Qiskit Global Summer School 2024

# Quantum Machine Learning

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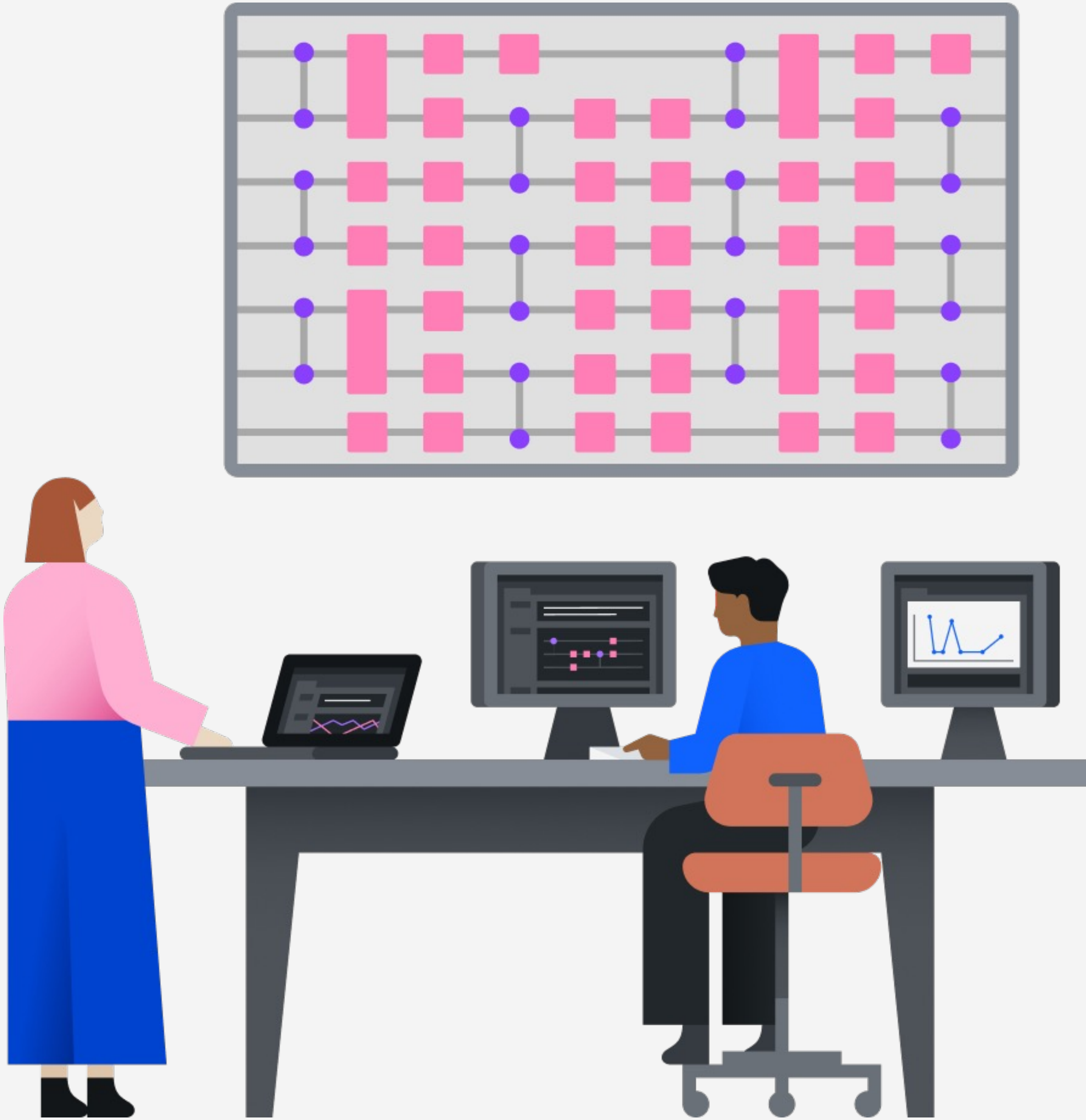
IBM Quantum



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# Overview

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Machine learning preliminaries

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Variational circuits and data encoding

3

Quantum kernels and support vector machines

4

Quantum neural networks

# Machine learning preliminaries

“Learning and adapting without following explicit instructions, by analyzing and drawing inferences from patterns in data”

