

# EfficientML.ai Lecture 23

## Quantum Machine Learning

Part II



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# Lecture Plan

Today we will:

1. Introduce Parameterized Quantum Circuit (PQC)
2. Introduce PQC Training
3. Introduce Quantum Classifiers
4. Introduce Noise Aware On-Chip Training (QOC) of PQC
5. Introduce TorchQuantum Library for QML
6. Introduce Robust Quantum Architecture Search

# Section 1

## Parameterized Quantum Circuit

# QML Approaches

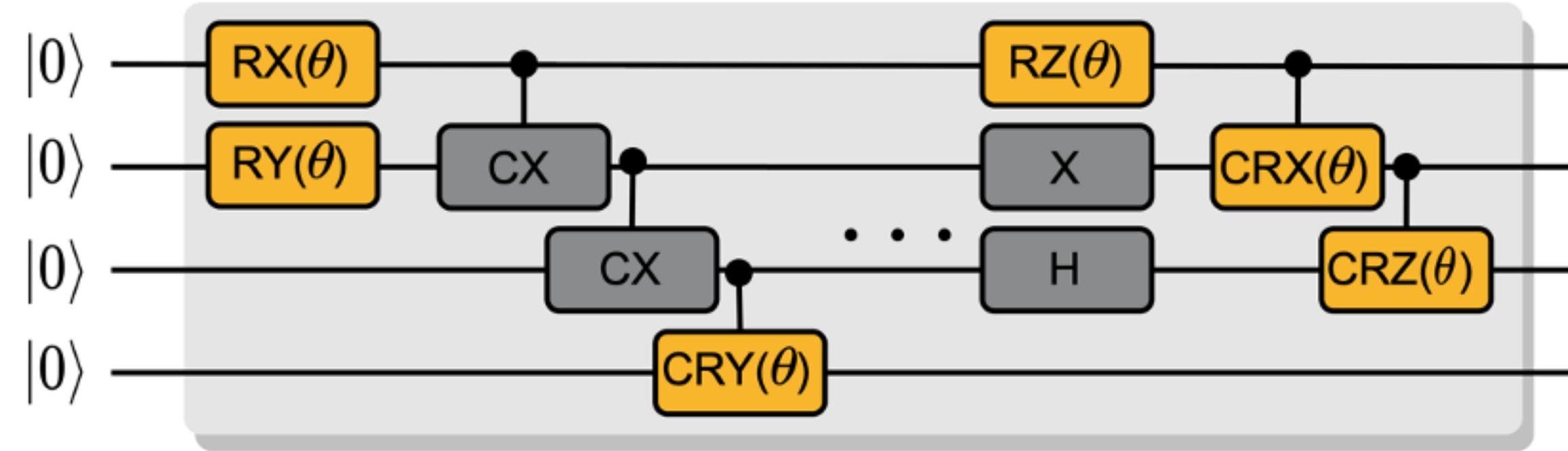
- CC: Classical Data, Classical algorithm: what we have learned from previous lectures
- CQ: Classical Data, Quantum algorithm: what we are going to introduce
- QC: Quantum Data, Classical algorithm: qubit control, calibration, readout...
- QQ: Quantum Data, Quantum algorithm: process quantum info with quantum machine

Type of algorithm	
Type of data	
CC	CQ
QC	QQ

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# Parameterized Quantum Circuits

- Circuit that contains fixed gates and parameterized gates

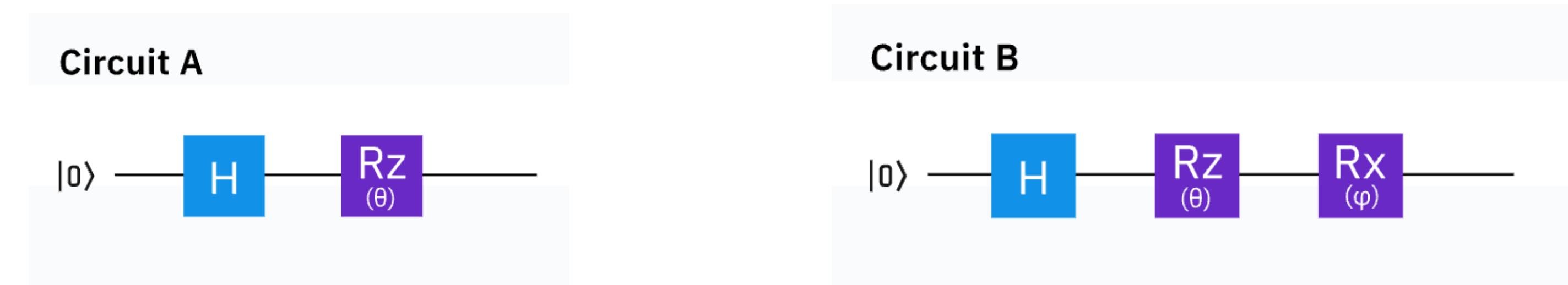


$$CNOT = \begin{array}{c|cccc} & \text{Input} & \text{00} & \text{01} & \text{10} & \text{11} \\ \hline & \text{00} & \begin{bmatrix} 1 & 0 & 0 & 0 \end{bmatrix} \\ & \text{01} & \begin{bmatrix} 0 & 1 & 0 & 0 \end{bmatrix} \\ & \text{10} & \begin{bmatrix} 0 & 0 & 0 & 1 \end{bmatrix} \\ & \text{11} & \begin{bmatrix} 0 & 0 & 1 & 0 \end{bmatrix} \end{array}$$

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

# Expressivity

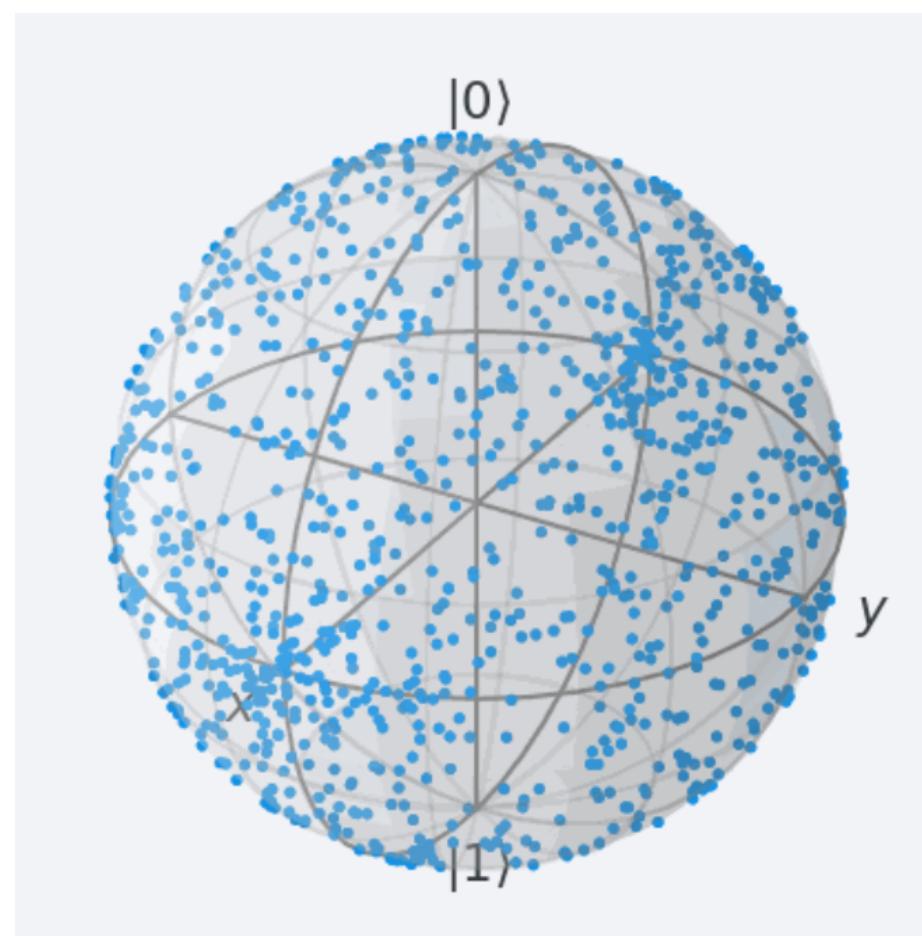
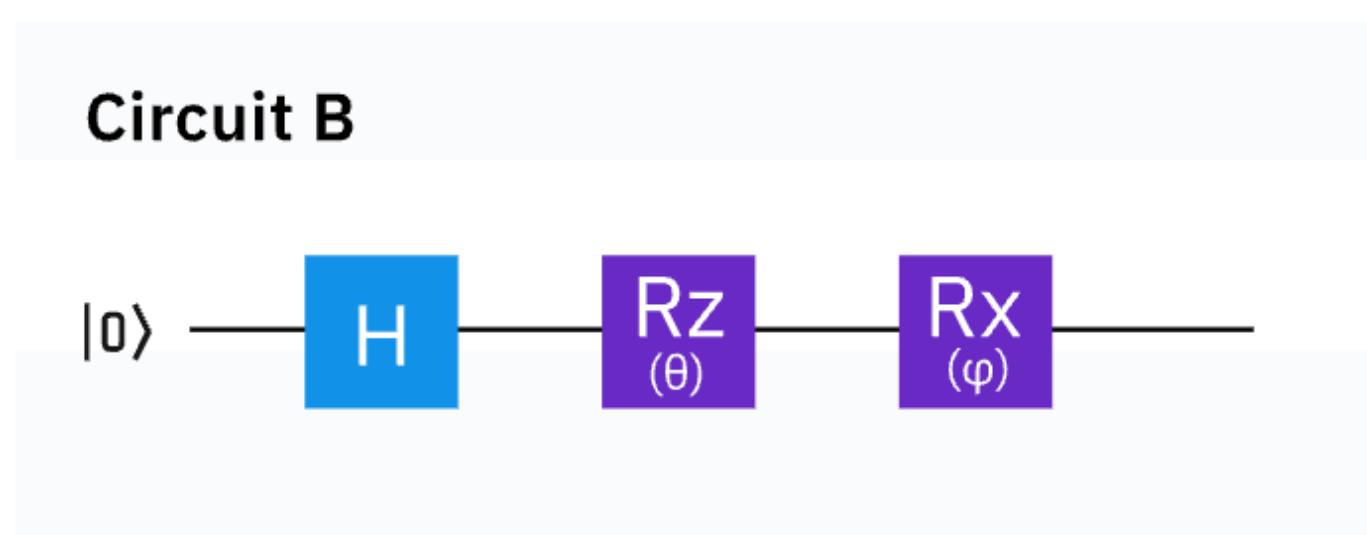
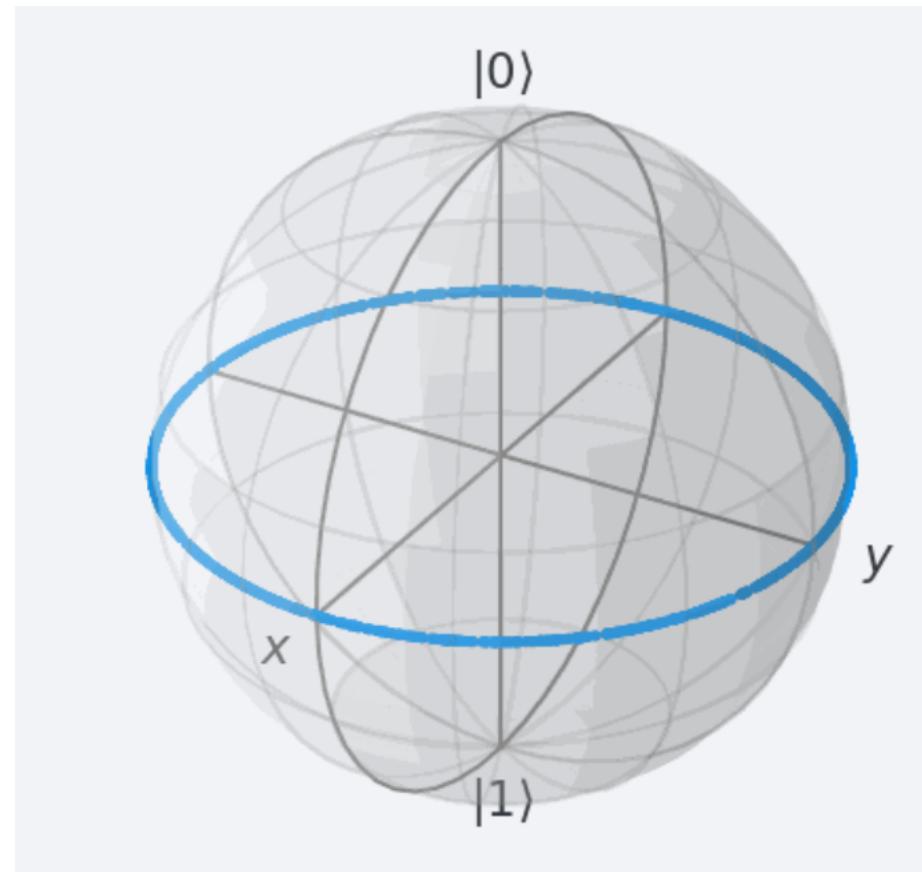
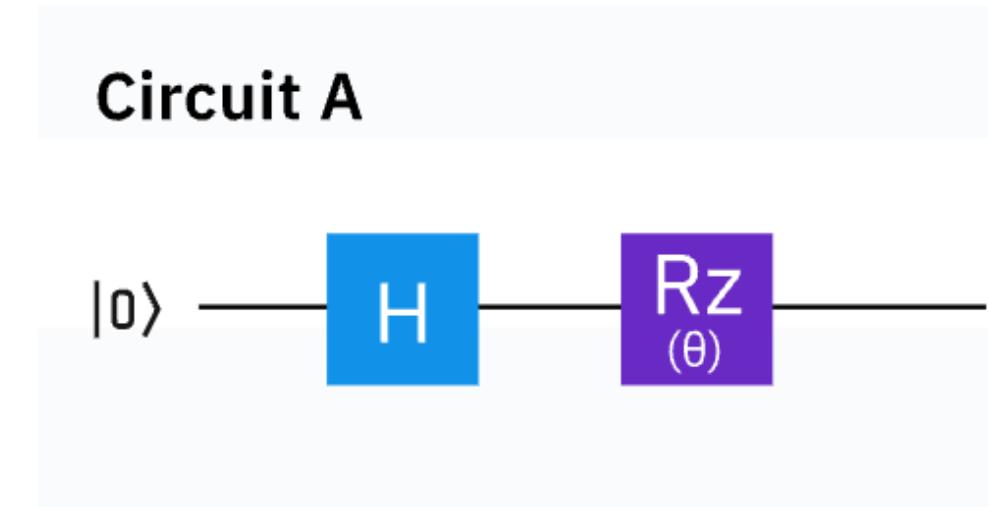
- How the quantum circuit can cover the **Hilbert space**?
- The extent to which the states generated from the circuit deviate from the **uniform** distribution
- Which circuit has **better expressivity** below?



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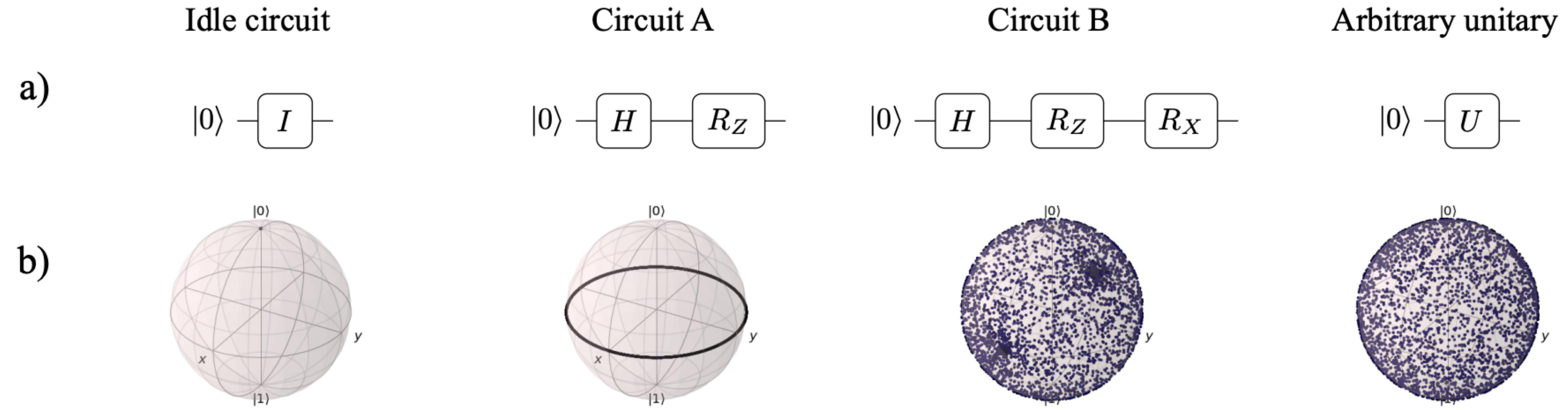
# Expressivity

- Circuit B has better **coverage** of Hilbert Space



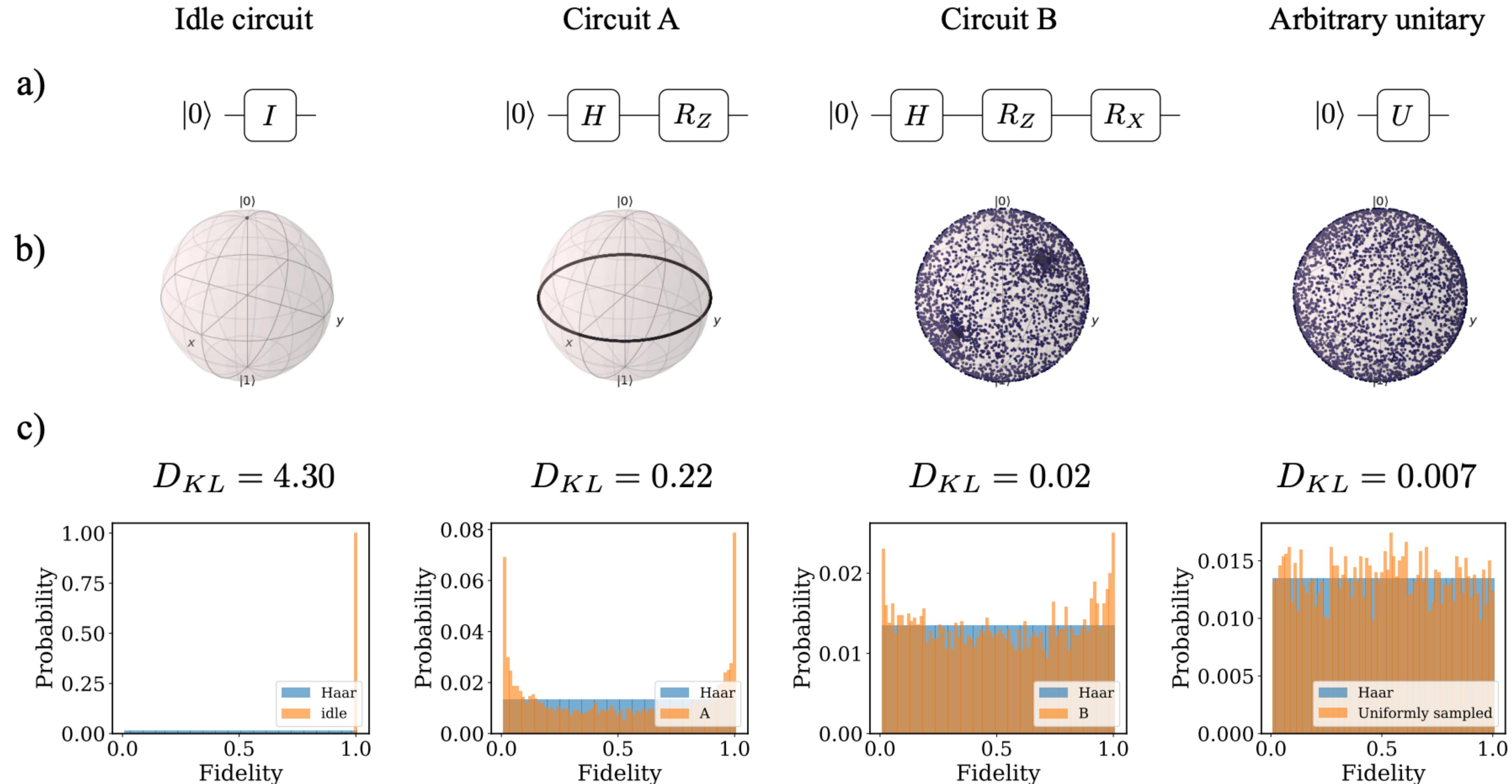
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# Expressivity



Expressibility and entangling capability of parameterized quantum circuits for hybrid quantum-classical algorithms

# Expressivity

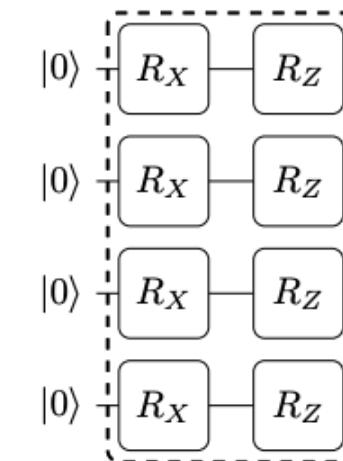


Expressivity and entangling capability of parameterized quantum circuits for hybrid quantum-classical algorithms

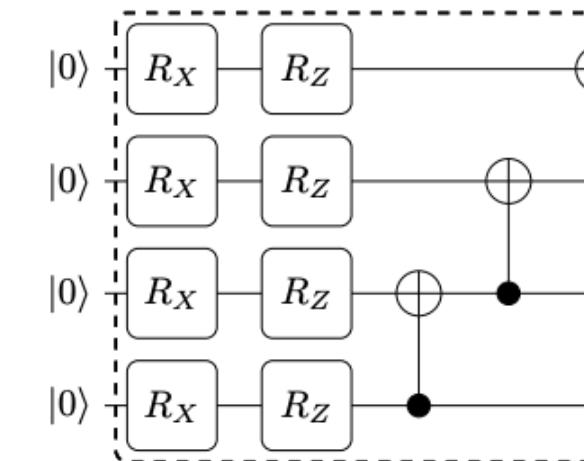
# Entanglement Capability

- The **Meyer-Wallach** measure tells how entangled a given state is; range [0, 1]
  - Unentangled state is 0
  - Full entangled state is 1
- We use **averaged MW** to measure the entanglement capability of circuit

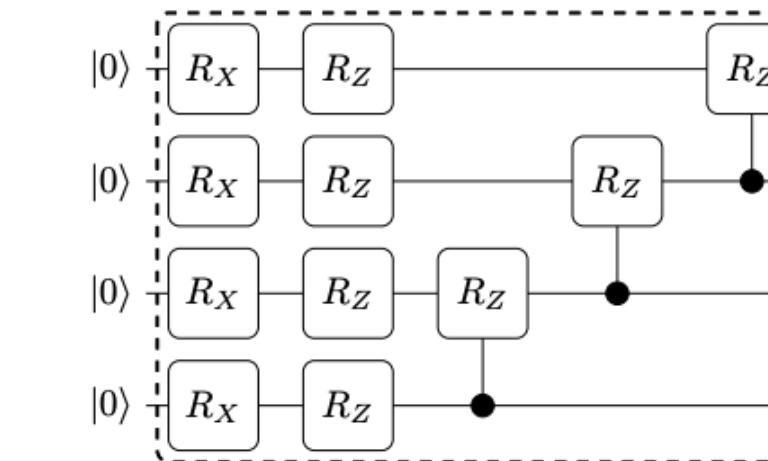
# Entanglement Capability



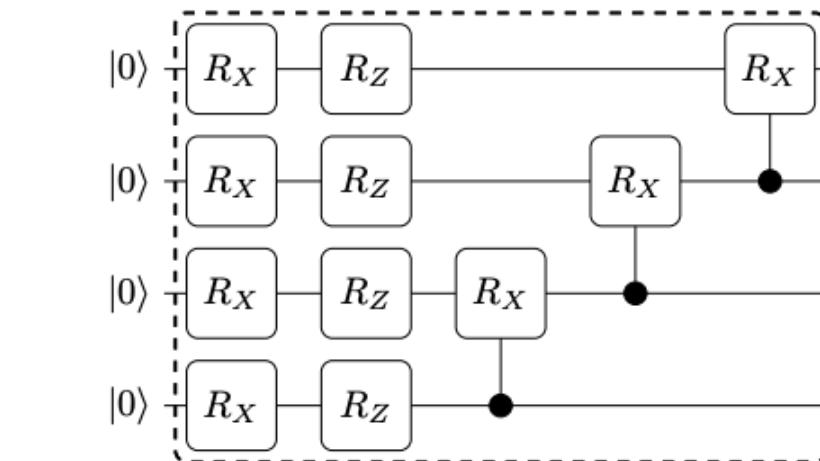
Circuit 1



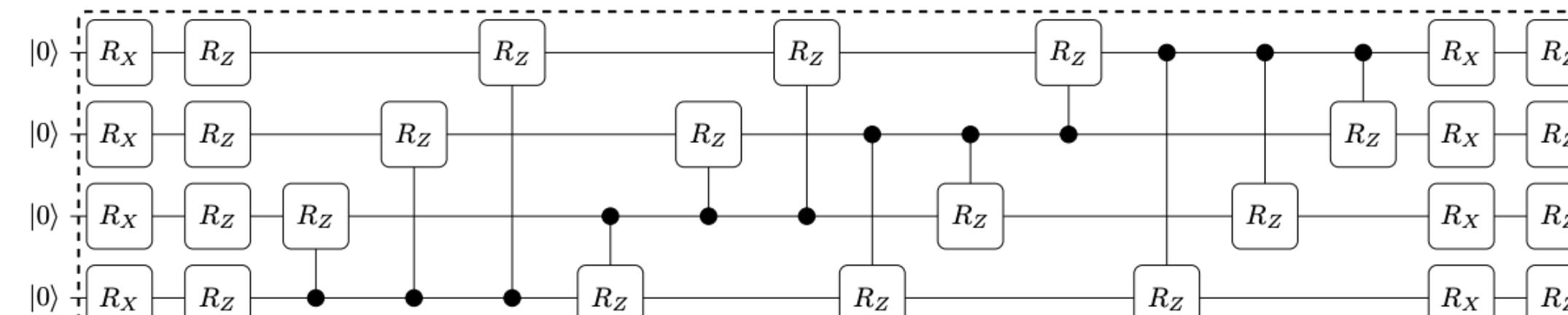
Circuit 2



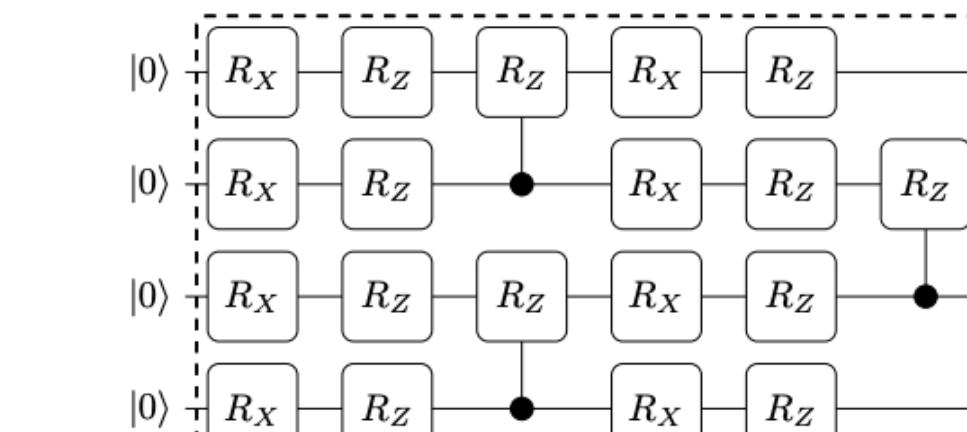
Circuit 3



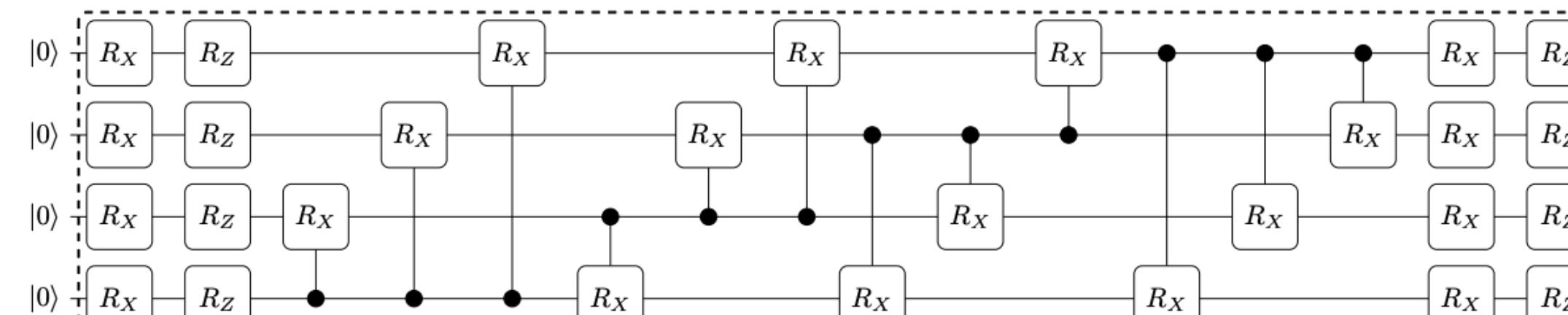
Circuit 4



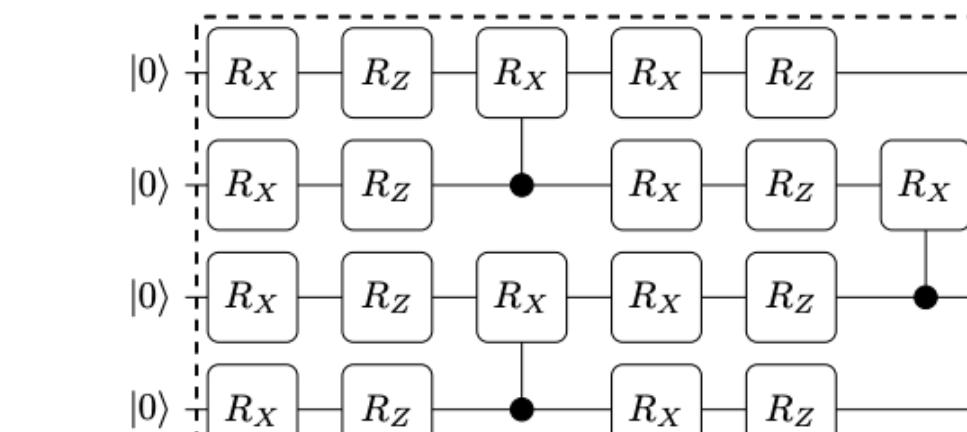
Circuit 5



Circuit 7



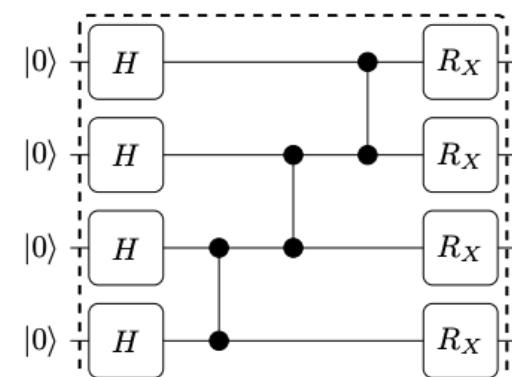
Circuit 6



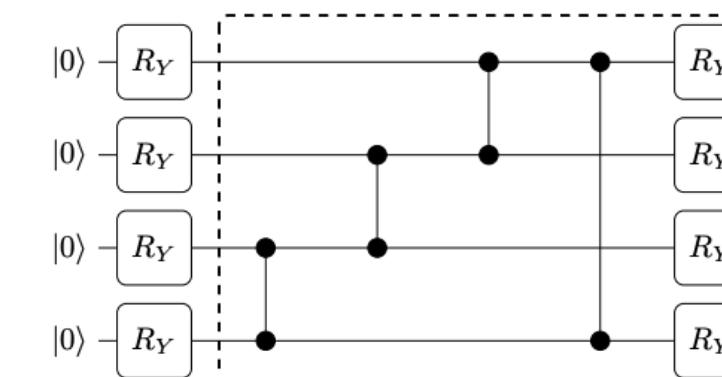
Circuit 8

Expressibility and entangling capability of parameterized quantum circuits for hybrid quantum-classical algorithms

