MIT HAN LAB

Lecture 22
Quantum Machine Learning

Part I

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Lecture Plan

Today we will:

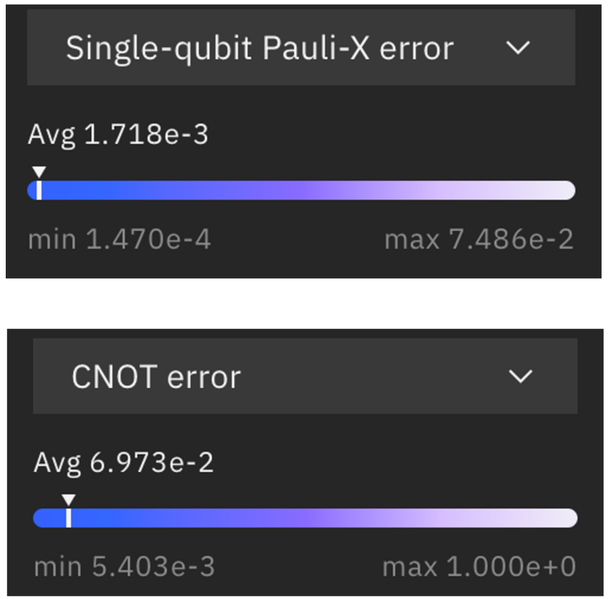
1. Continue to introduce NISQ devices
2. Introduce Parameterized Quantum Circuit (PQC)
3. Introduce PQC Training
4. Introduce Quantum Classifiers
5. Introduce Noise Aware On-Chip Training (QOC) of PQC
6. Introduce TorchQuantum Library for QML

Section 1

NISQ Devices

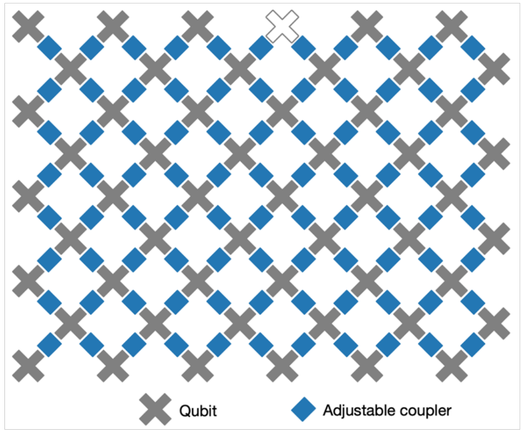
The NISQ Era

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



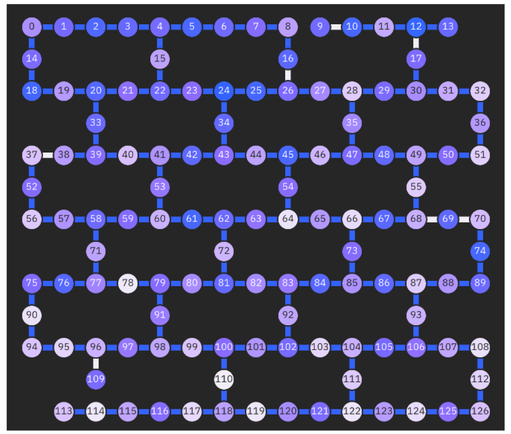
IBMQ Gate Error Rate

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



Google Sycamore 53Q

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

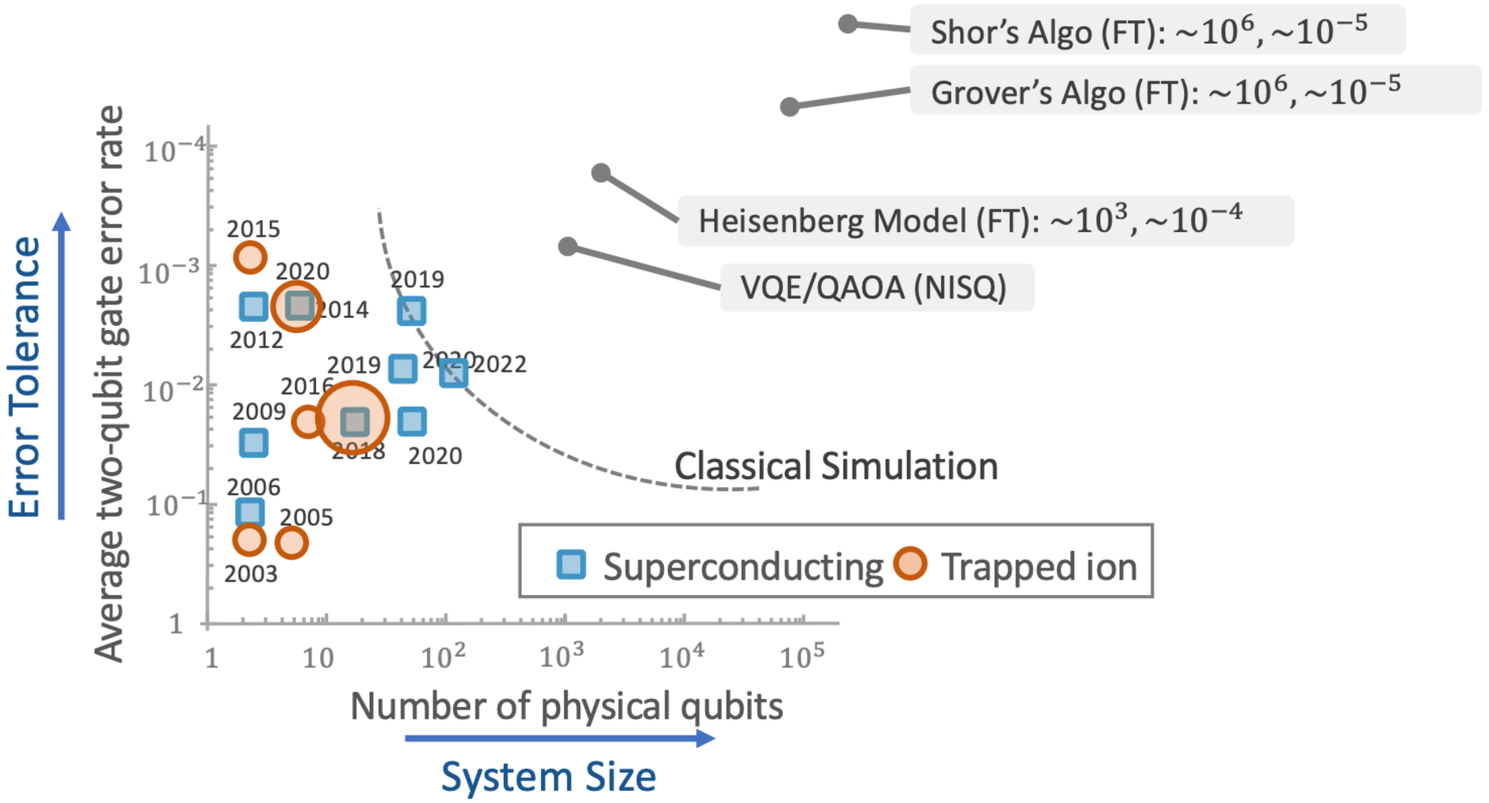


IBM Washington 127Q

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

Gap between the Algorithm and Device

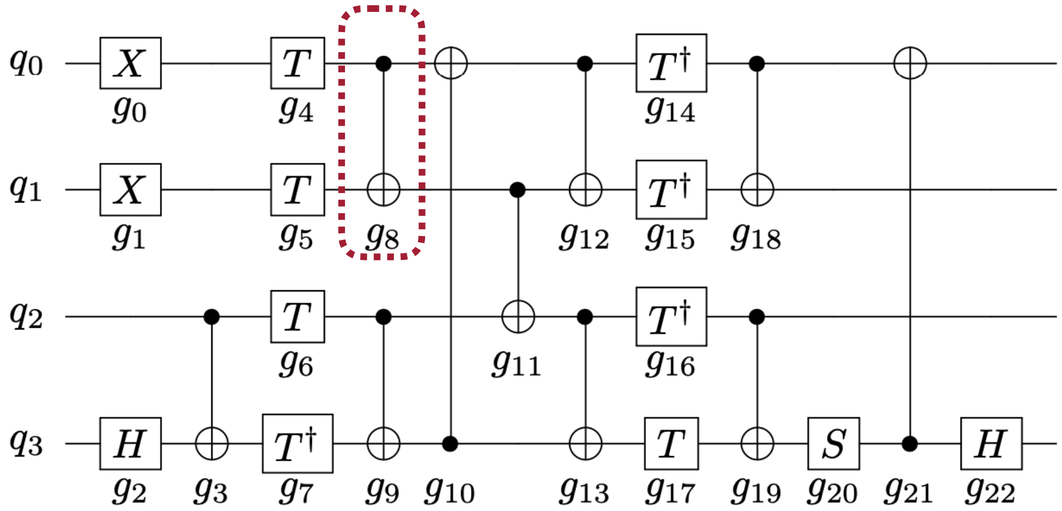
- Gap between algorithm and devices

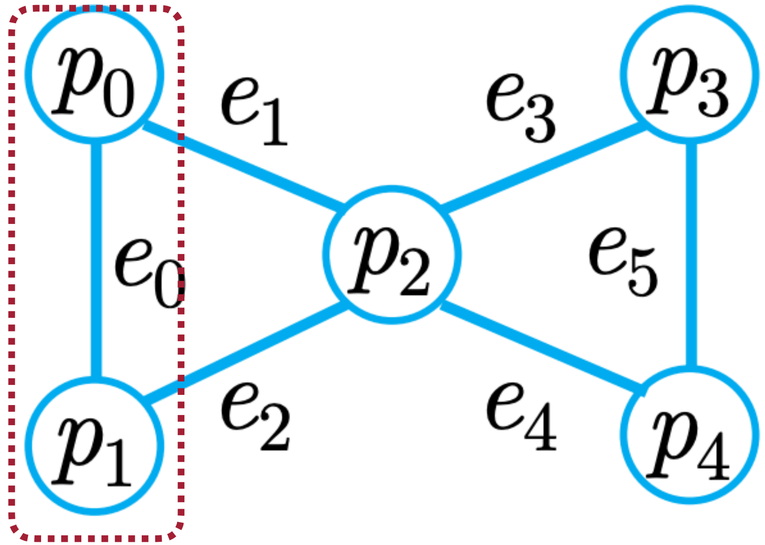


*Size of data point indicates connectivity; larger means denser connectivity.

Ding & Chong

Qubit Mapping





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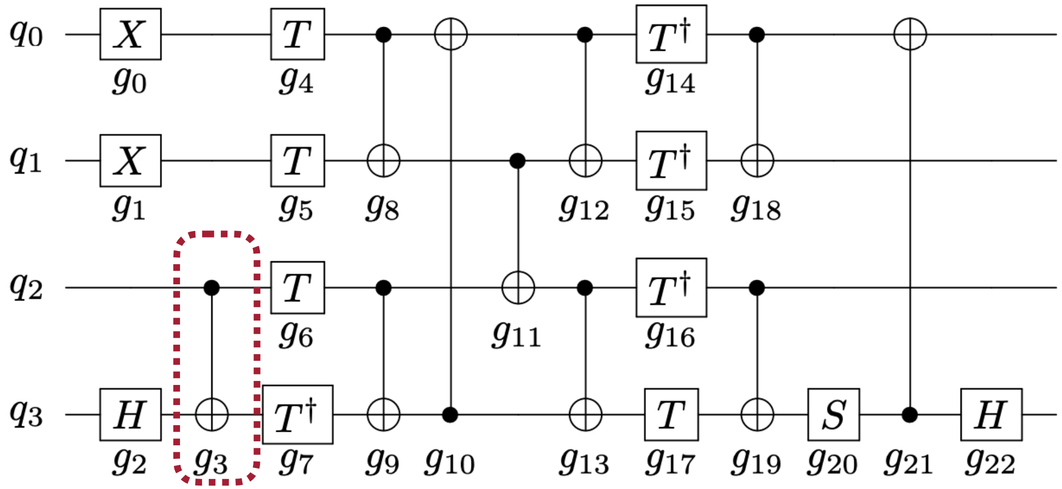
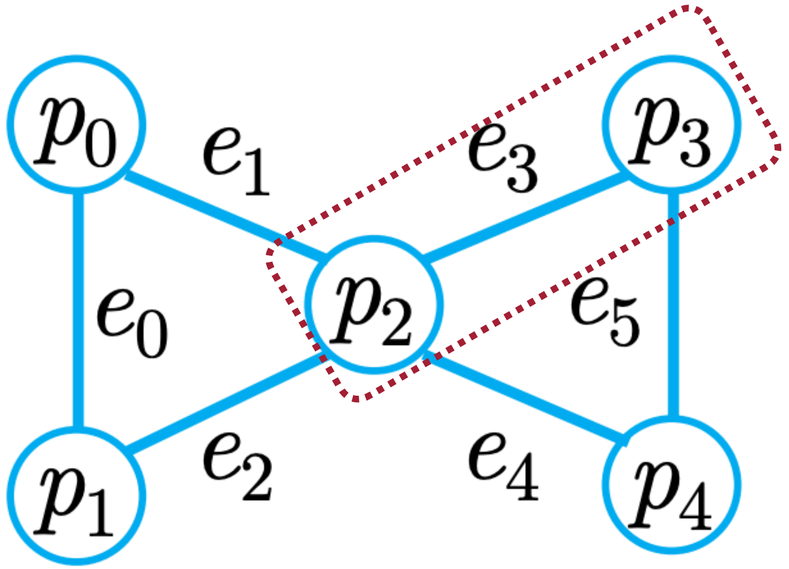
Qubit Mapping