# Machine learning overview

Function approximation and optimization

$$g(x)$$

true function

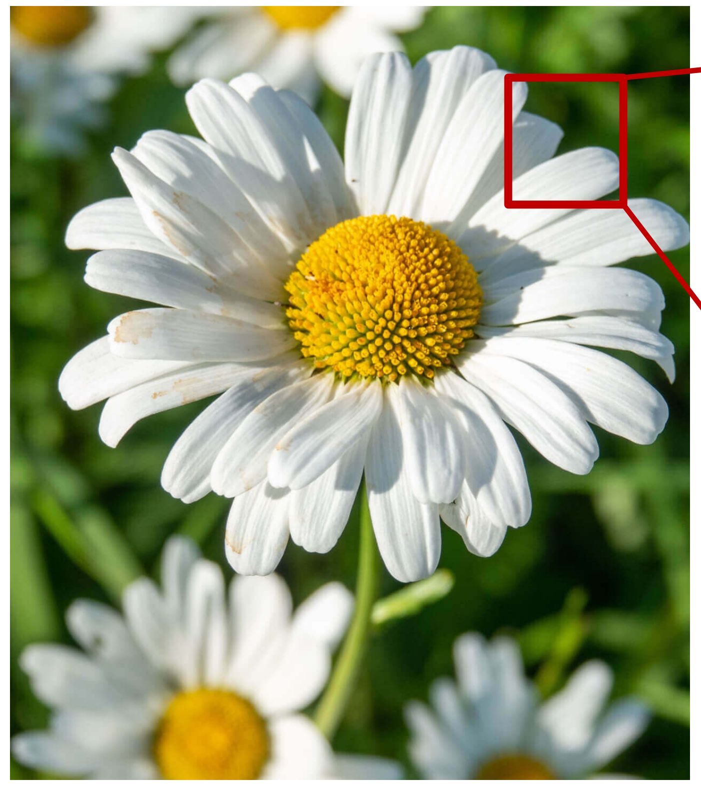
approximate $\longrightarrow$

$$f(\hat{x}, \vec{\theta})$$

mathematical model

$x$ : data features

e.g. pixel values of an image



| | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| 157 | 153 | 174 | 168 | 150 | 152 | 129 | 151 | 172 | 161 | 155 | 156 |
| 155 | 182 | 163 | 74 | 75 | 62 | 33 | 17 | 110 | 210 | 180 | 154 |
| 180 | 180 | 50 | 14 | 34 | 6 | 10 | 33 | 48 | 106 | 159 | 181 |
| 206 | 109 | 5 | 124 | 131 | 111 | 120 | 204 | 166 | 15 | 56 | 180 |
| 194 | 68 | 137 | 251 | 237 | 239 | 239 | 228 | 227 | 87 | 71 | 201 |
| 172 | 105 | 207 | 233 | 233 | 214 | 220 | 239 | 228 | 98 | 74 | 206 |
| 188 | 88 | 179 | 209 | 185 | 215 | 211 | 158 | 139 | 75 | 20 | 169 |
| 189 | 97 | 165 | 84 | 10 | 168 | 134 | 11 | 31 | 62 | 22 | 148 |
| 199 | 168 | 191 | 193 | 158 | 227 | 178 | 143 | 182 | 106 | 36 | 190 |
| 205 | 174 | 155 | 252 | 236 | 231 | 149 | 178 | 228 | 43 | 95 | 234 |
| 190 | 216 | 116 | 149 | 236 | 187 | 86 | 150 | 79 | 38 | 218 | 241 |
| 190 | 224 | 147 | 108 | 227 | 210 | 127 | 102 | 36 | 101 | 255 | 224 |
| 190 | 214 | 173 | 66 | 103 | 143 | 96 | 50 | 2 | 109 | 249 | 215 |
| 187 | 196 | 235 | 75 | 1 | 81 | 47 | 0 | 6 | 217 | 255 | 211 |
| 183 | 202 | 237 | 145 | 0 | 0 | 12 | 108 | 200 | 138 | 243 | 236 |
| 195 | 206 | 123 | 207 | 177 | 121 | 123 | 200 | 175 | 13 | 96 | 218 |

e.g. $h(x, \vec{\theta}) = \theta_0 + \theta_1 x + \theta_2 x^2 + \theta_3 x^3$

Goal:
- choose $f$
- train $\vec{\theta}$

## Machine learning types

1

### Supervised Learning

- Classification
- Regression

2

### Unsupervised Learning

- Dimensionality reduction
- Clustering
- Some generative models like GAN, autoencoder, etc.