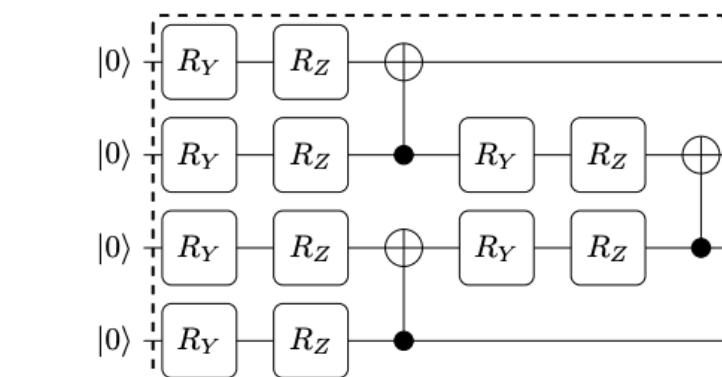
# Entanglement Capability



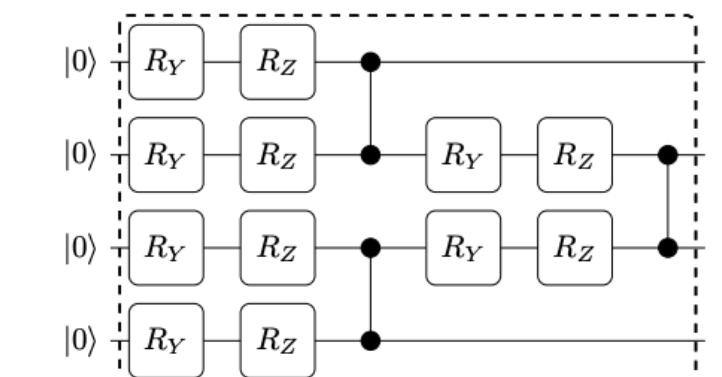
## Circuit 9



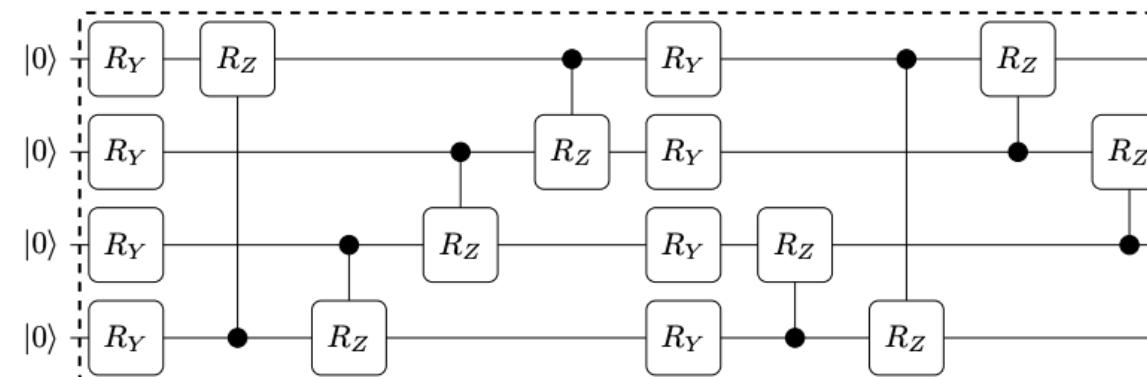
Circuit 10



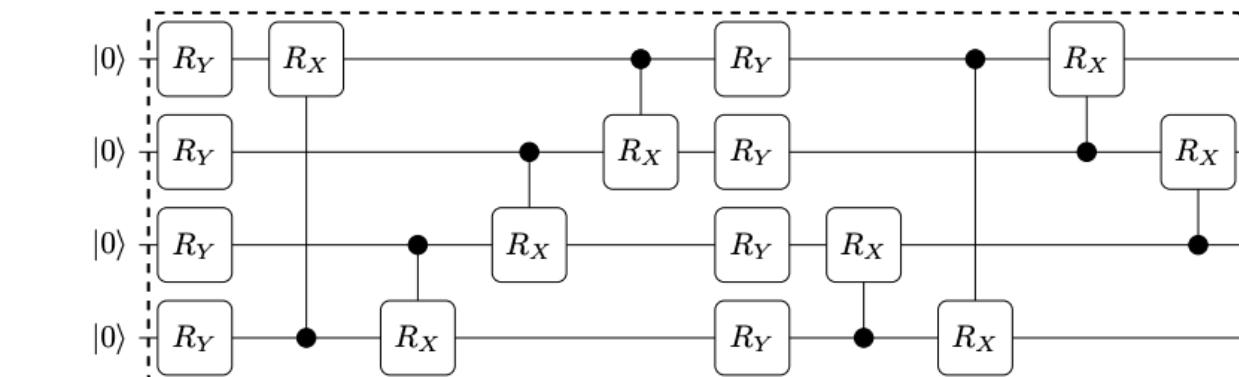
## Circuit 11



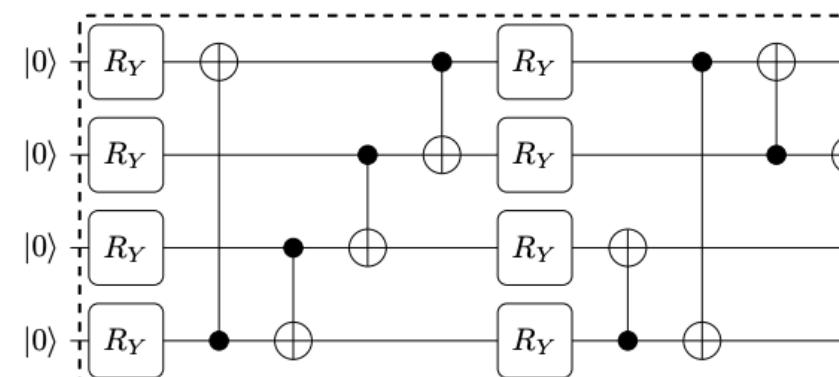
## Circuit 12



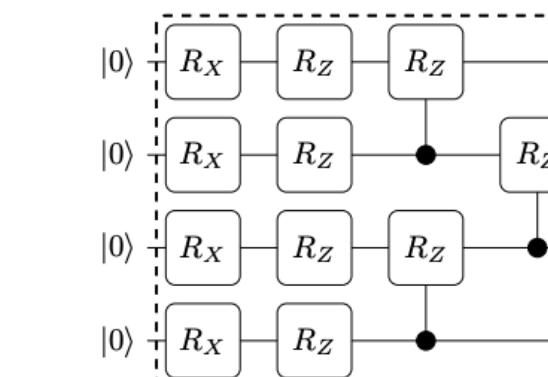
## Circuit 13



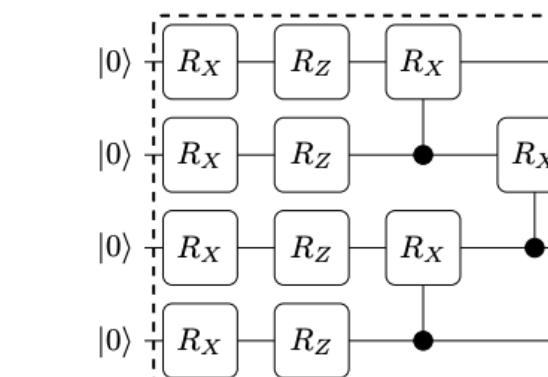
## Circuit 14



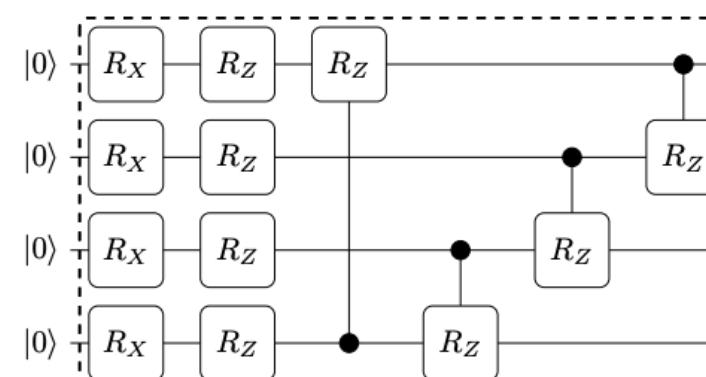
## Circuit 15



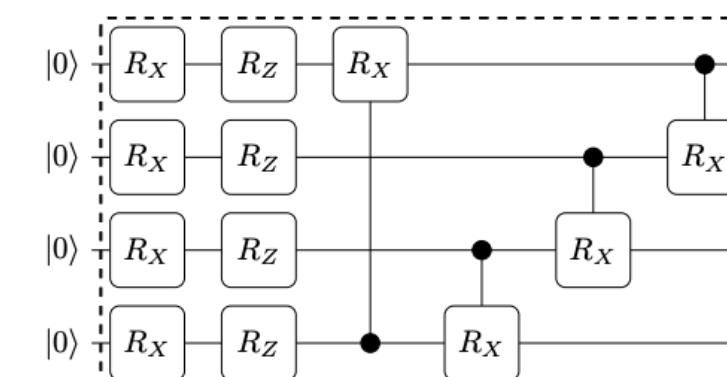
## Circuit 16



## Circuit 17



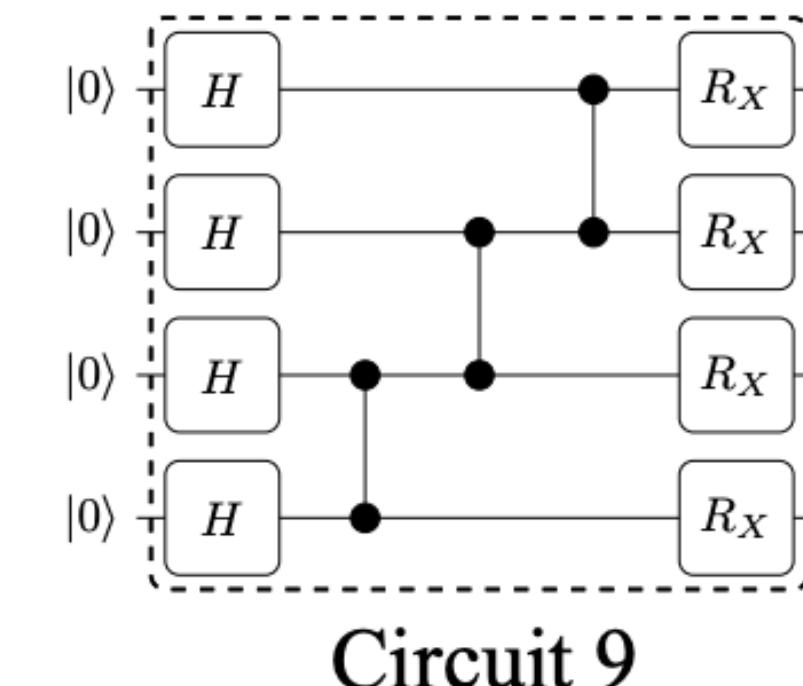
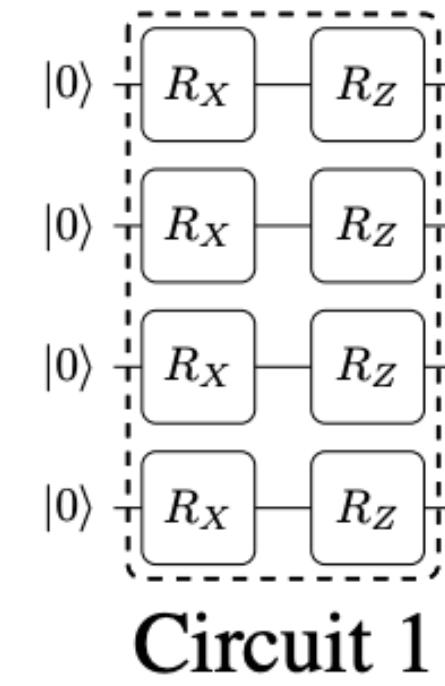
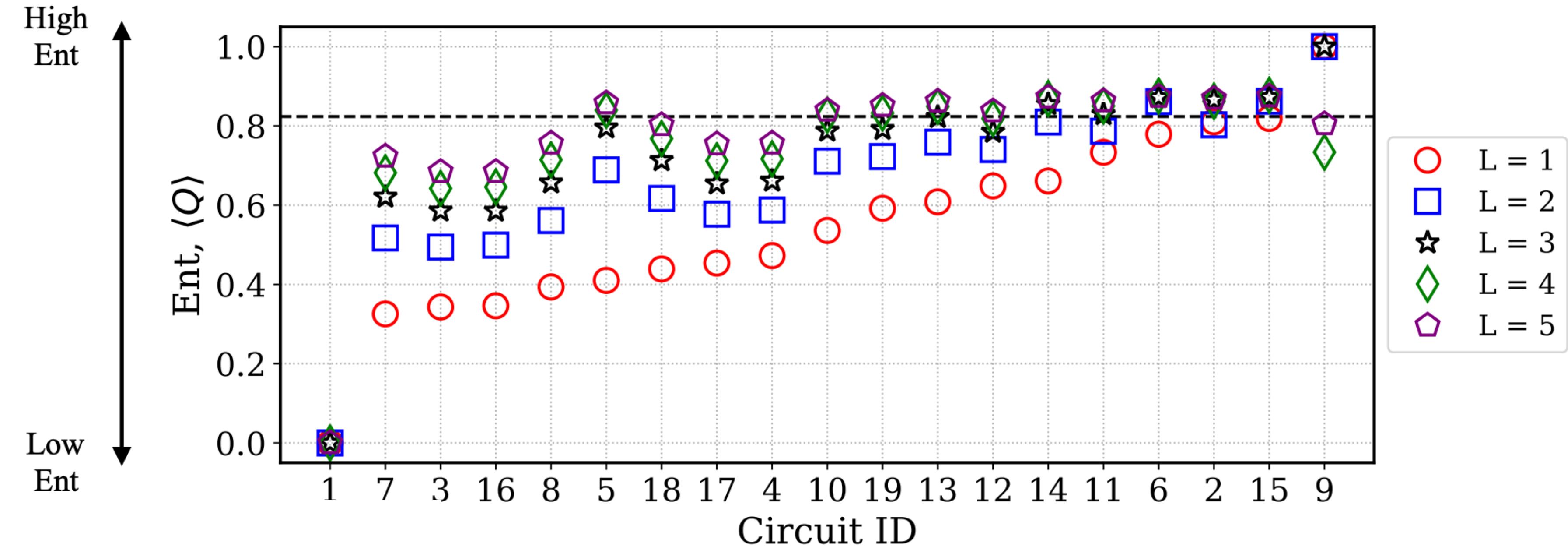
## Circuit 18



## Circuit 19

# Expressibility and entangling capability of parameterized quantum circuits for hybrid quantum-classical algorithms

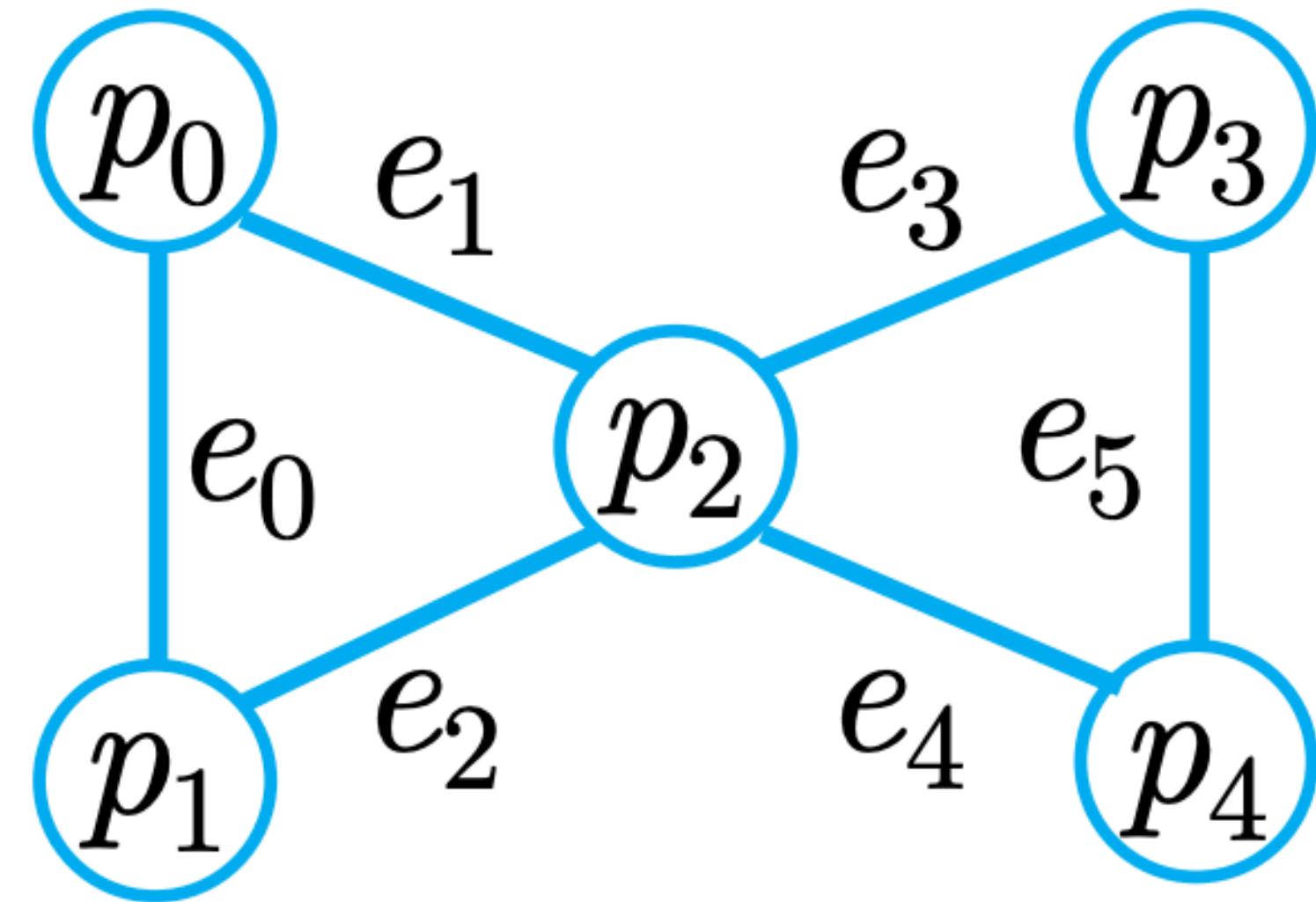
# Entanglement Capability



Expressibility and entangling capability of parameterized quantum circuits for hybrid quantum-classical algorithms

# Hardware Efficiency

- Whether the PQC design considers the qubit **connectivity**?
- Whether the gates are **native** gates?



# Data Encoding

- Consider a classical data set  $X$  consisting of  $M$  samples each with  $N$  features

$$\mathcal{X} = \{x^{(1)}, \dots, x^{(m)}, \dots, x^{(M)}\}$$

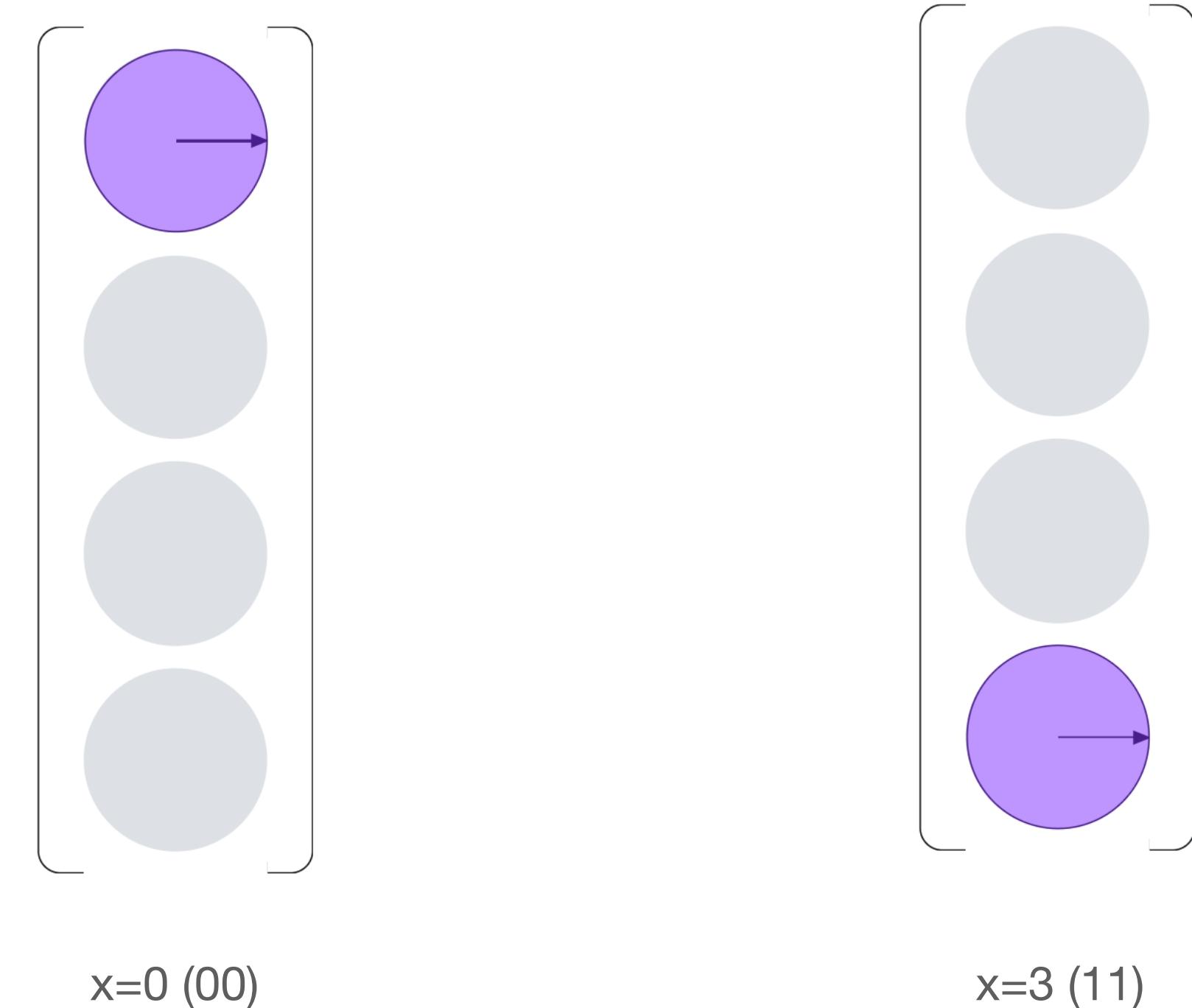
- **Encoding** methods:
  - Basis encoding
  - Amplitude encoding
  - Angle encoding
  - Arbitrary encoding

# Basis Encoding

- Similar to the **binary** representation in the classical machine
- $X = 2 \rightarrow$  binary “10”
- We create a quantum state with all energy on  $|10\rangle$

# Basis Encoding

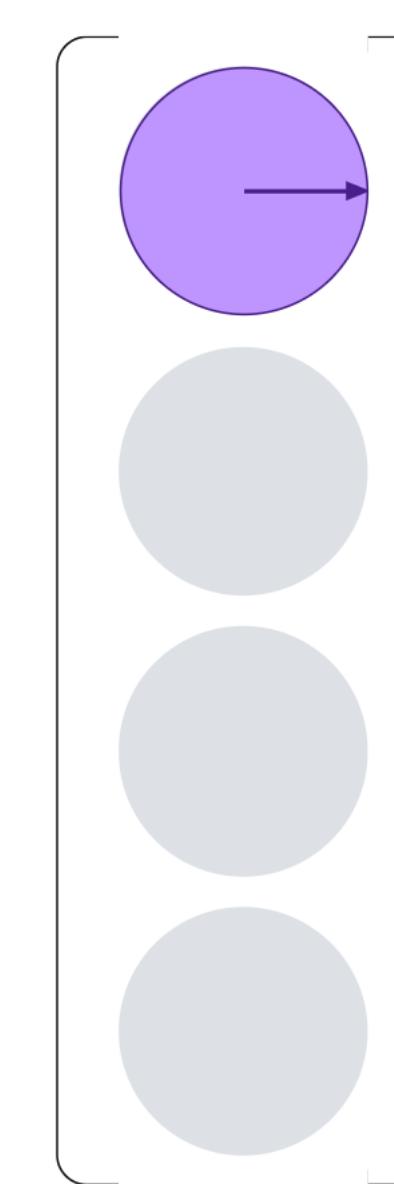
- Similar to the **binary** representation in the classical machine
- $X = 2 \rightarrow$  binary “10”
- Not efficient for one data



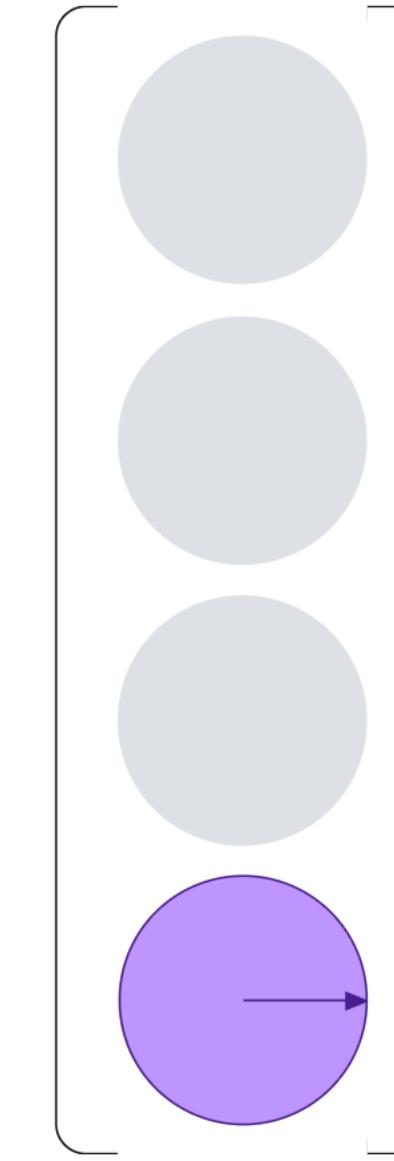
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# Basis Encoding

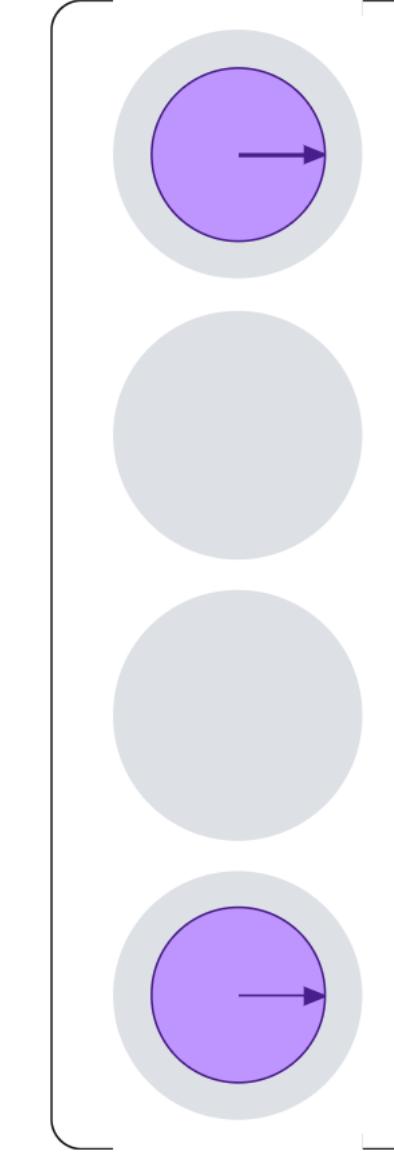
- Similar to the **binary** representation in the classical machine
- $X = 2 \rightarrow 10$
- Not efficient for one data but can be used to represent **multiple data simultaneously**



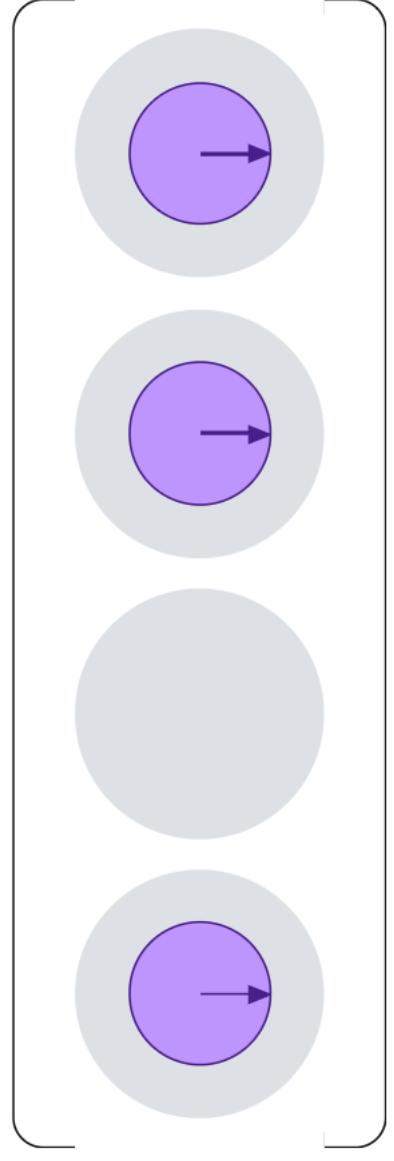
$x=0$  (00)



$x=3$  (11)



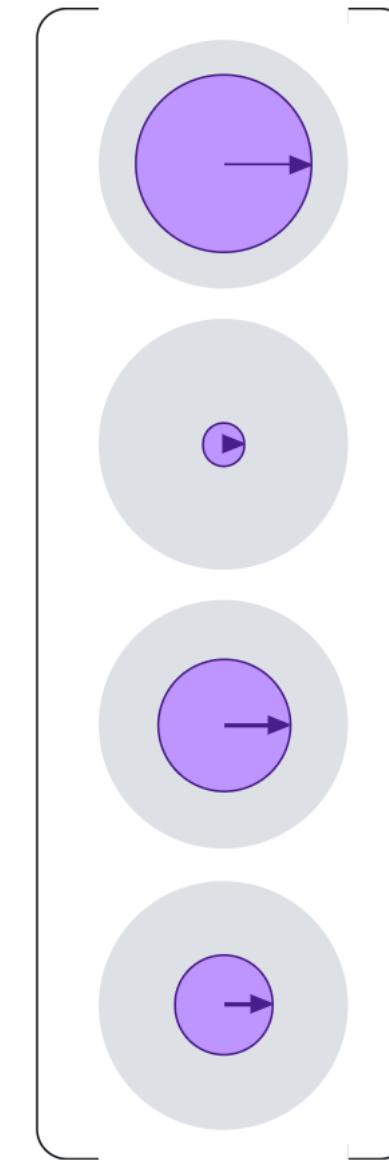
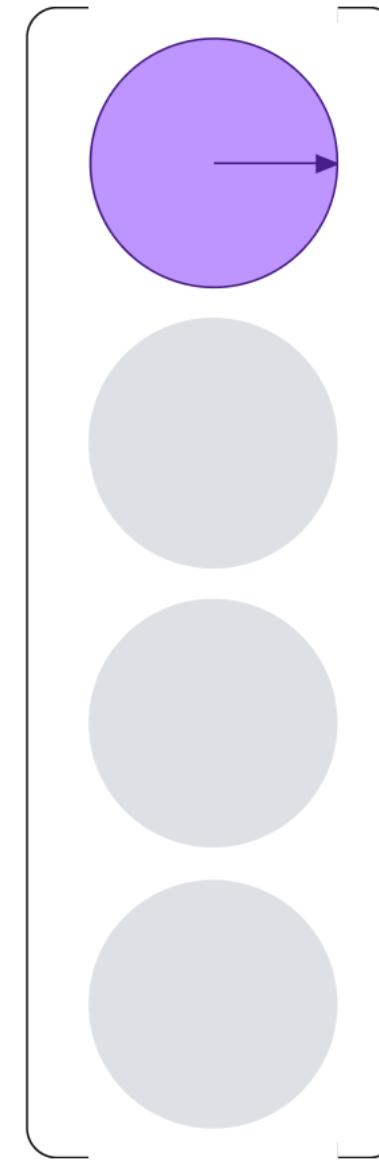
$x=0$  and  $3$  (00+11)



$x=0$  and  $1$  and  $3$  (00+ 01 +11)

# Amplitude Encoding

- The numbers are encoded as the **statevector** of the qubits
- input vector = [1, 0, 0, 0]                                      input vector = [0.8, 0.2, 0.6, 0.45]
- For N features, need **logN** qubits



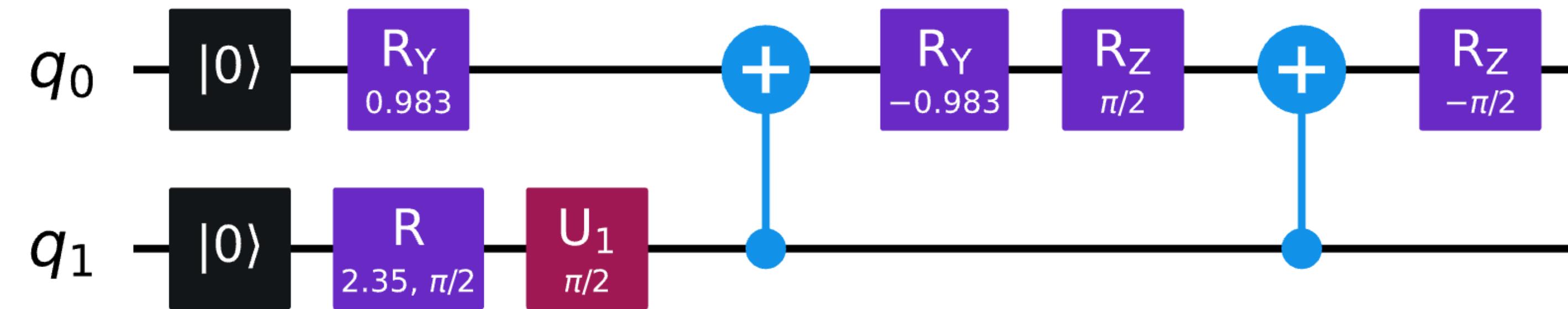
# Amplitude Encoding

- Also able to encode multiple data points together

$$\mathcal{X} = \{x^{(1)} = (1.5, 0), x^{(2)} = (-2, 3)\}$$

$$\alpha = \frac{1}{\sqrt{15.25}}(1.5, 0, -2, 3)$$

$$|\mathcal{X}\rangle = \frac{1}{\sqrt{15.25}}(1.5|00\rangle - 2|10\rangle + 3|11\rangle)$$