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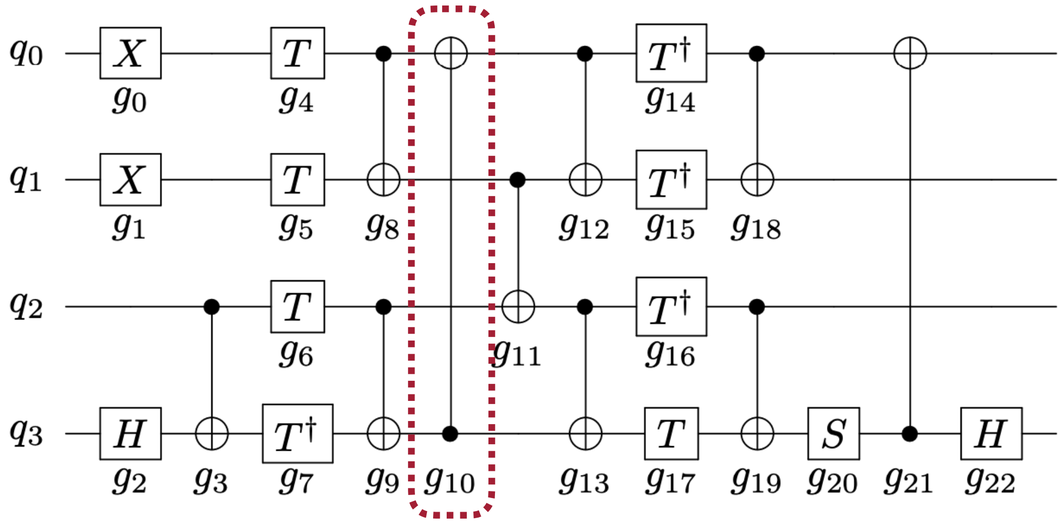
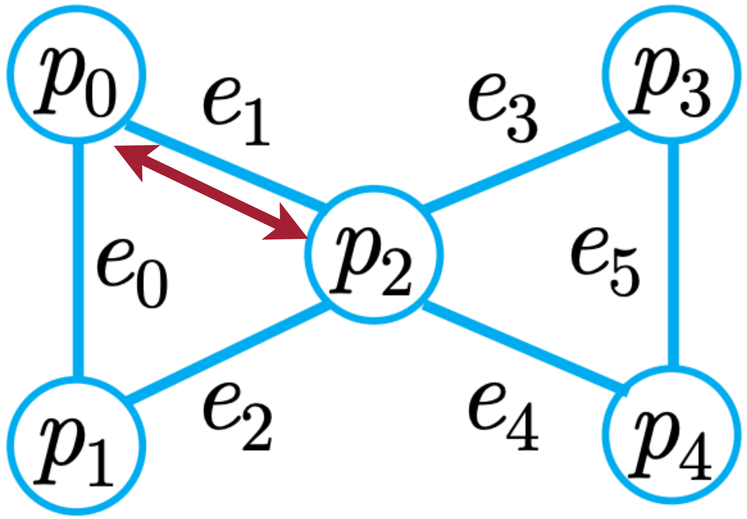
Qubit Mapping





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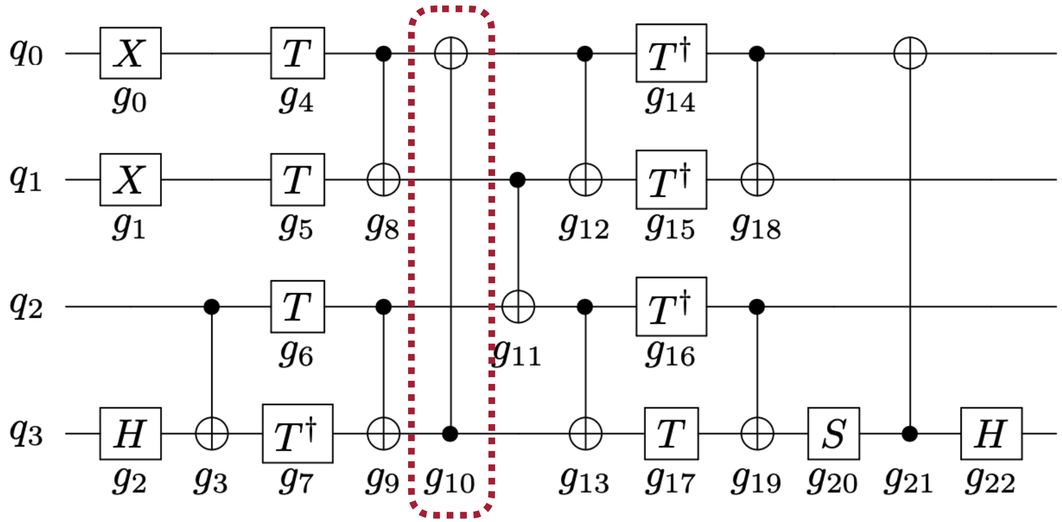
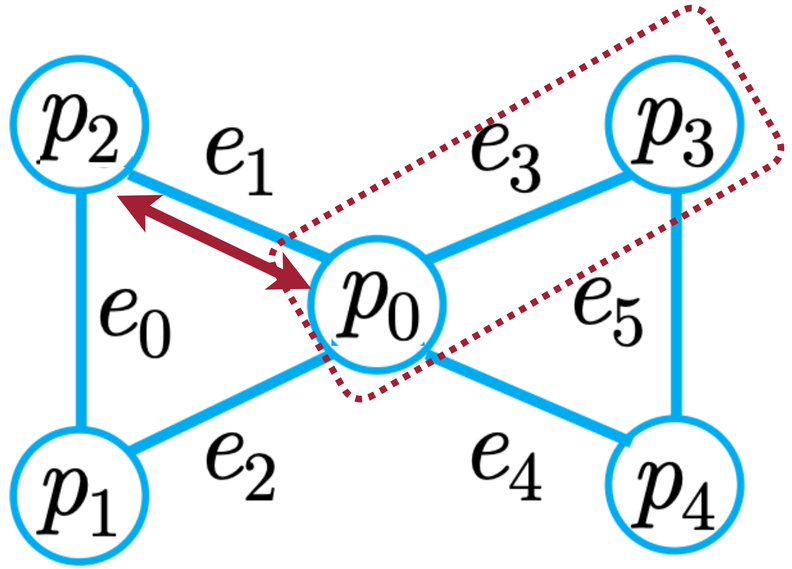
Qubit Mapping

- How to design the best scheduling? When to do the swap?





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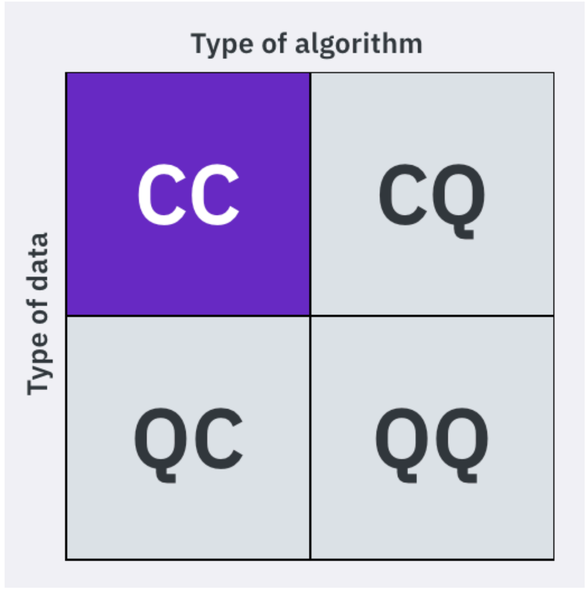
Section 2

Parameterized Quantum Circuit

QML Approaches

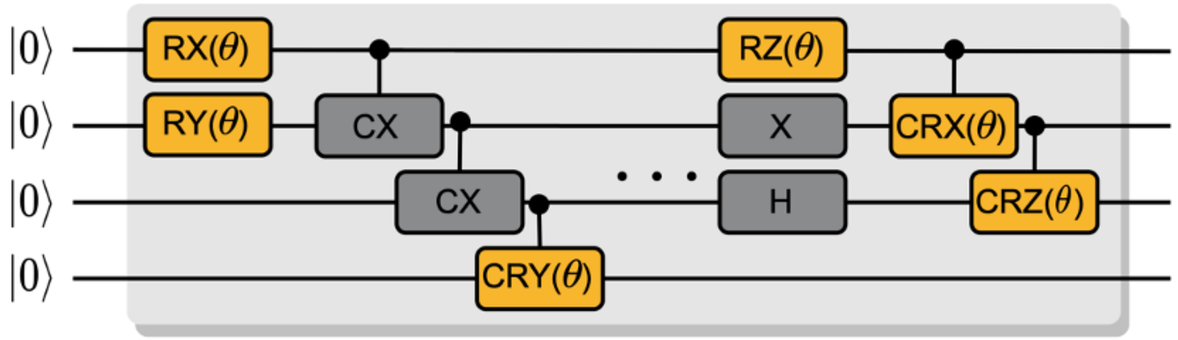
- CC: Classical Data, Classical algorithm: what we have learned from previous lectures
- CQ: Classical Data, Quantum algorithm: what we are going to introduce
- QC: Quantum Data, Classical algorithm: qubit control, calibration, readout…
- QQ: Quantum Data, Quantum algorithm: process quantum info with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



https://qiskit.org/learn/

Parameterized Quantum Circuits

- Circuit that contains fixed gates and parameterized gates

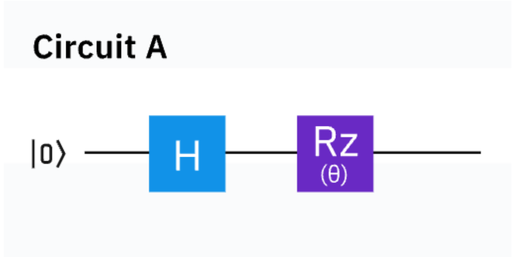


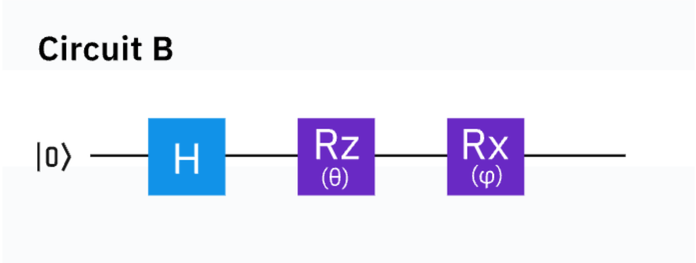
$$CNOT = \begin{array}{c} \\ \text{00} \\ \text{01} \\ \text{10} \\ \text{11} \end{array} \begin{array}{c} \begin{array}{cccc} \text{Output} & & & \\ \text{00} & \text{01} & \text{10} & \text{11} \end{array} \\ \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix}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

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

Expressivity

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





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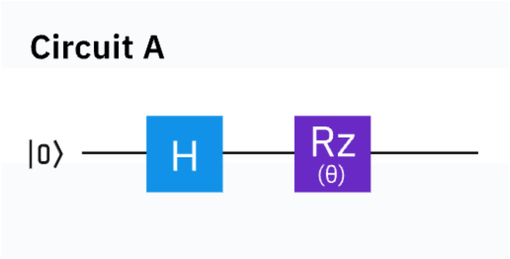
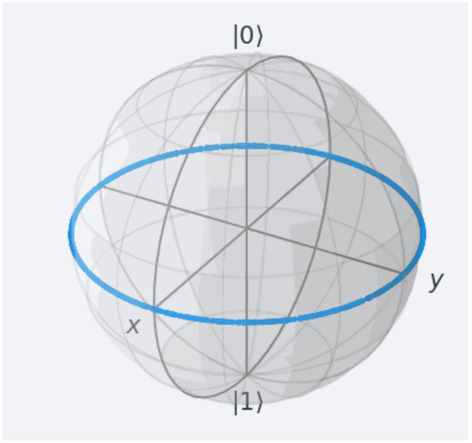
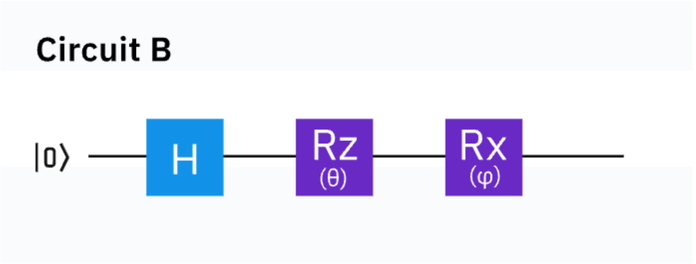
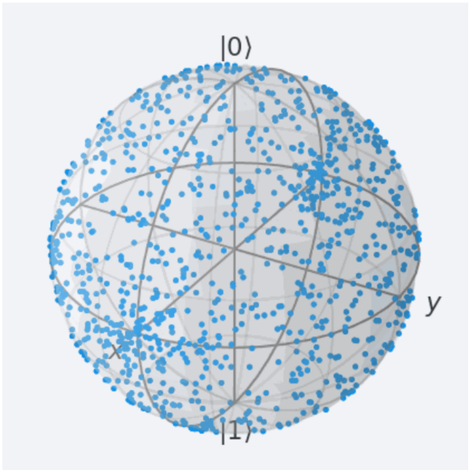
Expressivity

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









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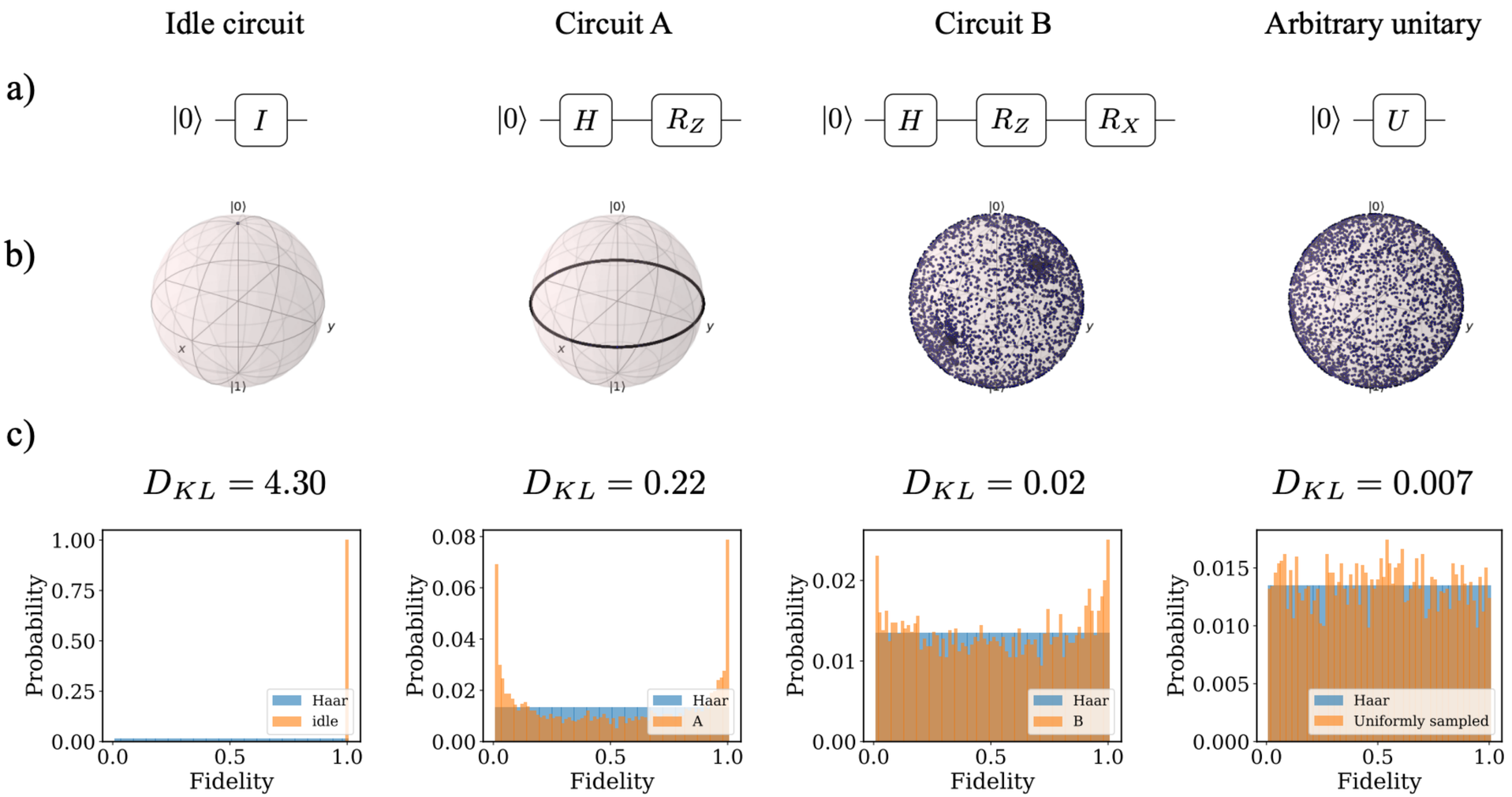
Expressivity