3

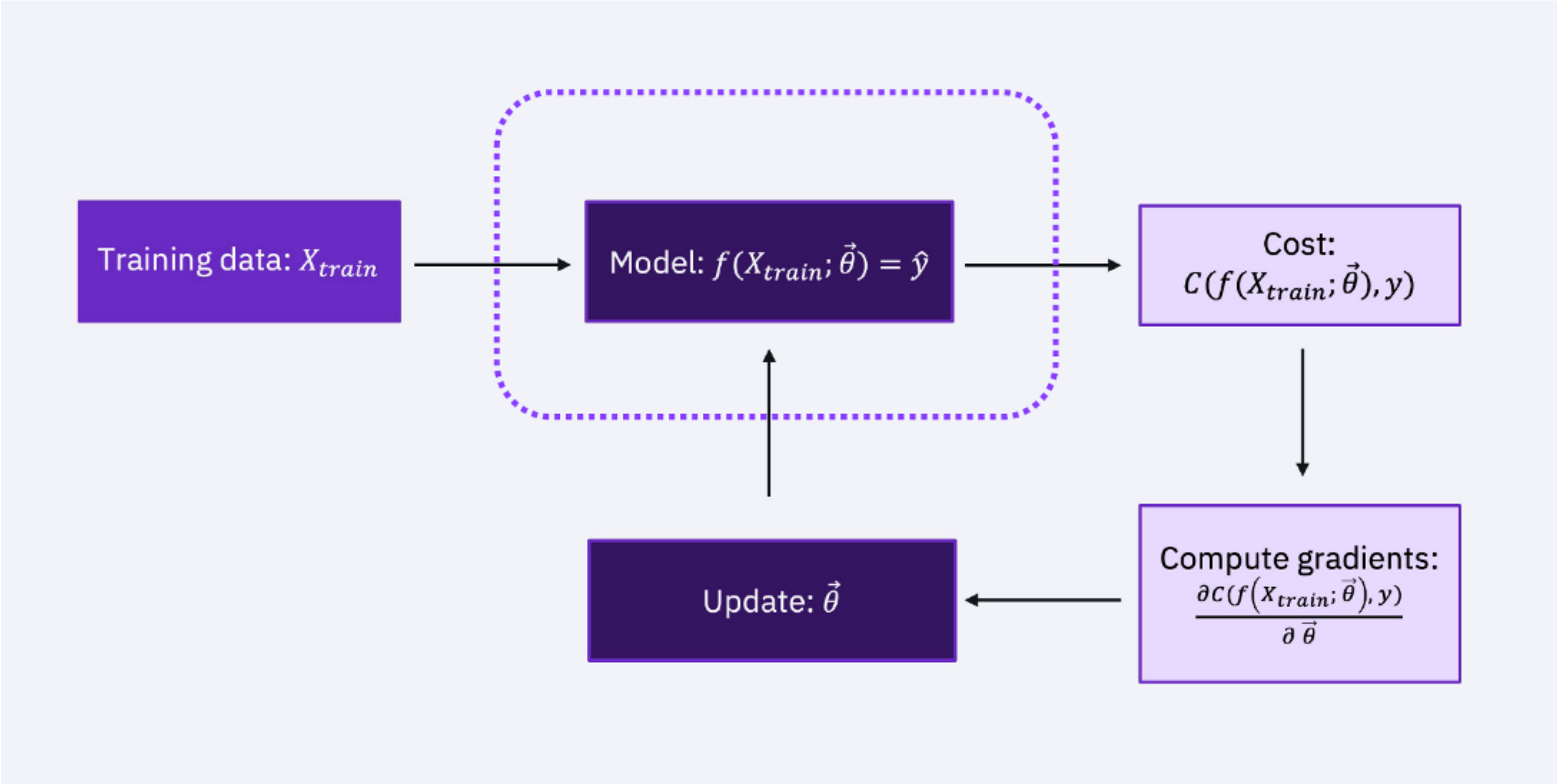
### Reinforcement Learning

Agent maximizing rewards in an environment



Source: https://www.ibm.com/blog/machine-learning-types/

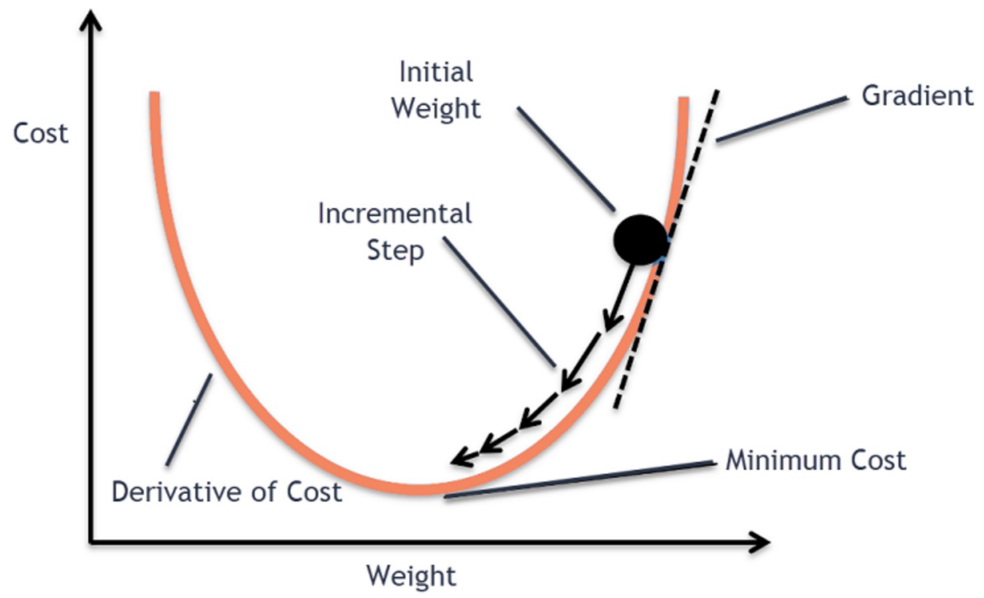