<https://qiskit.org/learn/>

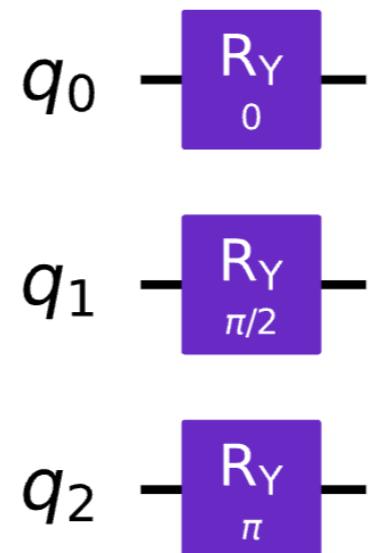
# Angle Encoding

- Encode the data in the **rotation** angles of the qubit gates
- For vector  $[0, \pi/2, \pi]$

$$|x\rangle = \bigotimes_{i=1}^N \cos(x_i)|0\rangle + \sin(x_i)|1\rangle$$

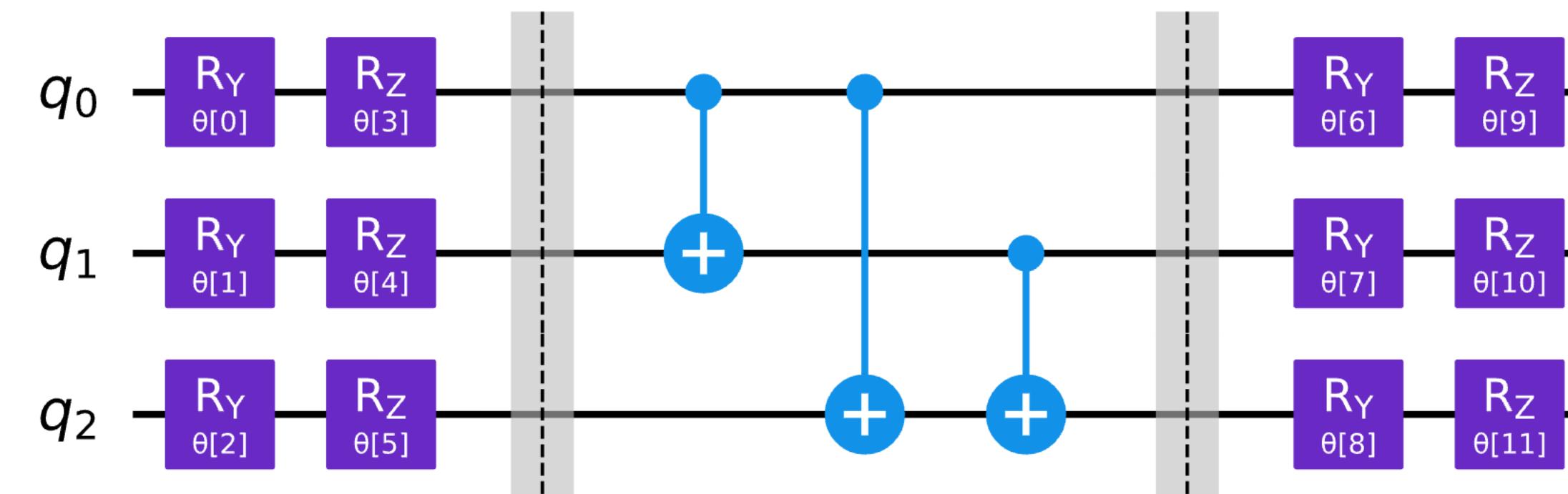
$$S_{x_j} = \bigotimes_{i=1}^N U(x_j^{(i)}) \quad U(x_j^{(i)}) = \begin{bmatrix} \cos(x_j^{(i)}) & -\sin(x_j^{(i)}) \\ \sin(x_j^{(i)}) & \cos(x_j^{(i)}) \end{bmatrix}$$

$$RY(\theta) = \exp(-i\frac{\theta}{2}Y) = \begin{pmatrix} \cos \frac{\theta}{2} & -\sin \frac{\theta}{2} \\ \sin \frac{\theta}{2} & \cos \frac{\theta}{2} \end{pmatrix}$$

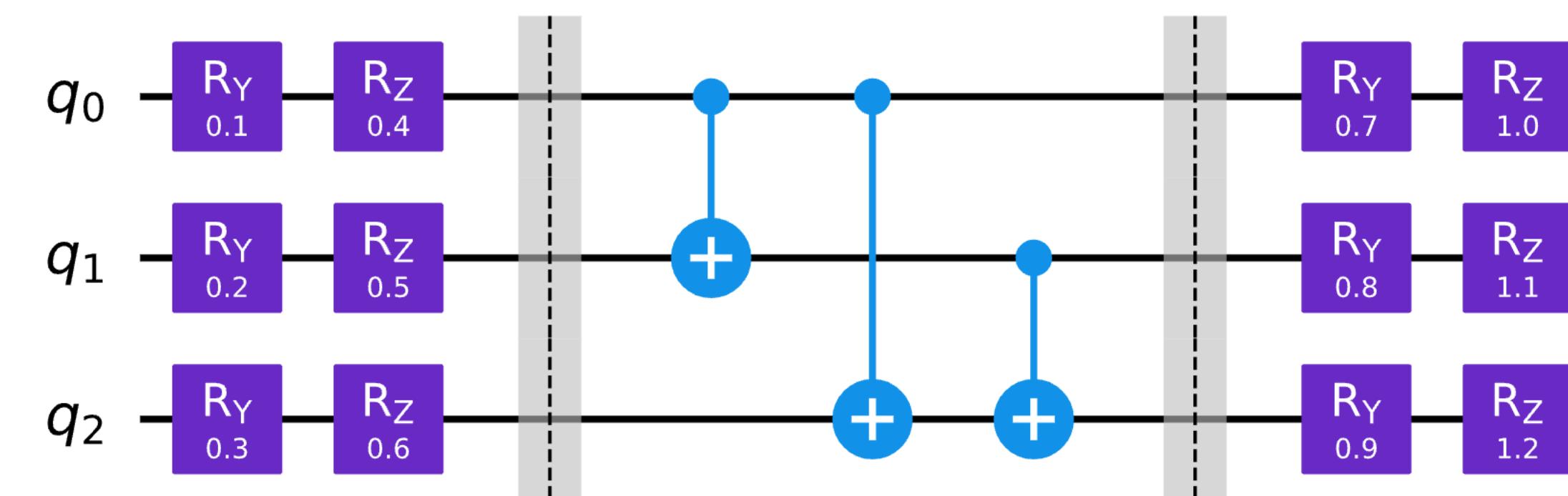


# Arbitrary Encoding

- Design **arbitrary** parameterized quantum circuit and let input data as the rotation angles



$$x = [0.1, 0.2, 0.3, 0.4, 0.5, 0.6, 0.7, 0.8, 0.9, 1.0, 1.1, 1.2]$$

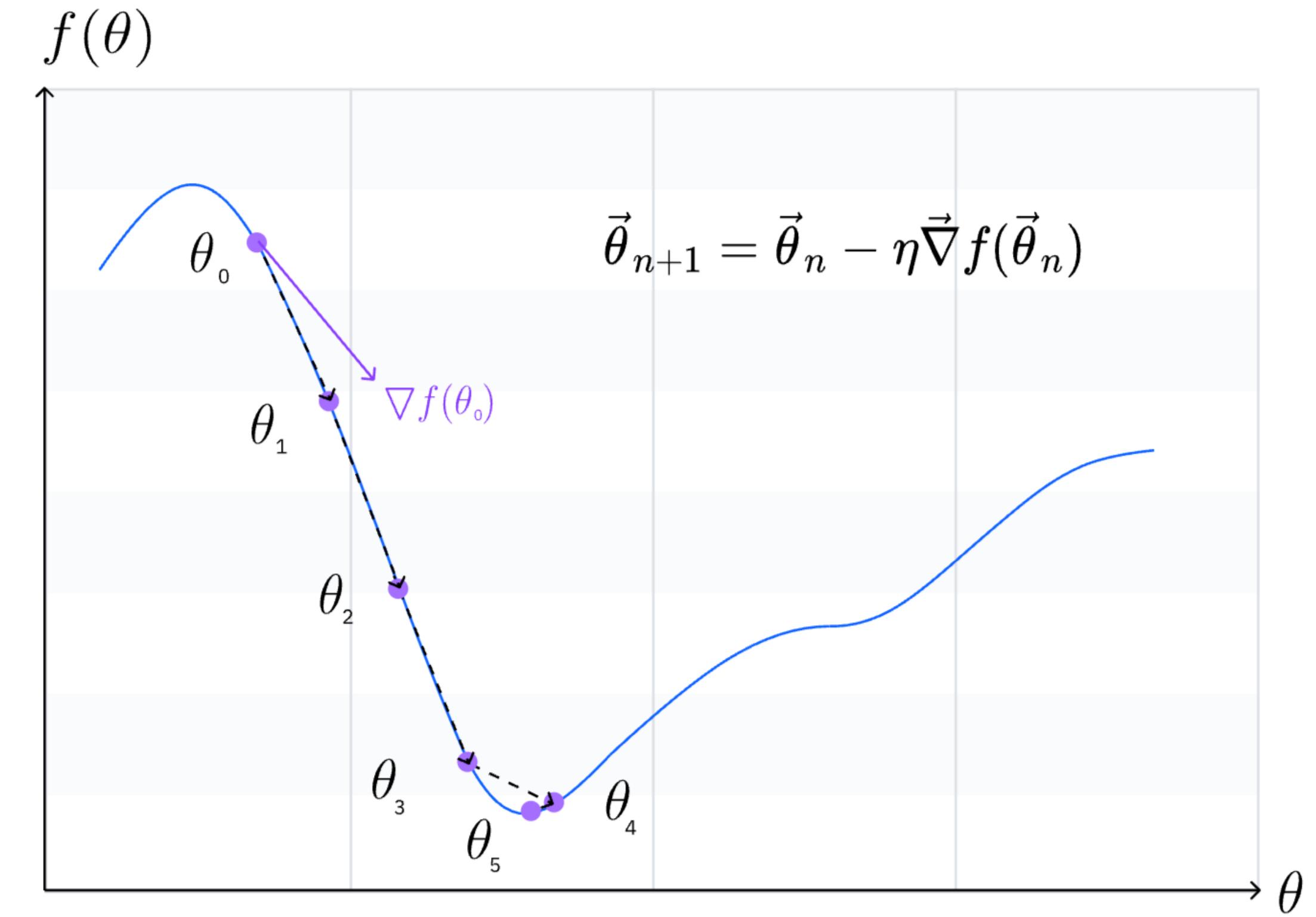
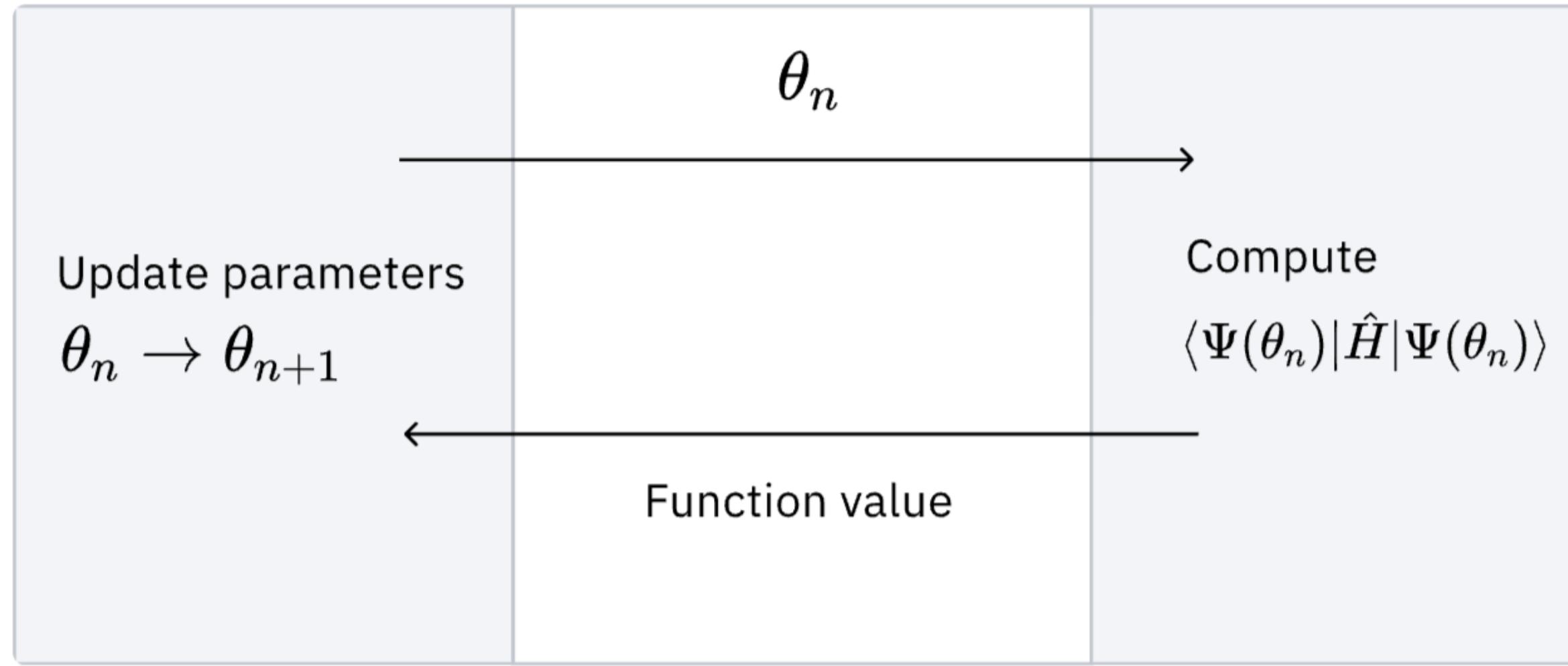


# Section 2

## PQC Training

# PQC Training

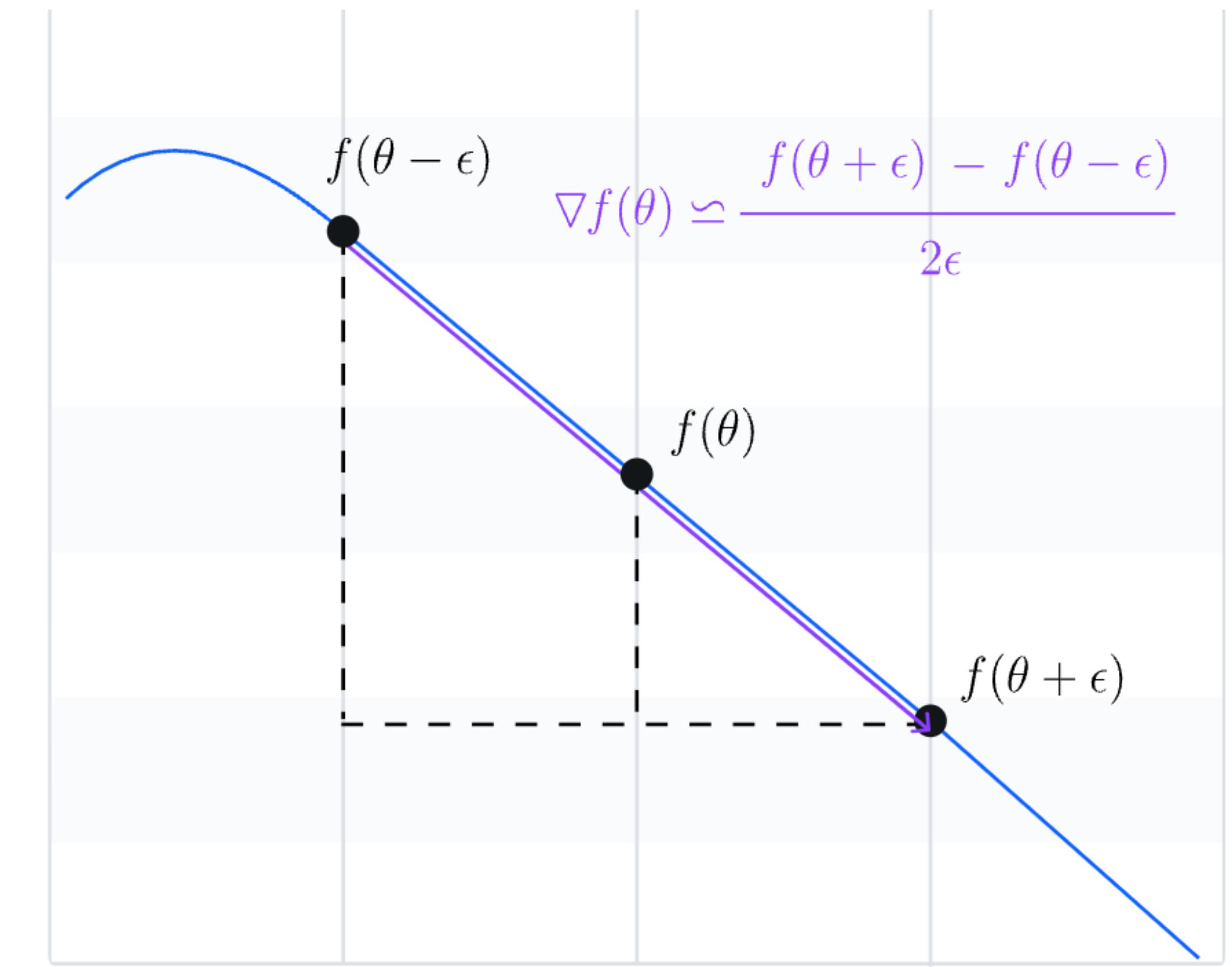
- Train parameters in parameterized quantum circuit to perform **data-driven** tasks



# Finite Difference Gradients

- Works **independently** of function's structure

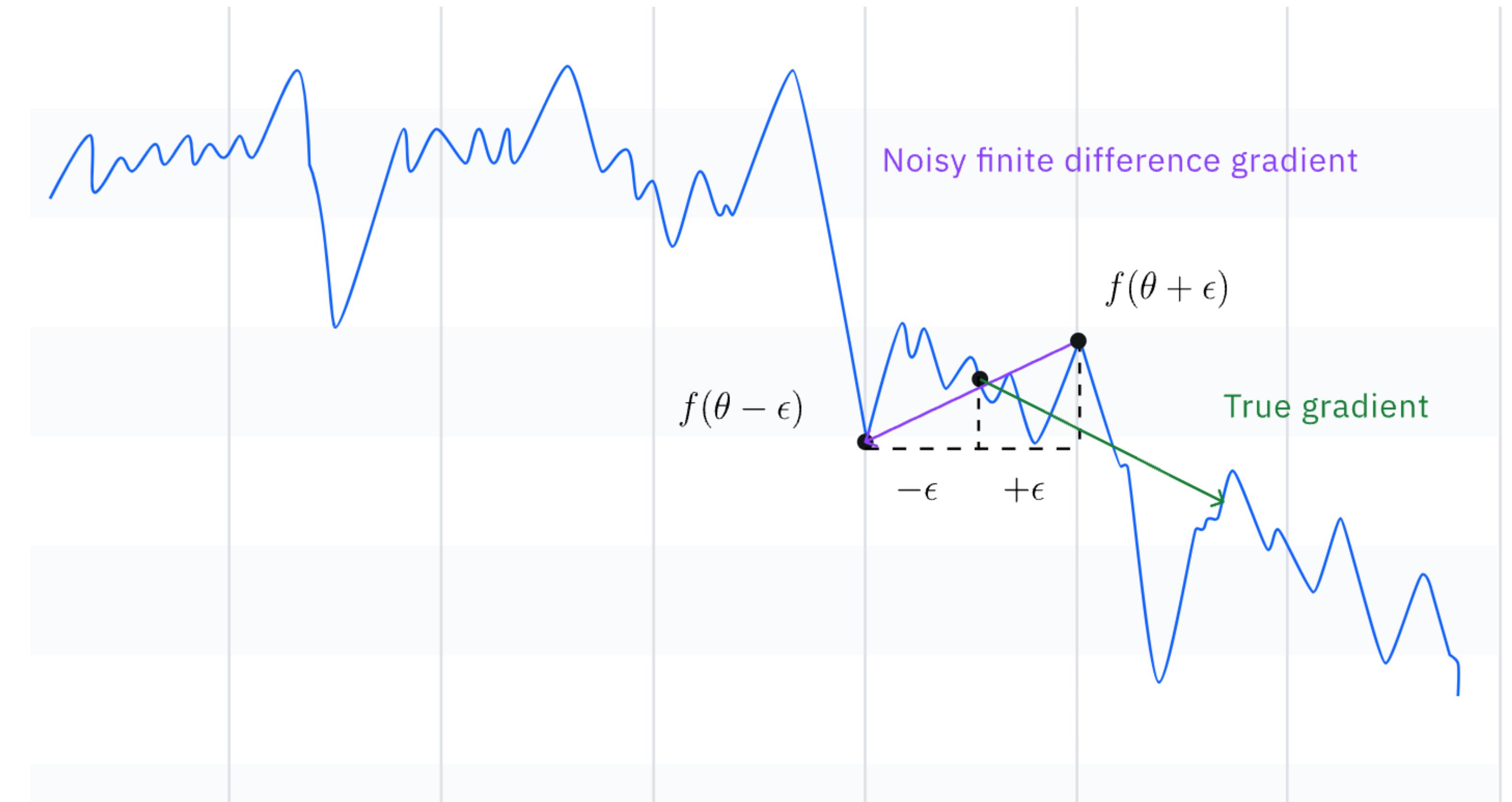
$$\vec{\nabla} f(\vec{\theta}) \approx \frac{1}{2\epsilon} \left( f(\vec{\theta} + \epsilon) - f(\vec{\theta} - \epsilon) \right)$$



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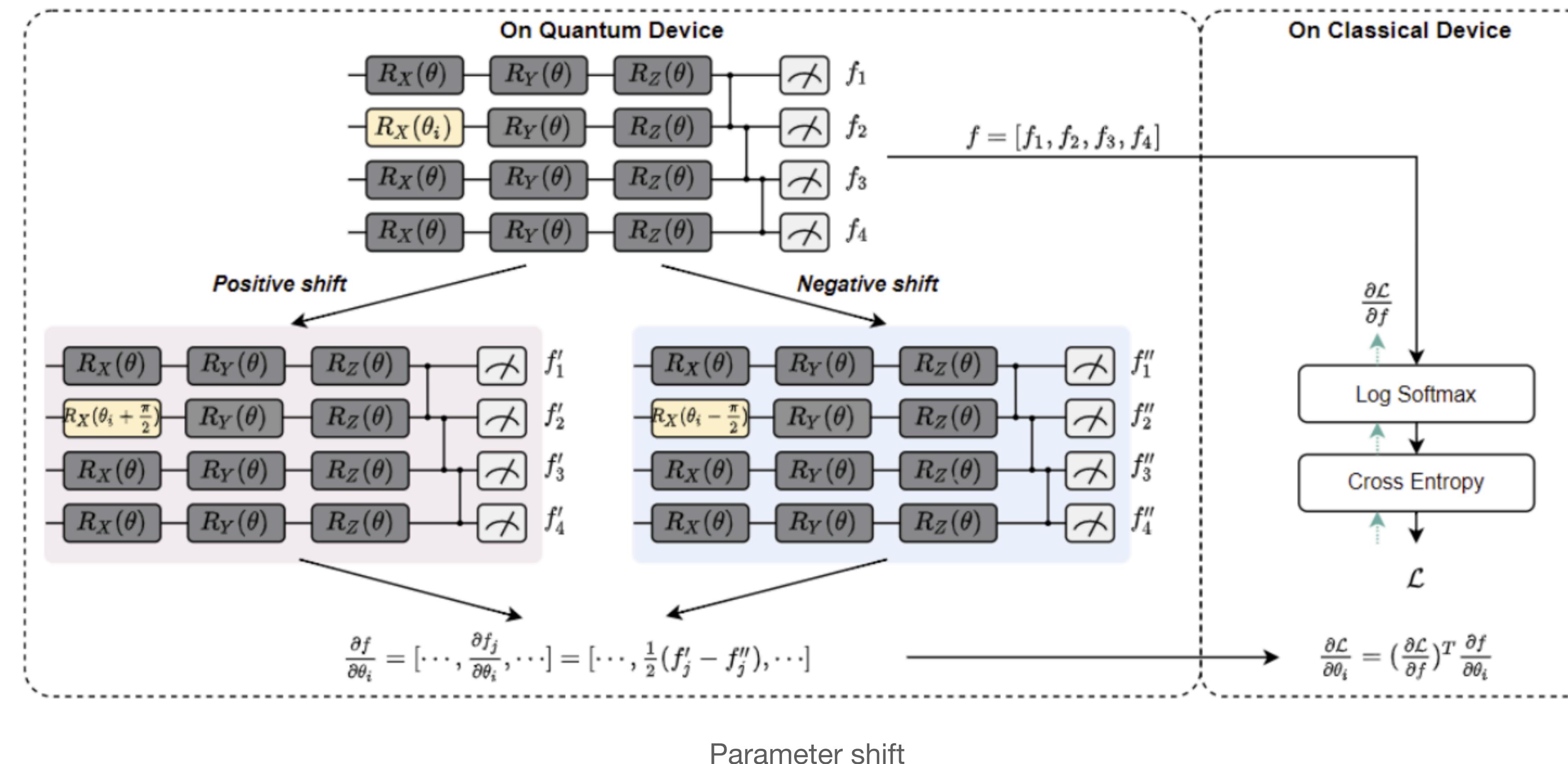
# Finite Difference Gradients

- The accuracy depends on the epsilon



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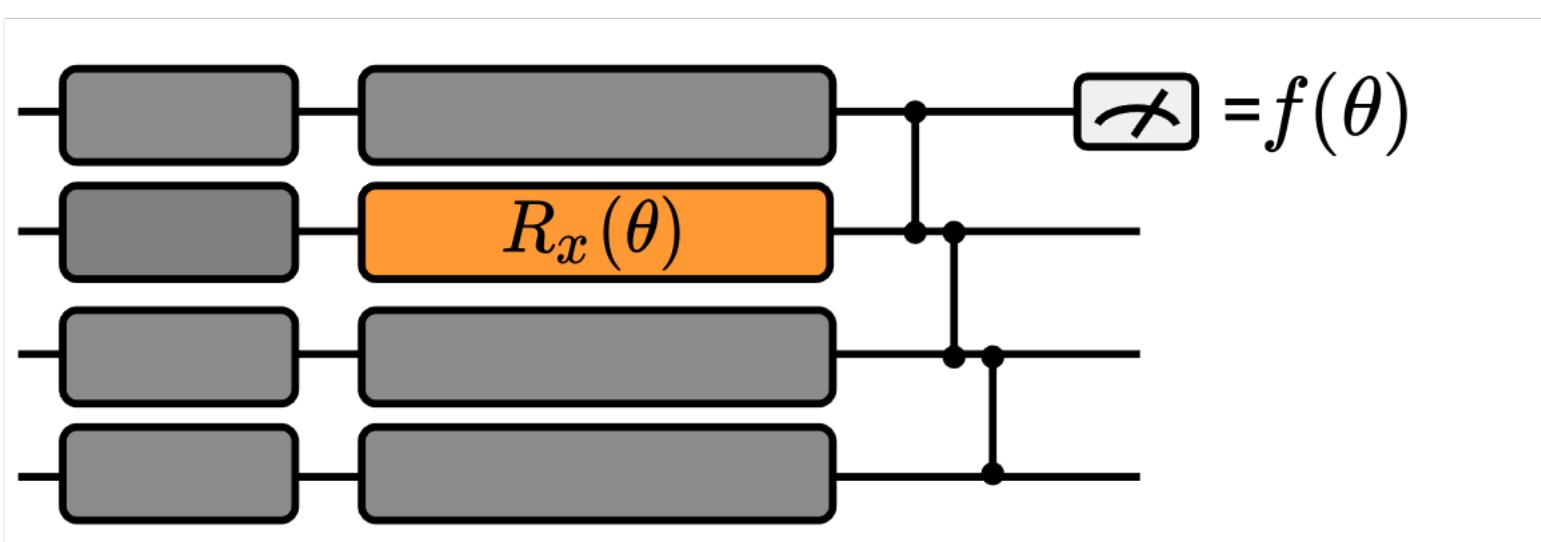
# Parameter-Shift Gradients



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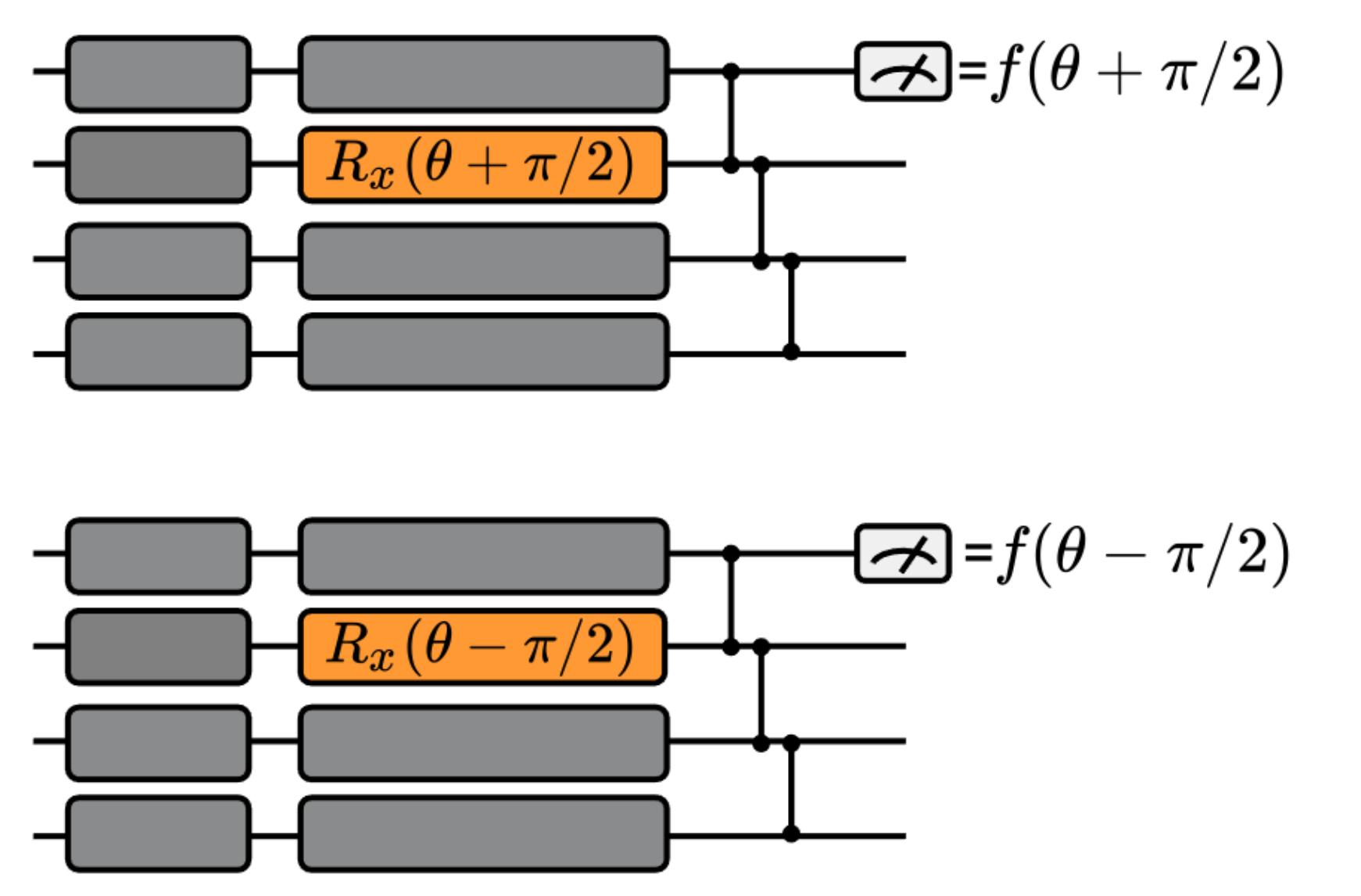
# Parameter-Shift

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



# Parameter-Shift

- Shift  $\theta$  twice



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

# Proof of the parameter shift rule

- Convert to the exponential representation of gates and prove

Assume  $U(\theta_i) = R_X(\theta_i)$ ,  $R_X(\alpha) = e^{-\frac{i}{2}\alpha X}$ , where  $X$  is the Pauli-X matrix.

Firstly, the RX gate is,

$$\begin{aligned} R_X(\alpha) &= e^{-\frac{i}{2}\alpha X} = \sum_{k=0}^{\infty} (-i\alpha/2)^k X^k / k! \\ &= \sum_{k=0}^{\infty} (-i\alpha/2)^{2k} X^{2k} / (2k)! + \sum_{k=0}^{\infty} (-i\alpha/2)^{2k+1} X^{2k+1} / (2k+1)! \\ &= \sum_{k=0}^{\infty} (-1)^k (\alpha/2)^{2k} I / (2k)! - i \sum_{k=0}^{\infty} (-1)^k (\alpha/2)^{2k+1} X / (2k+1)! \\ &= \cos(\alpha/2)I - i \sin(\alpha/2)X. \end{aligned}$$

# Proof of the parameter shift rule

Let  $\alpha = \frac{\pi}{2}$ ,  $R_X(\pm\frac{\pi}{2}) = \frac{1}{\sqrt{2}}(I \mp iX)$ .

