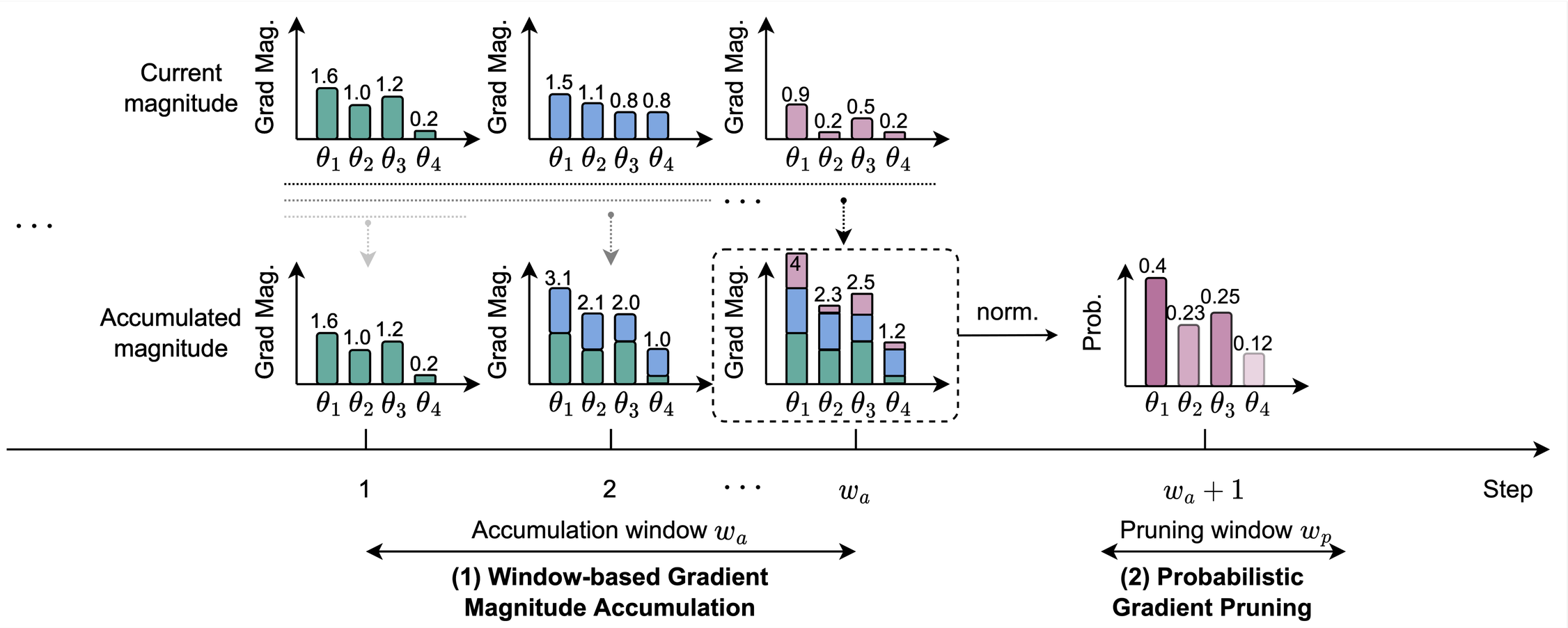
Accumulation Window

- Keep a record of accumulated gradient magnitude



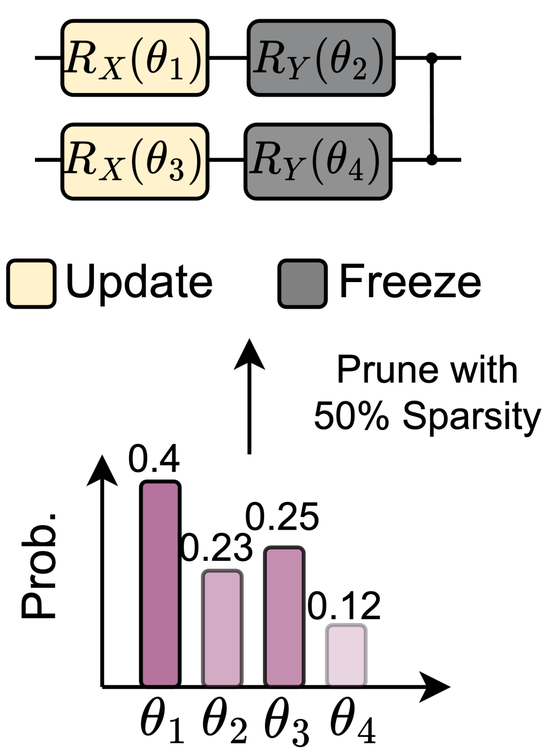