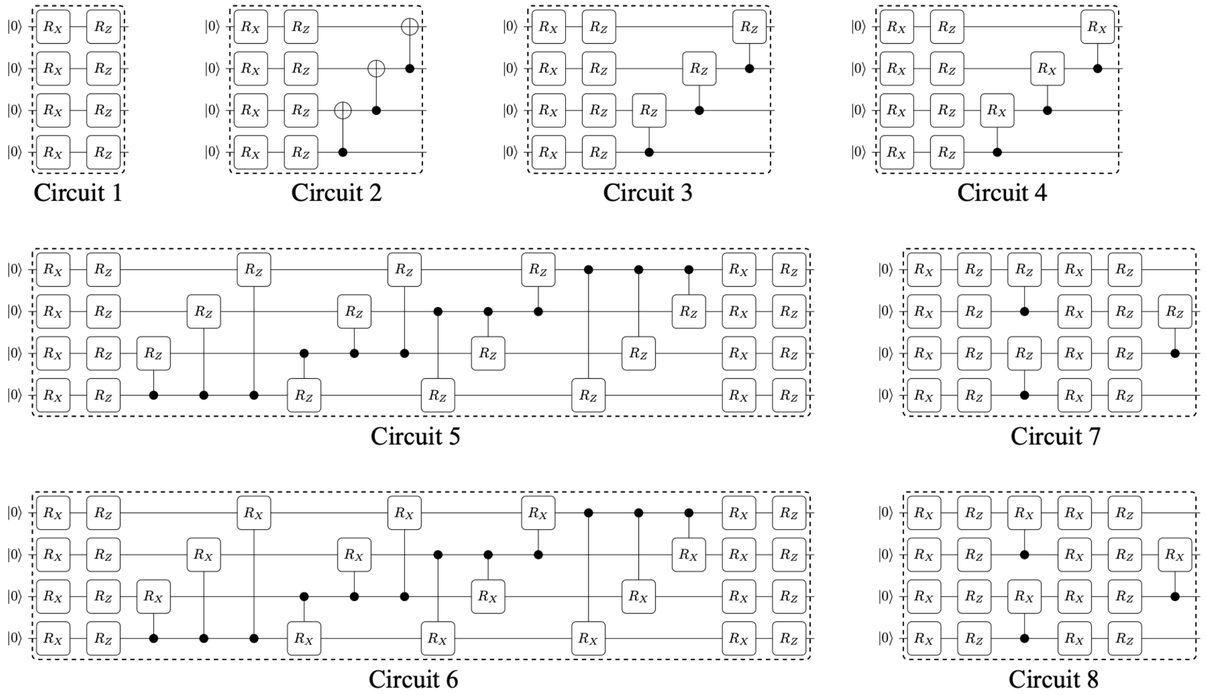


Expressibility and entangling capability of parameterized quantum circuits for hybrid quantum-classical algorithms

Entanglement Capability

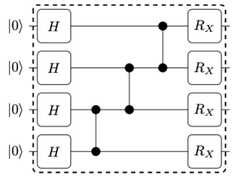
- The **Meyer-Wallach** measure tells how entangled a given state is. [0, 1]
  - Unentangled state is 0
  - Full entangled state is 1
- We use **averaged MW** to measure the entanglement capability of circuit

Entanglement Capability

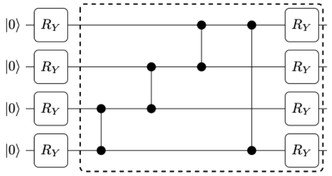


Expressibility and entangling capability of parameterized quantum circuits for hybrid quantum-classical algorithms

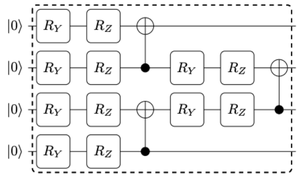
Entanglement Capability



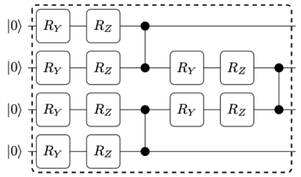
Circuit 9



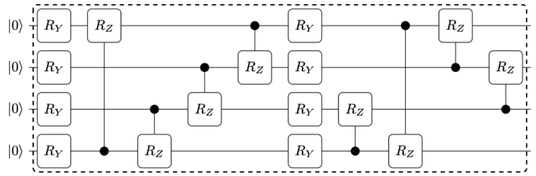
Circuit 10



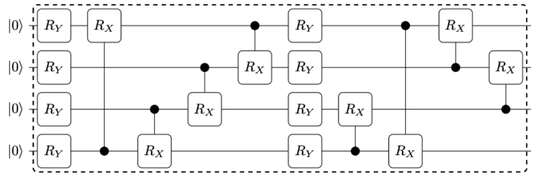
Circuit 11



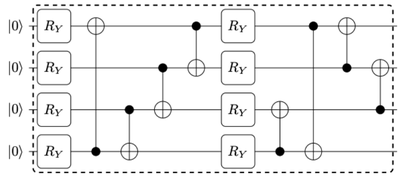
Circuit 12



Circuit 13



Circuit 14



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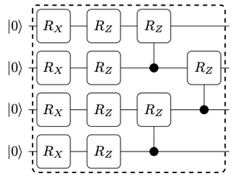

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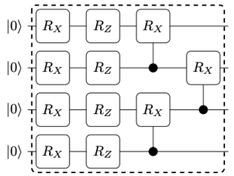
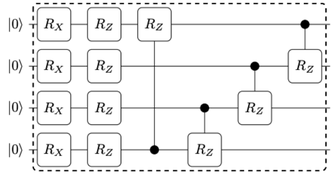
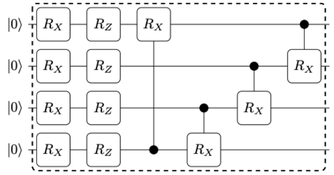


Circuit 17



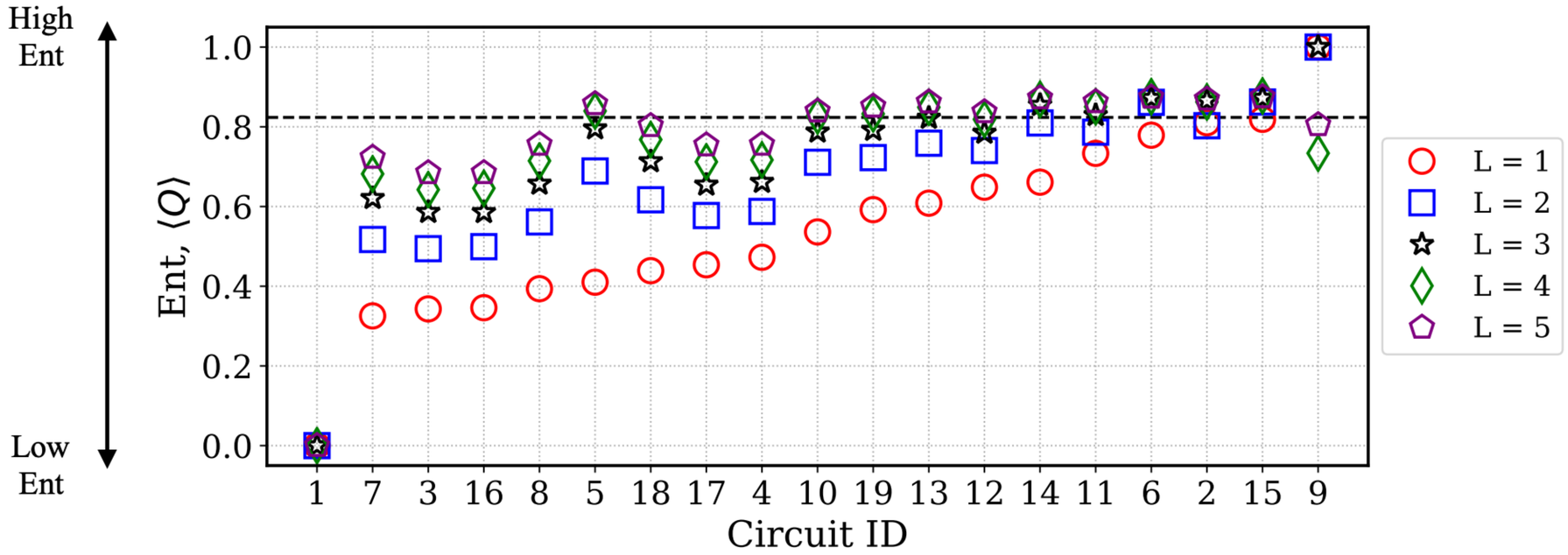
Circuit 18

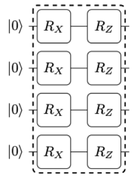


Circuit 19

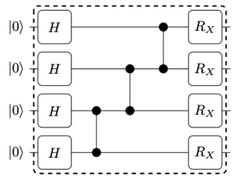
Expressibility and entangling capability of parameterized quantum circuits for hybrid quantum-classical algorithms

Entanglement Capability





Circuit 1

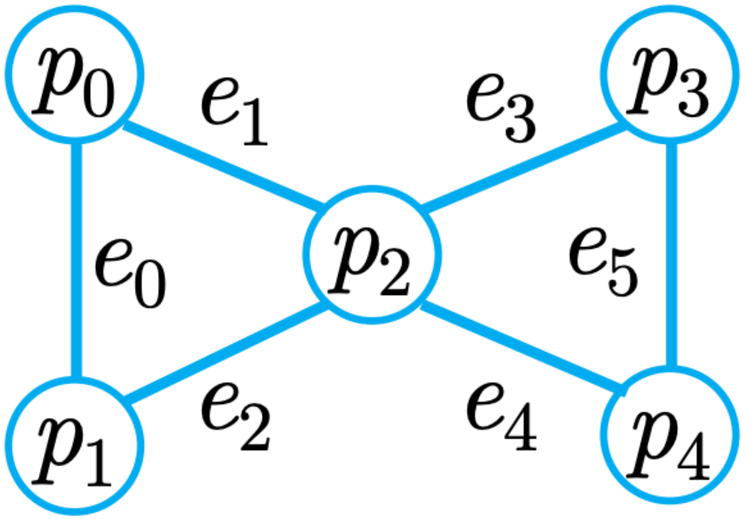


Circuit 9

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

$$\mathscr{X} = \{x^{(1)}, \ldots, x^{(m)}, \ldots, x^{(M)}\}$$

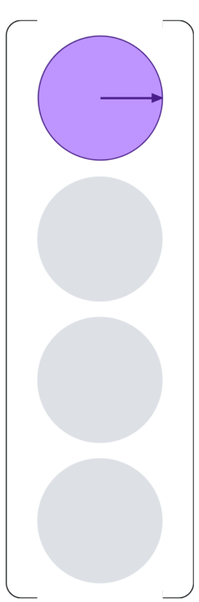
- **Encoding** methods:
  - Basis encoding
  - Amplitude encoding
  - Angle encoding
  - Arbitrary encoding

Basis Encoding

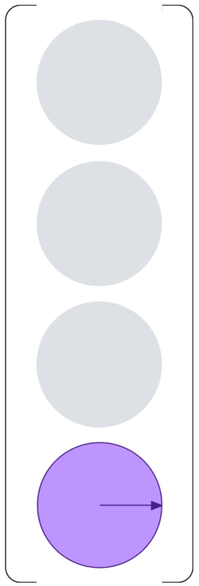
- Similar to the **binary** representation in the classical machine
- X = 2 -> 10
- We create a quantum state with all energy on |10>

Basis Encoding

- Similar to the **binary** representation in the classical machine
- X = 2 -> 10
- not efficiency for one data



x=0 (00)



x=3 (11)

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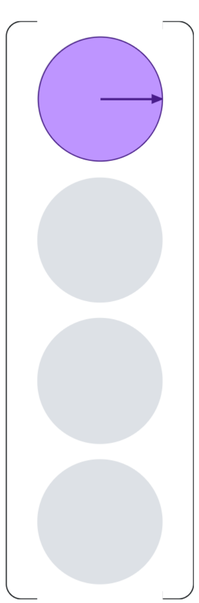
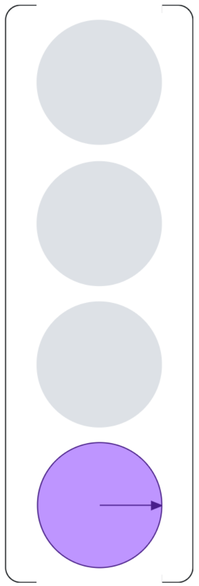
Basis Encoding

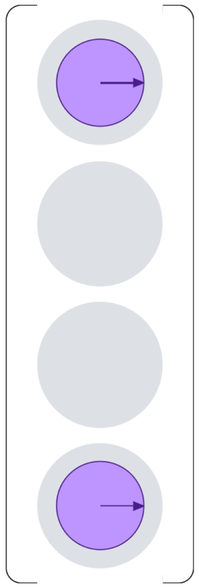
- Similar to the **binary** representation in the classical machine
- X = 2 -> 10
- not efficiency for one data but can be used to represent **multiple data simultaneously**



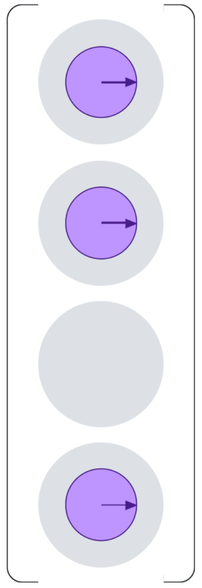
x=0 (00)



x=3 (11)



x=0 and 3 (00+11)