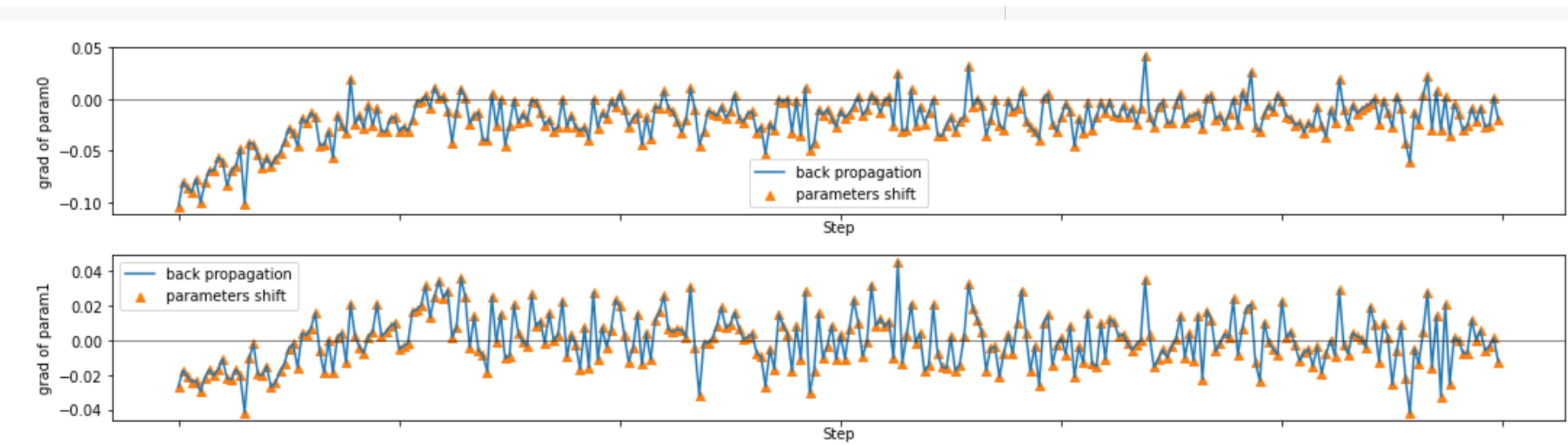
As  $f(\theta) = \langle \psi | R_X(\theta_i)^\dagger \widehat{Q} R_X(\theta_i) | \psi \rangle$ ,  $R_X(\alpha)R_X(\beta) = R_X(\alpha + \beta)$ , and  $\frac{\partial}{\partial \alpha} R_X(\alpha) = -\frac{i}{2} X R_X(\alpha)$ , we have

$$\begin{aligned}\frac{\partial f(\theta)}{\partial \theta_i} &= \langle \psi | R_X(\theta_i)^\dagger \left(-\frac{i}{2} X\right)^\dagger \widehat{Q} R_X(\theta_i) | \psi \rangle + \langle \psi | R_X(\theta_i)^\dagger \widehat{Q} \left(-\frac{i}{2} X\right) R_X(\theta_i) | \psi \rangle \\ &= \frac{1}{4} (\langle \psi | R_X(\theta_i)^\dagger (I - iX)^\dagger \widehat{Q} (I - iX) R_X(\theta_i) | \psi \rangle \\ &\quad - \langle \psi | R_X(\theta_i)^\dagger (I + iX)^\dagger \widehat{Q} (I + iX) R_X(\theta_i) | \psi \rangle) \\ &= \frac{1}{2} (\langle \psi | R_X(\theta_i)^\dagger R_X(\frac{\pi}{2})^\dagger \widehat{Q} R_X(\frac{\pi}{2}) R_X(\theta_i) | \psi \rangle \\ &\quad - \langle \psi | R_X(\theta_i)^\dagger R_X(-\frac{\pi}{2})^\dagger \widehat{Q} R_X(-\frac{\pi}{2}) R_X(\theta_i) | \psi \rangle) \\ &= \frac{1}{2} (f(\theta_+) - f(\theta_-)).\end{aligned}$$

i --

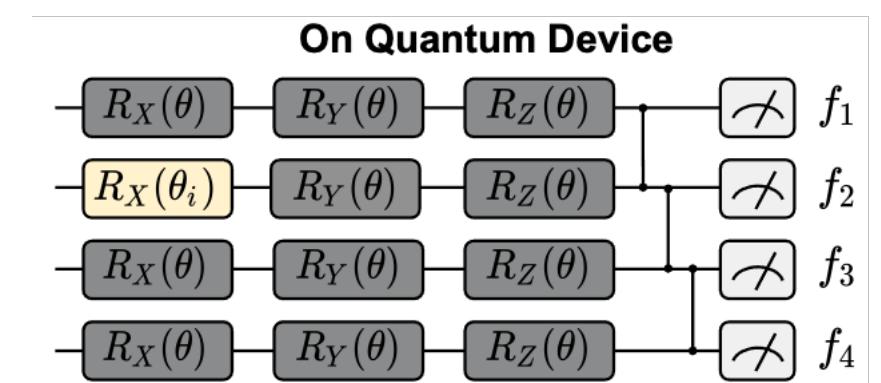
# Back-Propagation

- The gradients can also be calculated with back-propagation
- Can only be used on **classical simulator**
- All computation are essentially differentiable linear algebra



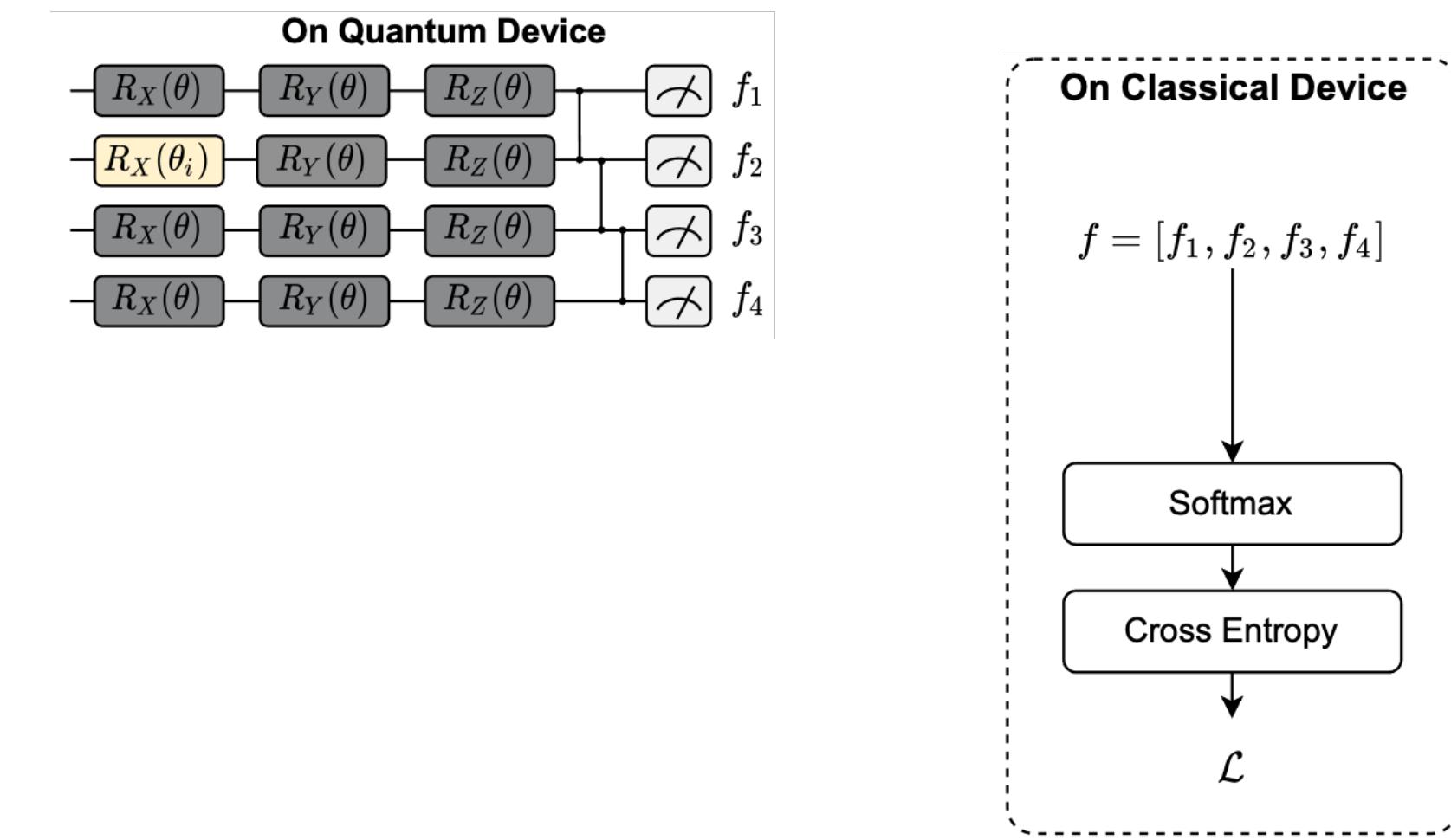
# General Flow to calculate PQC gradients

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



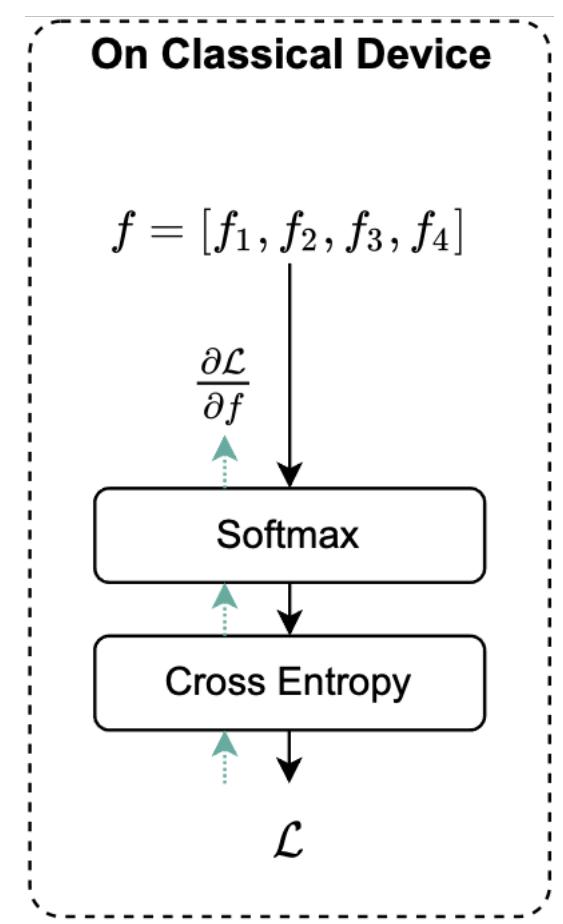
# General Flow to calculate PQC gradients

- Step 2: Further forward to get Loss



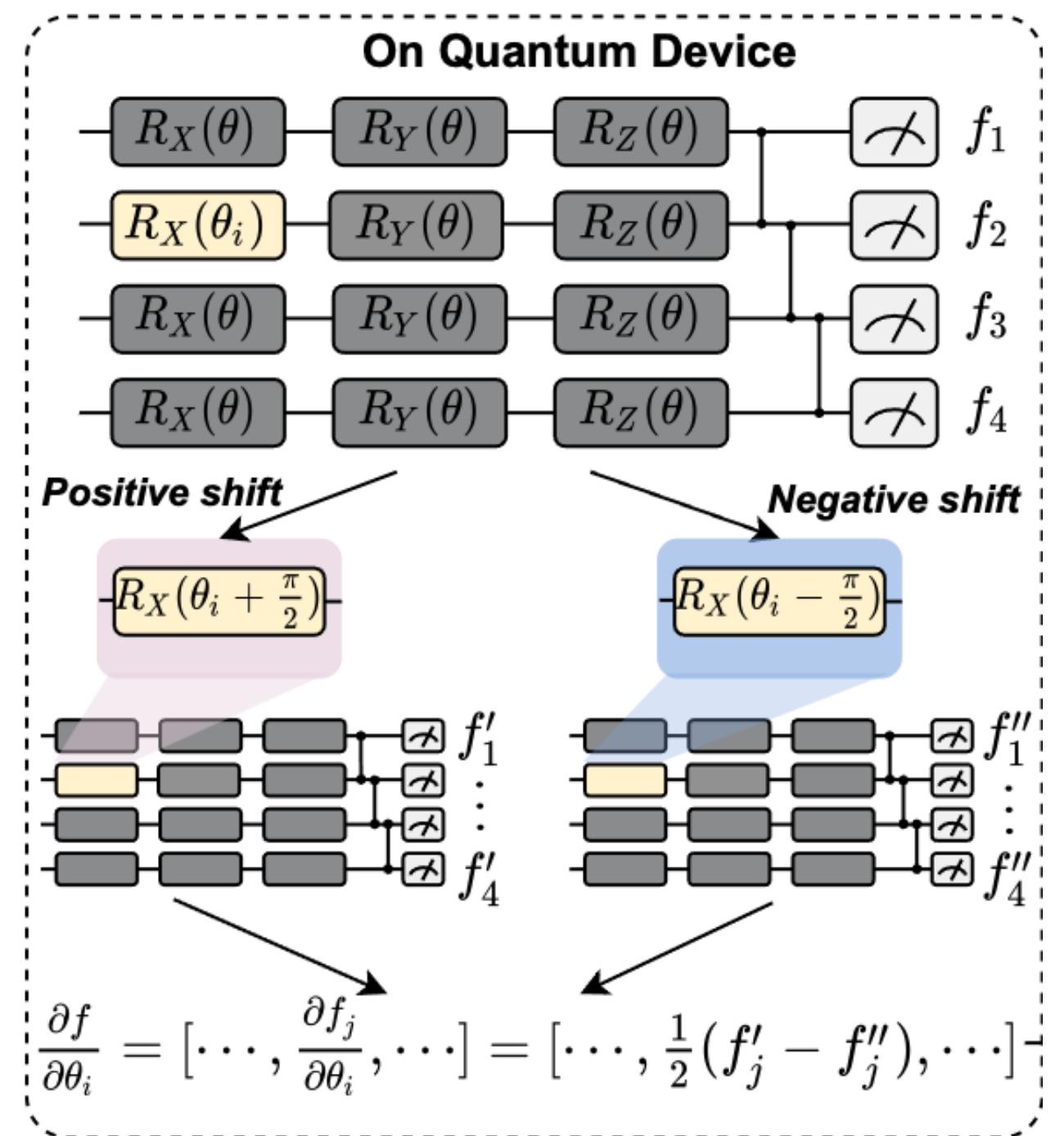
# General Flow to calculate PQC gradients

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



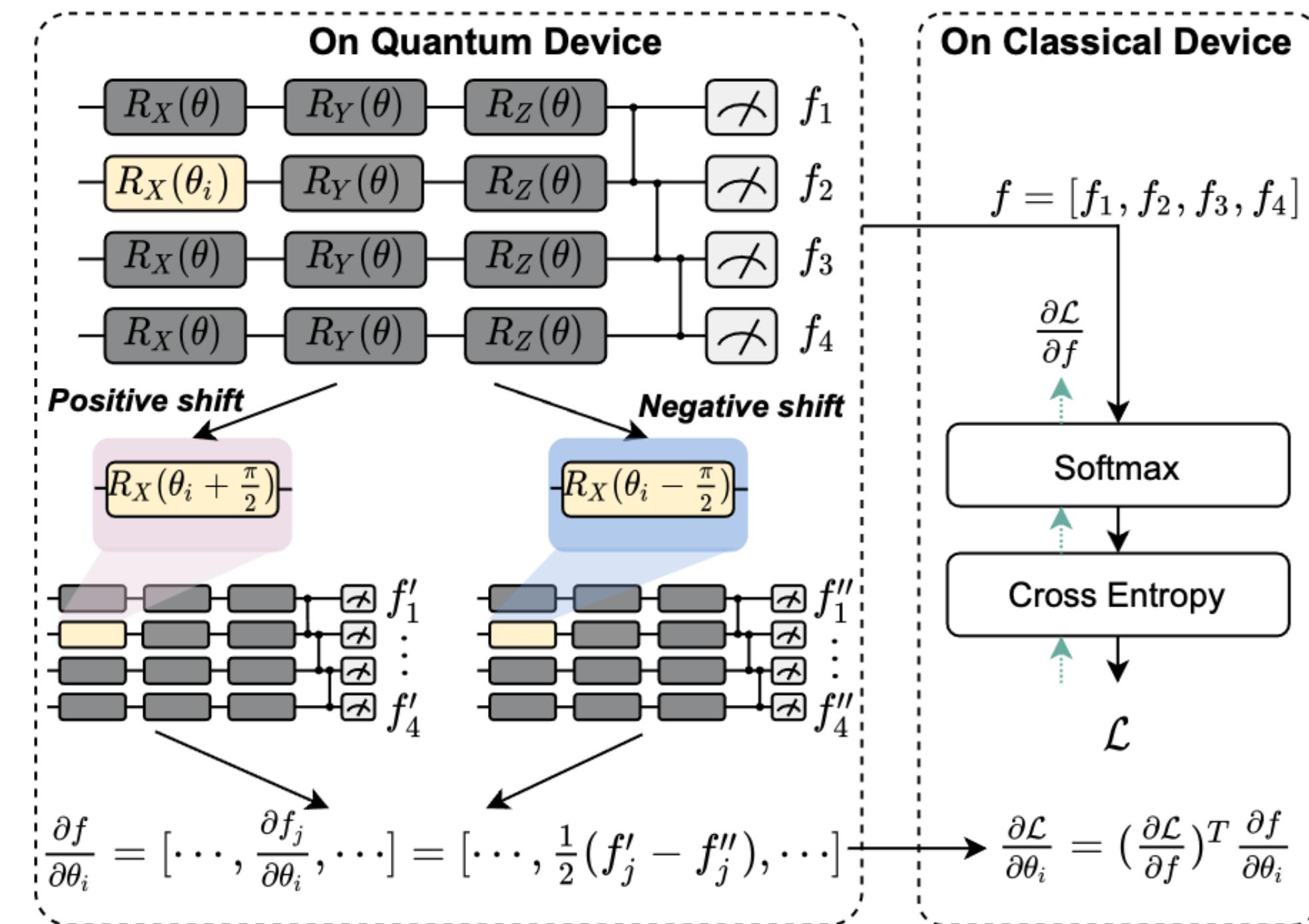
# General Flow to calculate PQC gradients

- Step 4: Shift twice and run on QC to calculate  $(\partial f(\theta)) / (\partial \theta_i)$ 
  - Or use finite differentiate

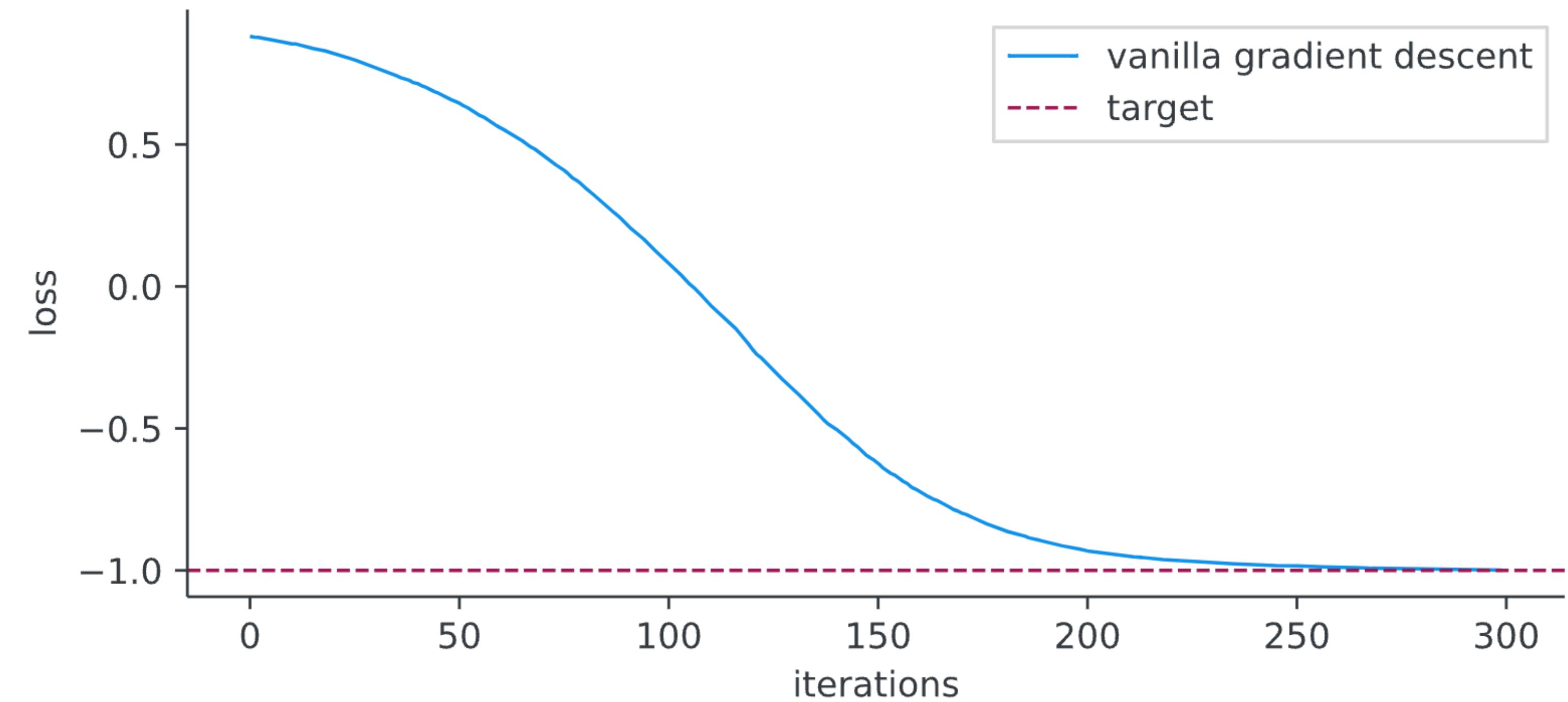


# General Flow to calculate PQC gradients

- Step 5: By Chain Rule, sum over 4 passes (4 qubits)
- Only forward on quantum device



# Training Techniques



# Training Techniques

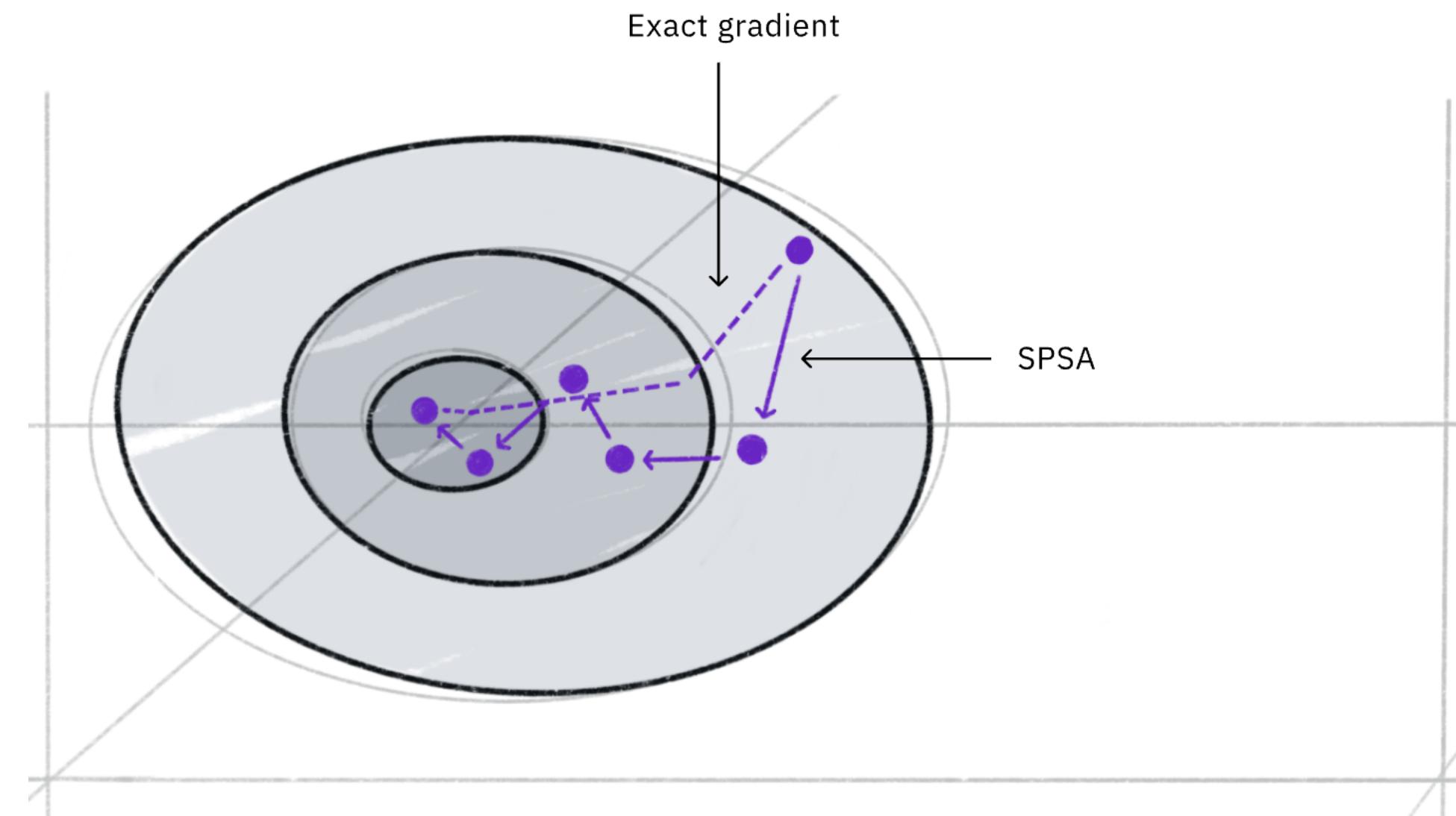
## SPSA

- Simultaneous Perturbation Stochastic Approximation
- How **many** circuit run for the original methods?  $2N$

$$\vec{\nabla} f(\vec{\theta}) = \begin{pmatrix} \frac{\partial f}{\partial \theta_1} \\ \vdots \\ \frac{\partial f}{\partial \theta_n} \end{pmatrix} \simeq \frac{1}{2\epsilon} \underbrace{\begin{pmatrix} f(\vec{\theta} + \epsilon \vec{e}_1) - f(\vec{\theta} - \epsilon \vec{e}_1) \\ \vdots \\ f(\vec{\theta} + \epsilon \vec{e}_n) - f(\vec{\theta} - \epsilon \vec{e}_n) \end{pmatrix}}_{\text{Finite difference:  
Perturb each dim once}} \simeq \frac{f(\vec{\theta} + \epsilon \vec{\Delta}) - f(\vec{\theta} - \epsilon \vec{\Delta})}{2\epsilon} \vec{\Delta}^{-1}$$

Random perturbation  $\vec{\Delta} \in \{+1, -1\}^n$

SPSA:  
simultaneously  
perturb all dims at once!

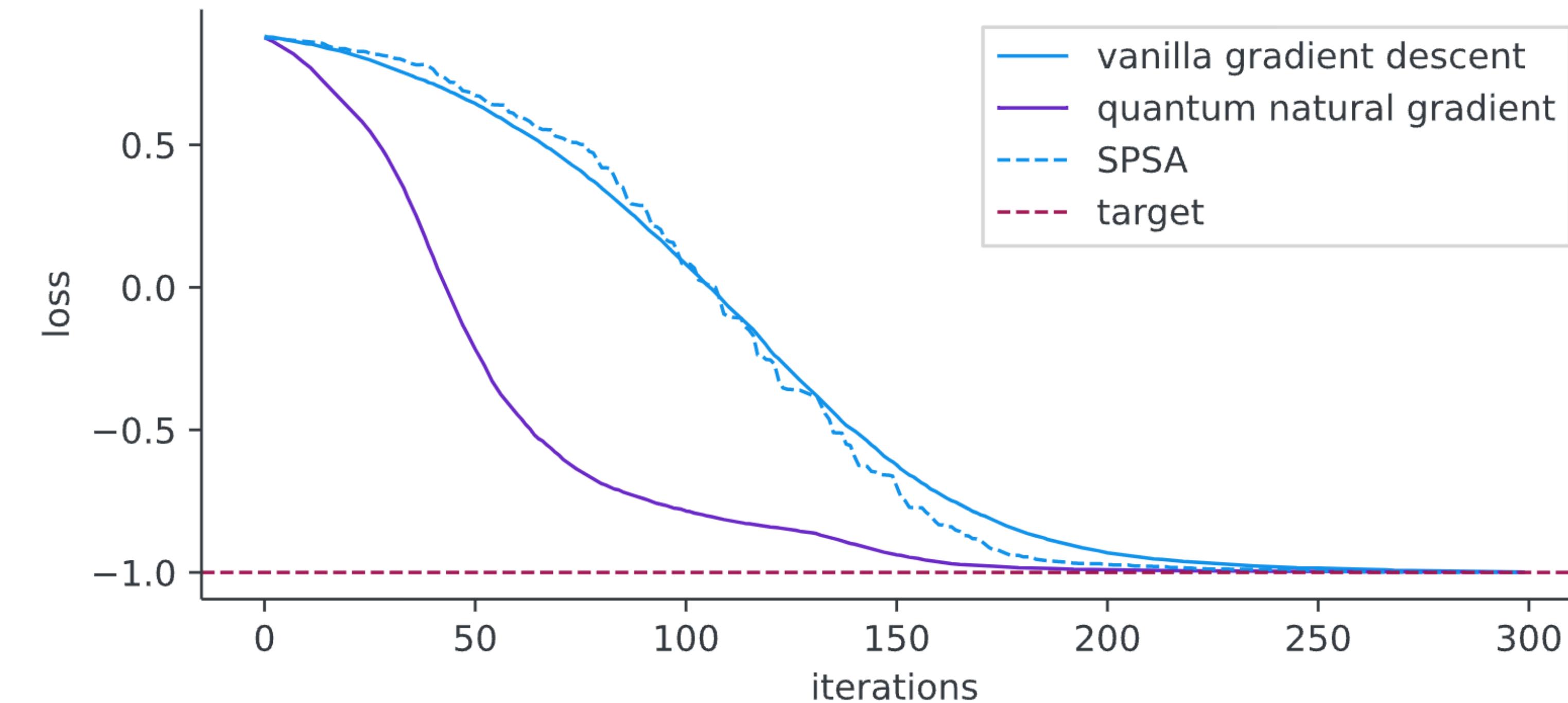


<https://qiskit.org/learn/>

# Training Techniques

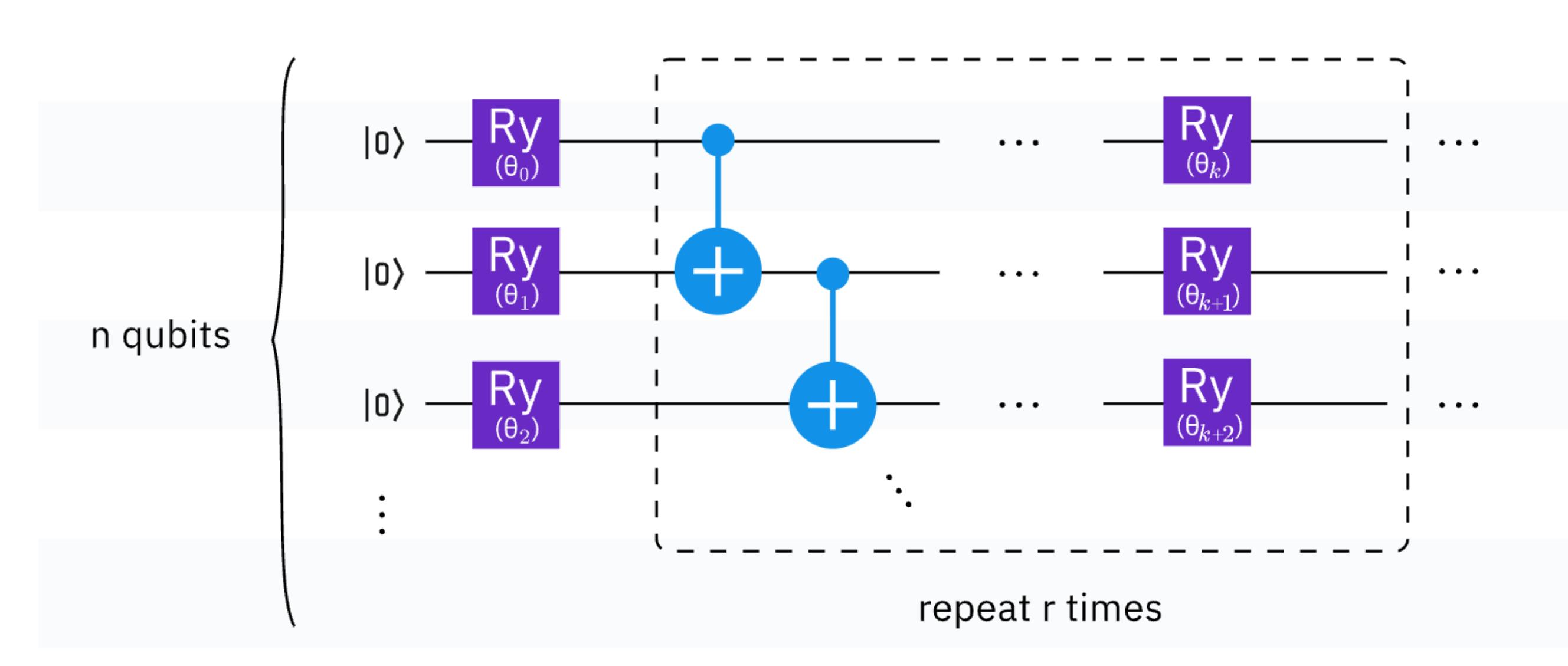
## SPSA

- The SPSA has similar convergence as the gradient descent



# Barren Plateaus

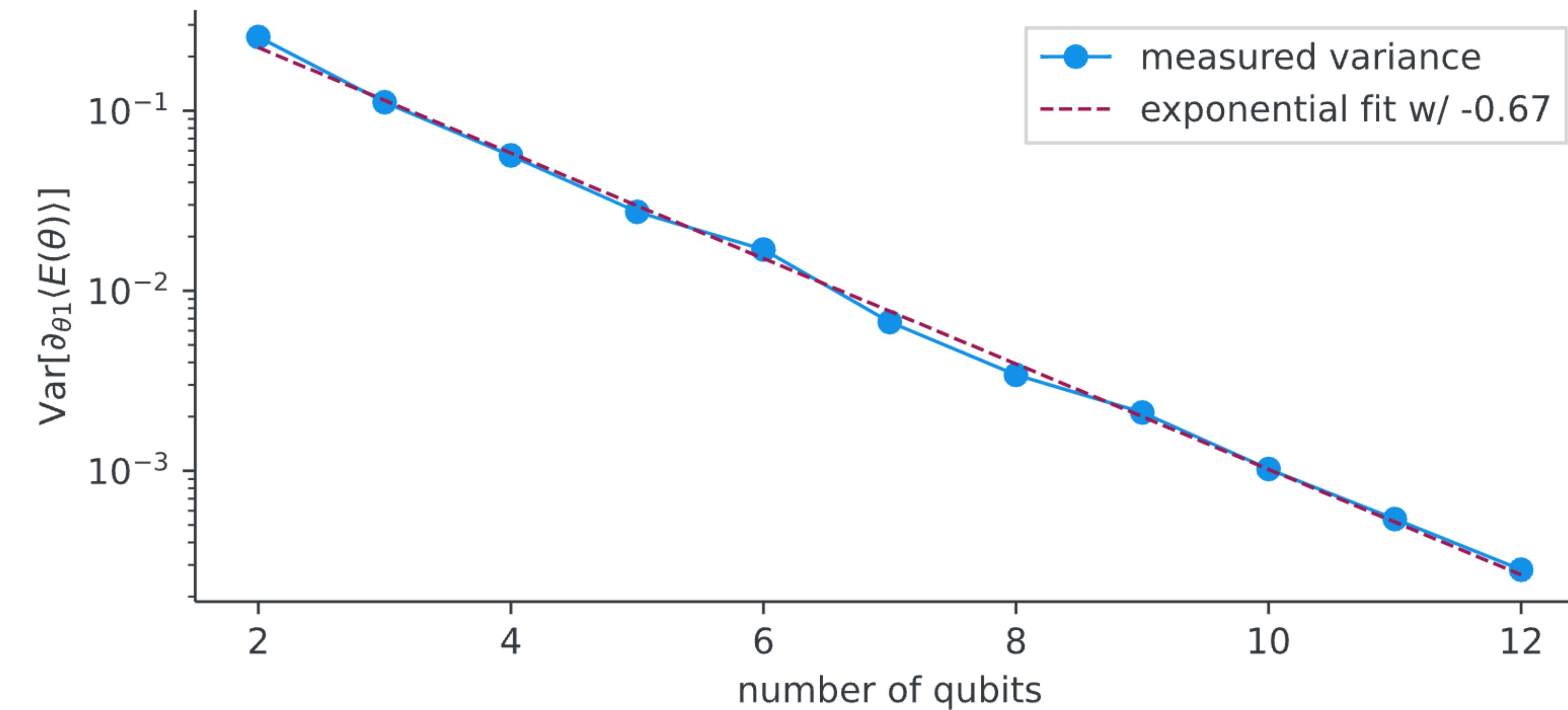
- Vanishing Gradients problem when circuit goes larger