Accumulation Window

- Normalize the accumulated gradient magnitude to a probability distribution



Accumulation Window

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



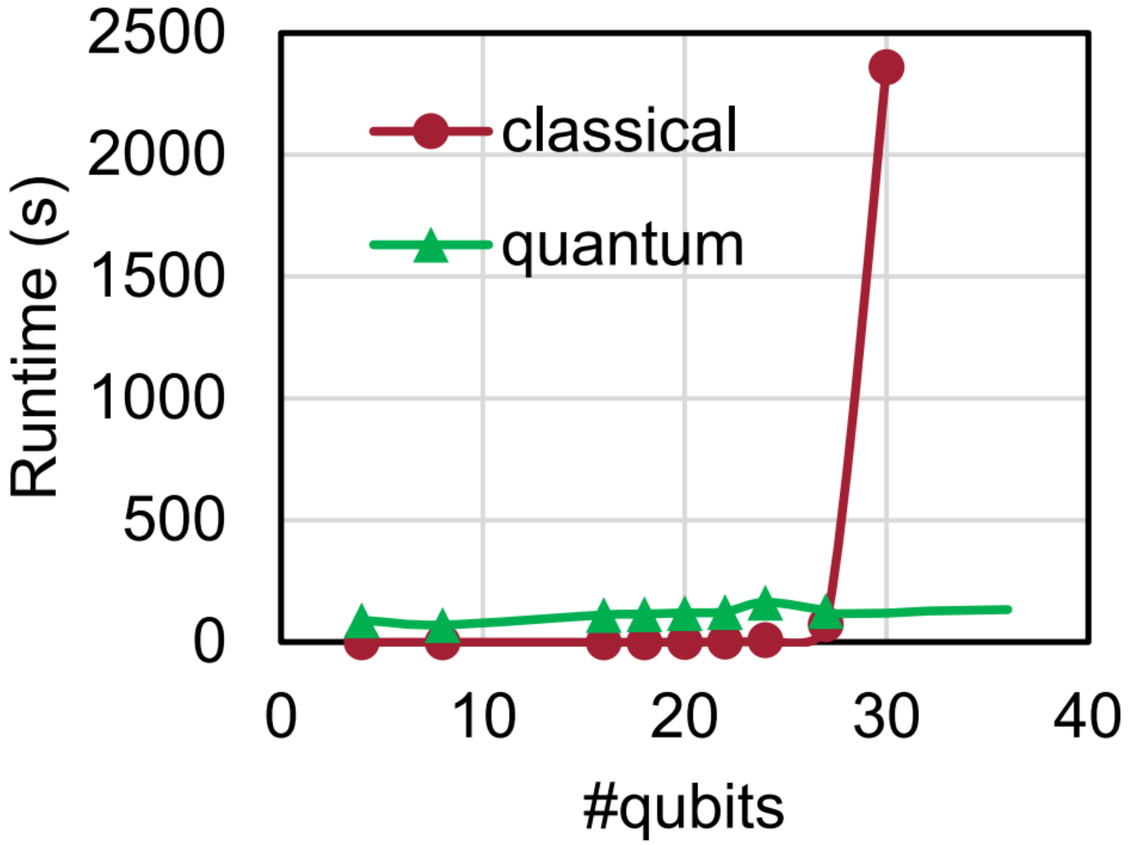
QNN results

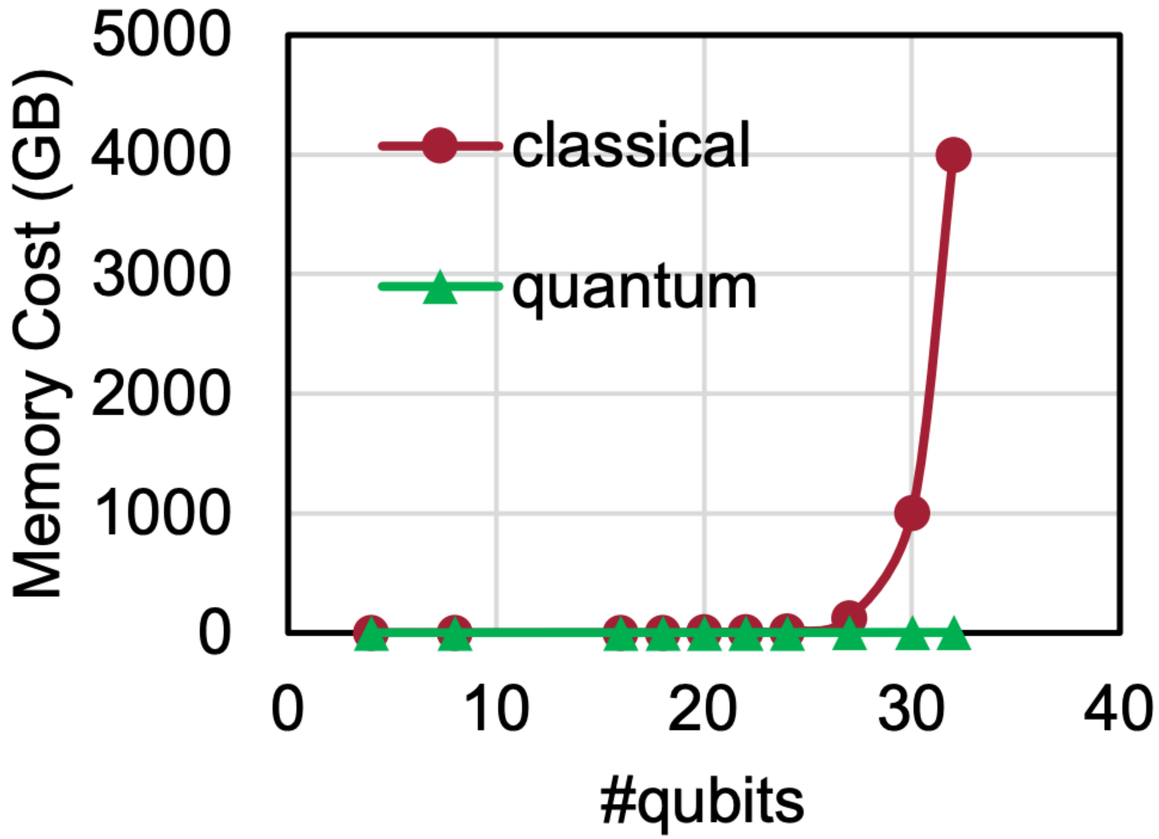
- QOC achieved similar results to classical simulation