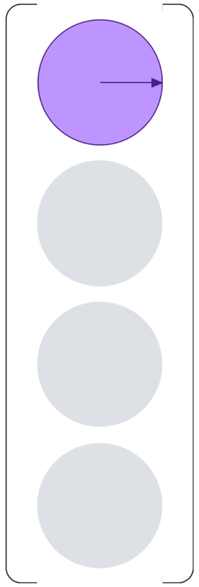


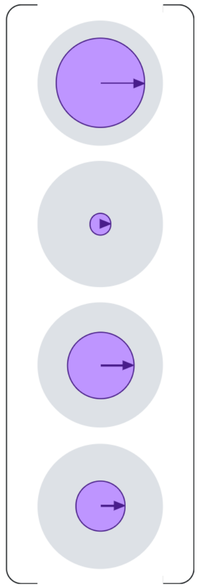
x=0 and 1 and 3 (00+ 01 +11)

Amplitude Encoding

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

input vector = [0.8, 0.2, 0.6, 0.45]





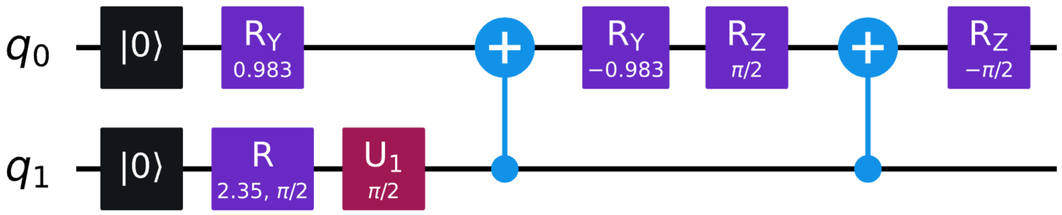
Amplitude Encoding

- Also possible to encoder multiple data points together

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

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

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



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Angle Encoding

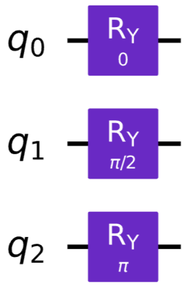
- Encode the data in the **rotation** angles of the qubit gates
- For vector [0, pi/4, pi/2]

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

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

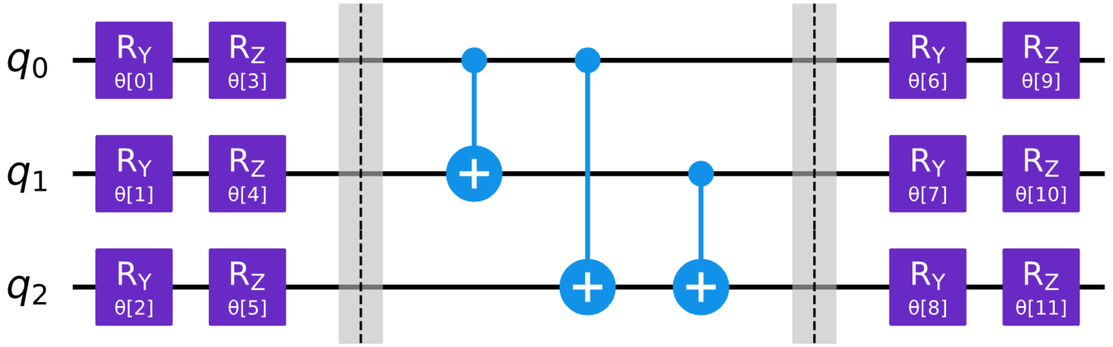
.

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

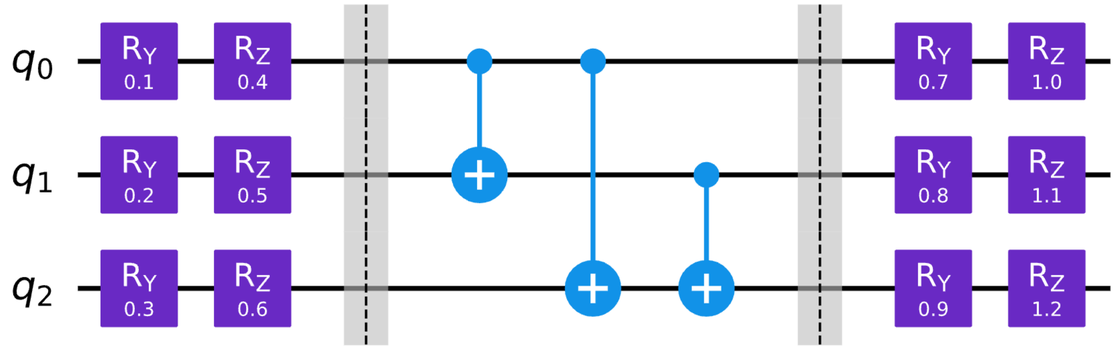


Arbitrary Encoding

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



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

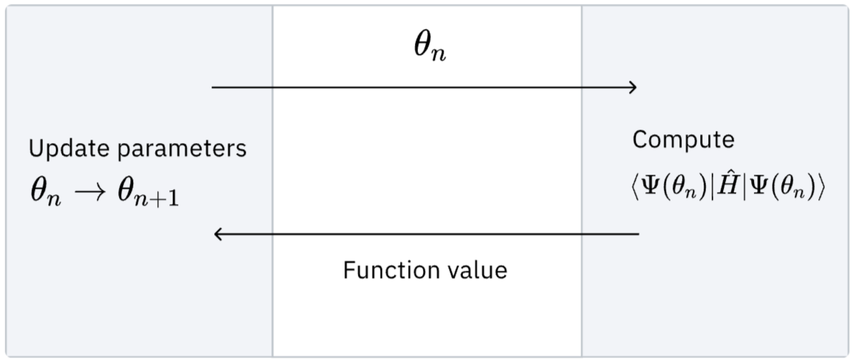


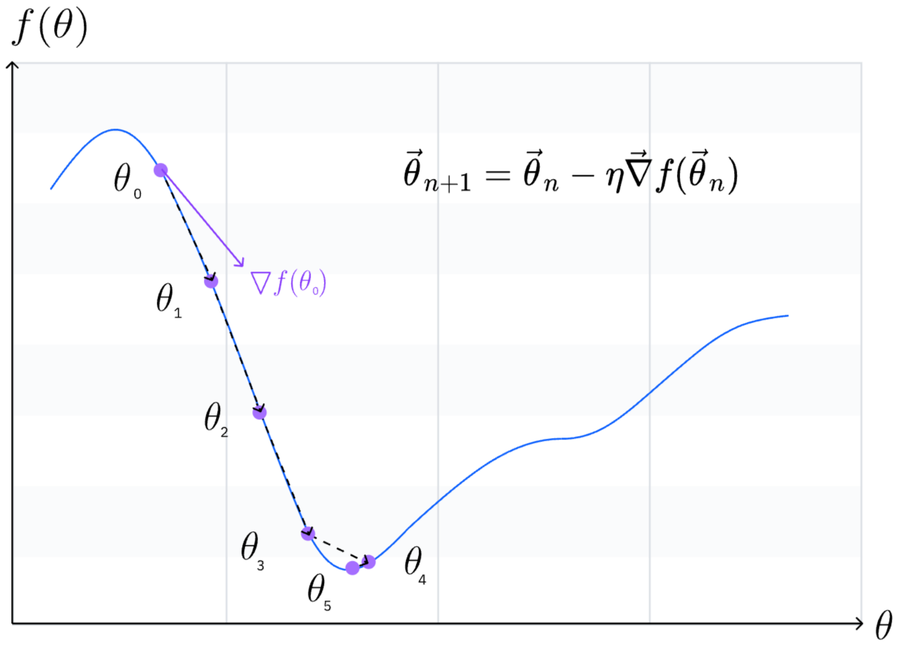
Section 3

PQC Training

PQC Training

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





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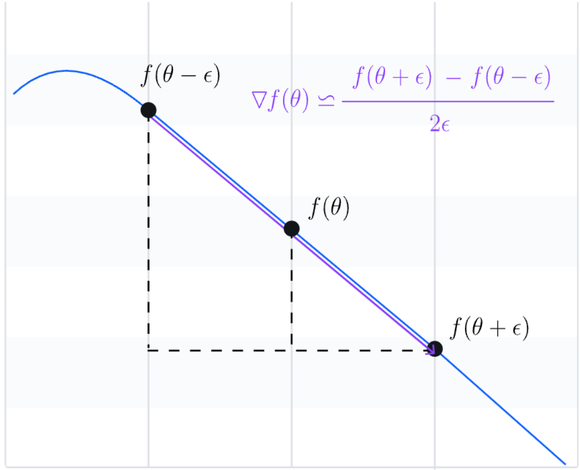
Finite Difference Gradients

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



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

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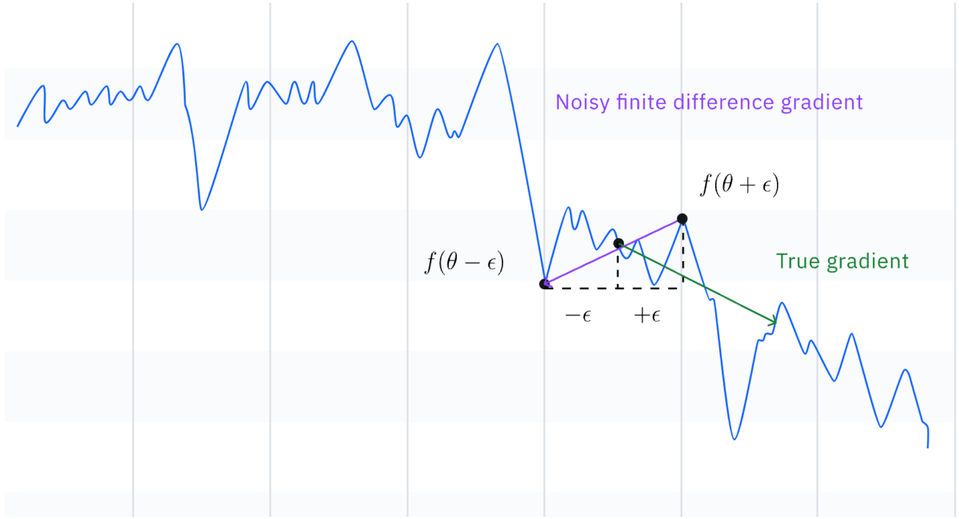
Finite Difference Gradients

- The accuracy depends on the epsilon



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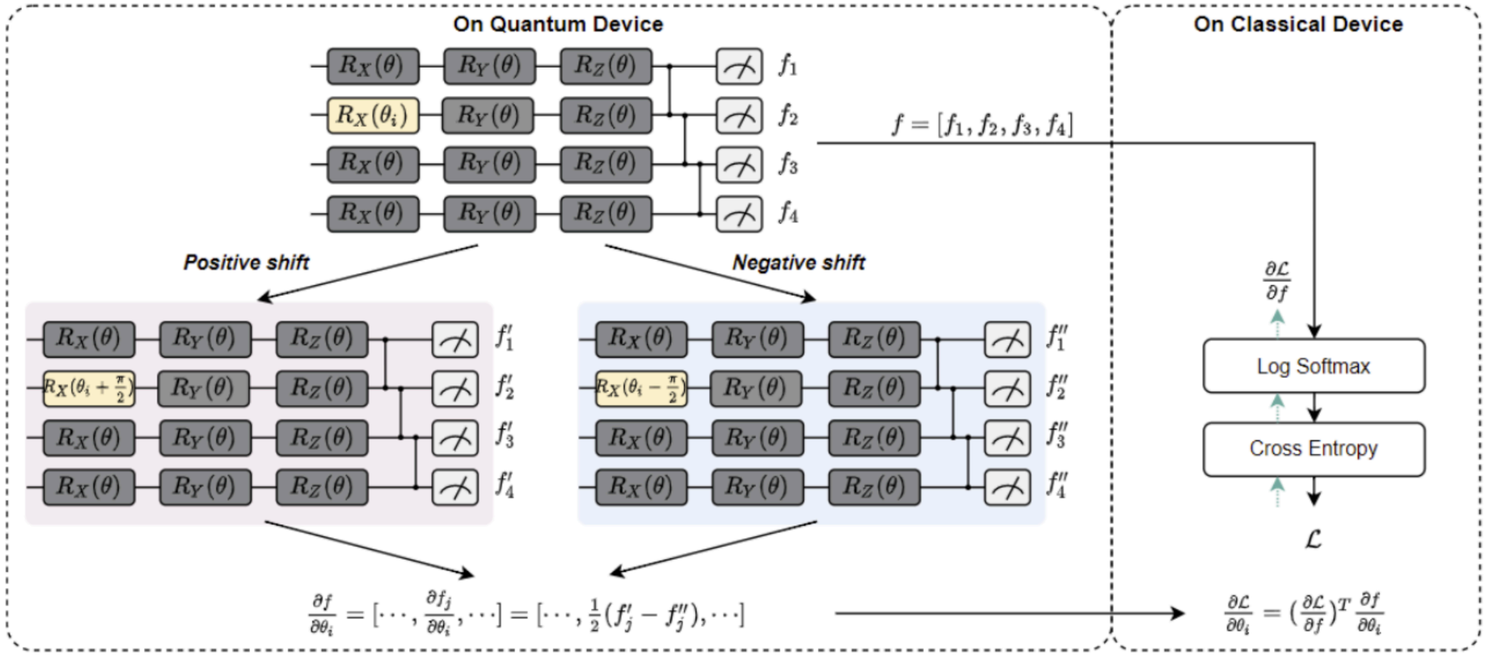
Parameter-Shift Gradients



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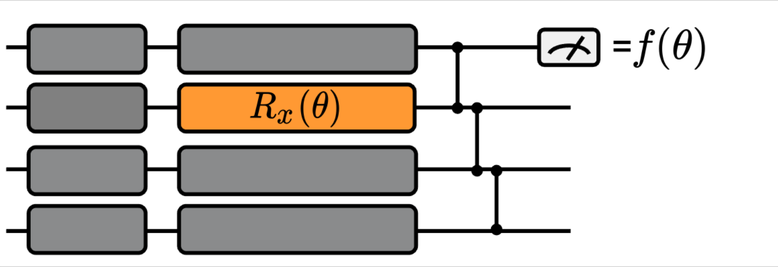
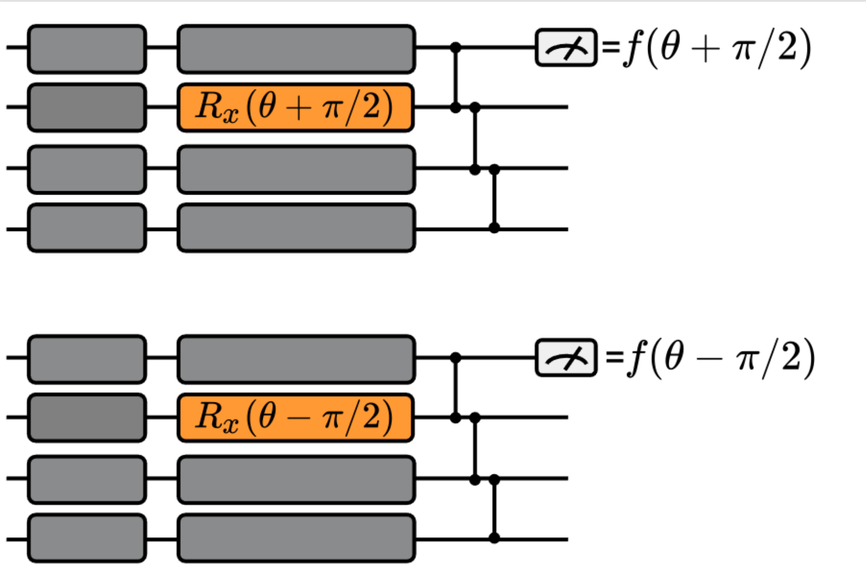
Parameter-Shift