<https://qiskit.org/learn/>

# Barren Plateaus

- Gradient **variance** reduces drastically

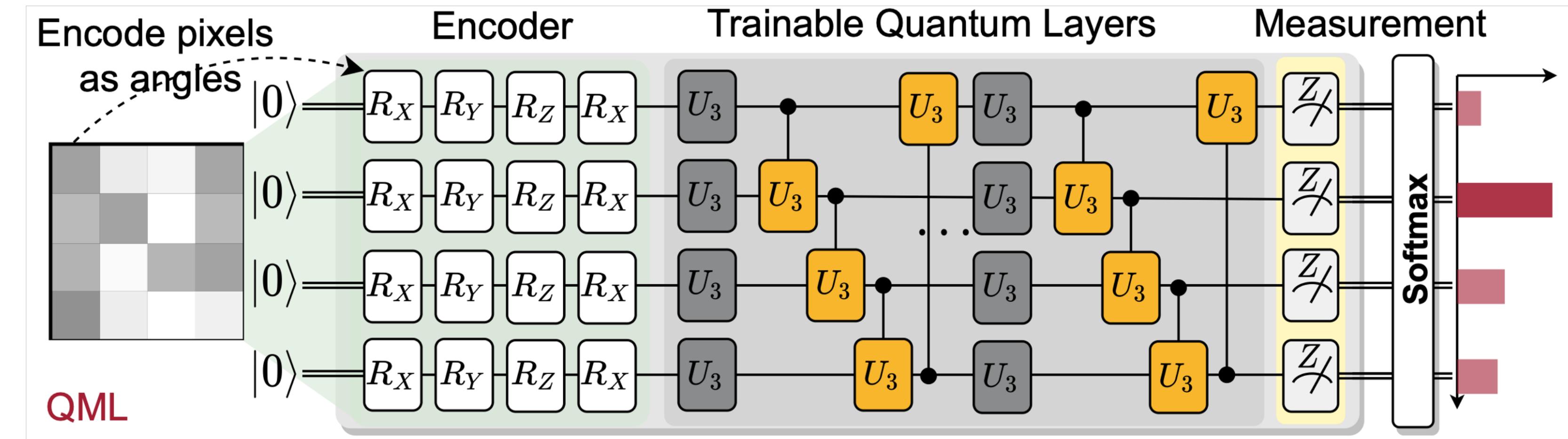


# Section 3

## Quantum Classifiers

# Quantum Classifiers

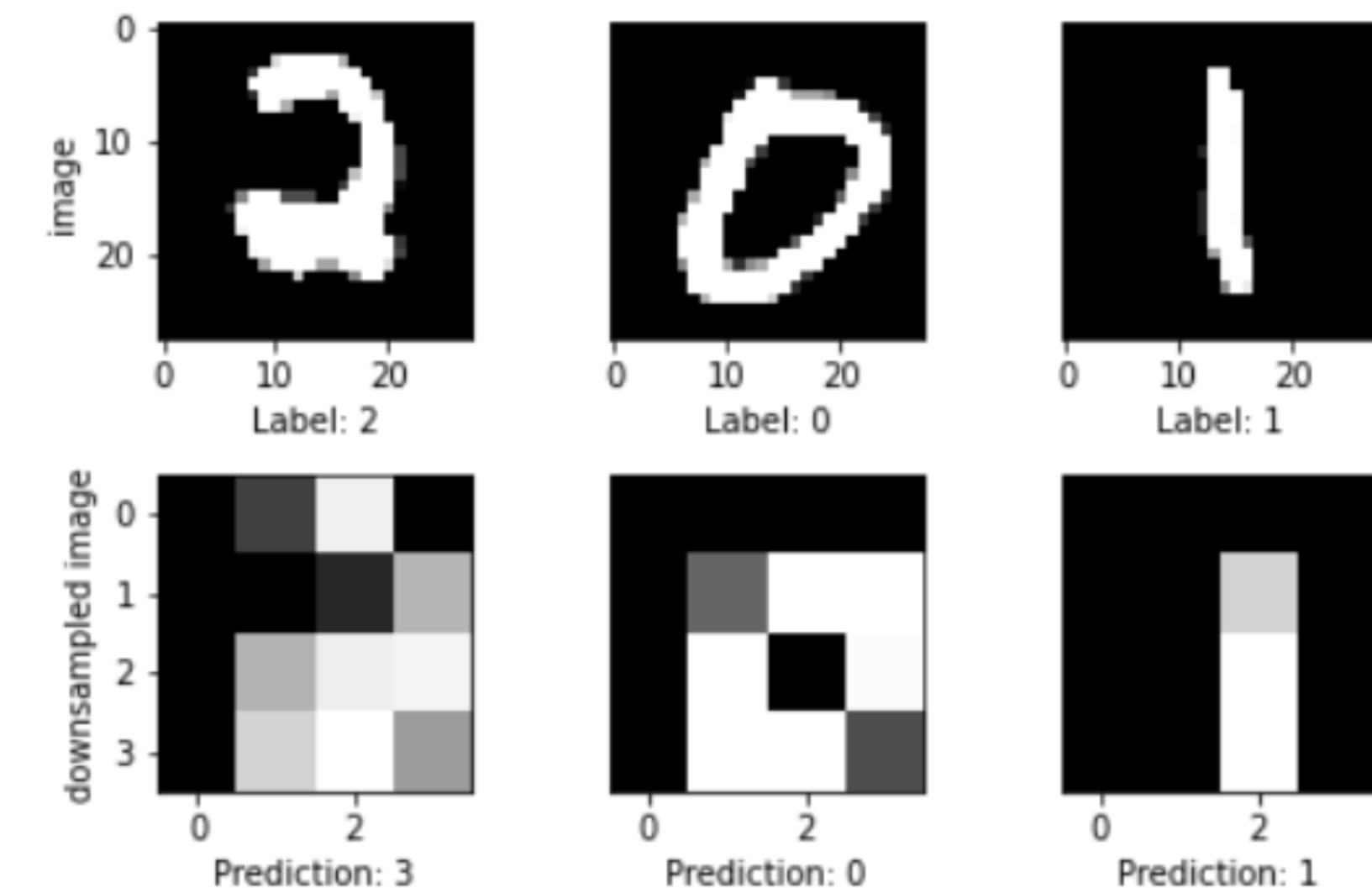
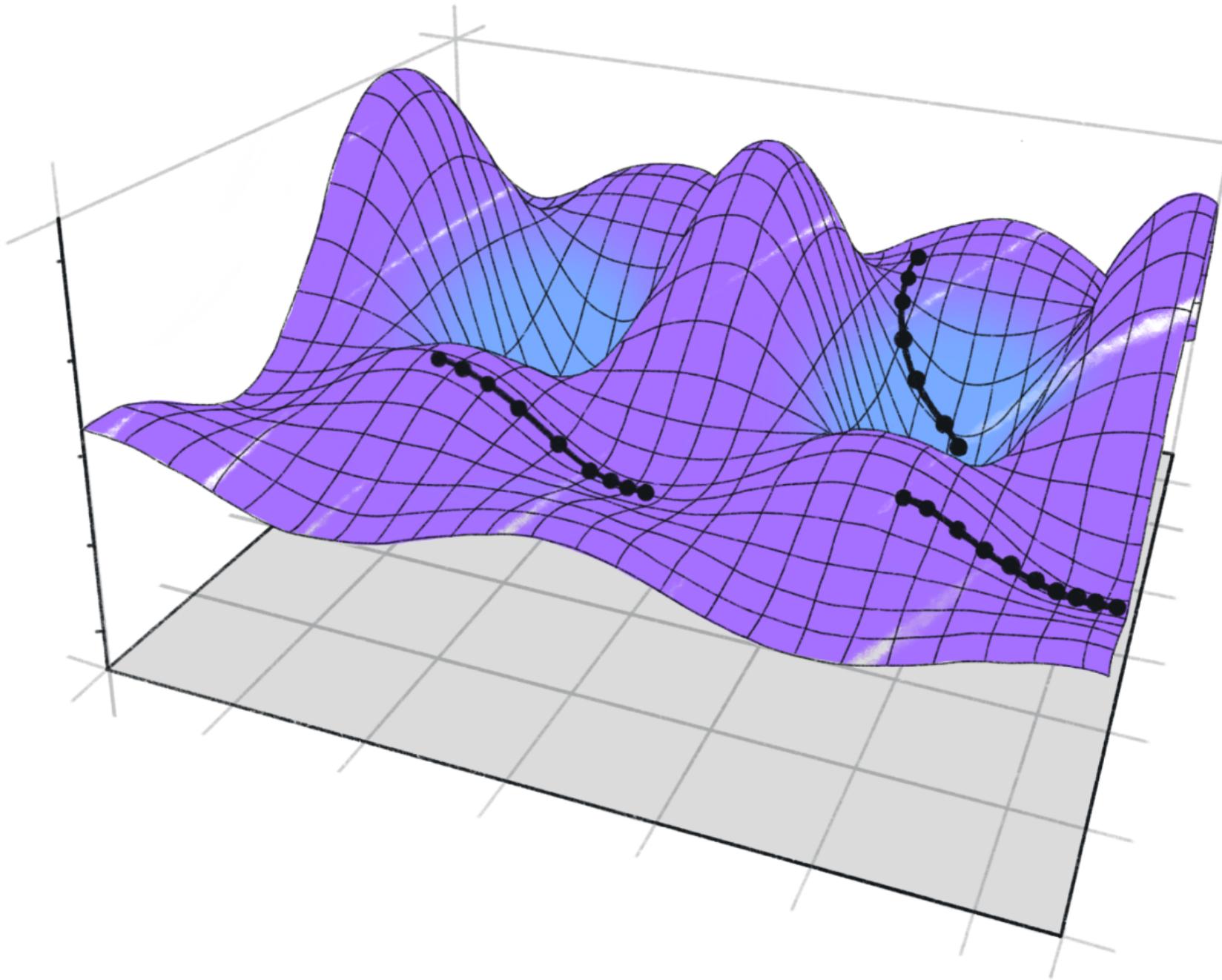
## With Quantum Neural Networks



# Quantum Classifiers

## With Quantum Neural Networks

- Training

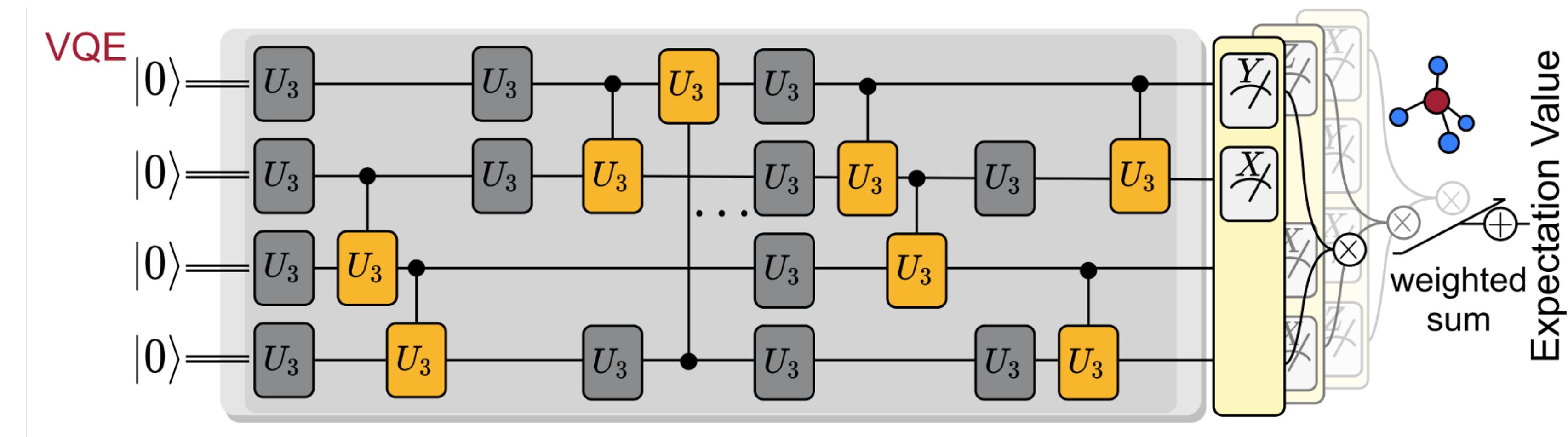


<https://qiskit.org/learn/>

# PQC for Other tasks

## VQE and QAOA

- Variational Quantum eigensolver
- Quantum Approximate Optimization Algorithm (QAOA)

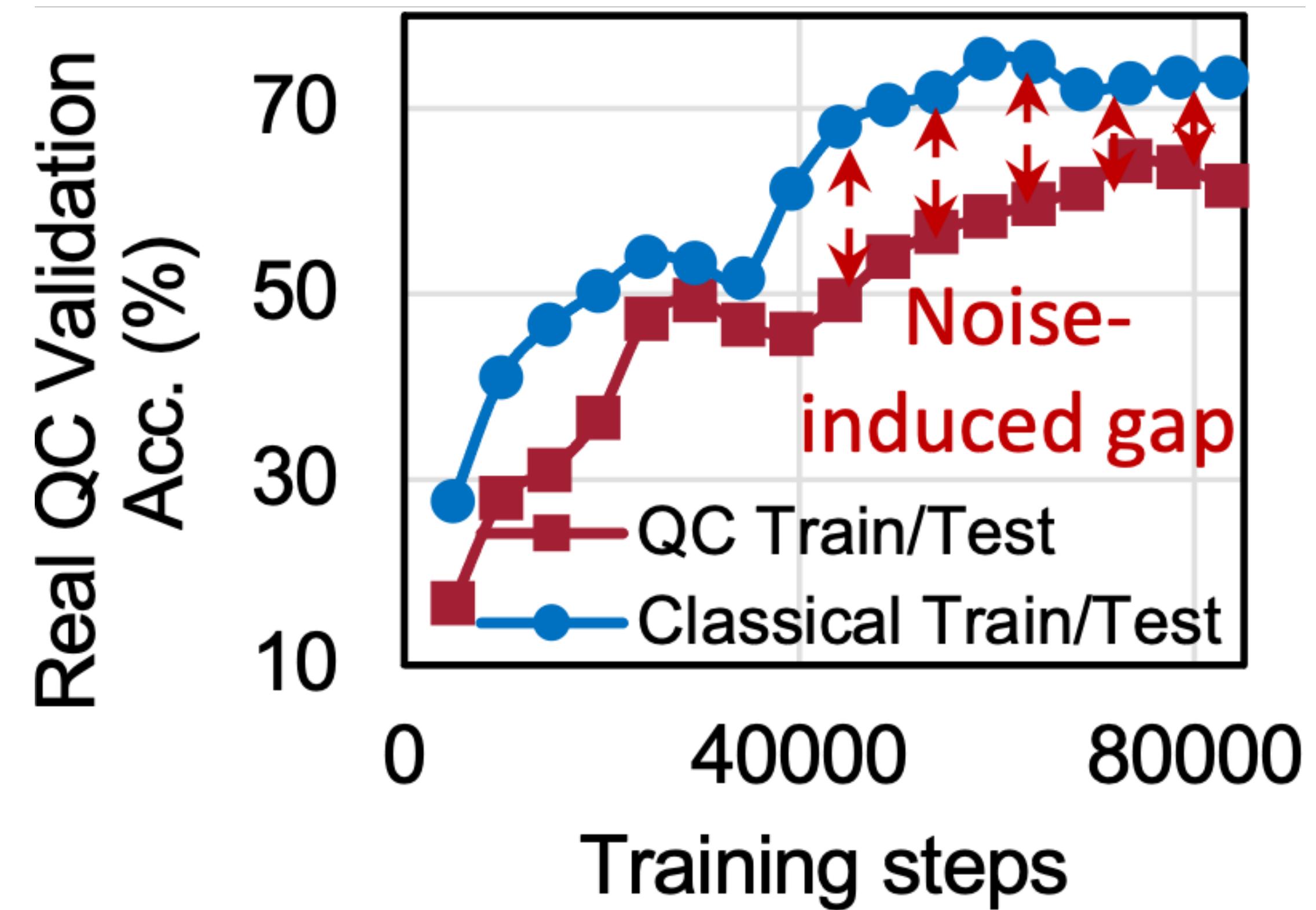


# Section 4

## Noise-Aware On-Chip Training (QOC)

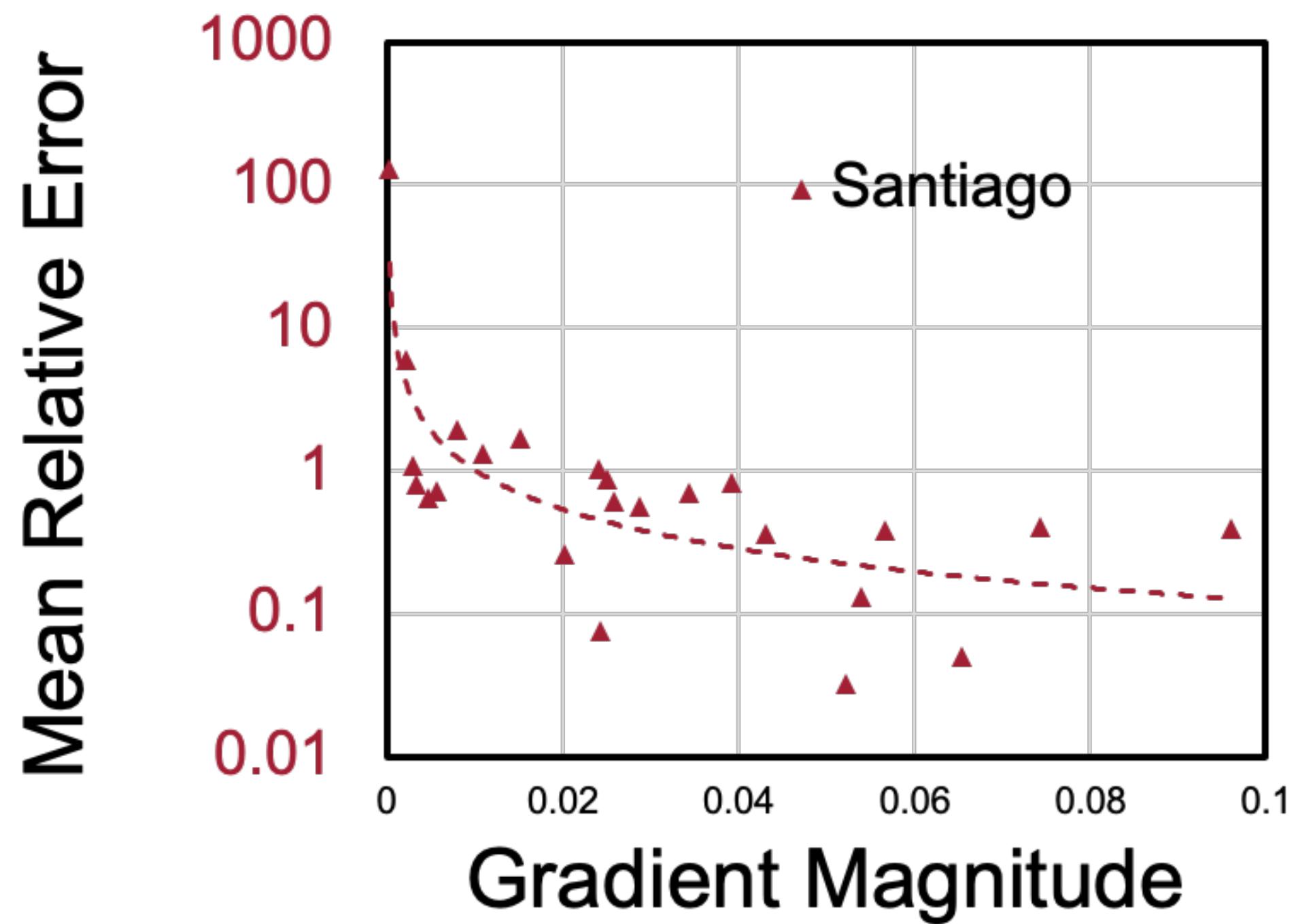
# The impact of noise on gradient computation