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**

Scalability Improvements

- On-chip Training is scalable





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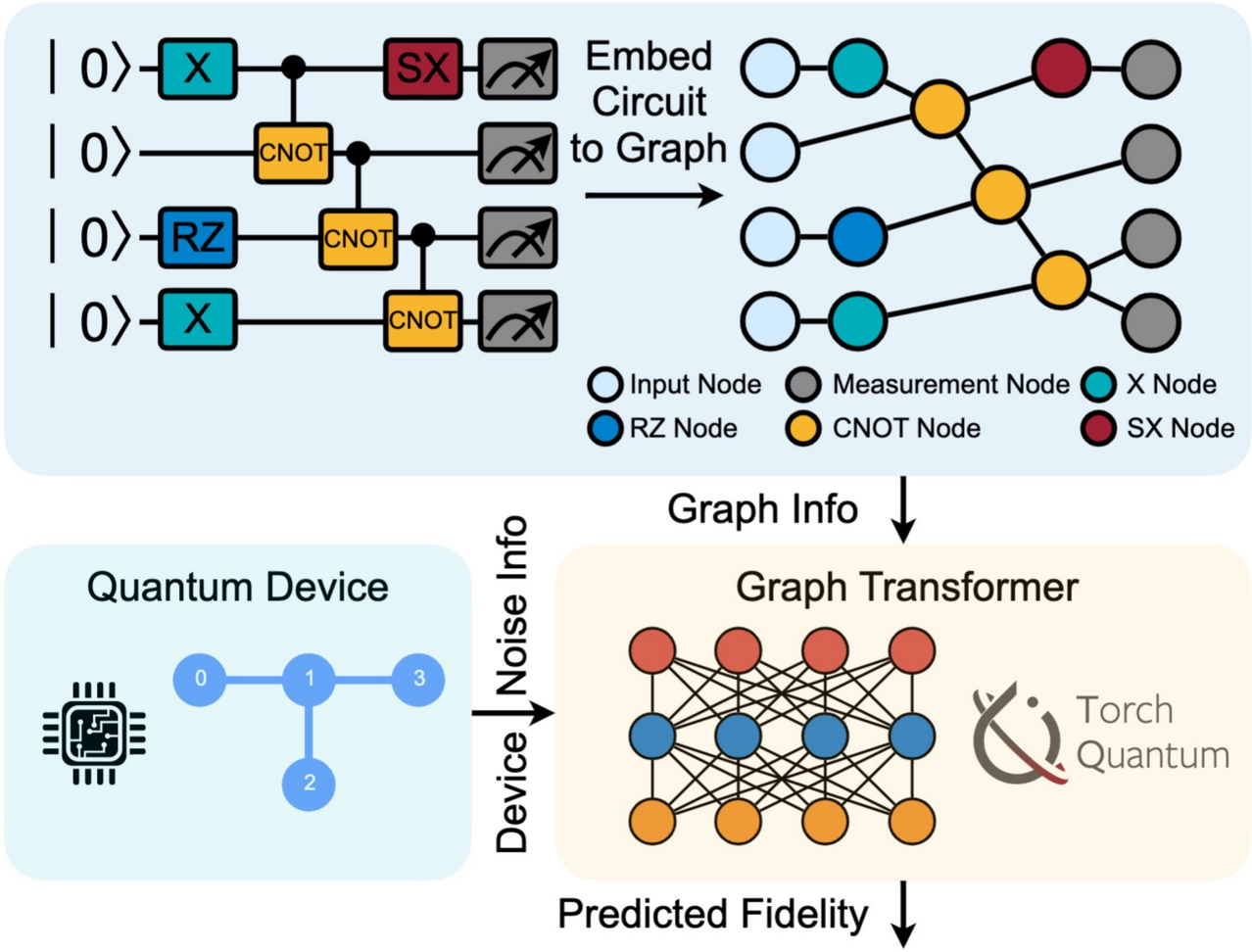
Transformer for Quantum Circuit Reliability Prediction