# Supervised learning workflow




e.g. Mean squared error

$$\mathrm{MSE} = \frac{1}{n}\sum_{i=1}^{n}\left(Y_i - \hat{Y}_i\right)^2.$$

e.g. Gradient descent

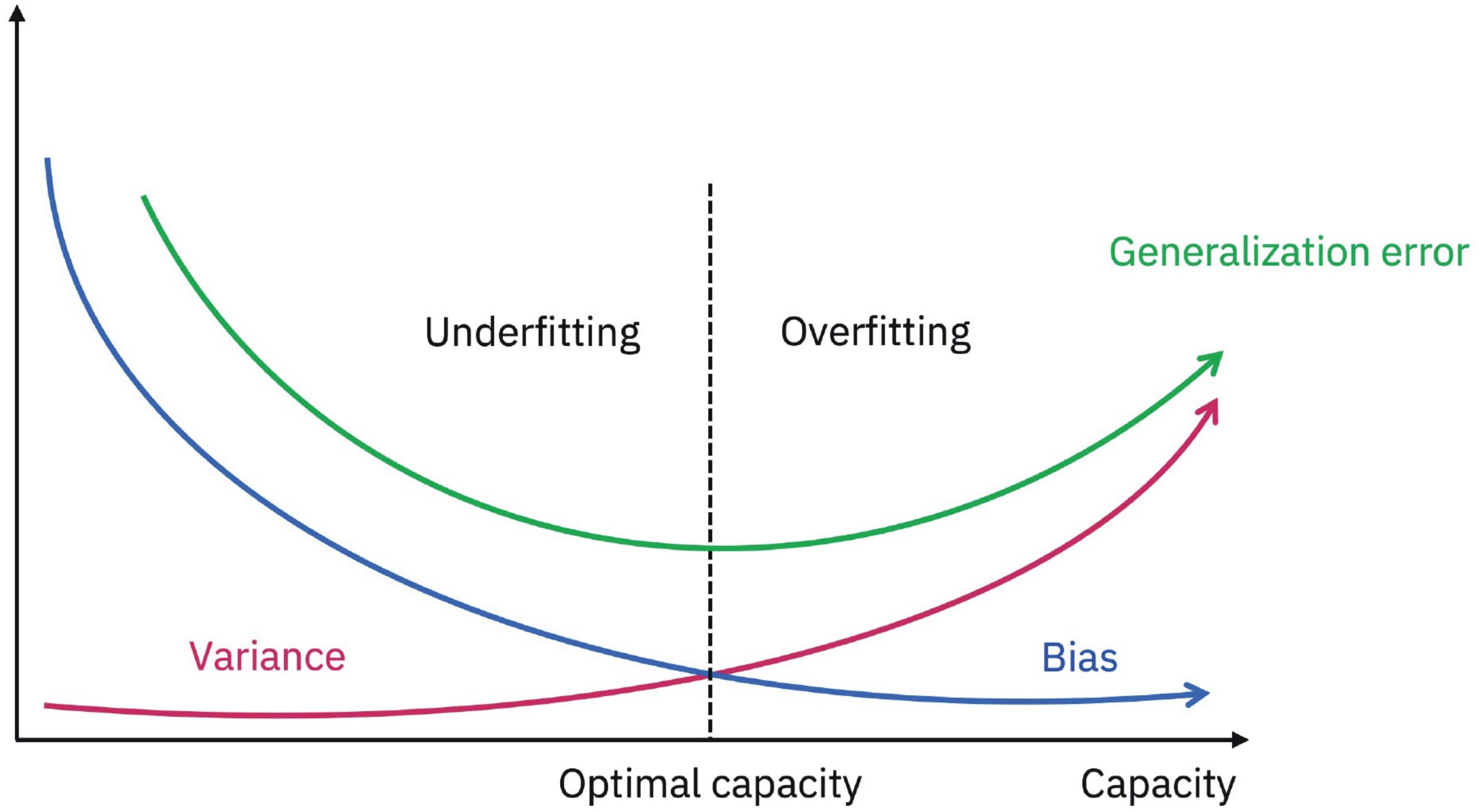