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



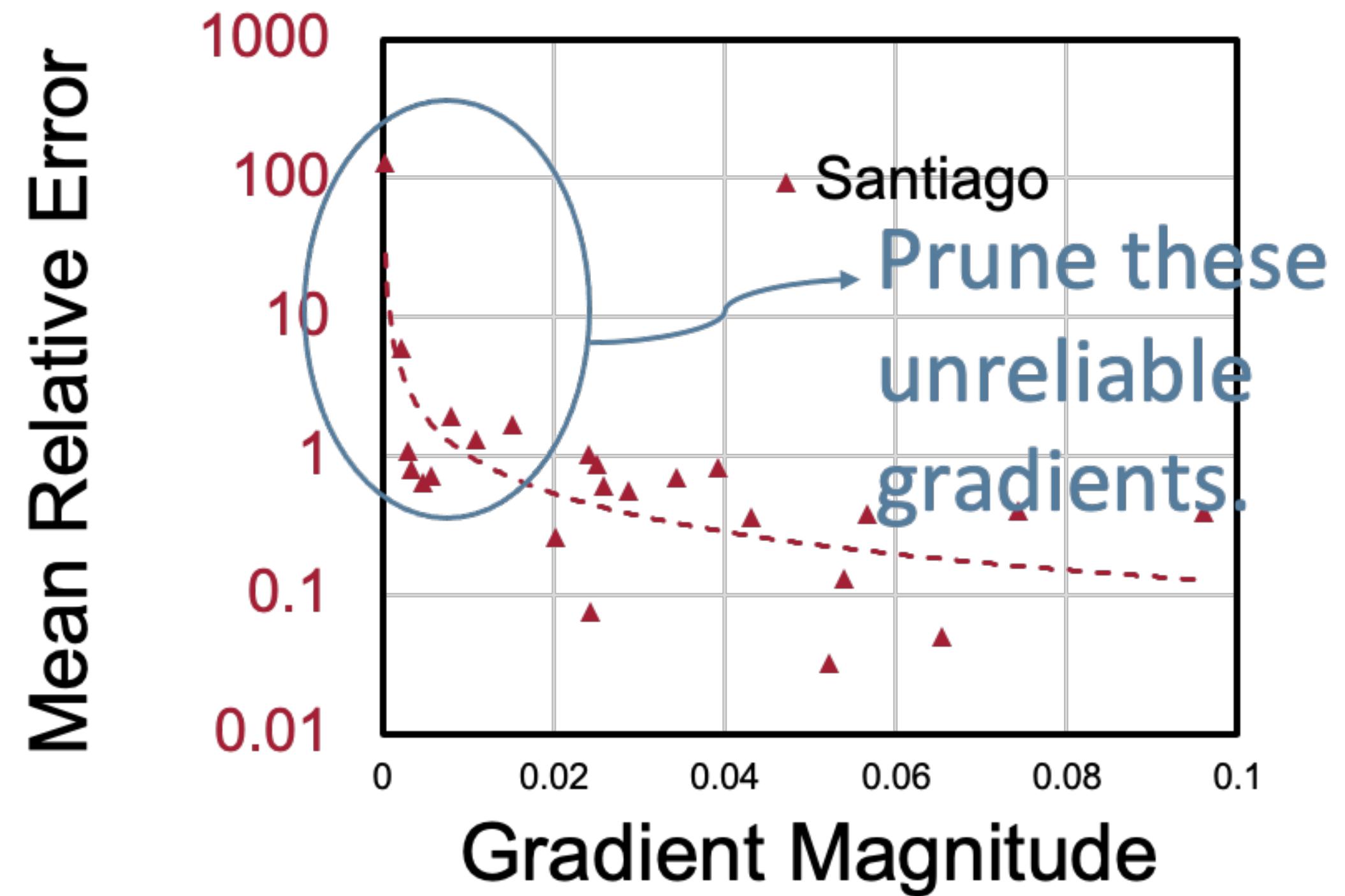
# Noise Impact

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



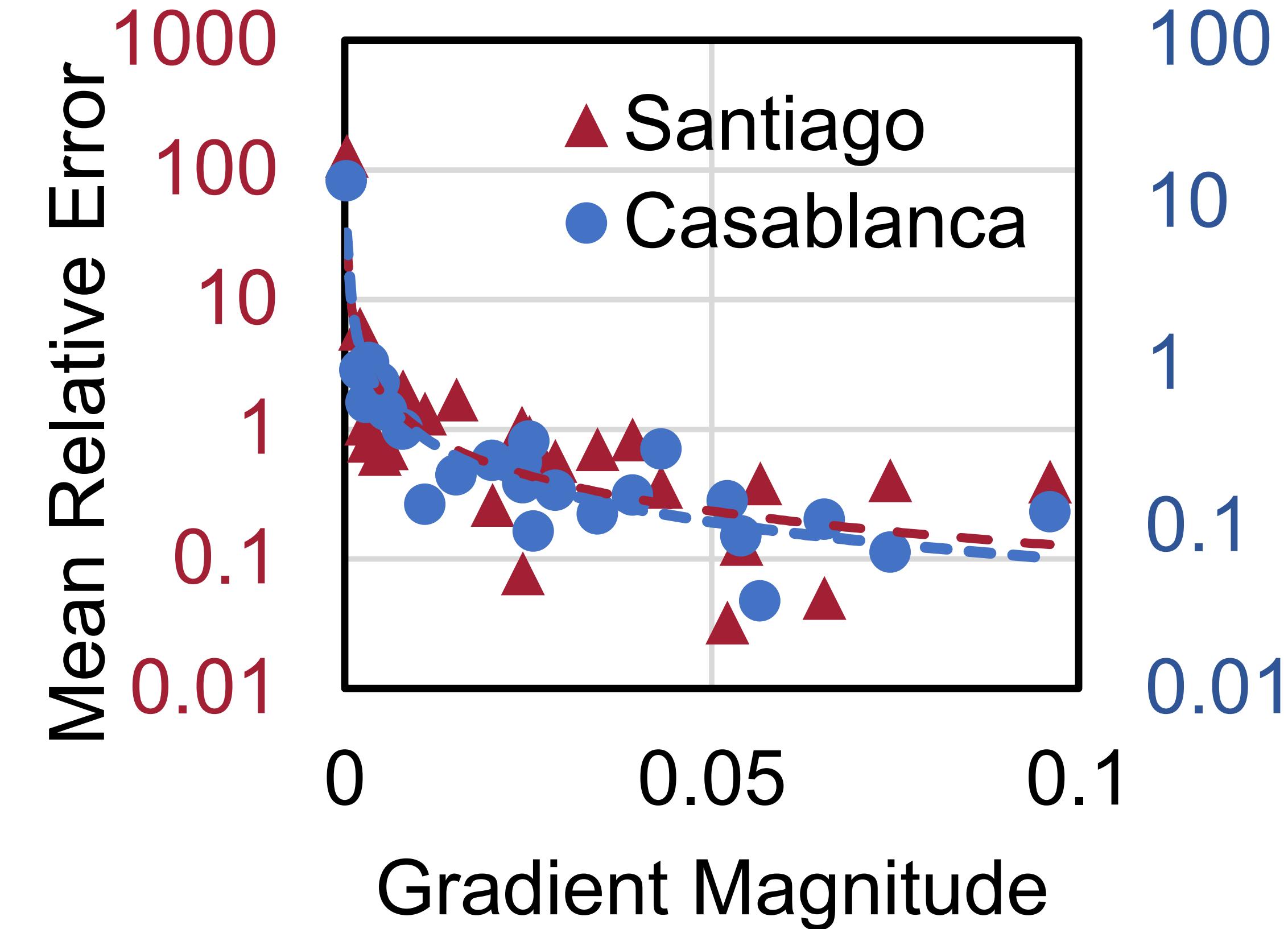
# Noise Impact

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



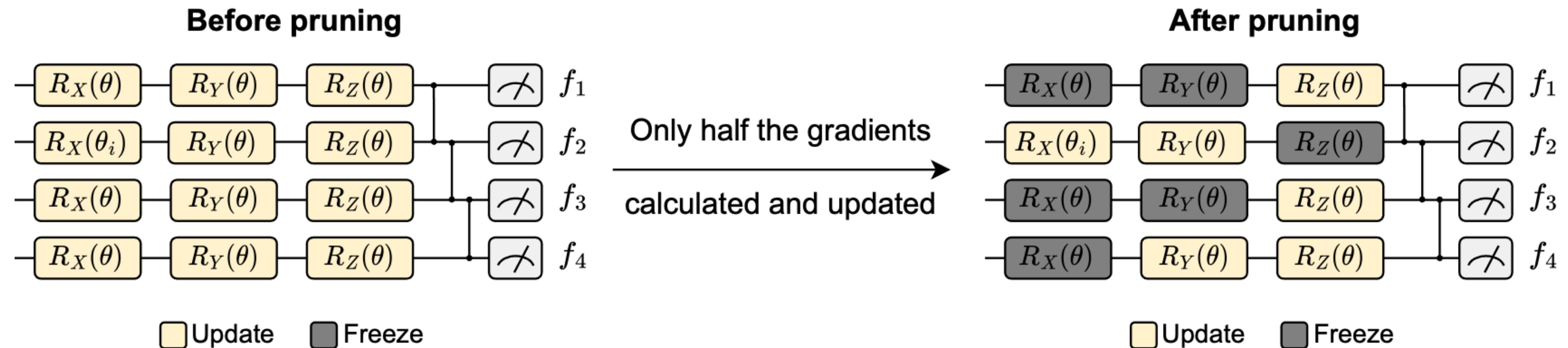
# Probabilistic Gradient Pruning

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



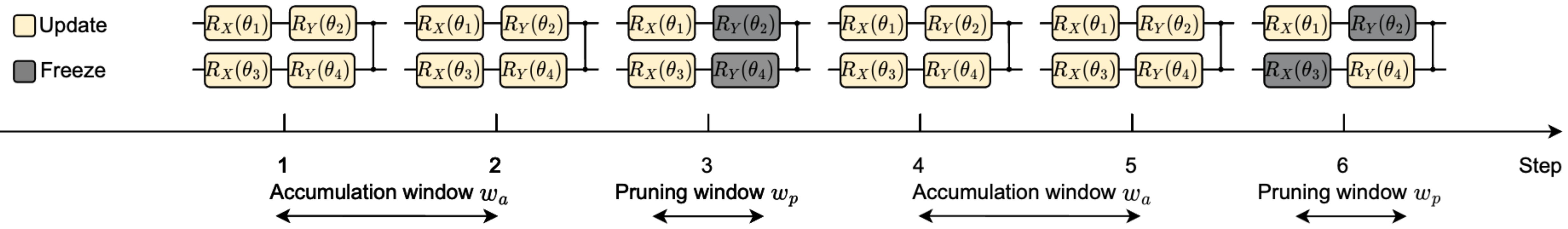
# Probabilistic Gradient Pruning

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



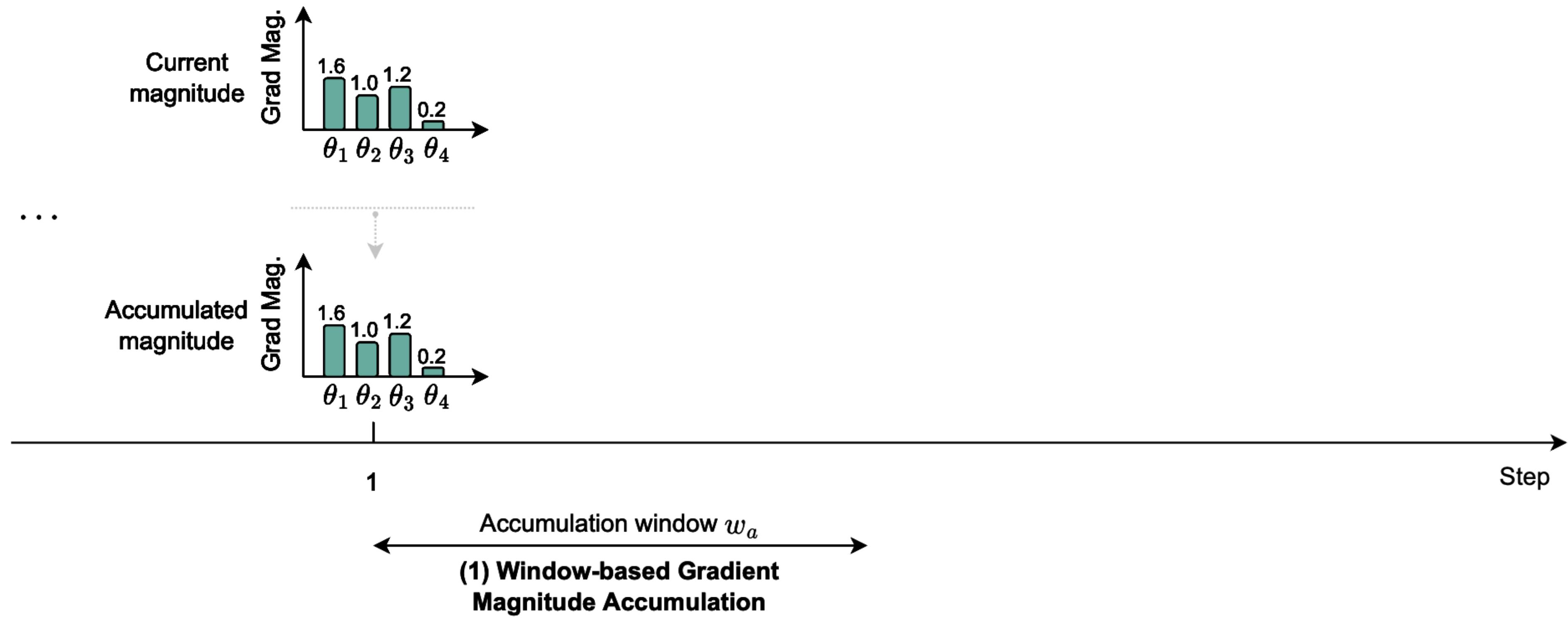
# Probabilistic Gradient Pruning

- **Accumulation Window** followed by **Pruning Window** repeatedly



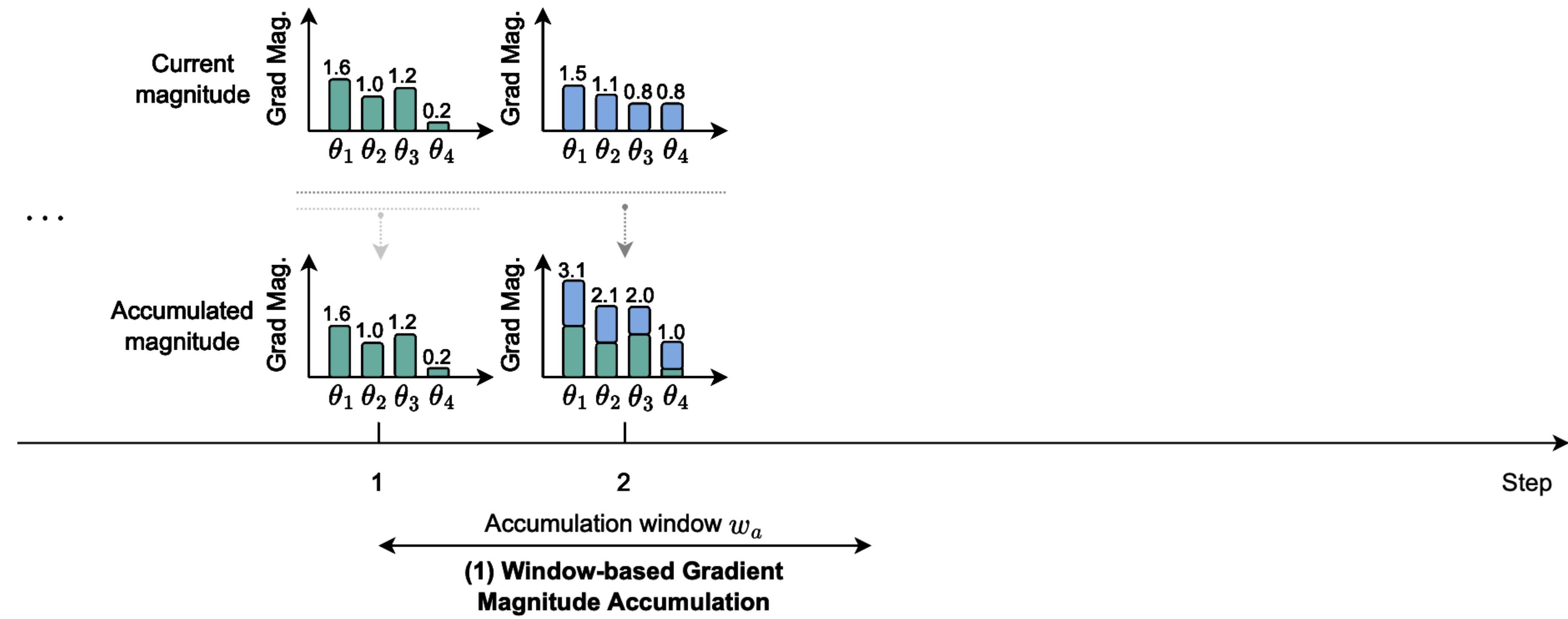
# Accumulation Window

- Keep a **record** of accumulated gradient magnitude



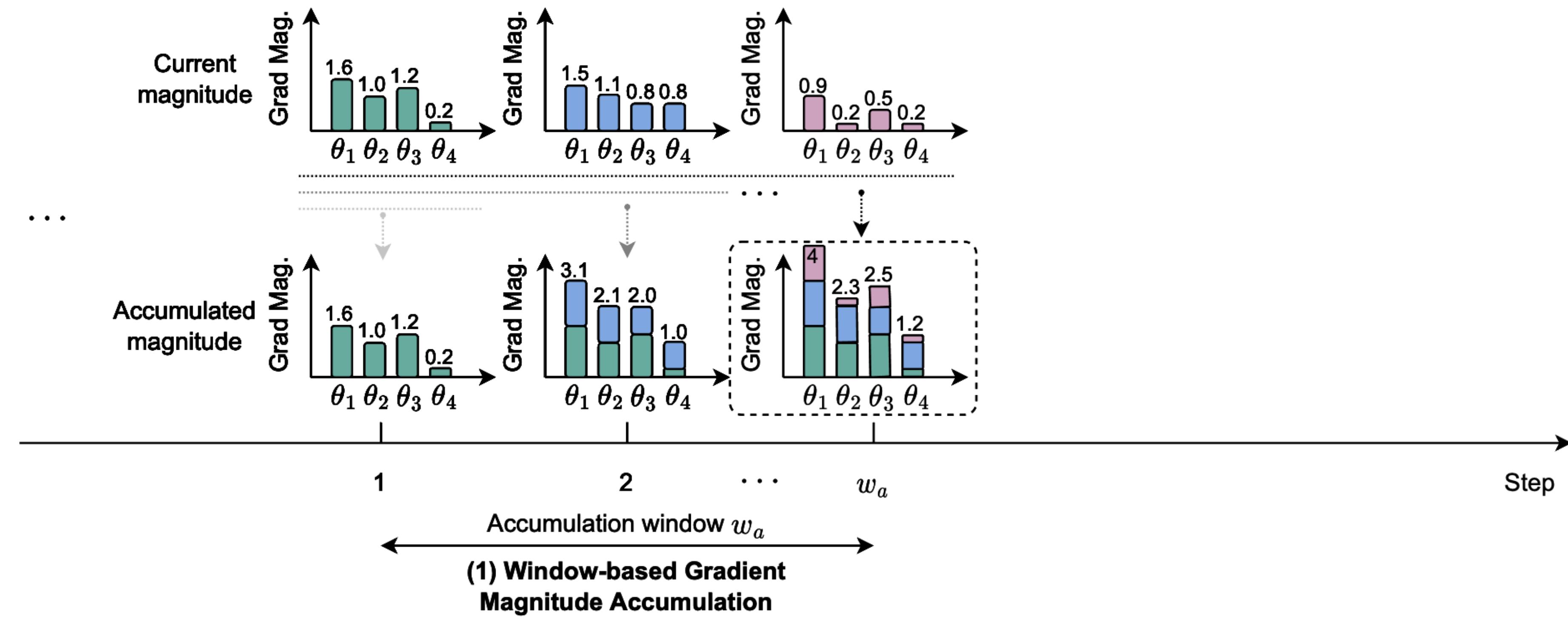
# Accumulation Window

- Keep a **record** of accumulated gradient magnitude.



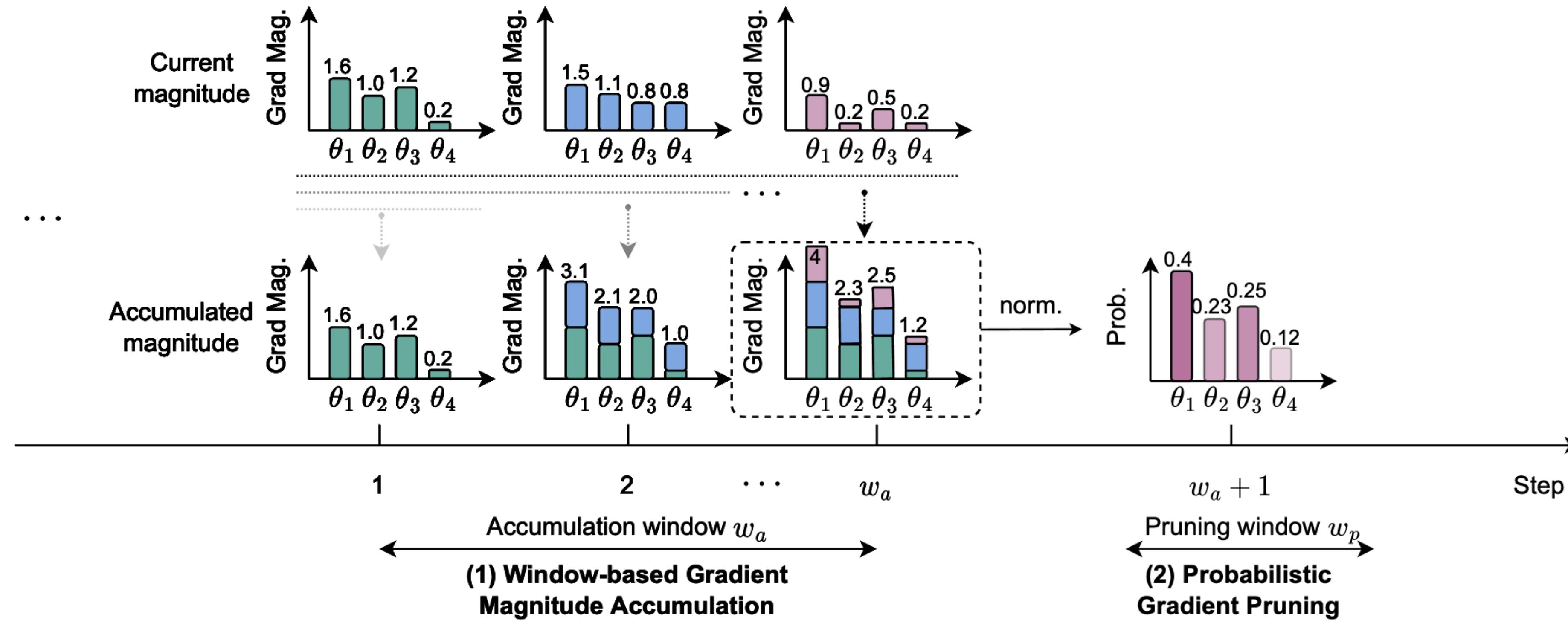
# Accumulation Window

- Keep a **record** of accumulated gradient magnitude



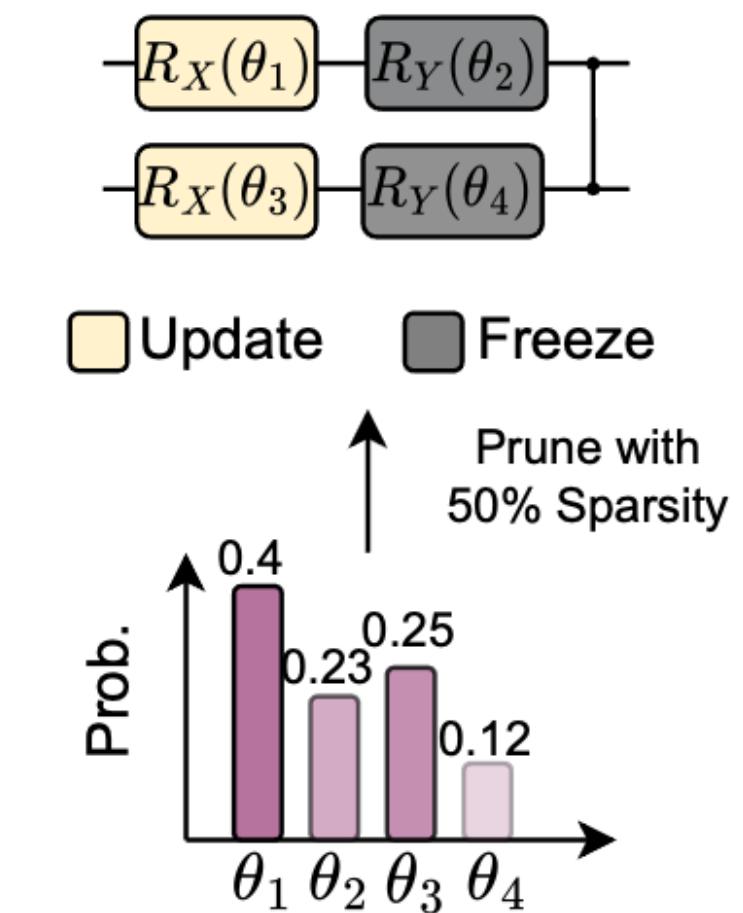
# Pruning Window

- Normalize the accumulated gradient magnitude to a probability distribution



# Pruning Window

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



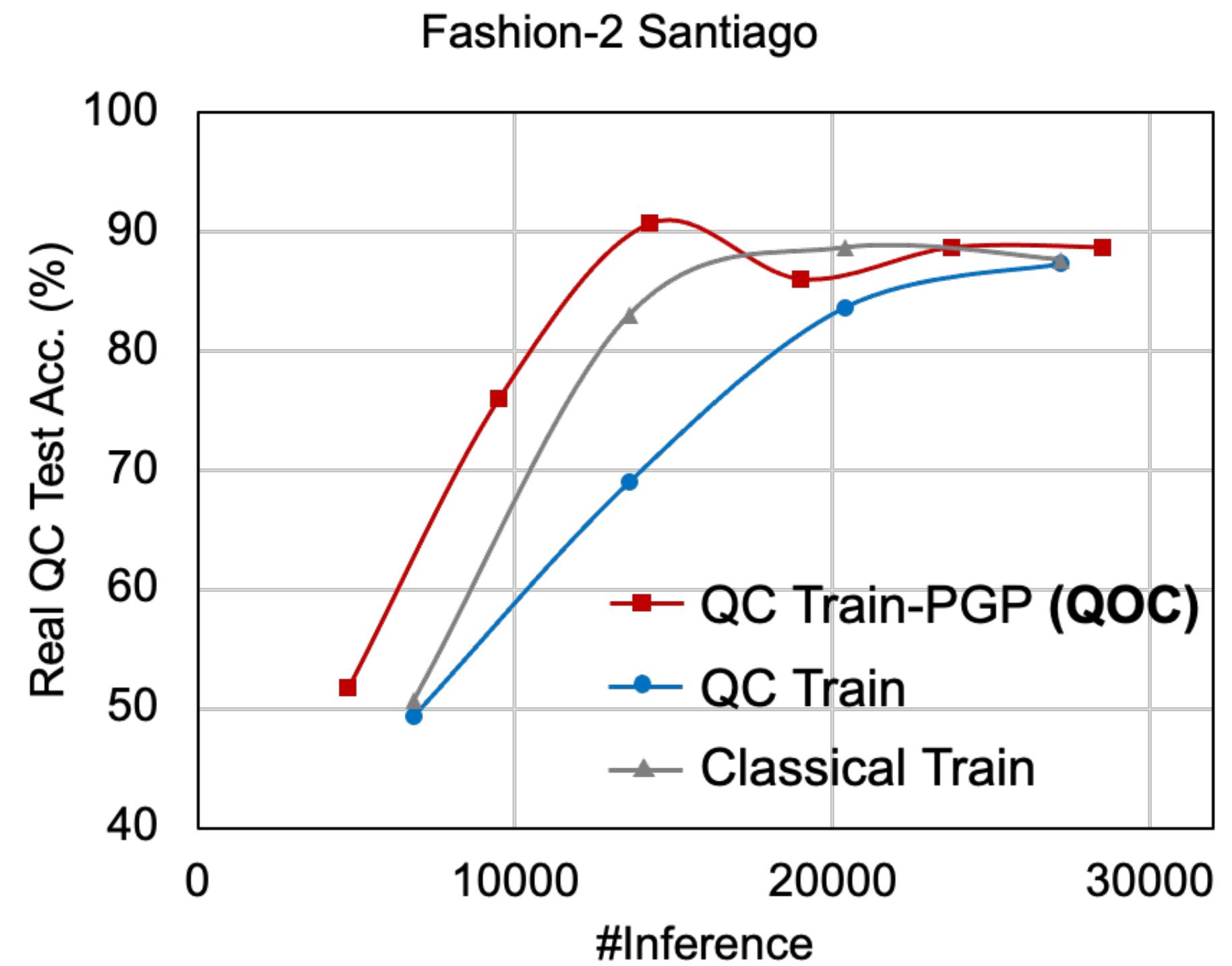
# Classification Results

- Gradient achieves similar results to classical simulation

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

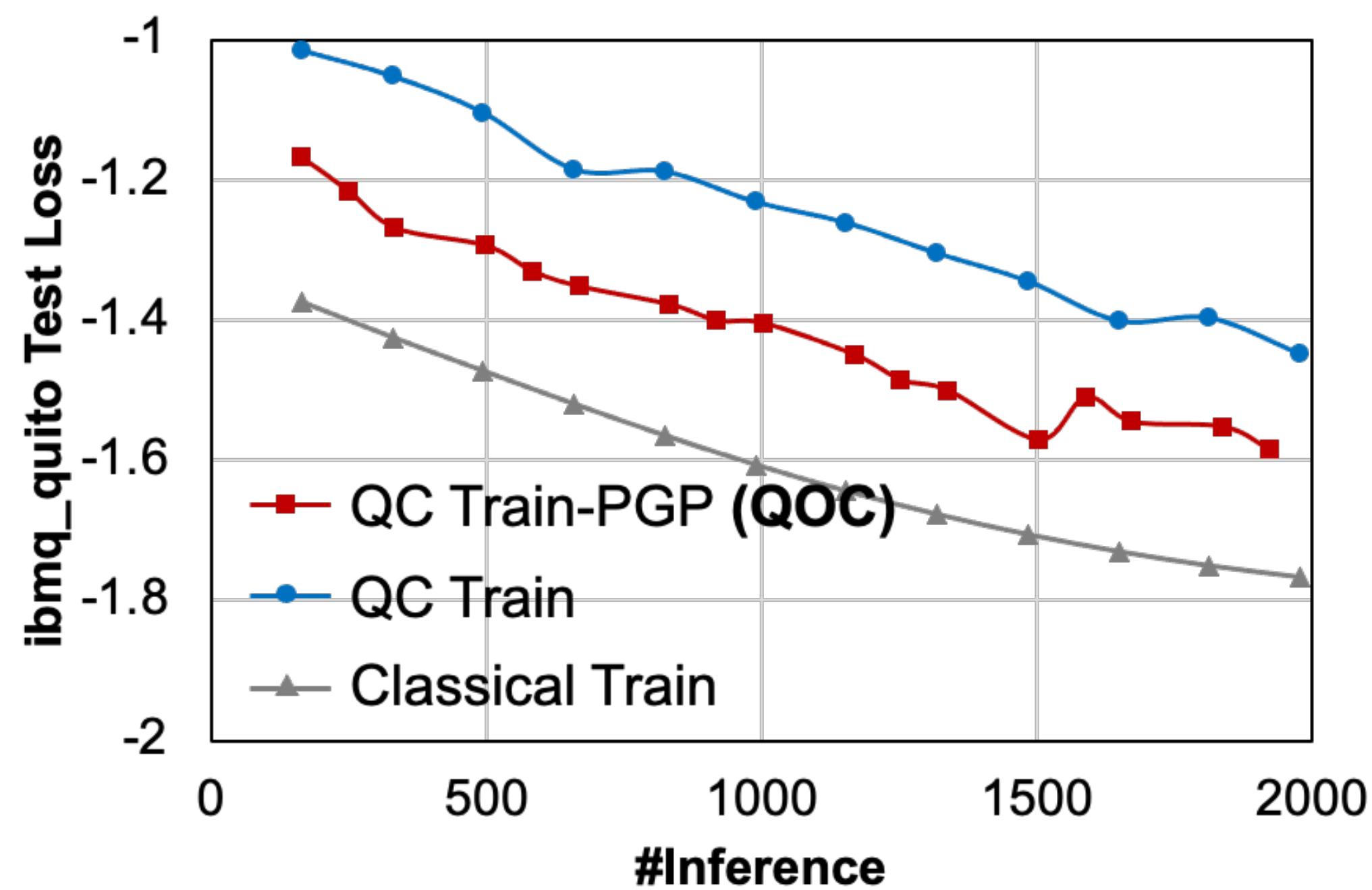
# Classification Results

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



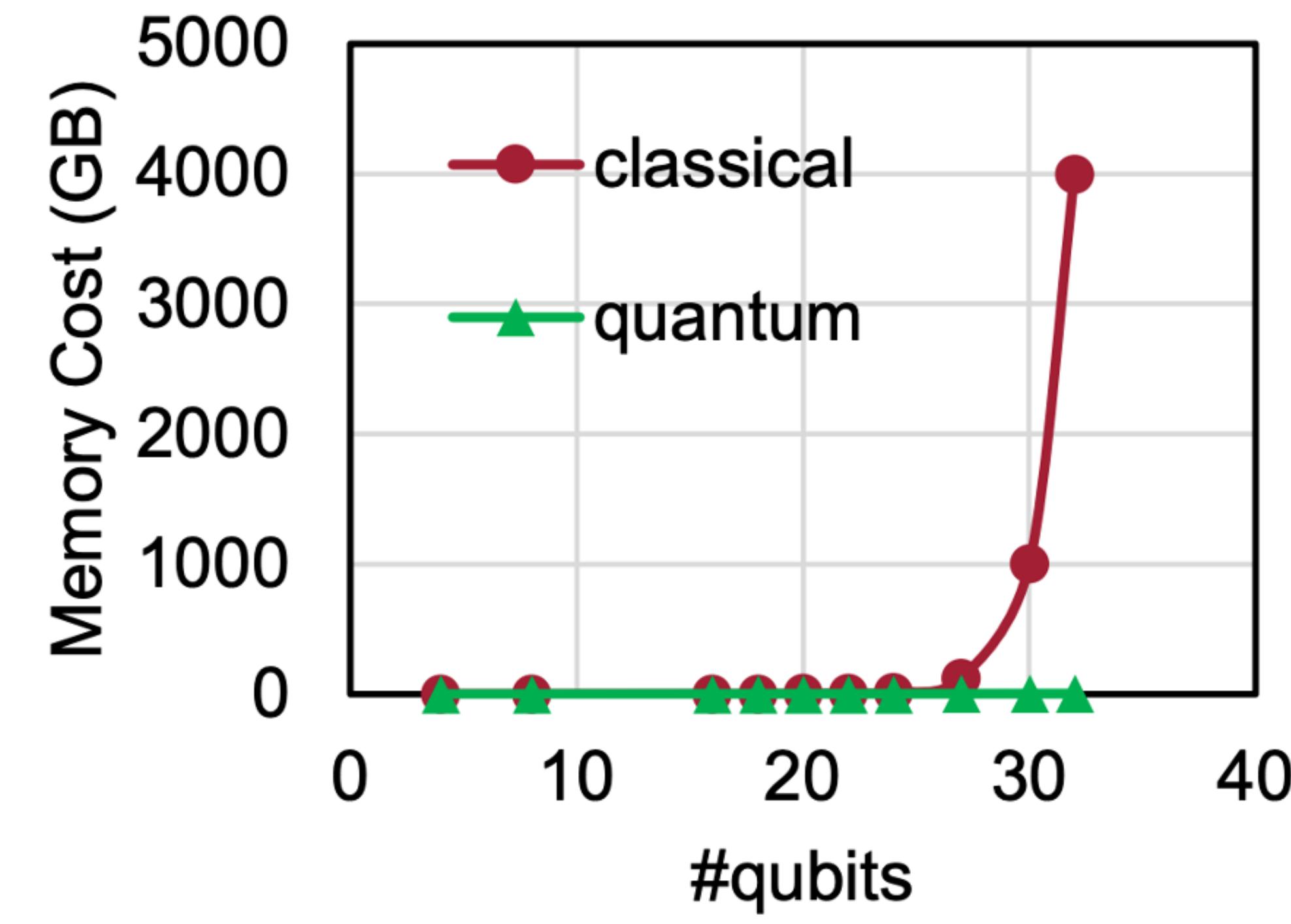
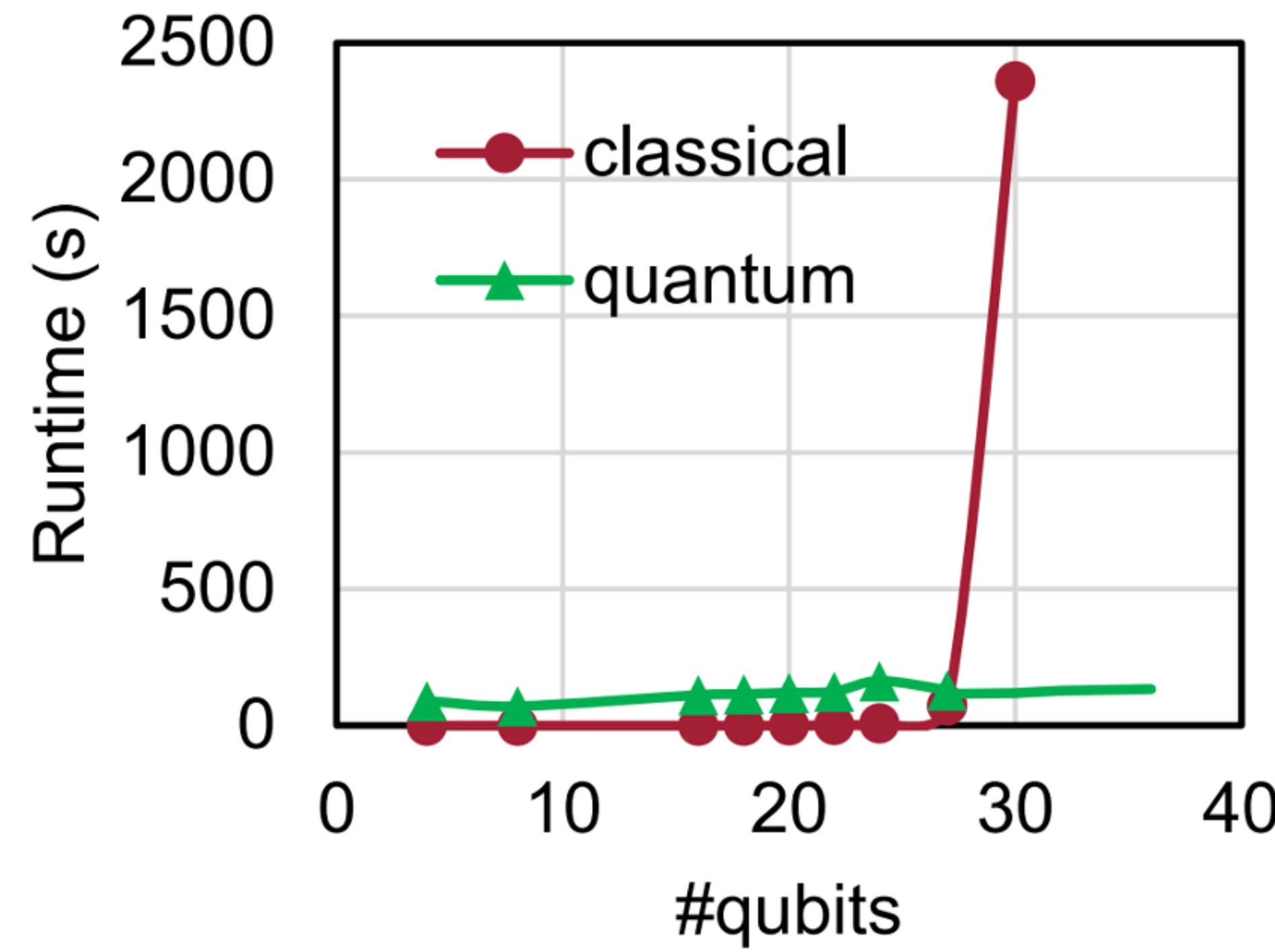
# VQE Results

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



# Scalability

- On-chip Training is scalable



# Probabilistic Pruning

- Probabilistic pruning can provide better results

Method	MNIST-4	MNIST-2	Fashion-4	Fashion-2
Deterministic	0.61	0.82	0.72	0.89
Probabilistic	<b>0.62</b>	<b>0.85</b>	<b>0.79</b>	<b>0.90</b>

# Section 5

## TorchQuantum Library for QML

# TorchQuantum

Good Infrastructure is Critical



Torch  
Quantum

# TorchQuantum

## 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

## Good Infrastructure is Critical

- 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
  - And so on...