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



Parameter-Shift

- Shift θ twice



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

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

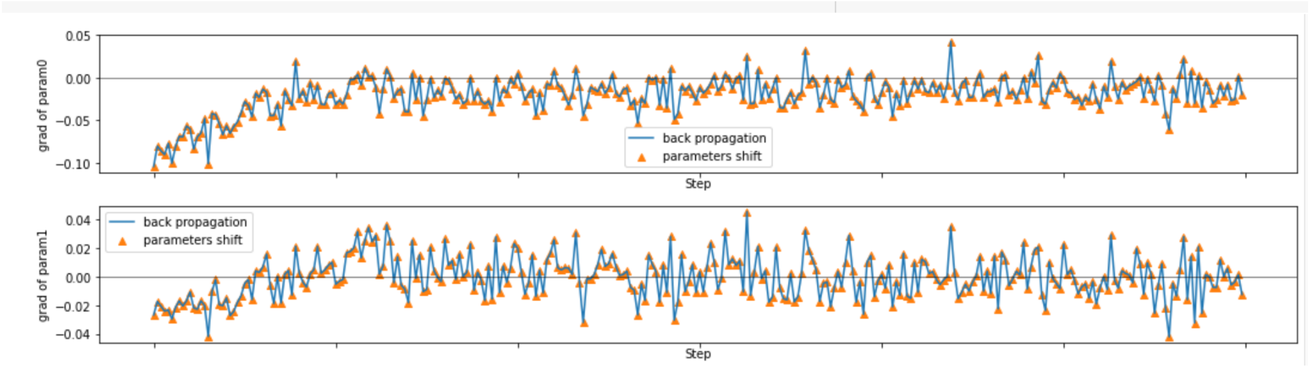
Let $\alpha = \frac{\pi}{2}$, $R_X(\pm\frac{\pi}{2}) = \frac{1}{\sqrt{2}}(I \mp iX)$.

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 $\frac{\partial}{\partial\alpha}R_X(\alpha) = -\frac{i}{2}XR_X(\alpha)$, we have

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

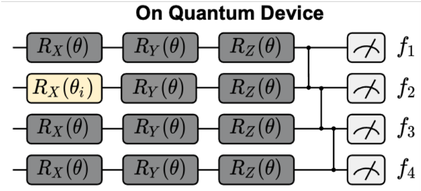
Back-Propagation

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



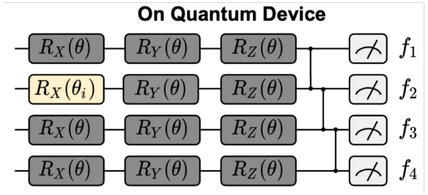
General Flow to calculate PQC gradients

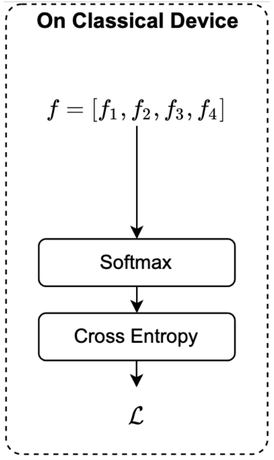
- Step 1: Run on QC without shift to obtain f



General Flow to calculate PQC gradients

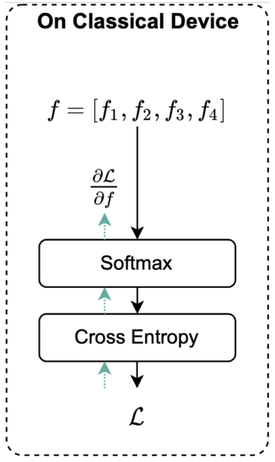
- Step 2: Further forward to get Loss





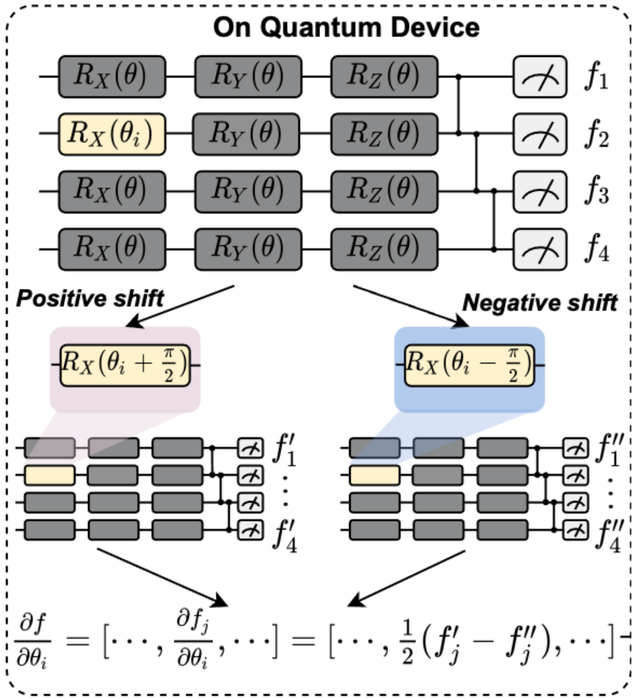
General Flow to calculate PQC gradients

- Step 3: Backpropagation to calculate ∂(Loss)/∂f(θ)



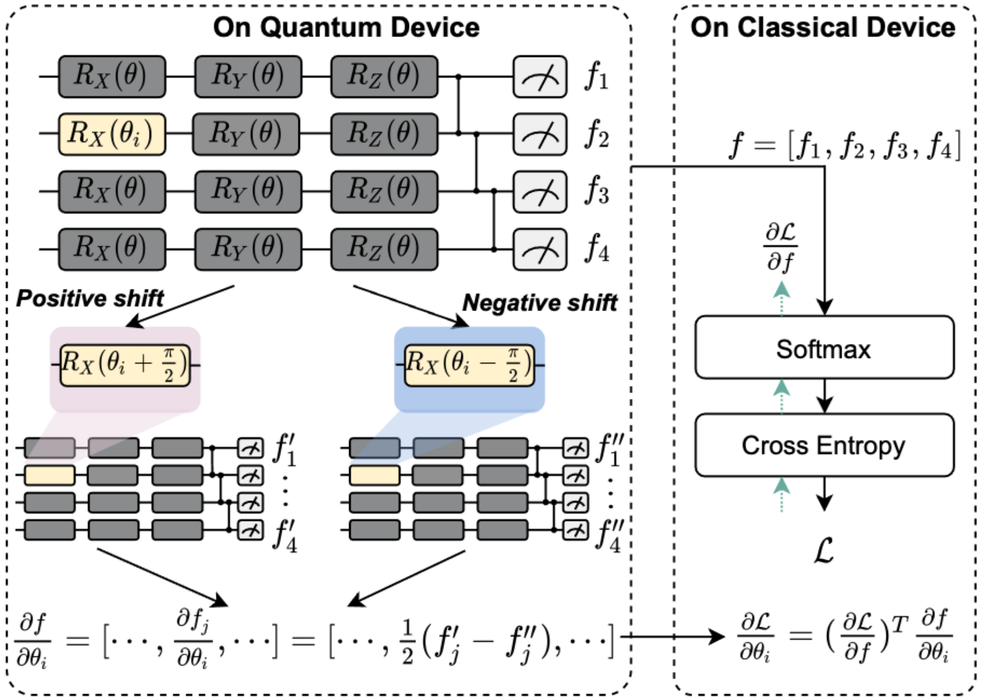
General Flow to calculate PQC gradients

- Step 4: Shift twice and run on QC to calculate (∂f(θ))/(∂θ_i)
  - Or use finite differentiate

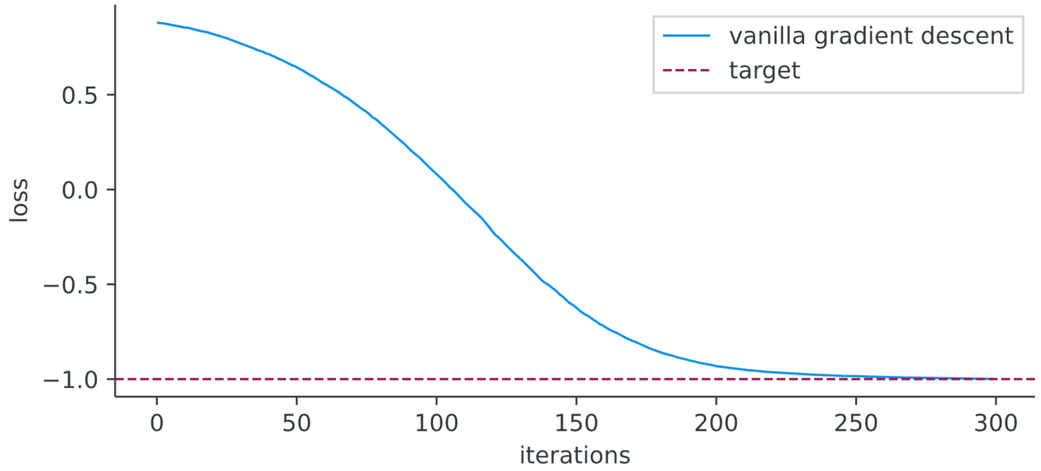


General Flow to calculate PQC gradients

- Step 5: By Chain Rule: ∂Loss/∂f(θ) · ∂f(θ)/∂θ_i = ∂Loss/(∂θ_i), sum over 4 passes (4 qubits)
- Only forward on quantum device



Training Techniques



Training Techniques

SPSA

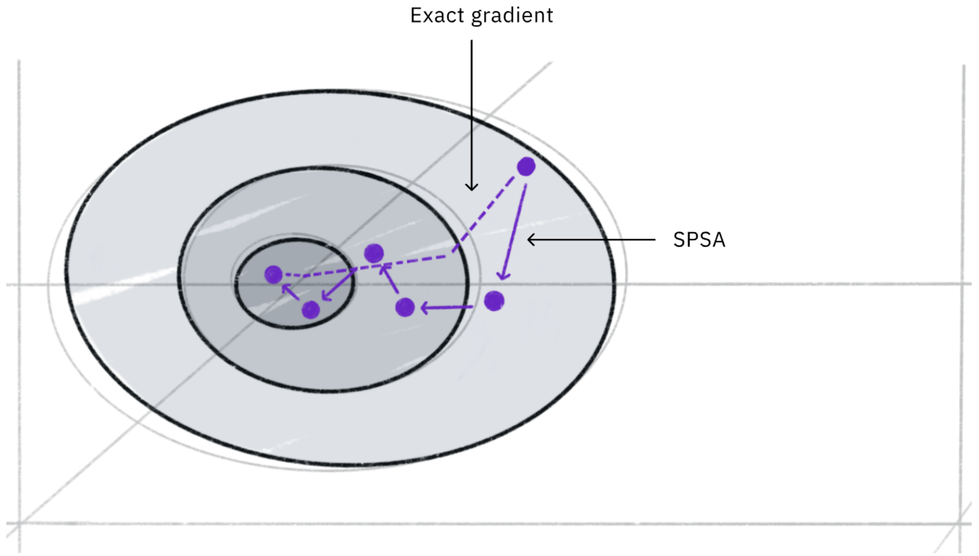
- Simultaneous Perturbation Stochastic Approximation
- How **many** circuit run for the original methods? 2N

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

$$\vec{\nabla} f(\vec{\theta}) = \begin{pmatrix} \frac{\partial f}{\partial \theta_1} \\ \vdots \\ \frac{\partial f}{\partial \theta_n} \end{pmatrix} \simeq \frac{1}{2\epsilon} \begin{pmatrix} f(\vec{\theta}+\epsilon\vec{e}_1) - f(\vec{\theta}-\epsilon\vec{e}_1) \\ \vdots \\ f(\vec{\theta}+\epsilon\vec{e}_n) - f(\vec{\theta}-\epsilon\vec{e}_n) \end{pmatrix} \simeq \frac{f(\vec{\theta}+\epsilon\vec{\Delta}) - f(\vec{\theta}-\epsilon\vec{\Delta})}{2\epsilon} \vec{\Delta}^{-1}$$

Finite difference:
Perturb each dim once

SPSA:
simultaneously
perturb all dims at once!