# Model validation

Model should work well both on training and the test data

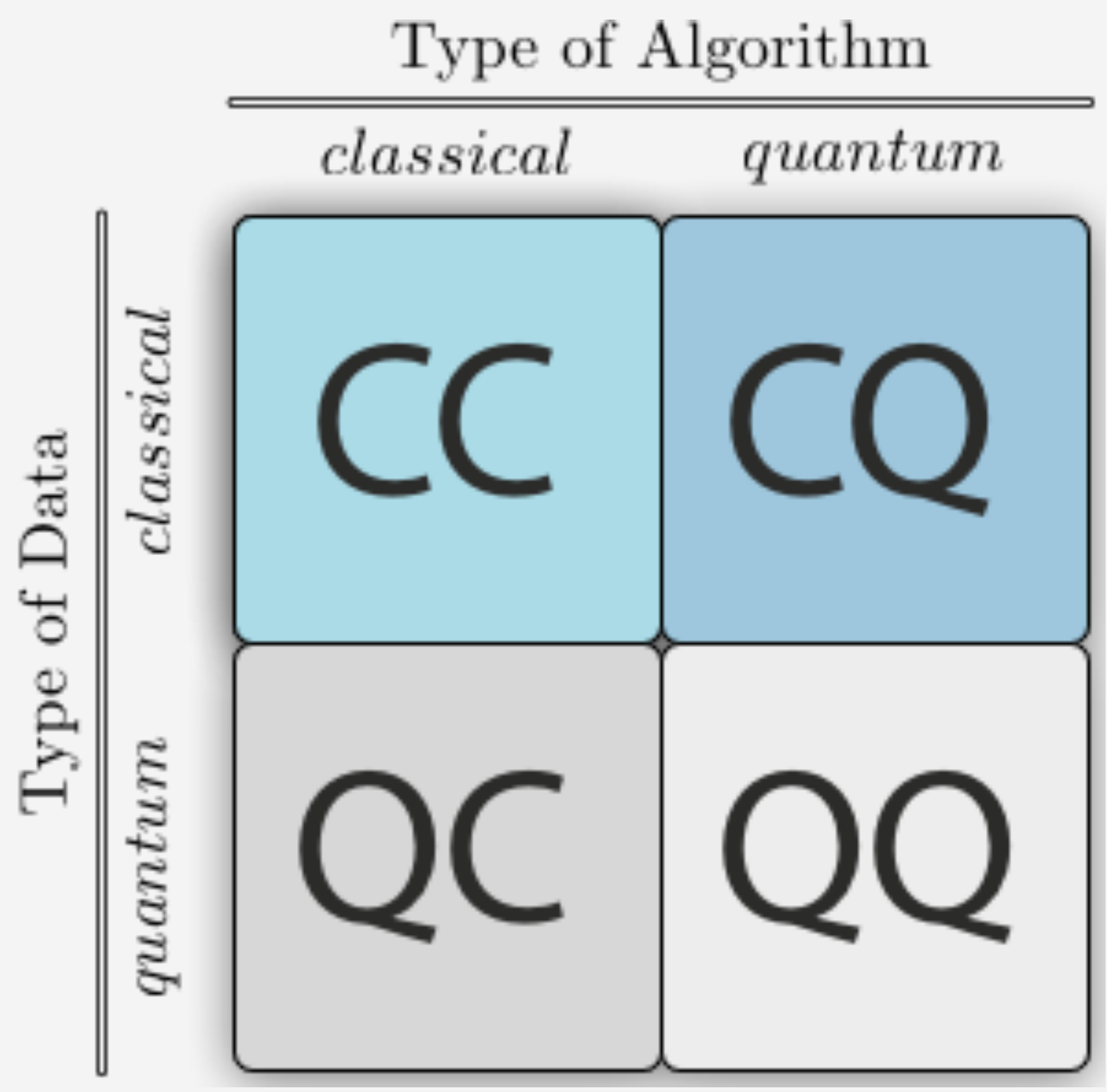
The model should not overfit or underfit to training data (poor generalization)