# Construct a QNN with TorchQuantum

Initialize a quantum device

```
import torch.nn as nn
import torch.nn.functional as F
import torchquantum as tq
import torchquantum.functional as tqf

class QFCModel(nn.Module):
    def __init__(self):
        super().__init__()
        self.n_wires = 4
        self.q_device = tq.QuantumDevice(n_wires=self.n_wires)
        self.measure = tq.MeasureAll(tq.PauliZ)
```

Specify encoder gates

```
self.encoder_gates = [tqf.rx] * 4 + [tqf.ry] * 4 + \
                     [tqf.rz] * 4 + [tqf.rx] * 4
```

Specify trainable gates

```
self.rx0 = tq.RX(has_params=True, trainable=True)
self.ry0 = tq.RY(has_params=True, trainable=True)
self.rz0 = tq.RZ(has_params=True, trainable=True)
self.crx0 = tq.CRX(has_params=True, trainable=True)
```

# Construct a QNN with TorchQuantum

Reset statevector

```
def forward(self, x):
    bsz = x.shape[0]
    # down-sample the image
    x = F.avg_pool2d(x, 6).view(bsz, 16)

    # reset qubit states
    self.q_device.reset_states(bsz)
```

Encode classical pixels

```
# encode the classical image to quantum domain
for k, gate in enumerate(self.encoder_gates):
    gate(self.q_device, wires=k % self.n_wires, params=x[:, k])
```

Apply the trainable gates

```
# add some trainable gates (need to instantiate ahead of time)
self.rx0(self.q_device, wires=0)
self.ry0(self.q_device, wires=1)
self.rz0(self.q_device, wires=3)
self.crx0(self.q_device, wires=[0, 2])
```

Apply some non-trainable gates

```
# add some more non-parameterized gates (add on-the-fly)
tqf.hadamard(self.q_device, wires=3)
tqf.sx(self.q_device, wires=2)
tqf.cnot(self.q_device, wires=[3, 0])
tqf.qubitunitary(self.q_device0, wires=[1, 2], params=[[1, 0, 0, 0],
                                                       [0, 1, 0, 0],
                                                       [0, 0, 0, 1j],
                                                       [0, 0, -1j, 0]])
```

Measure to get classical values

```
# perform measurement to get expectations (back to classical domain)
x = self.measure(self.q_device).reshape(bsz, 2, 2)

# classification
x = x.sum(-1).squeeze()
x = F.log_softmax(x, dim=1)

return x
```

# 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 1:
    - `import torchquantum.functional as tqf`
    - `tqf.h(q_dev, wires=1)`
  - 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