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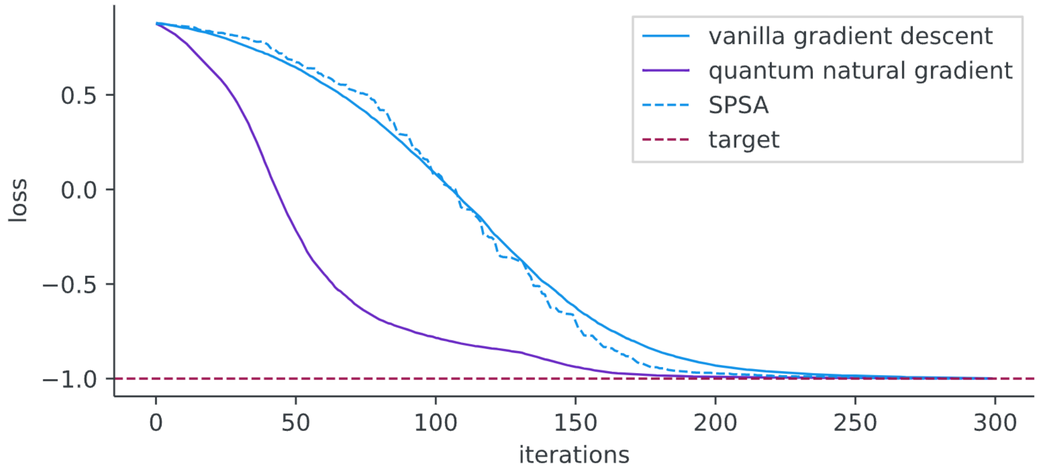
Training Techniques

SPSA

- The SPSA has similar convergence as the gradient descent



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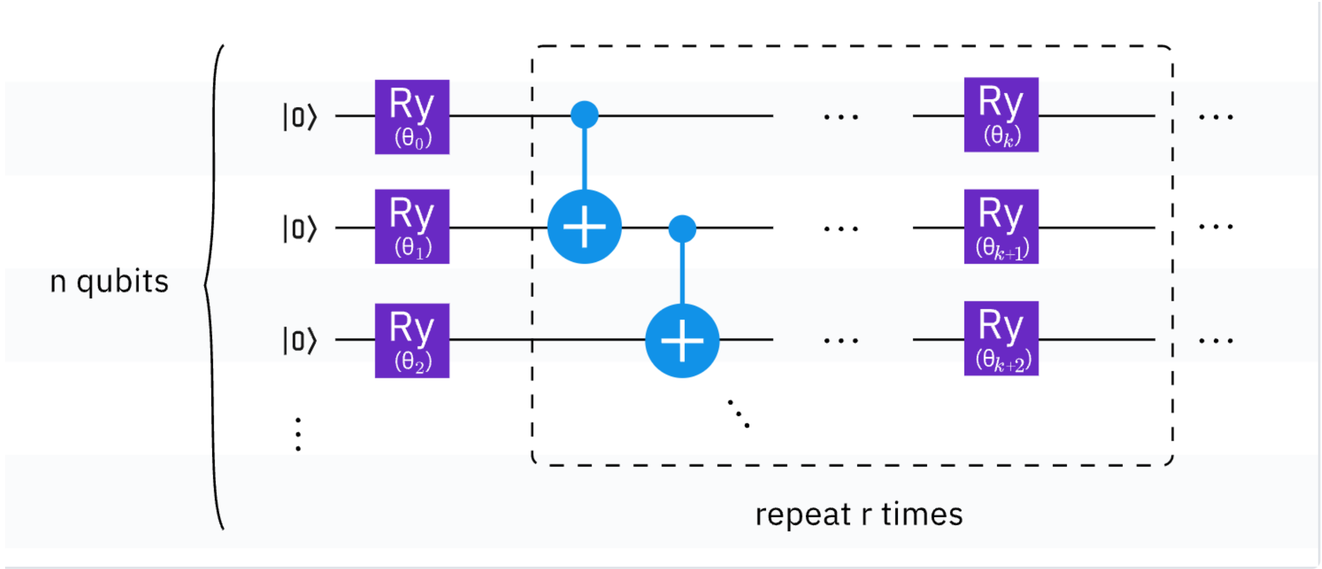
Barren Plateaus

- Vanishing Gradients problem when circuit goes larger



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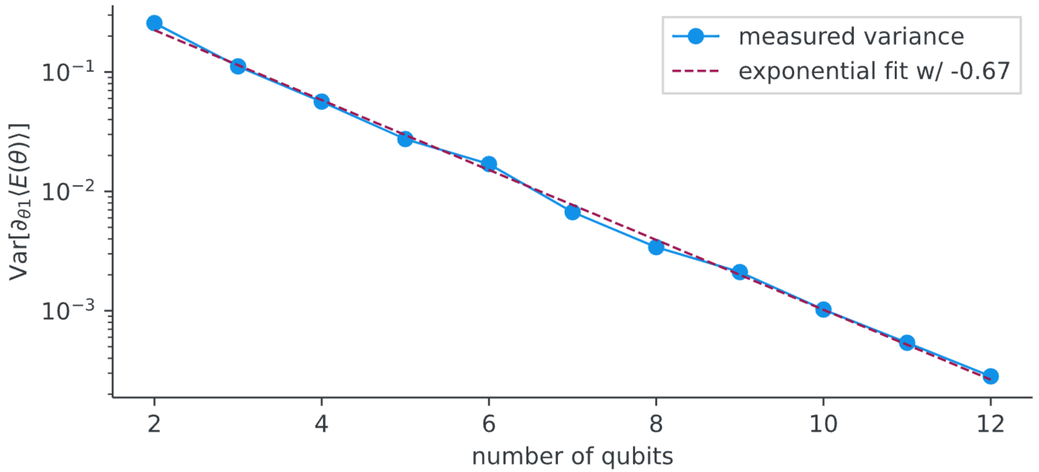
Barren Plateaus

- Gradient **variance** reduces drastically



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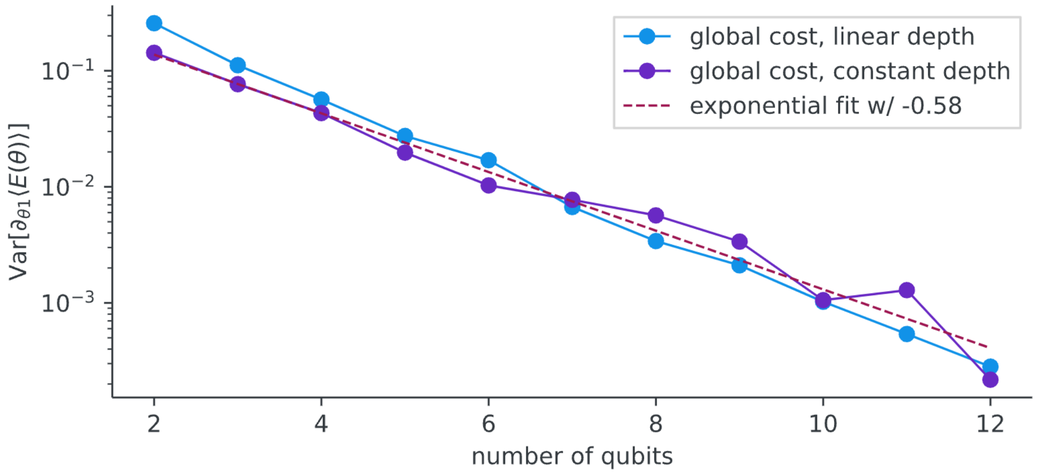
Barren Plateaus

- Gradient **variance** reduces drastically



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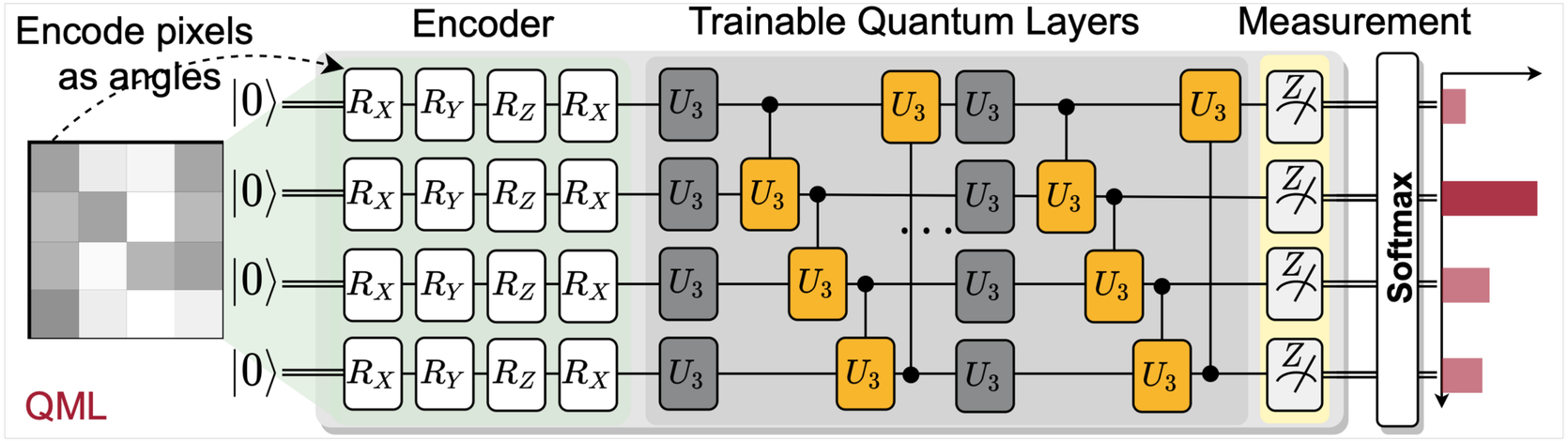
Section 4

Quantum Classifiers

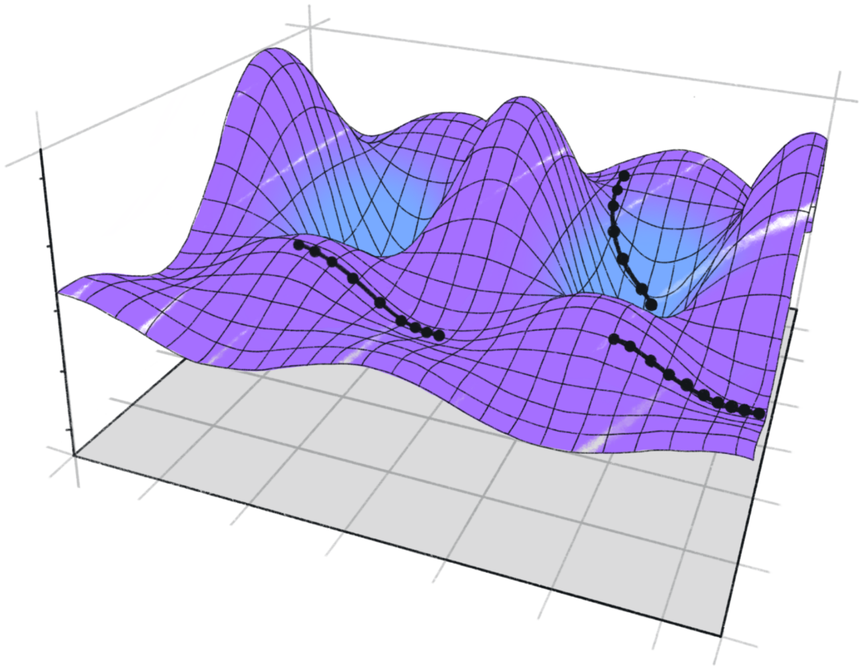
Quantum Classifiers

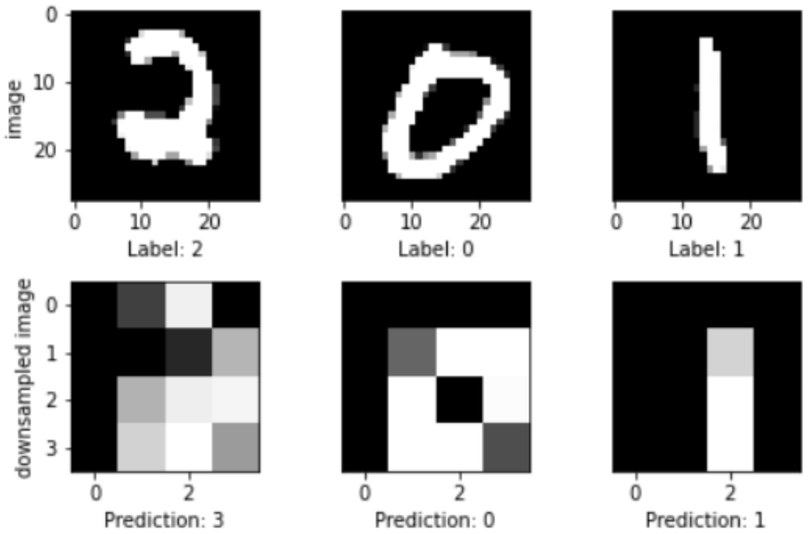
With Quantum Neural Networks



Quantum Classifiers

- Training





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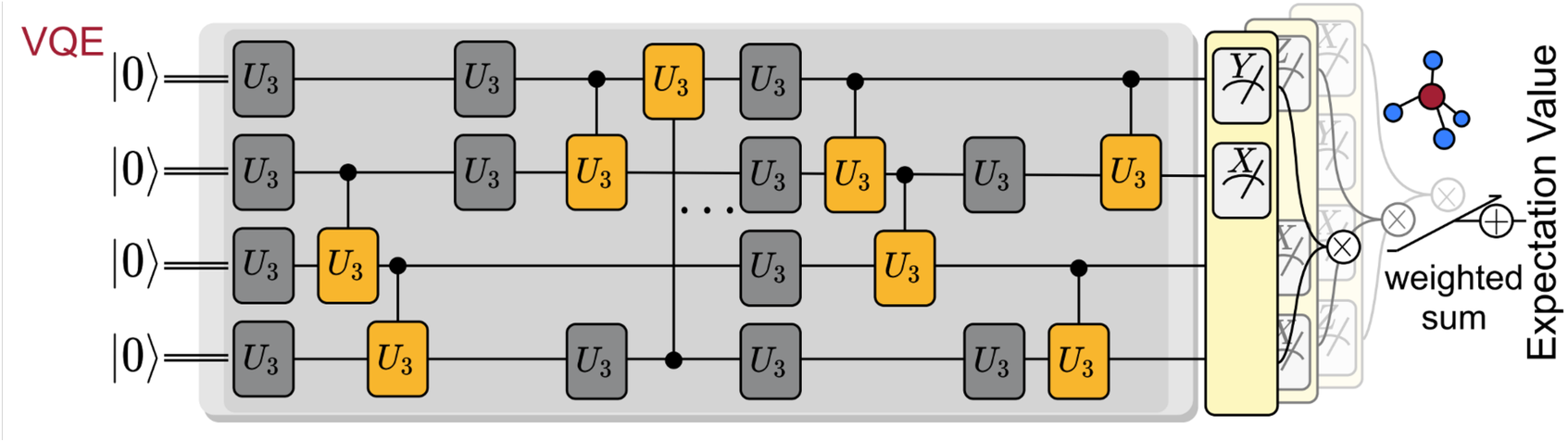
PQC for Other tasks

VQE and QAOA

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

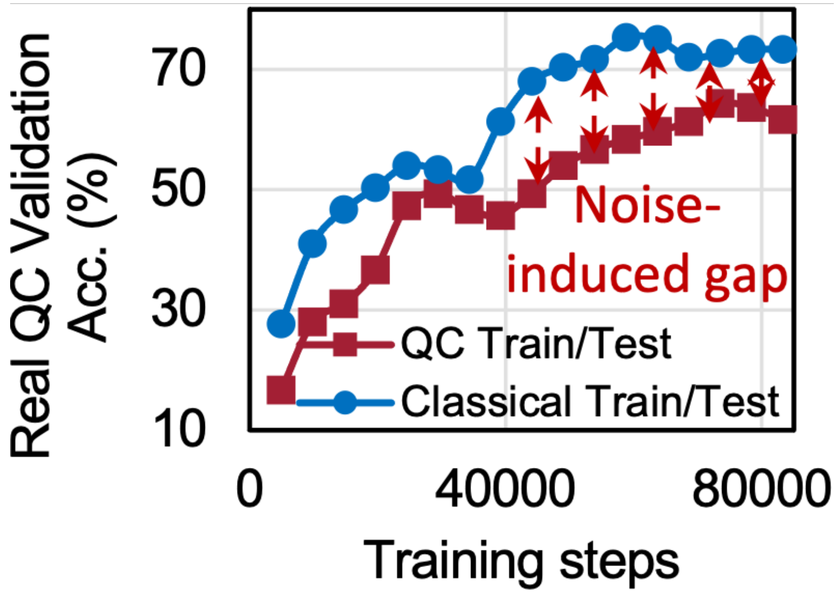


Section 5

Noise Aware On-Chip Training (QOC)