- Use the circuit graph information



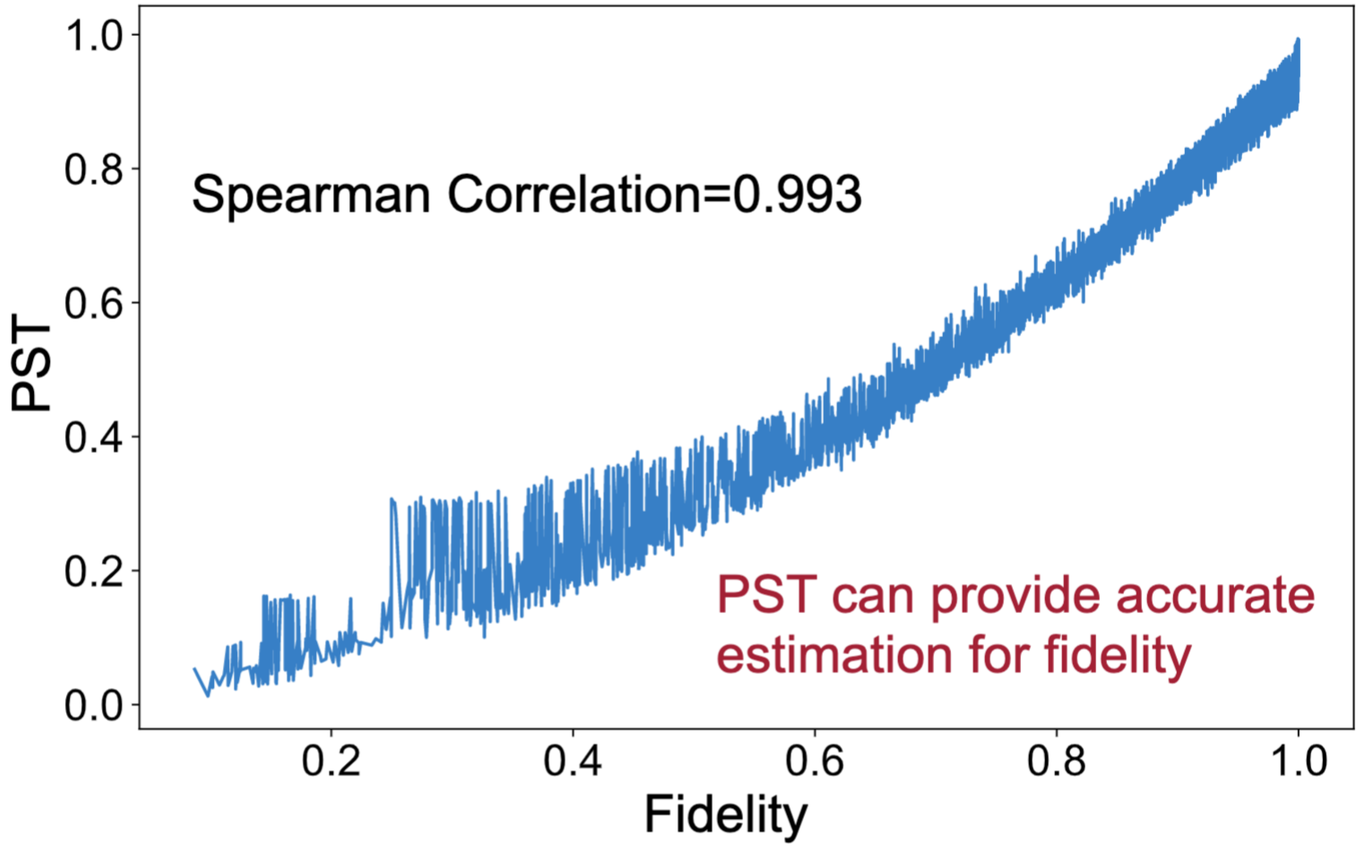
Torch Quantum

Materials at: https://torchquantum.org

Transformer for Quantum Circuit Reliability Prediction

- Use PST as the metrics

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



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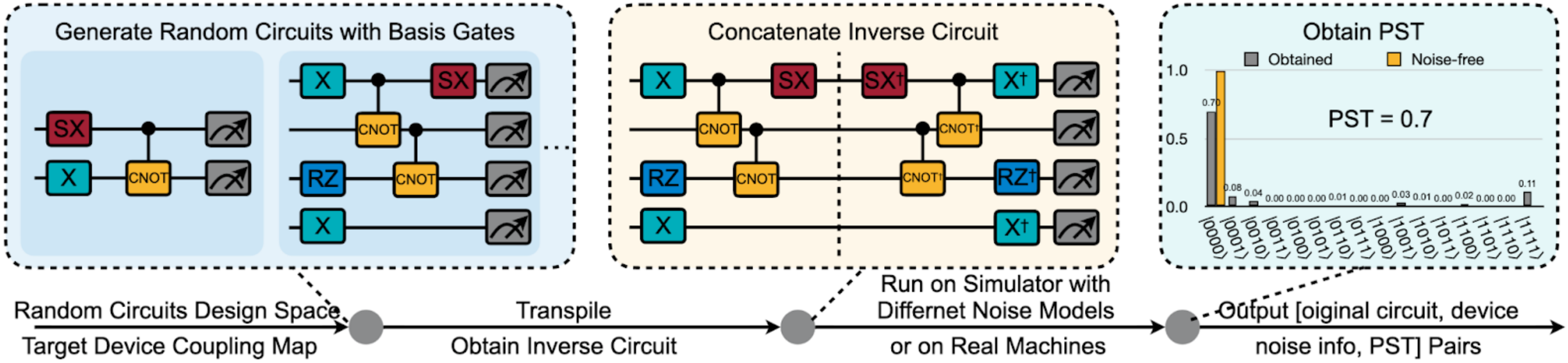
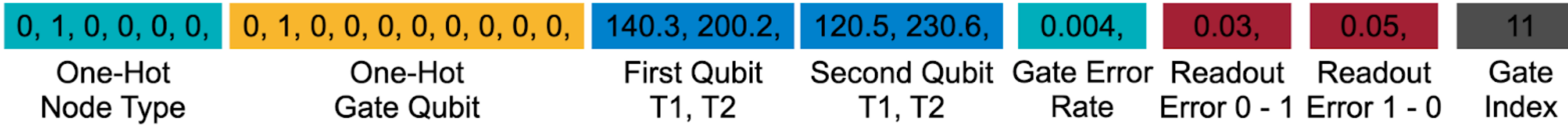
Dataset collection