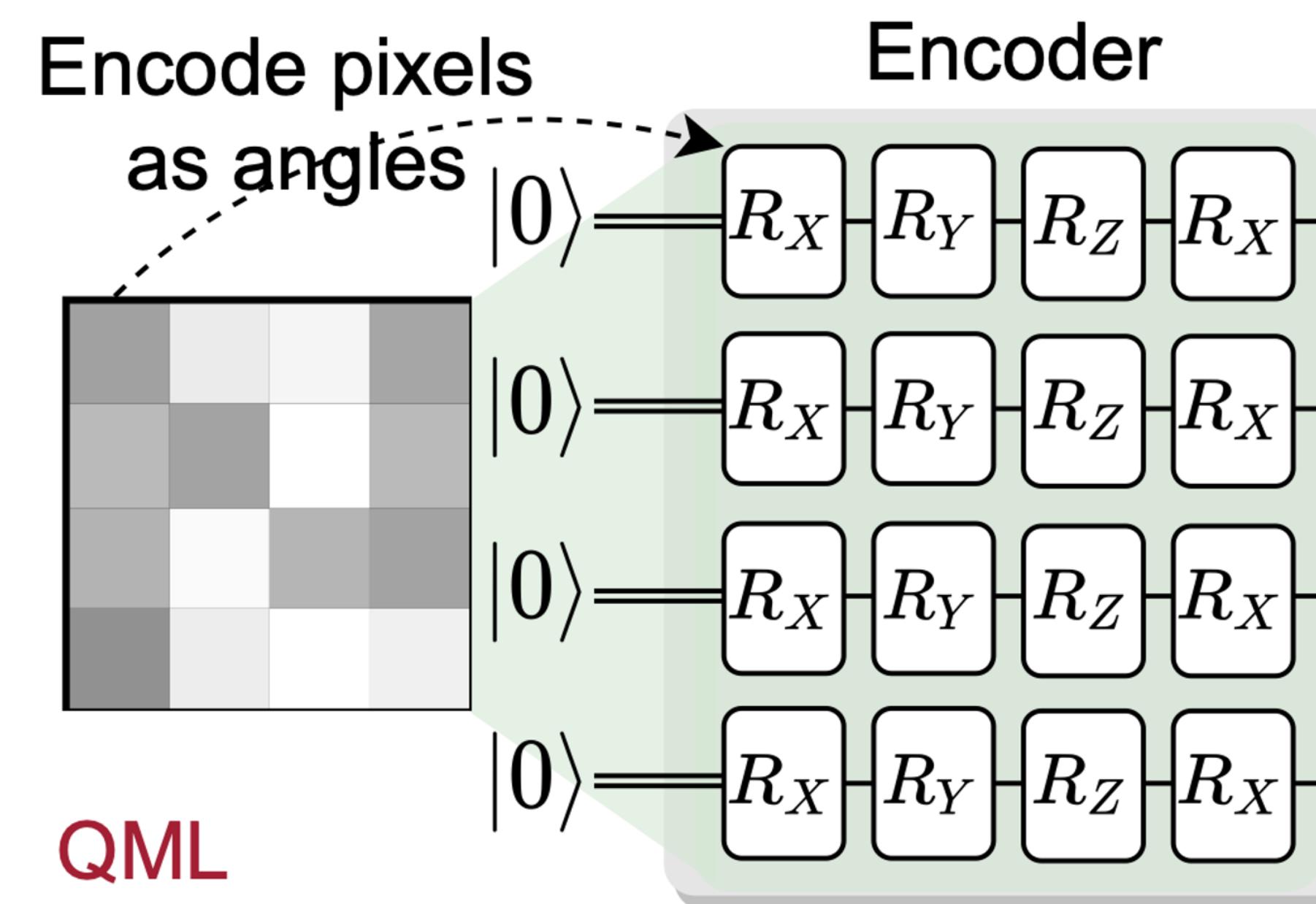
```
_state = torch.zeros(2 ** self.n_wires, dtype=C_DTYPE)
_state[0] = 1 + 0j

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

# 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



# Convert tq Model to Other Frameworks

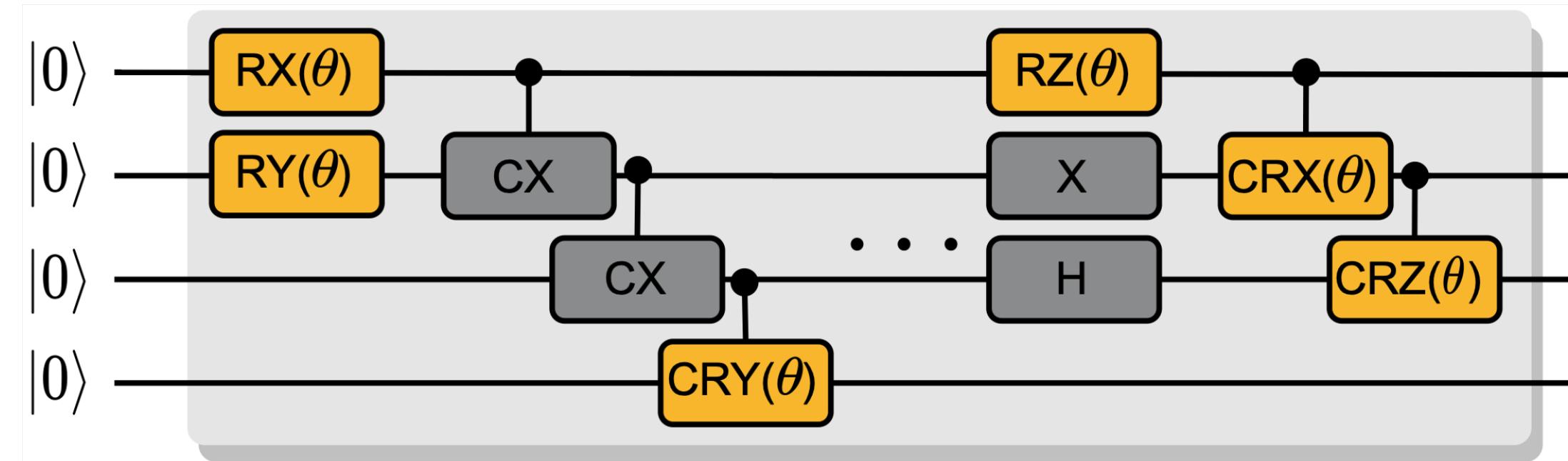
- Convert the `tq.QuantumModule` to other frameworks such as Qiskit
  - `from torchquantum.plugins.qiskit_plugin import tq2qiskit`
  - `circ = tq2qiskit(q_dev, q_model)`
  - `circ.draw('mpl')`

# Section 6

## **Robust Quantum Circuit Architecture Search**

# Parameterized Quantum Circuits

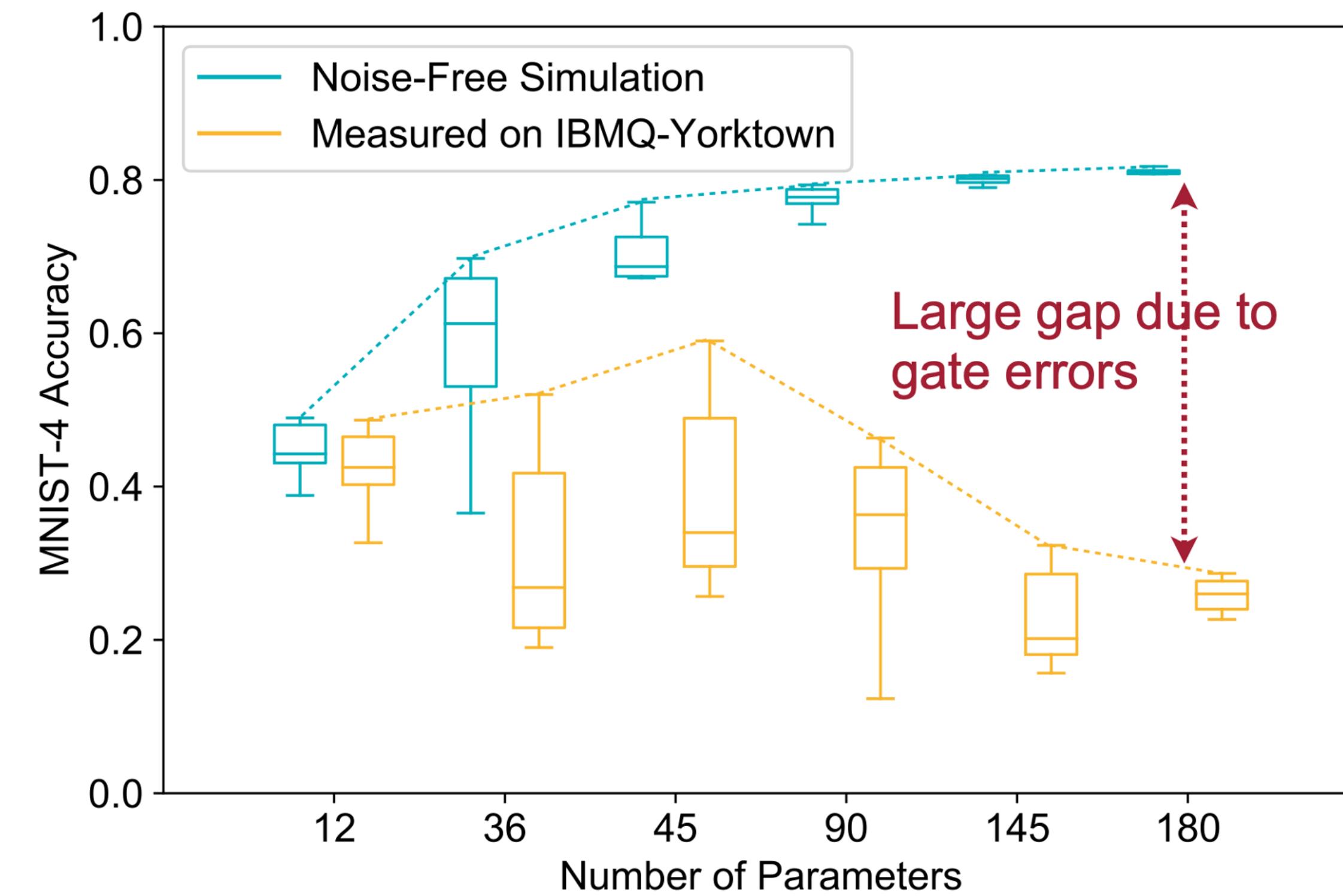
- Parameterized Quantum Circuits (PQC)
- Quantum circuit with fixed gates and parameterized gates



- PQCs are commonly used in **hybrid classical-quantum models** and show promises to achieve quantum advantage
  - Variational Quantum Eigensolver (VQE)
  - Quantum Neural Networks (QNN)
  - Quantum Approximate Optimization Algorithm (QAOA)

# Challenges of PQC — Noise

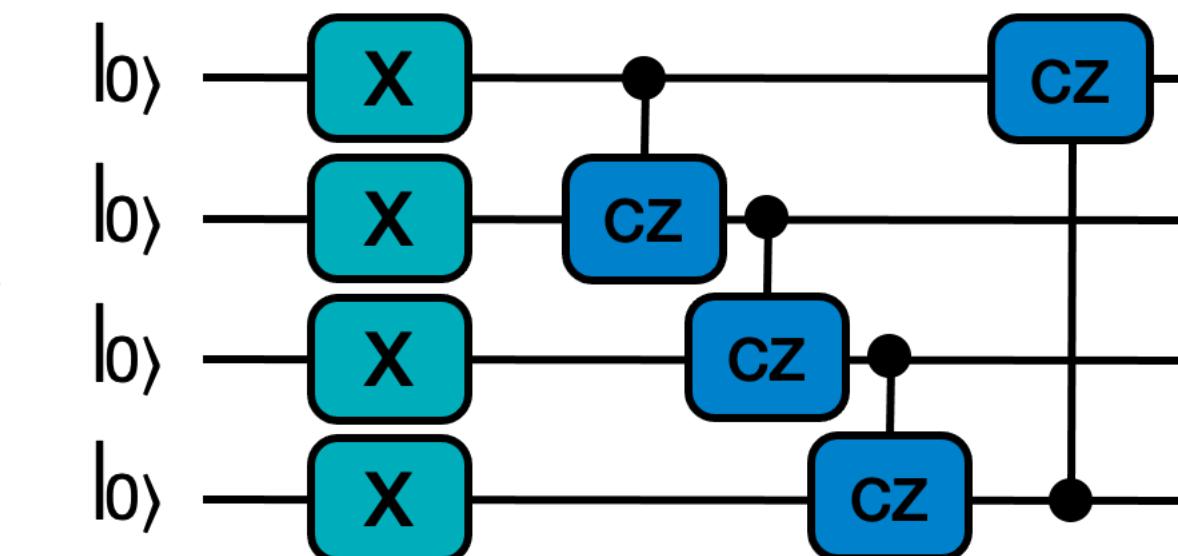
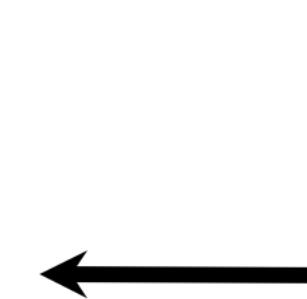
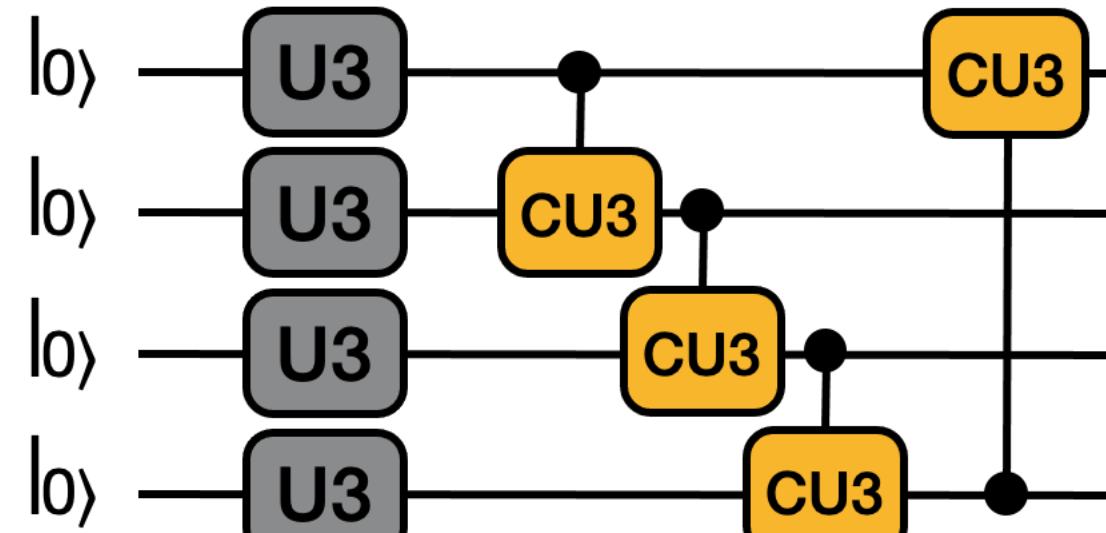
- Noise **degrades** PQC reliability
- More parameters increase the noise-free accuracy but degrade the measured accuracy
- Therefore, circuit architecture is critical



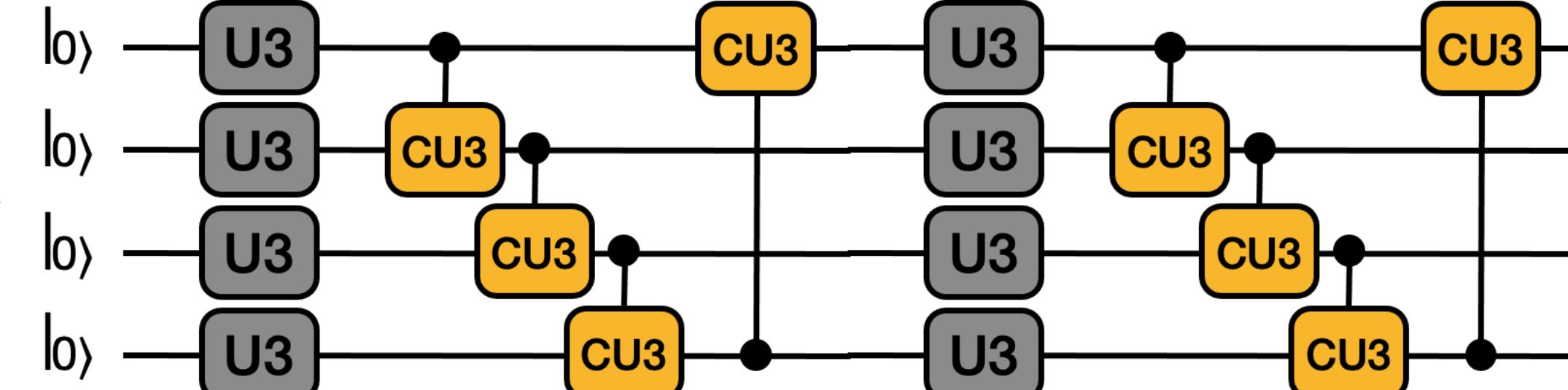
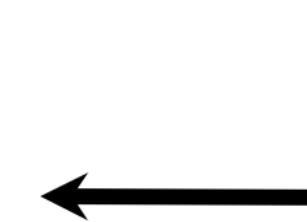
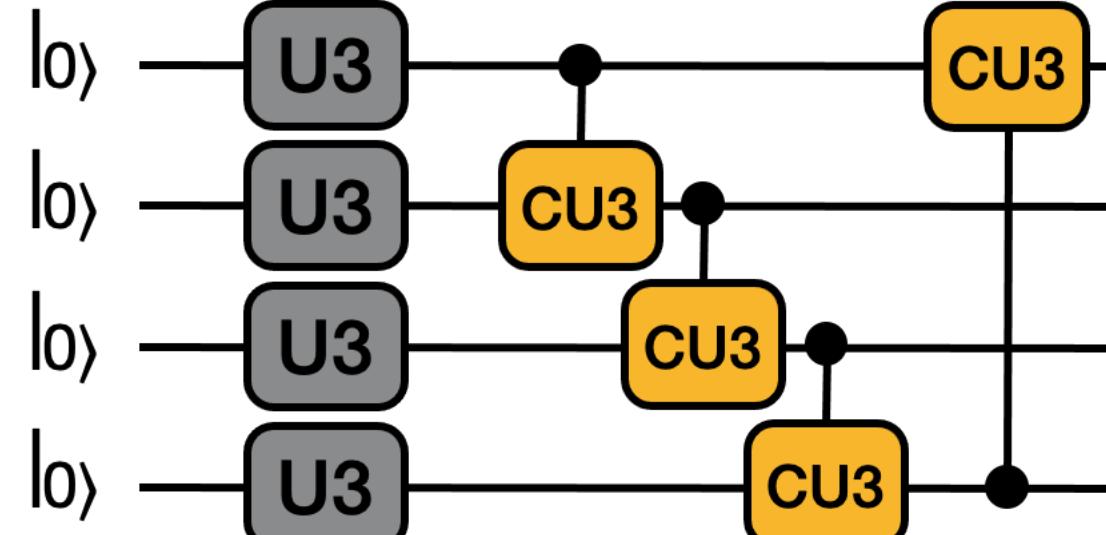
# Challenges of PQC — Large Design Space

- Large design space for circuit architecture

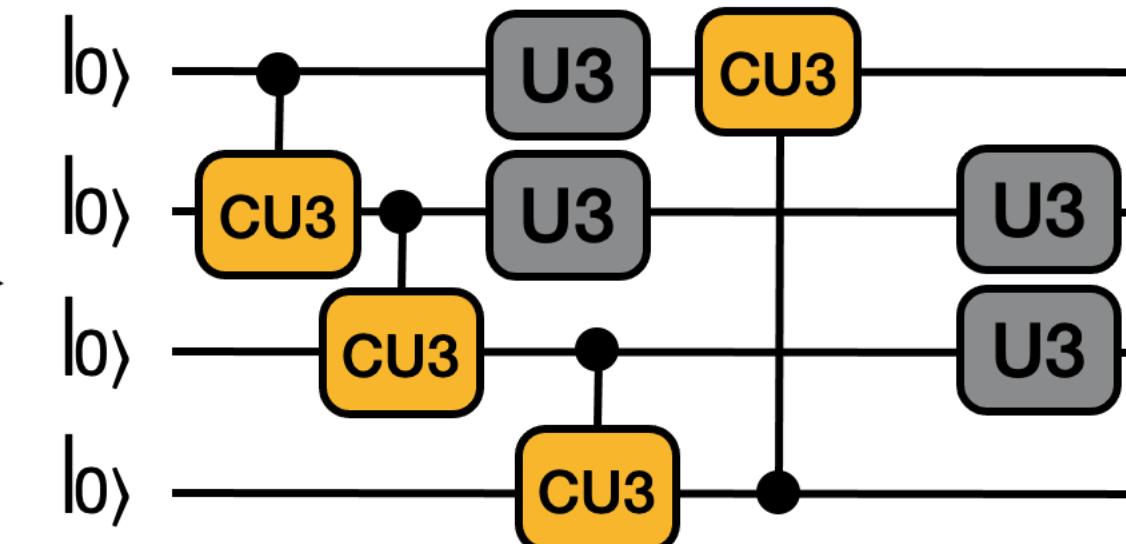
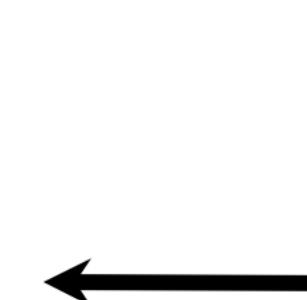
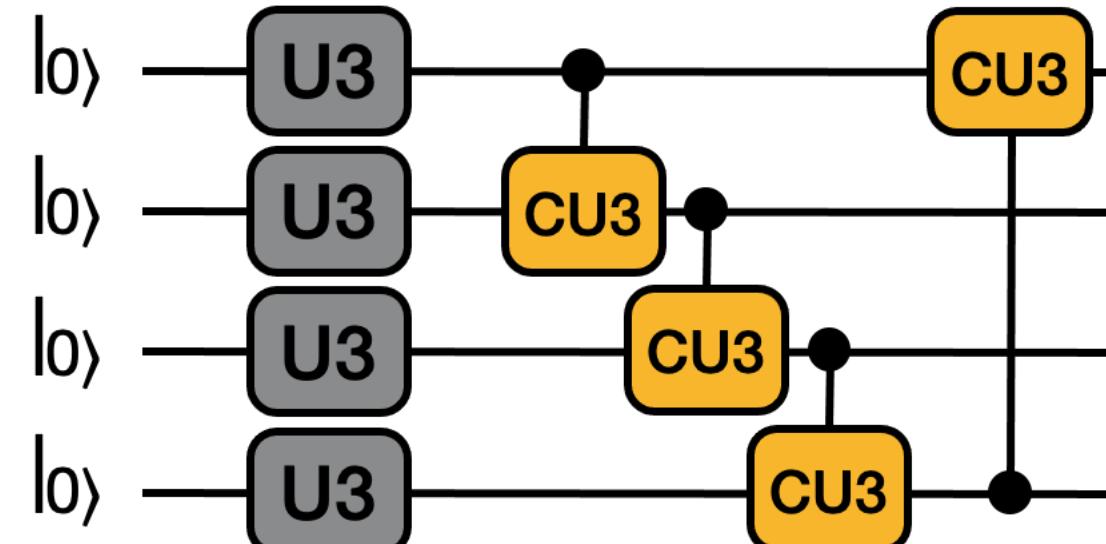
- Type of gates



- Number of gates



- Position of gates



# QuantumNAS Framework

## 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

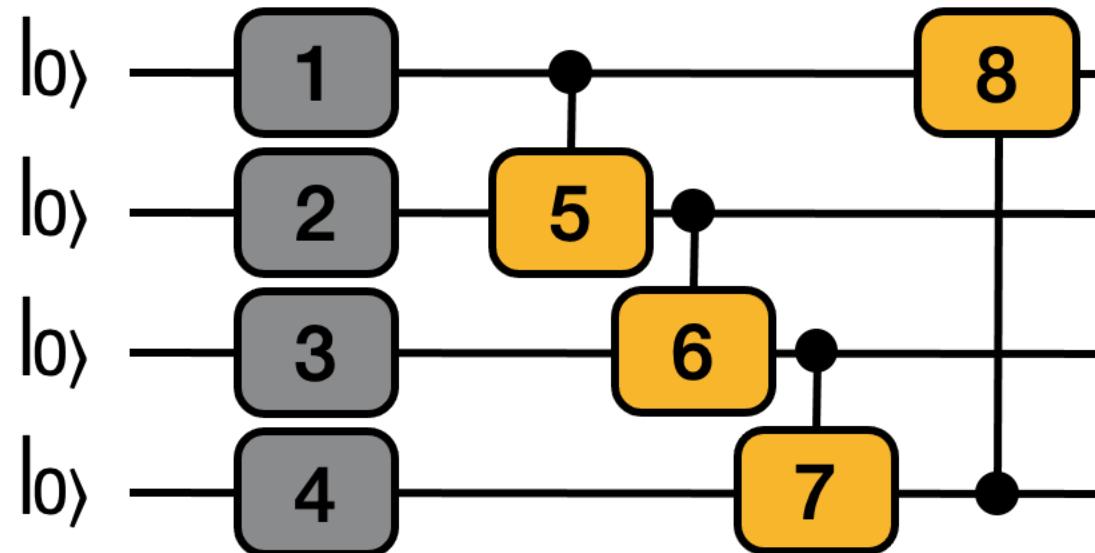
# QuantumNAS Framework

## Four Steps

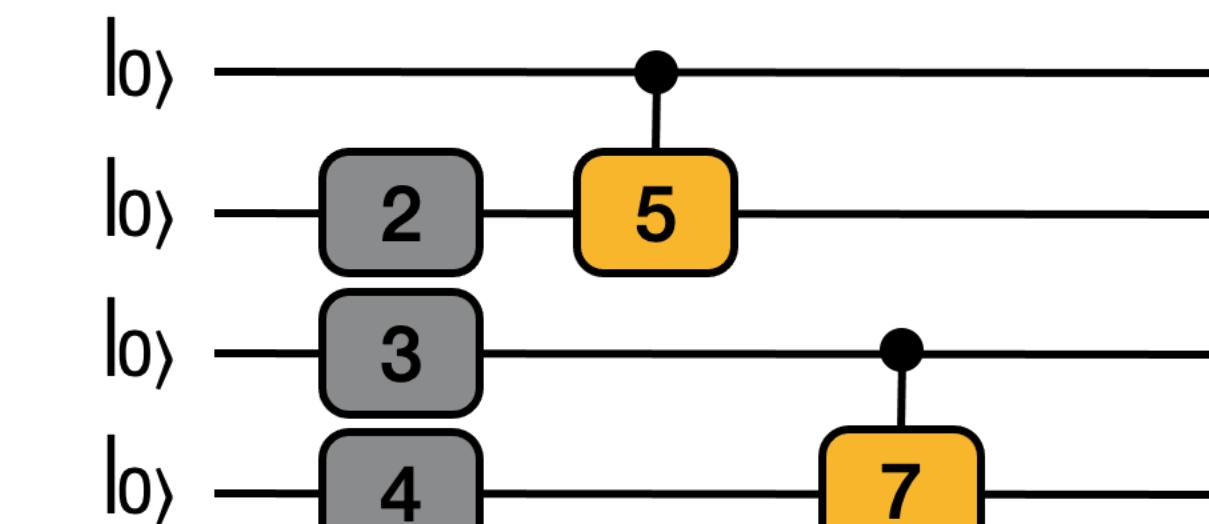
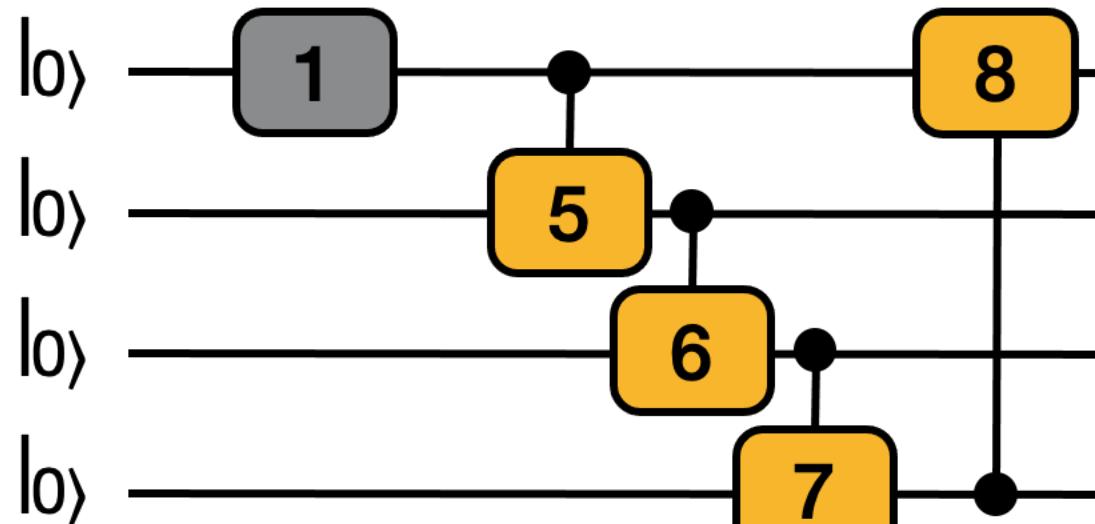
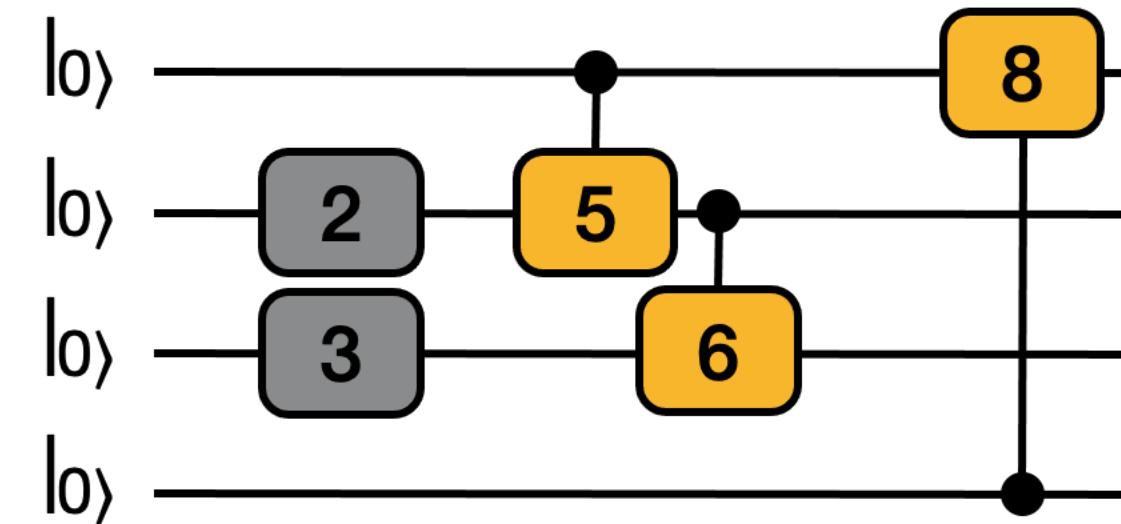
- SuperCircuit Construction and Training
- Noise-Adaptive Evolutionary Co-Search of SubCircuit and Qubit Mapping
- Train the Searched SubCircuit
- Iterative Quantum Gate Pruning

# 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: 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

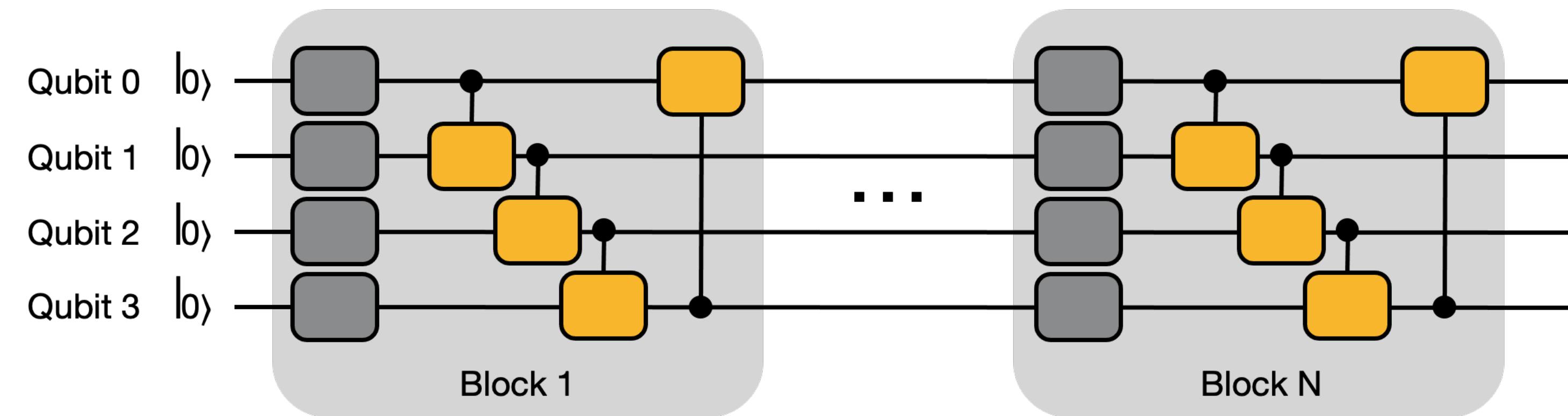
- Why use a SuperCircuit?
  - Enables **efficient** search of architecture candidates without training each
  - SubCircuit inherits parameters from SuperCircuit
  - With **inherited** parameters, we find some good SubCircuits, we find that they **are also good SubCircuits** with parameters **trained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

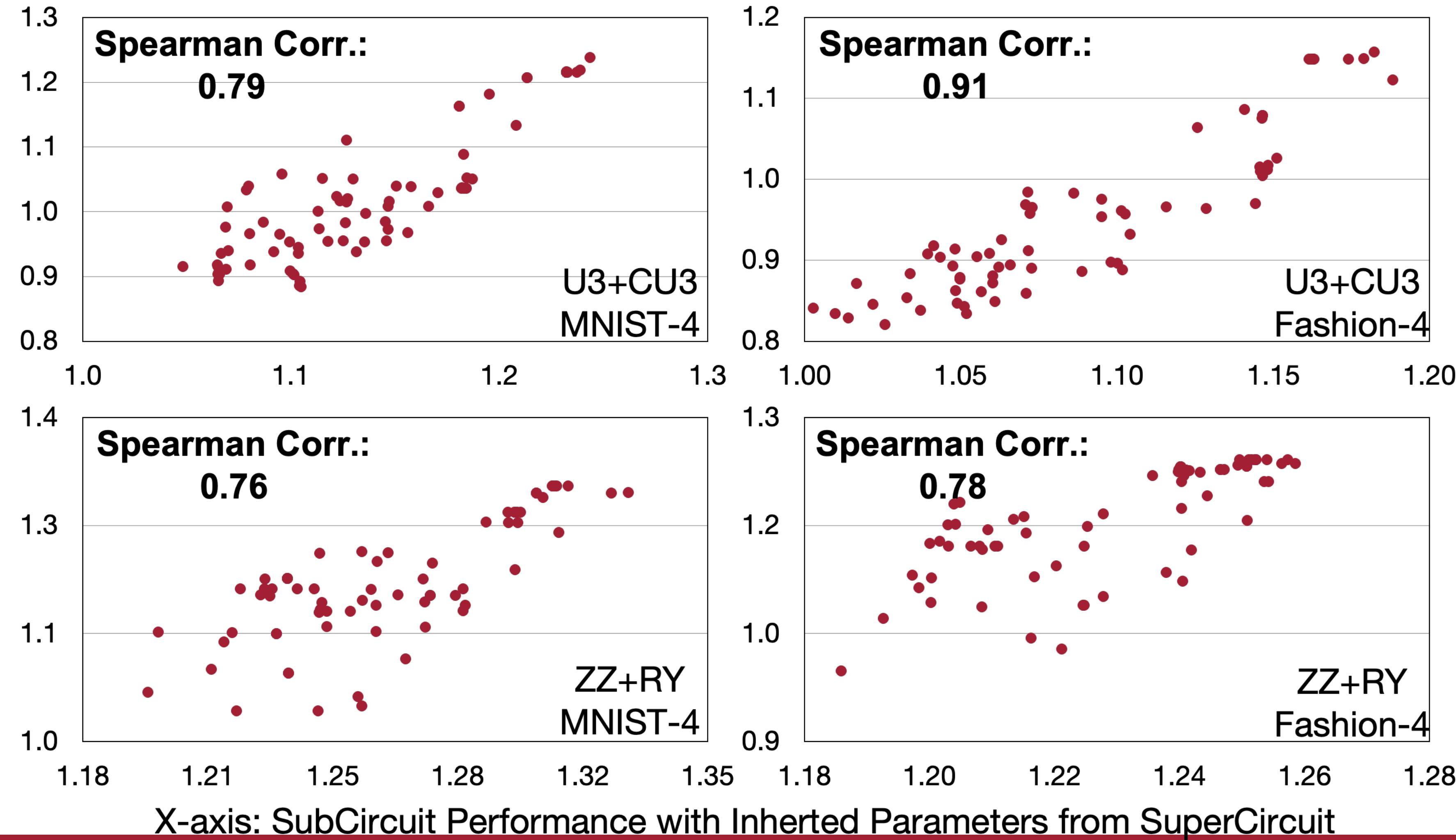
# Train SuperCircuit for Multiple Steps

- In one SuperCircuit Training step: Sample and Train



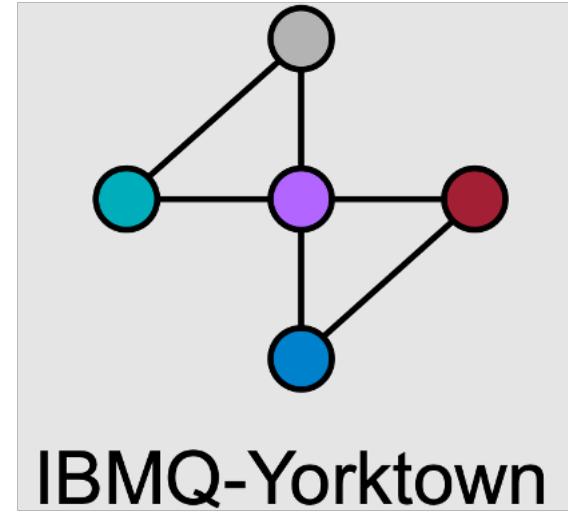
# How Reliable is the SuperCircuit?

- Inherited parameters from SuperCircuit can provide accurate **relative performance**



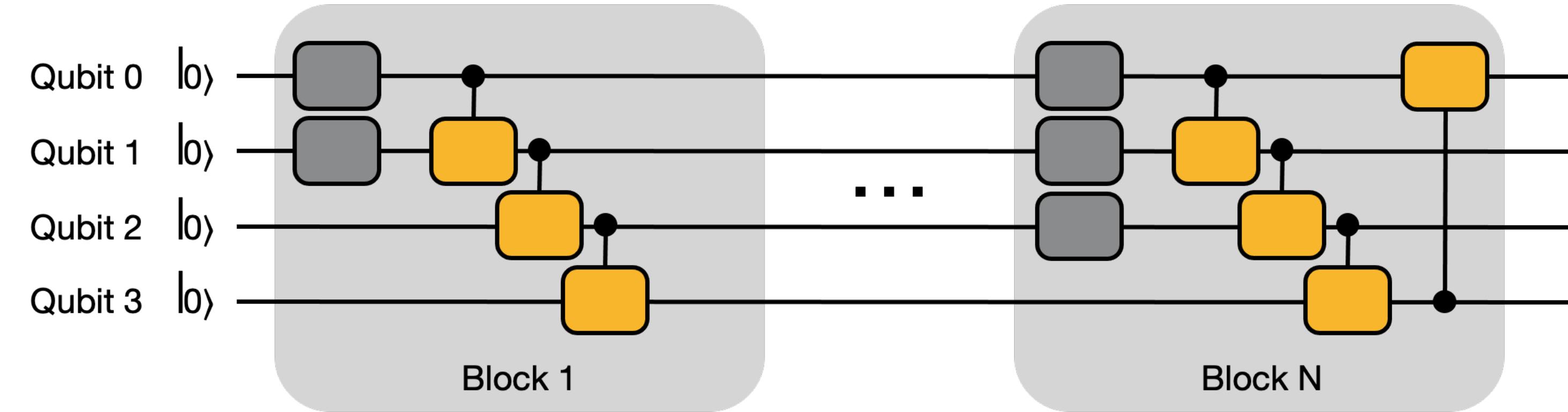
# Noise-Adaptive Evolutionary Search

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



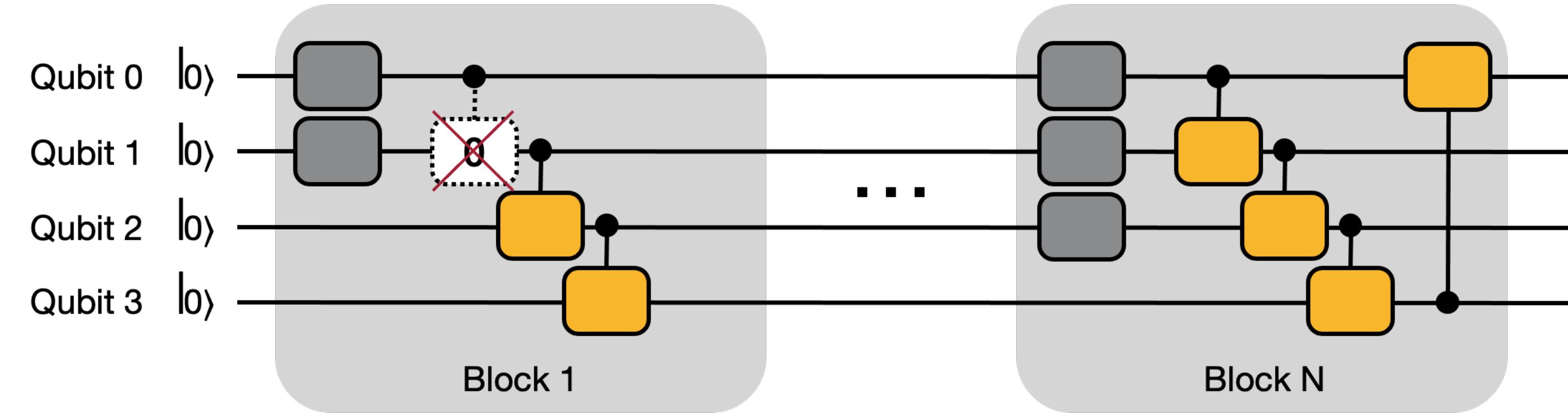
# Iterative Quantum Gate Pruning

- 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



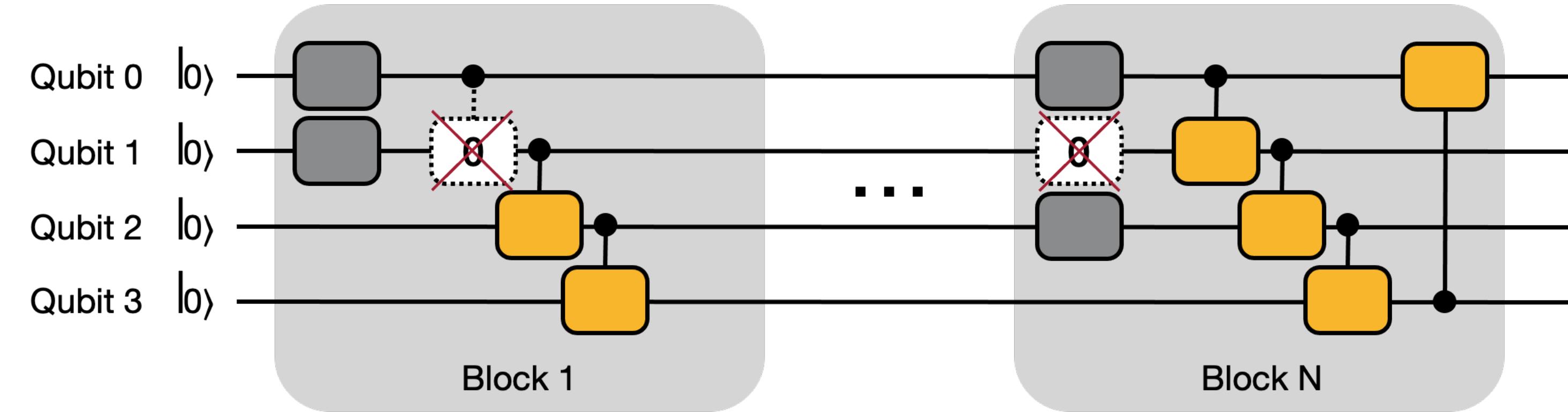
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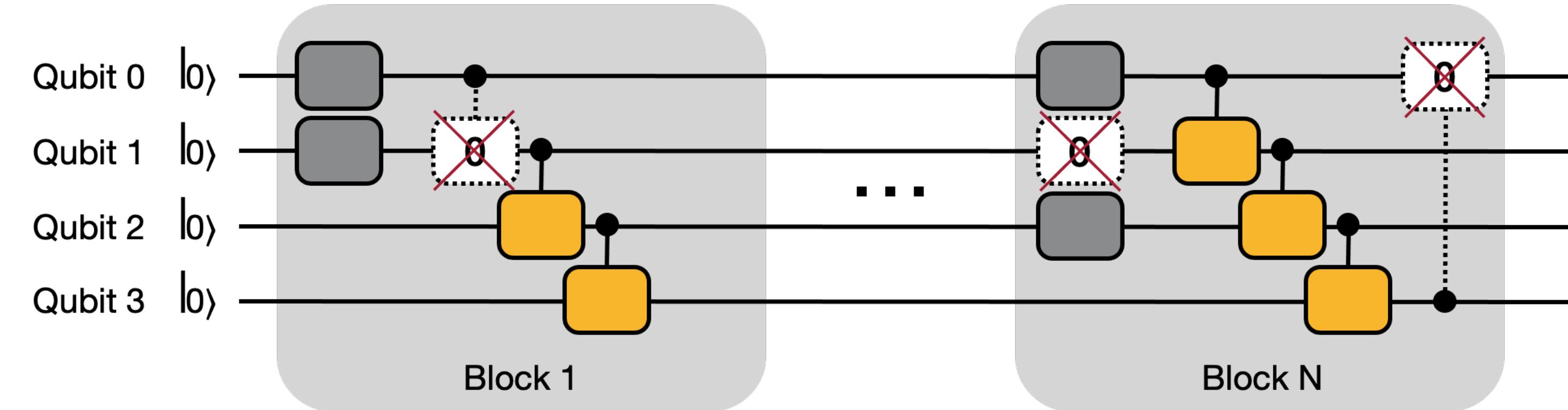
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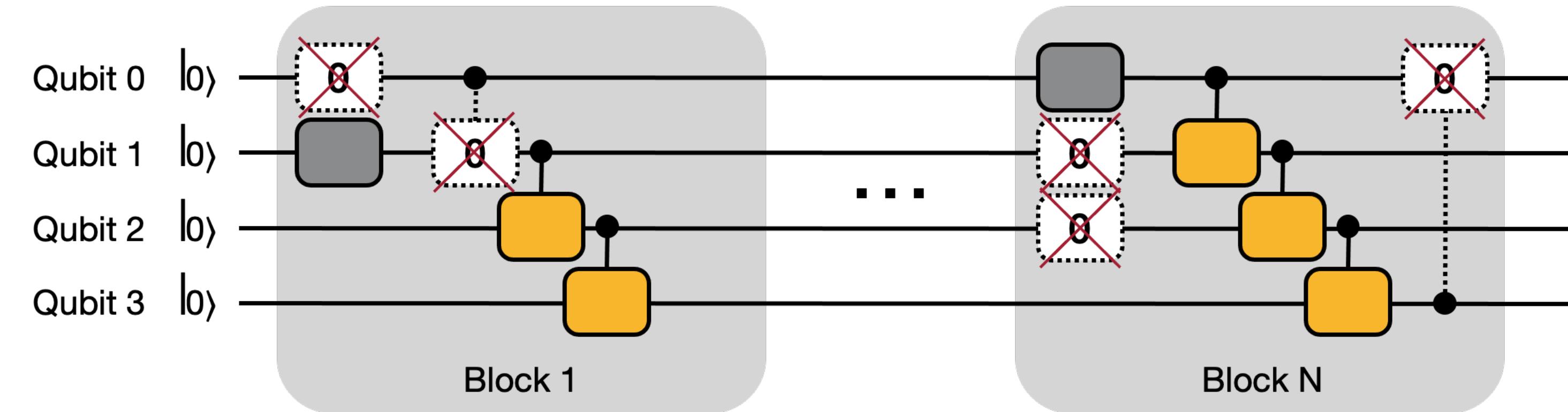
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# Iterative Quantum Gate Pruning

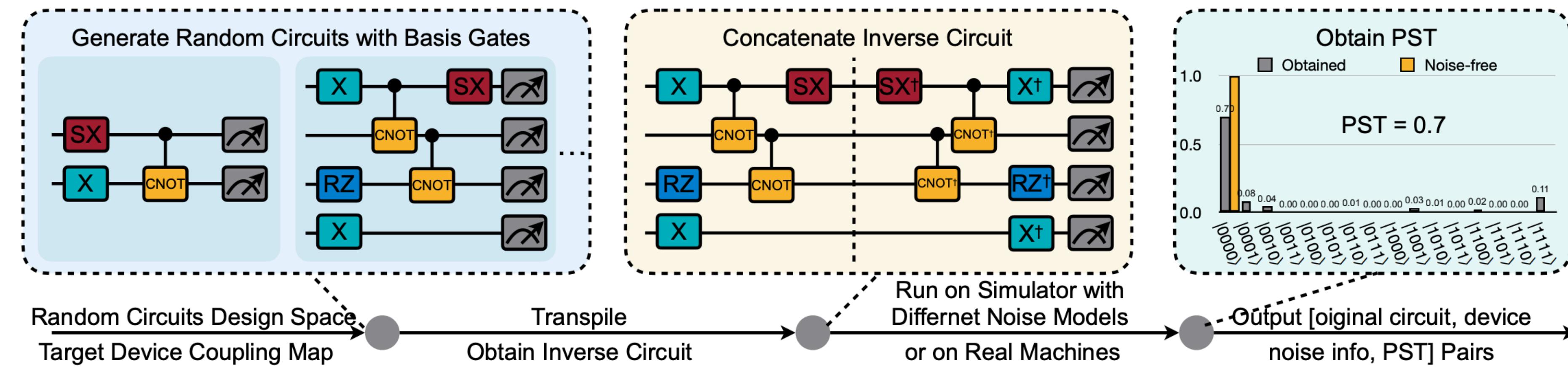
- Some gates have parameters **close to 0**
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# Other Search Frameworks

## Faster method to evaluate real device performance

- Graph transformer for circuit fidelity estimation

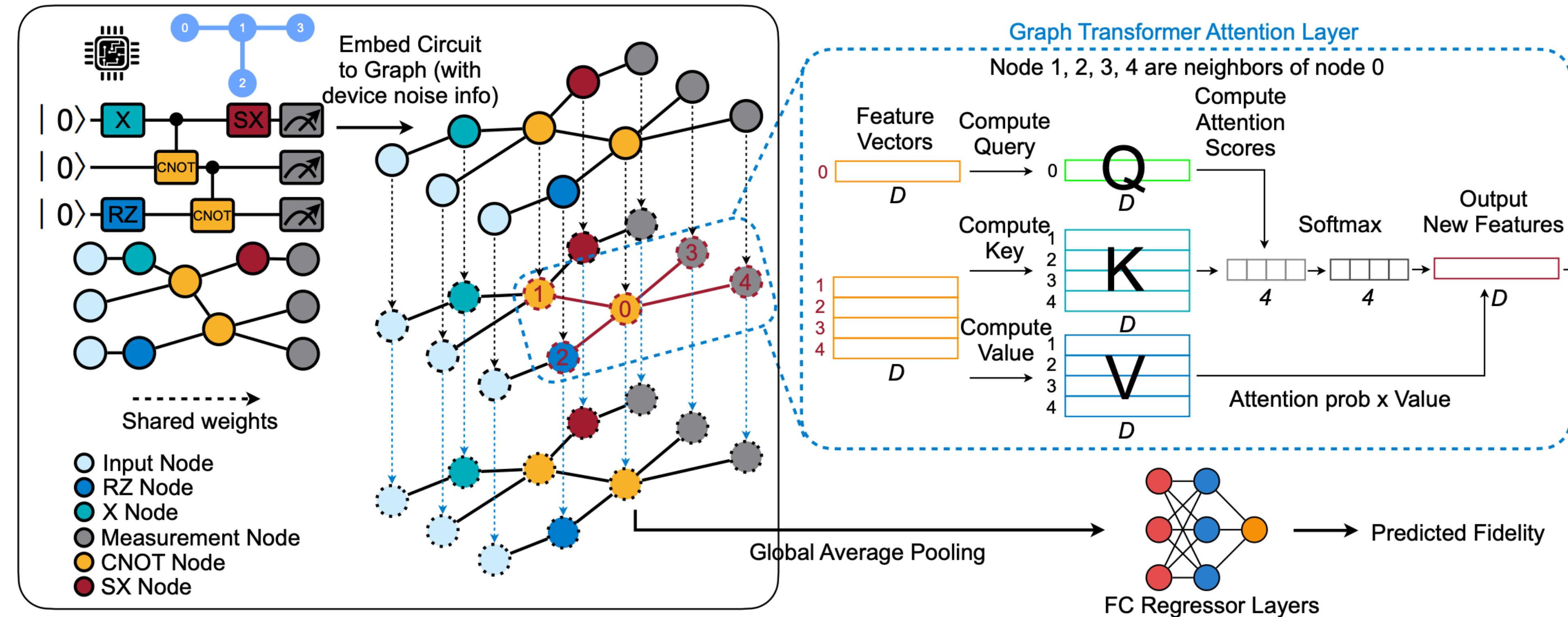


QuEst: Graph Transformer for Quantum Circuit Reliability Estimation

# Other Search Frameworks

## Faster method to evaluate real device performance

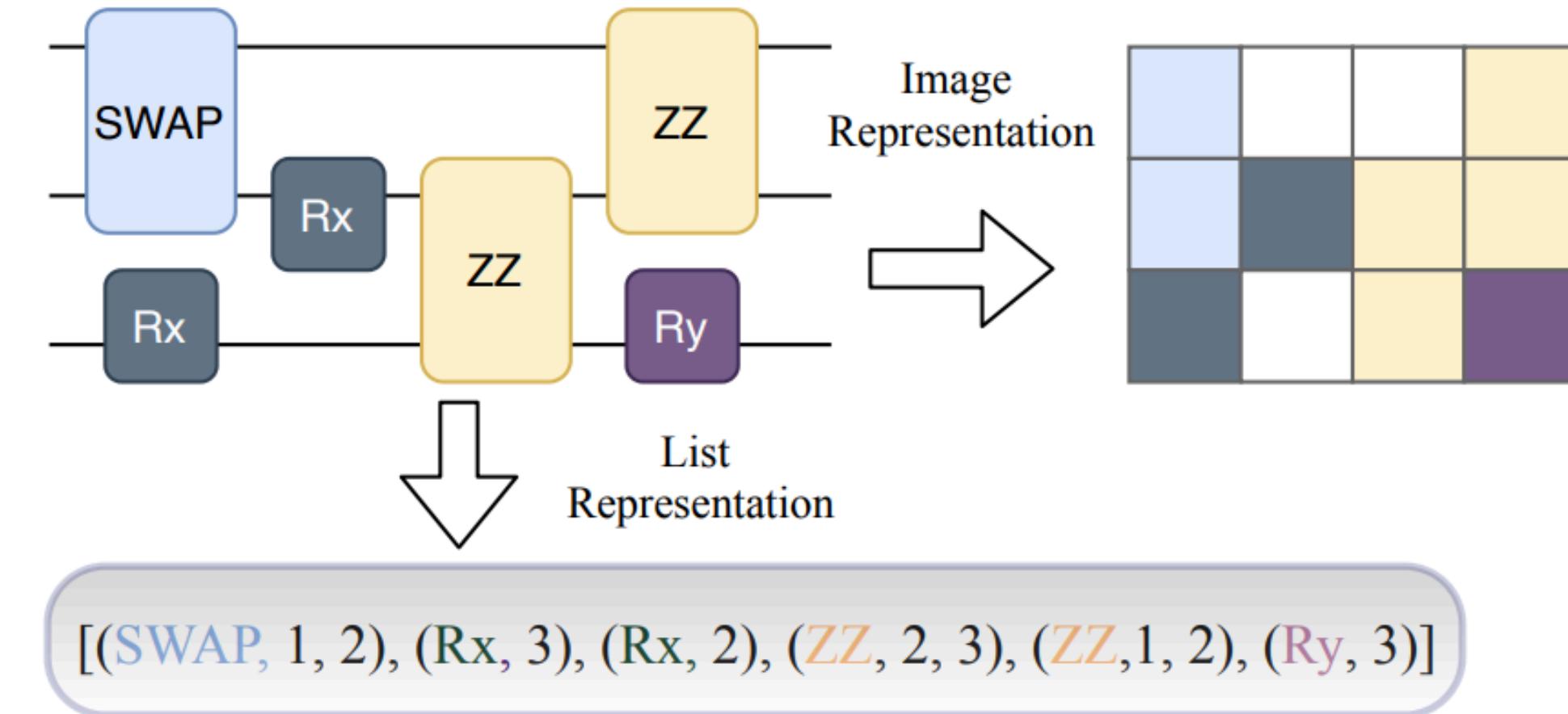
- Graph transformer for circuit fidelity estimation



QuEst: Graph Transformer for Quantum Circuit Reliability Estimation

# Other Search Frameworks

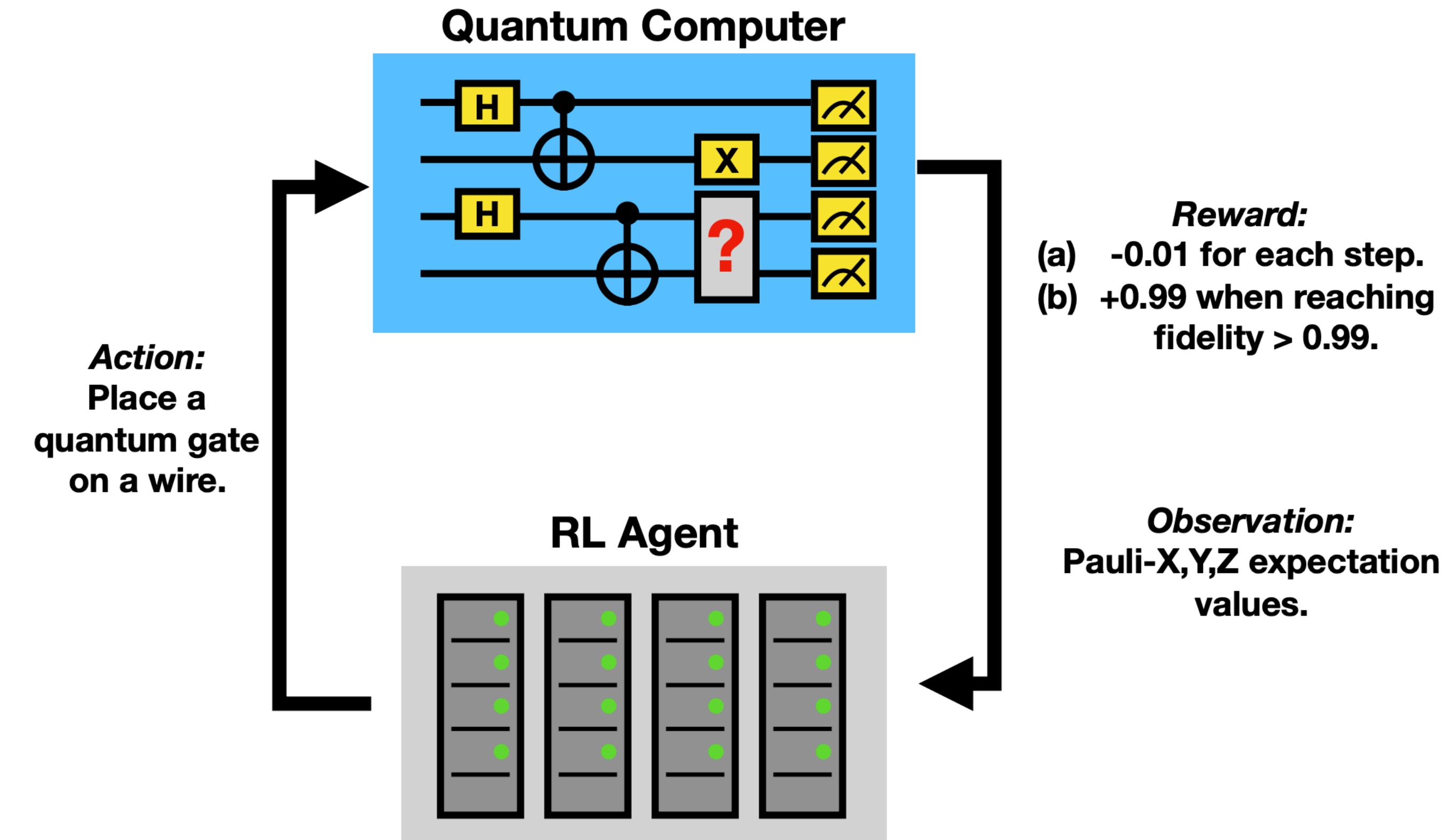
Faster method to evaluate real device performance



Neural Predictor based Quantum Architecture Search

# Other Search Frameworks

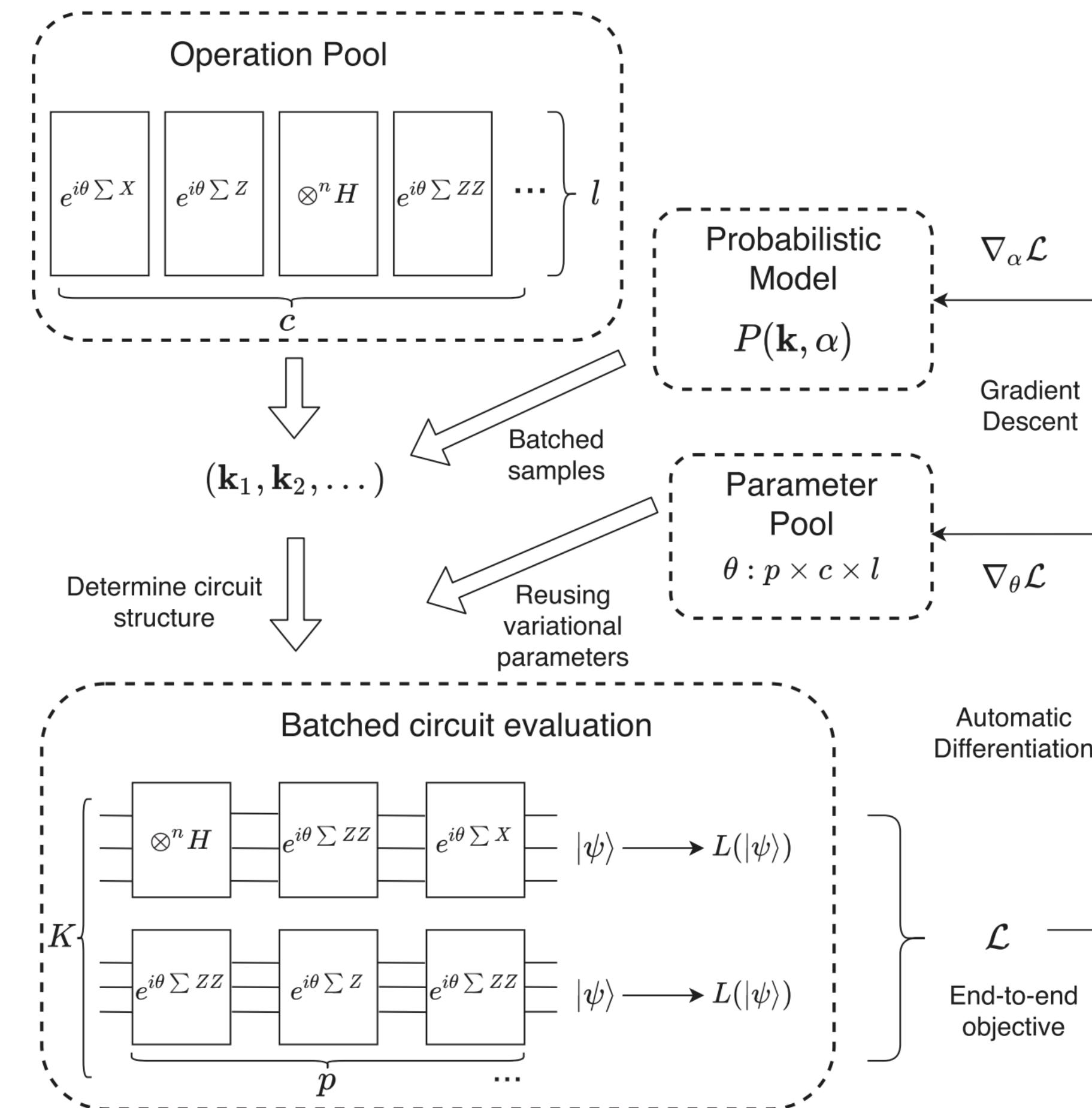
## RL for Architecture Search



Quantum Architecture Search via Deep Reinforcement Learning

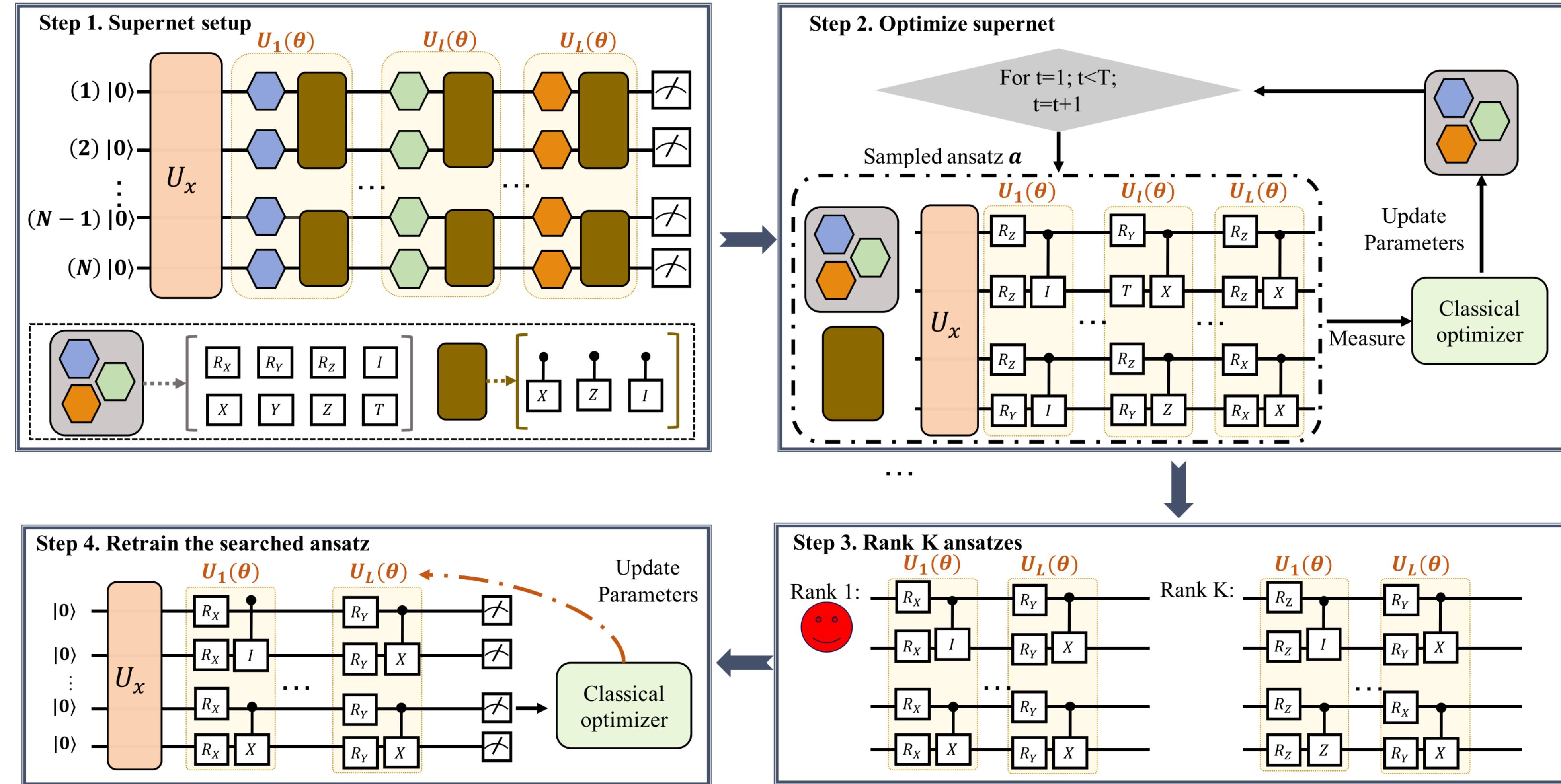
# Other Search Frameworks

## Differentiable Search



Differentiable quantum architecture search

# Other Search Frameworks



Quantum circuit architecture search for variational quantum algorithms

# Summary of Today's Lecture

- We learned
  - Parameterized Quantum Circuit (PQC)
  - PQC Training
  - Quantum Classifiers
  - Noise Aware On-Chip Training of PQC
  - TorchQuantum Library for QML
  - Robust Quantum Architecture Search