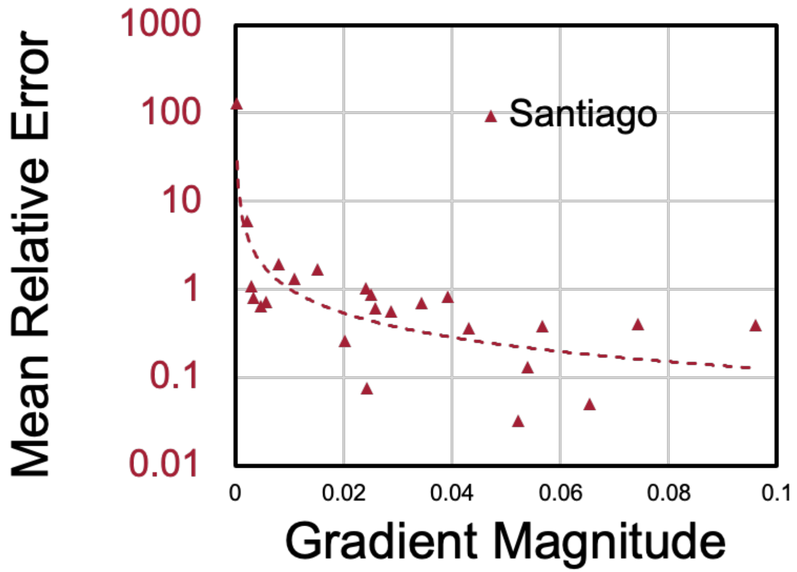
The impact of noise on gradient computation

- 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

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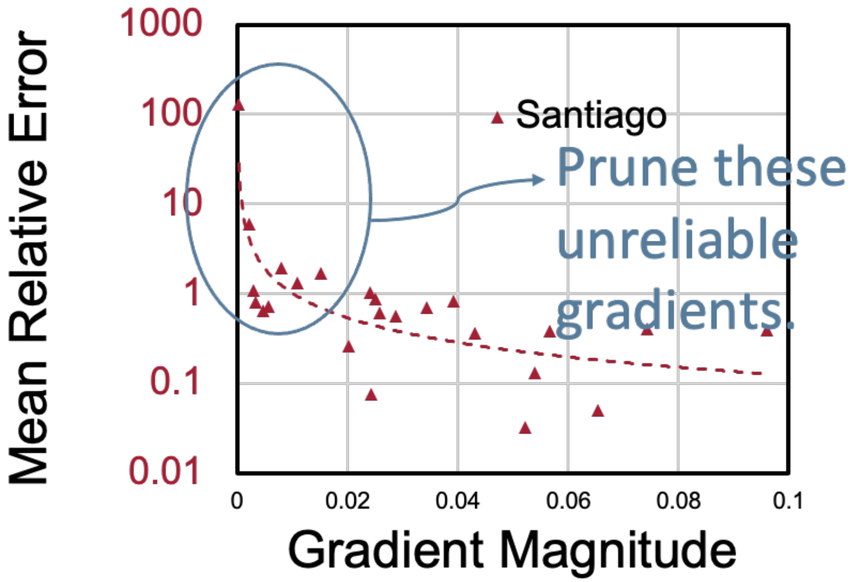
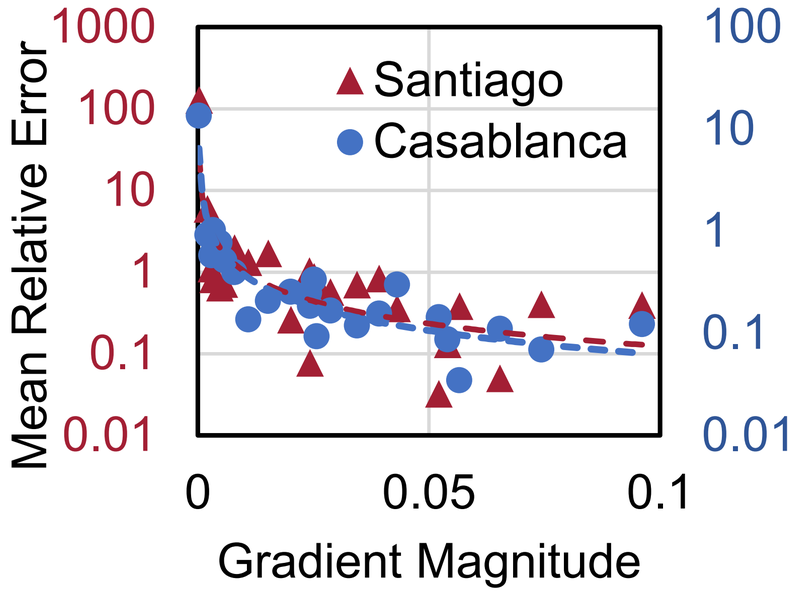