- Collect dataset on real machine / noisy simulator

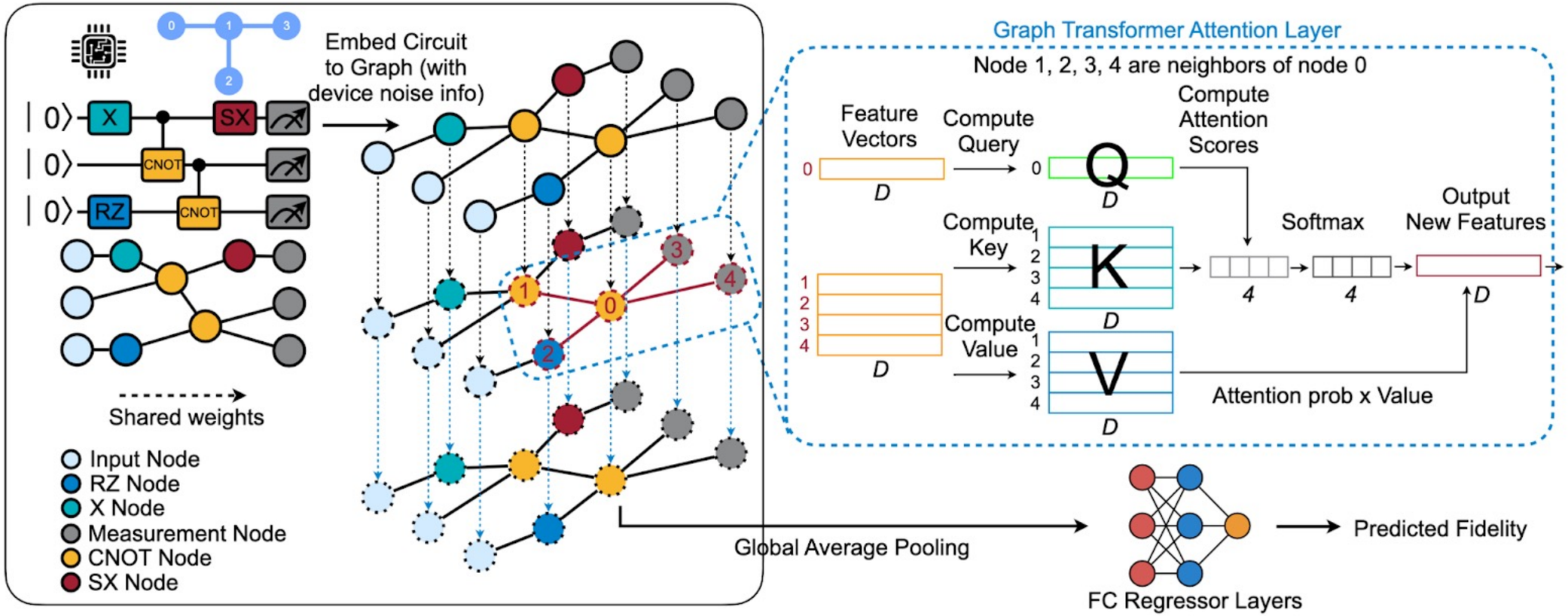


Features on each node



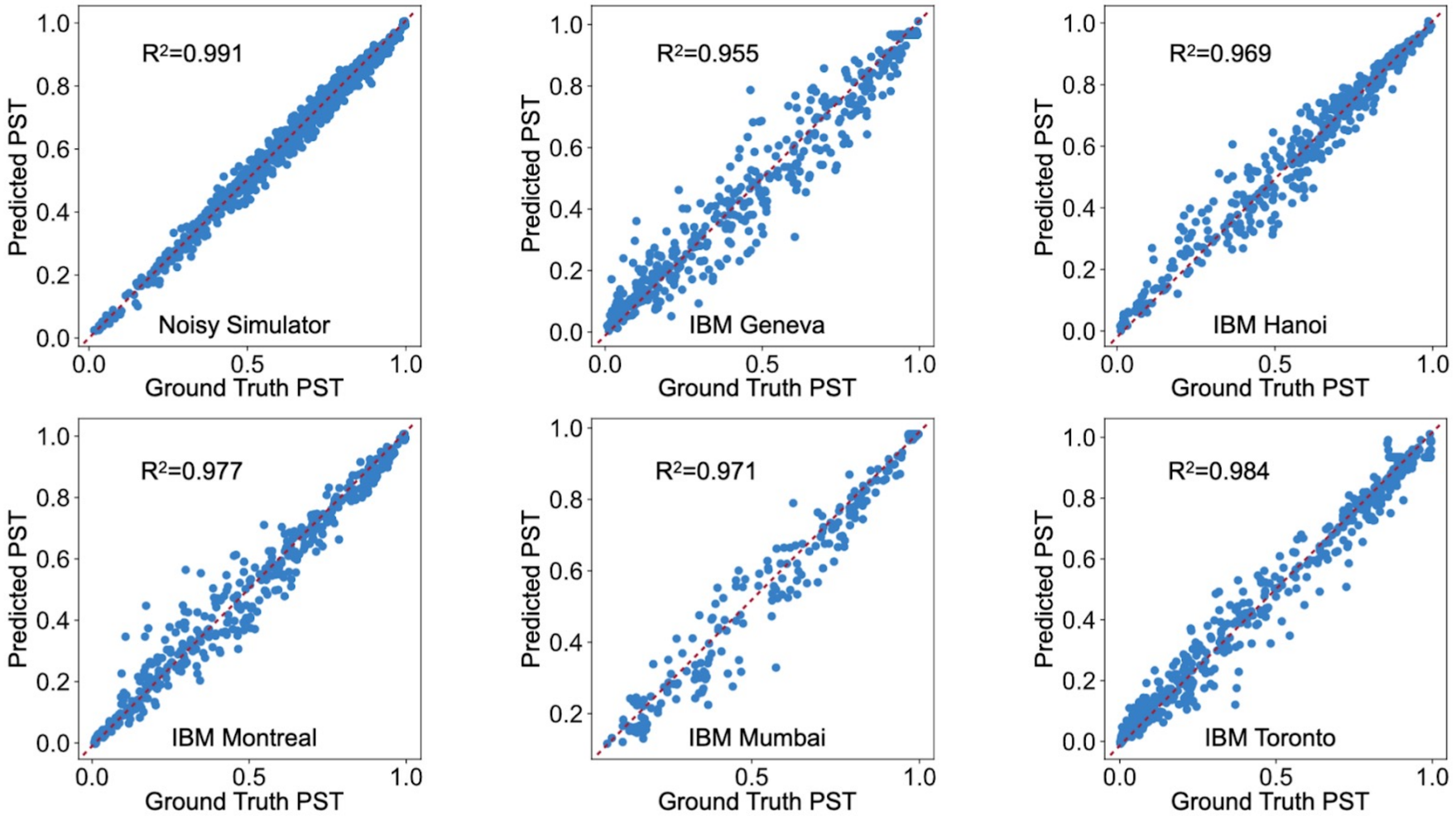
Graph Transformer

- Graph Transformer



Evaluation

- On random generated circuit



Torch Quantum

Materials at: https://torchquantum.org

TorchQuantum Tutorial Outline

Section 1

Quantum Basics and TorchQuantum Usage

1.1 Introduction to Quantum Computing (Prof. Yongshan Ding)

1.2 TorchQuantum API and examples (Hanrui Wang)

Section 2

Use TorchQuantum on Gate Level Optimization

2.1 QuantumNAS Ansatz Search and On-Chip Training (Hanrui Wang)

2.2 Variational Quantum Circuit Compression (Prof. Weiwen Jiang)

2.3 Various VQA Gradient Estimation Methods (Dantong Li)

Section 3

Use TorchQuantum on Pulse Level Optimization

3.1 Intro to Pulse Level Quantum Control (Zhiding Liang)

3.2 Variational Pulse Learning & Optimal Control (Jinglei Cheng)

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Materials at: https://torchquantum.org

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Thank you for listening!

Torch Quantum

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

qmlsys.mit.edu