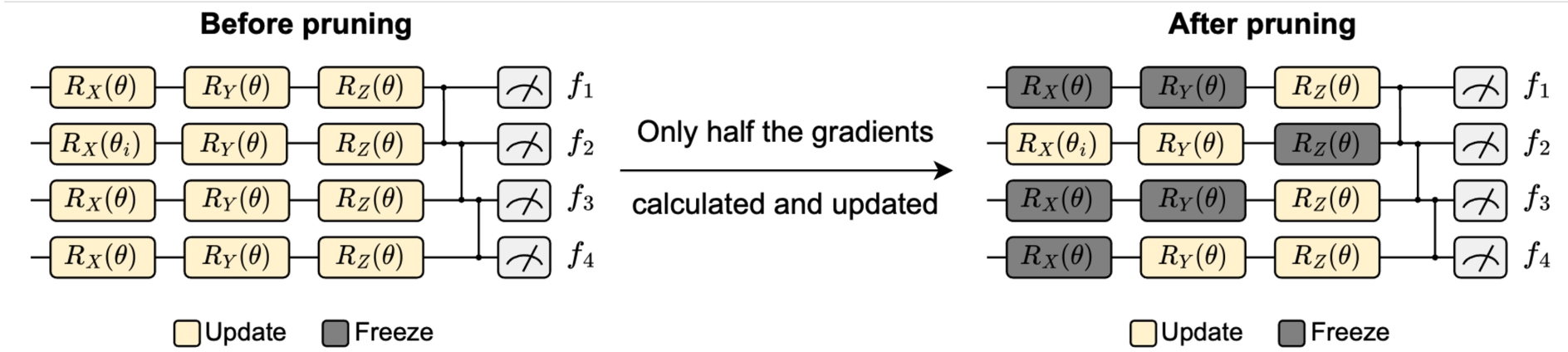
Probabilistic Gradient Pruning

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



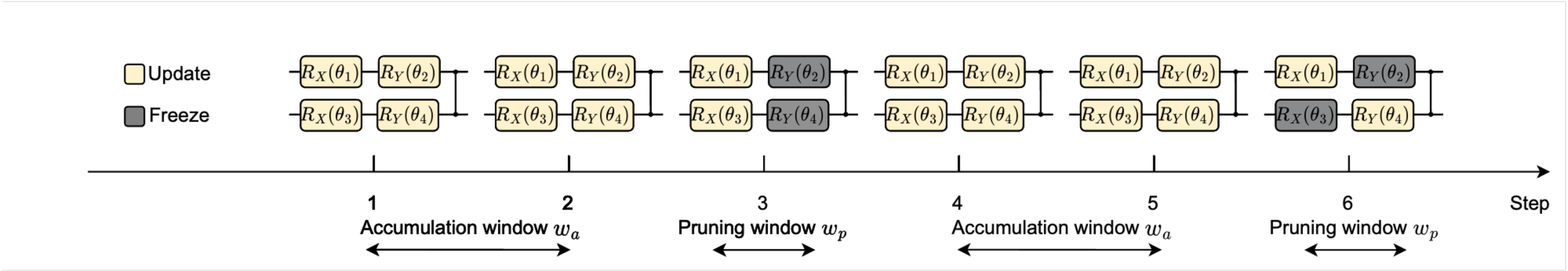
Probabilistic Gradient Pruning

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



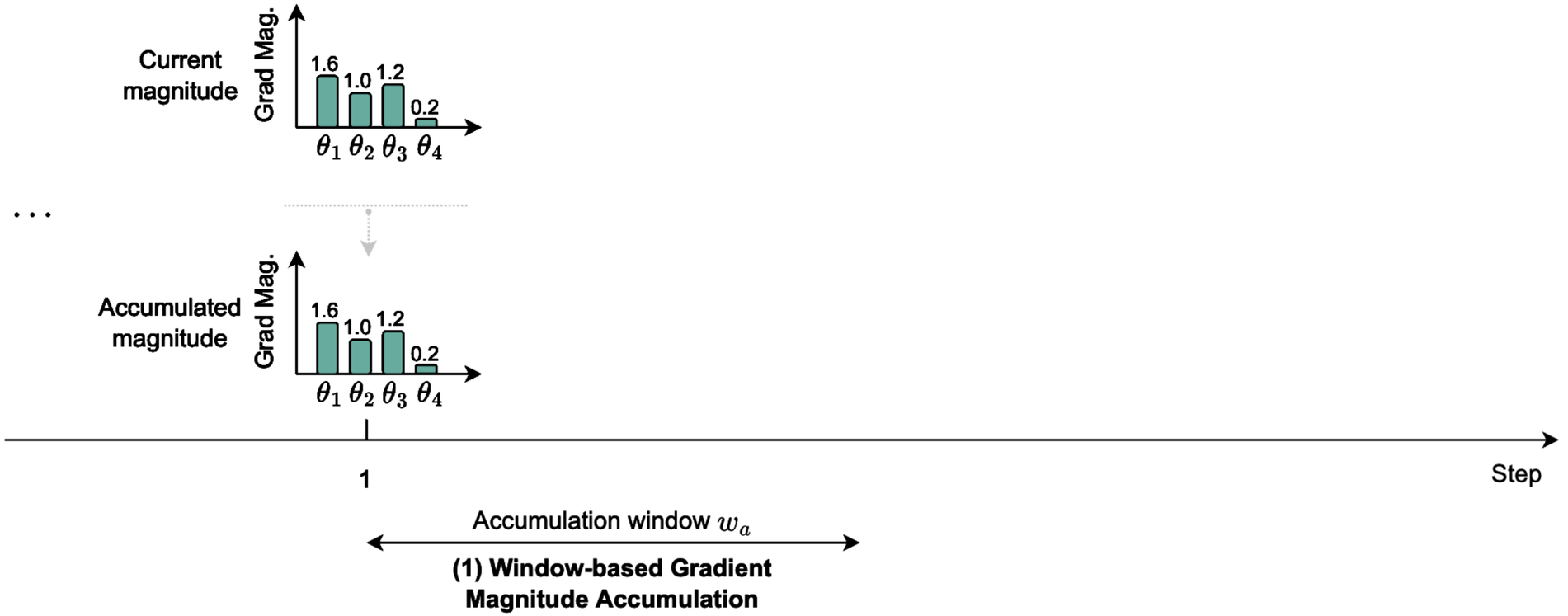
Probabilistic Gradient Pruning

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



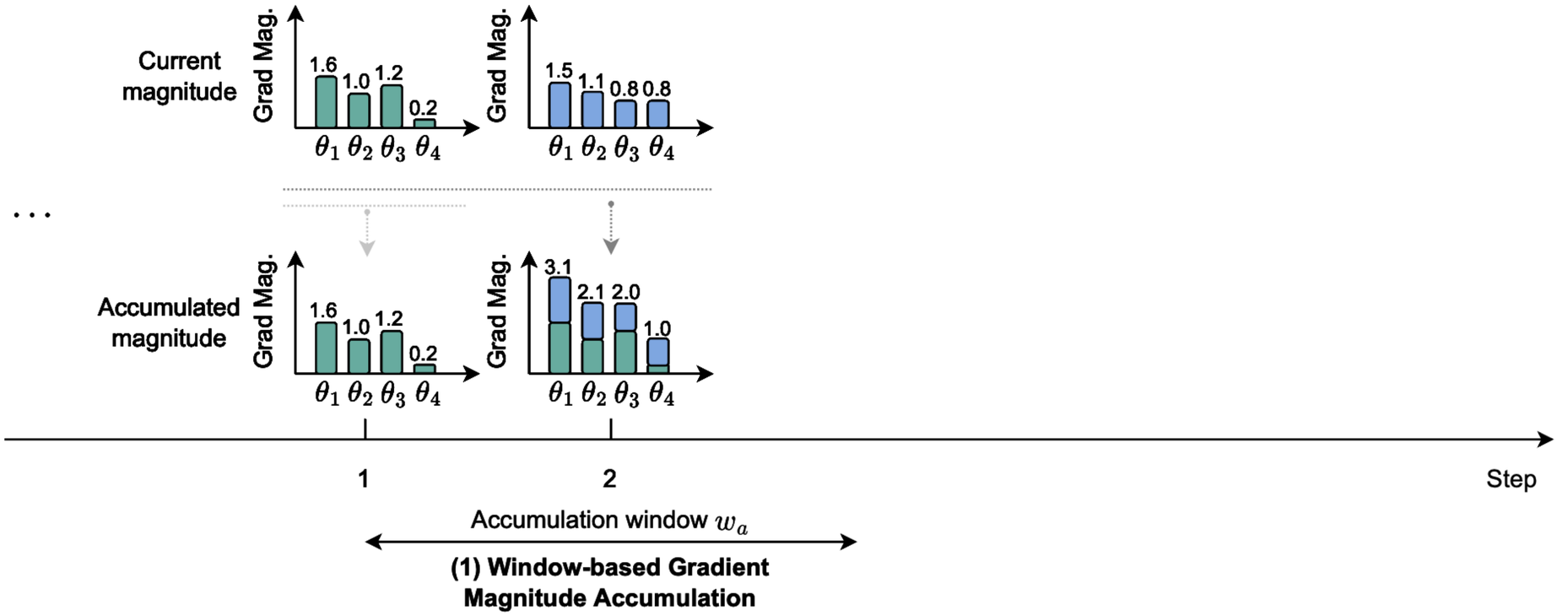
Accumulation Window

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



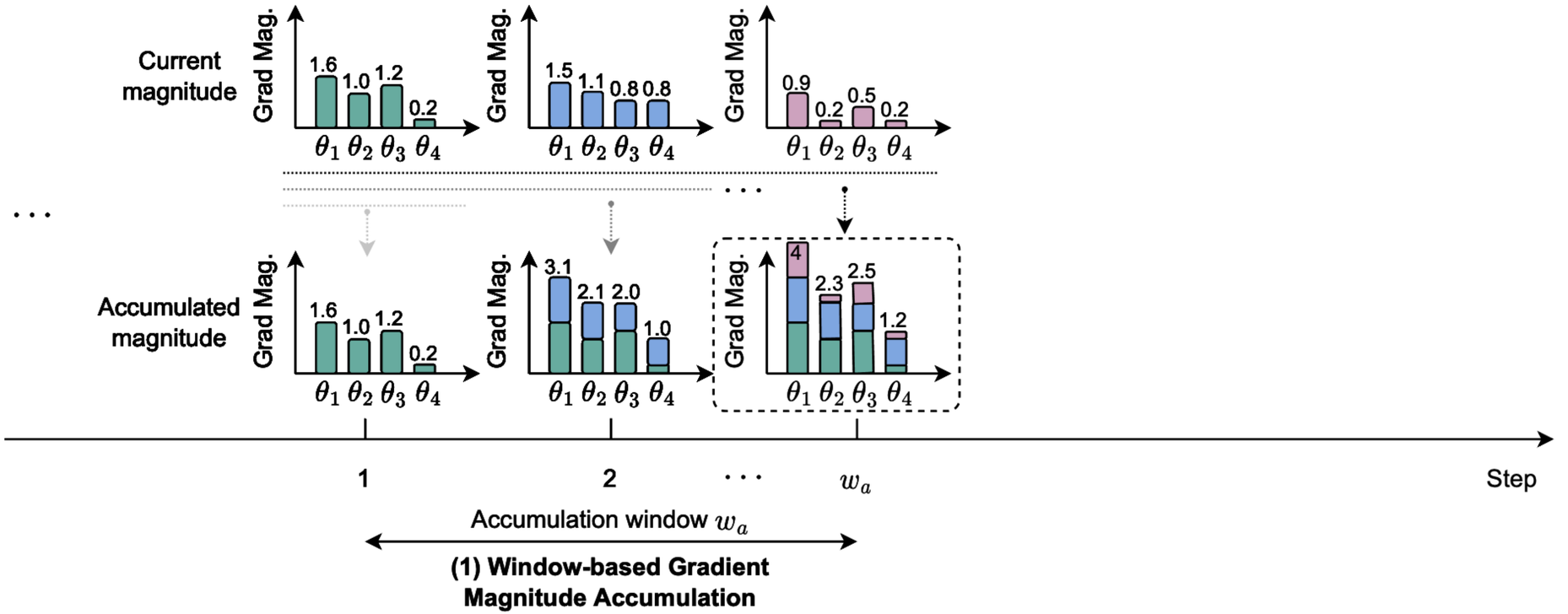
Accumulation Window

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



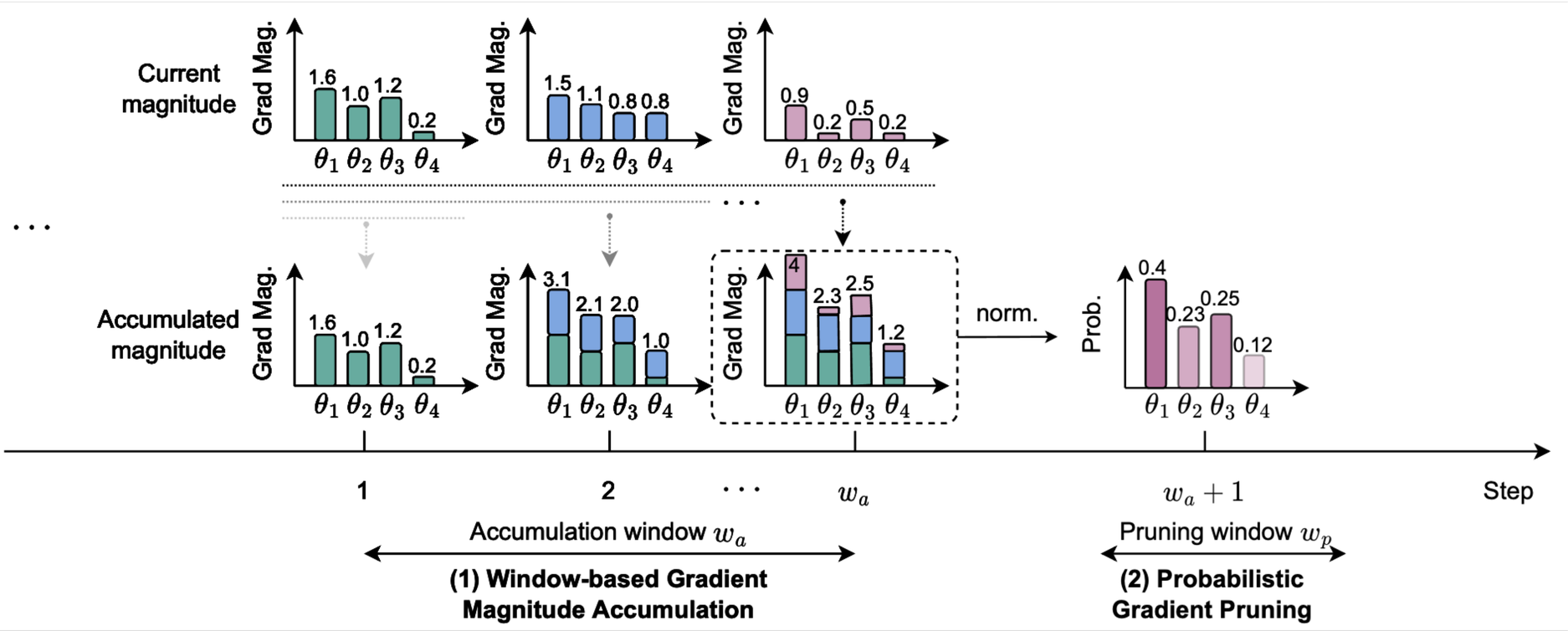
Accumulation Window

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



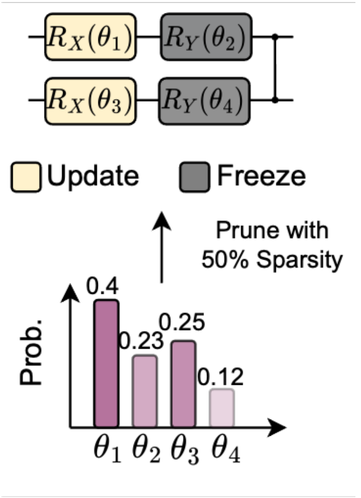
Pruning Window

- **Normalize** the accumulated gradient magnitude to a probability distribution



Pruning Window

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



Evaluation of the Gradient Pruning

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

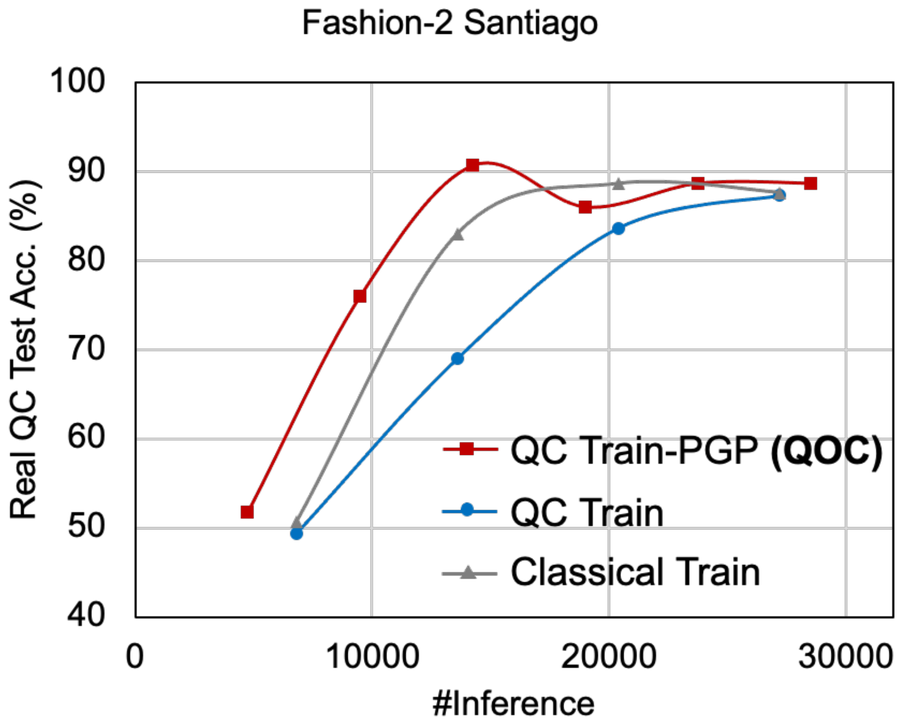
Classification Results

- Gradient achieves 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**

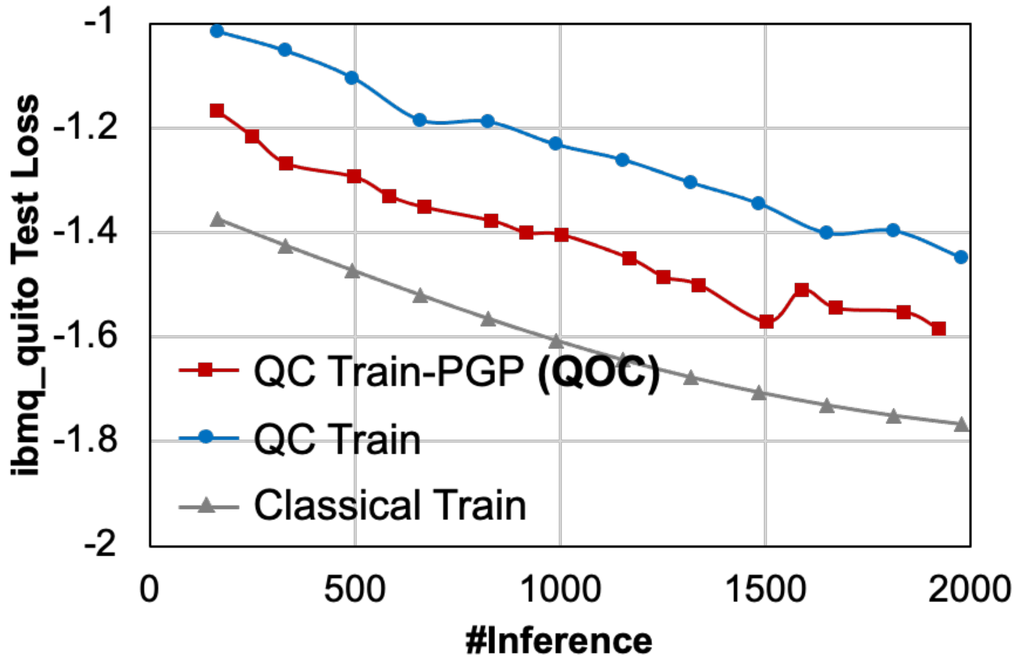
Classification Results

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



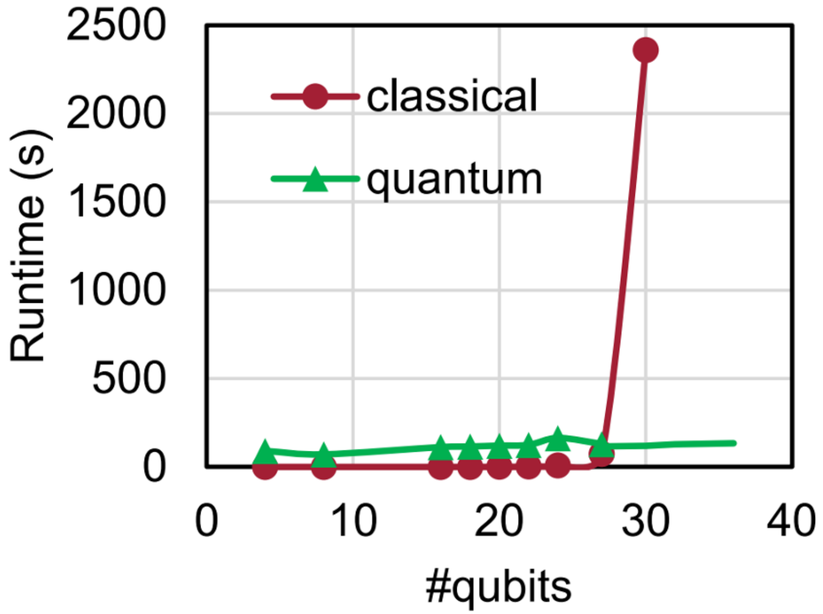
VQE Results

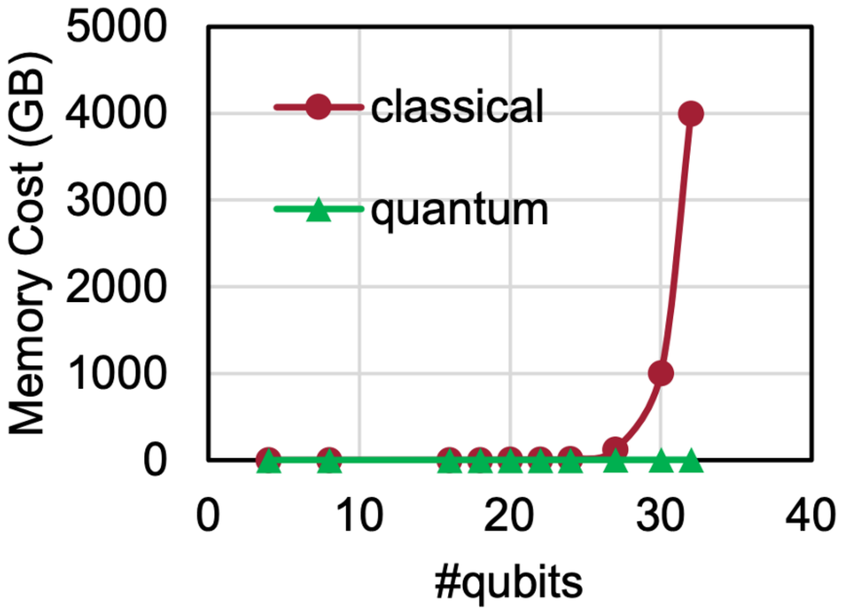
- Gradient pruning can **reduce the gap** between quantum and classical



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	**0.62**	**0.85**	**0.79**	**0.90**

TorchQuantum

Good Infrastructure is Critical

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

Specify encoder gates

Specify trainable gates

```
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)

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

ctor

cal pixels

able gates

-trainable gates

classical values

```
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 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])

  # 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])

  # 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]])

  # 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
```

Summary of Today's Lecture

- We learned
  - Continue to introduce NISQ devices
  - Introduce Parameterized Quantum Circuit (PQC)
  - Introduce PQC Training
  - Introduce Quantum Classifiers
  - Introduce Noise Aware On-Chip Training (QOC) of PQC
  - Introduce TorchQuantum Library for QML

In next lecture, we will introduce:

Noise Robust QML