”bias-variance” trade-off

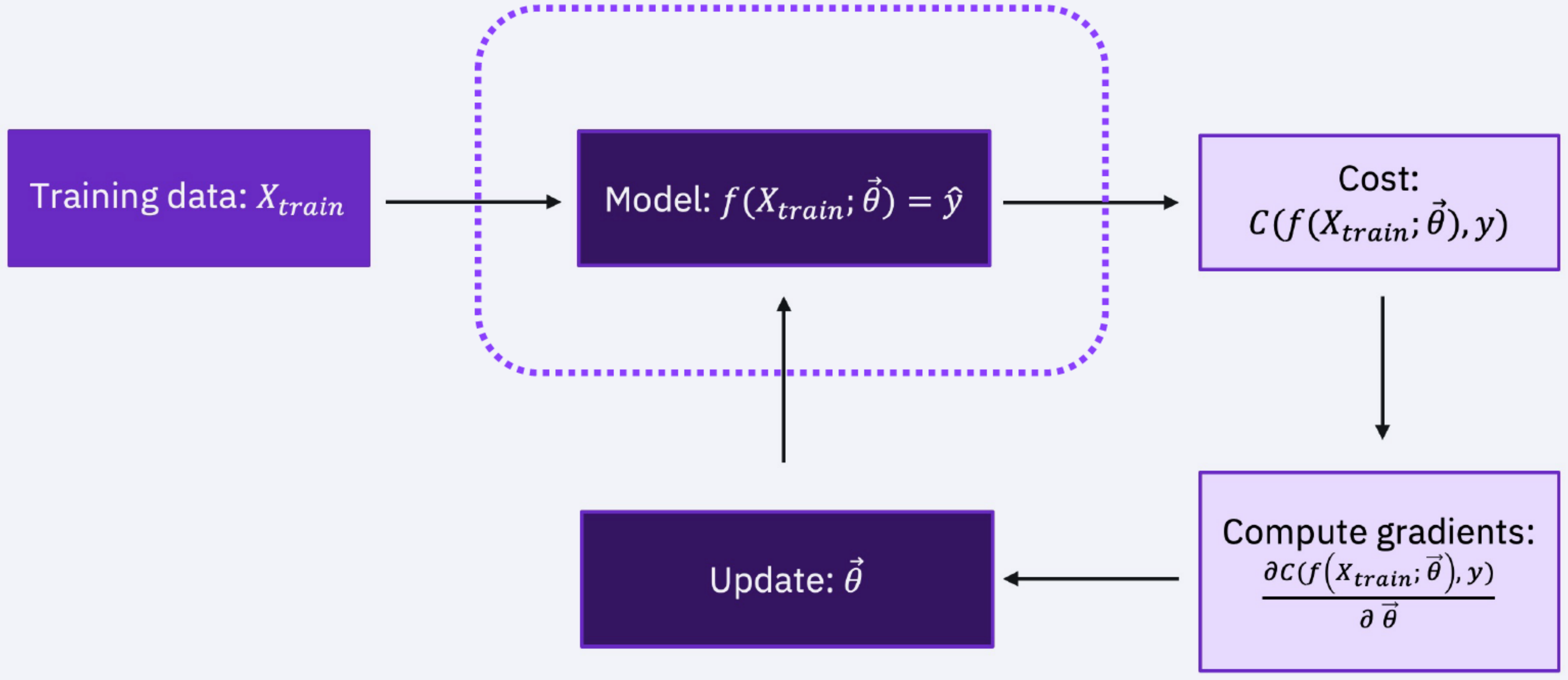


# Variational circuits and data encoding

# Quantum machine learning




Schuld, Maria, and Francesco Petruccione. Supervised learning with quantum computers. Vol. 17. Berlin: Springer, 2018.

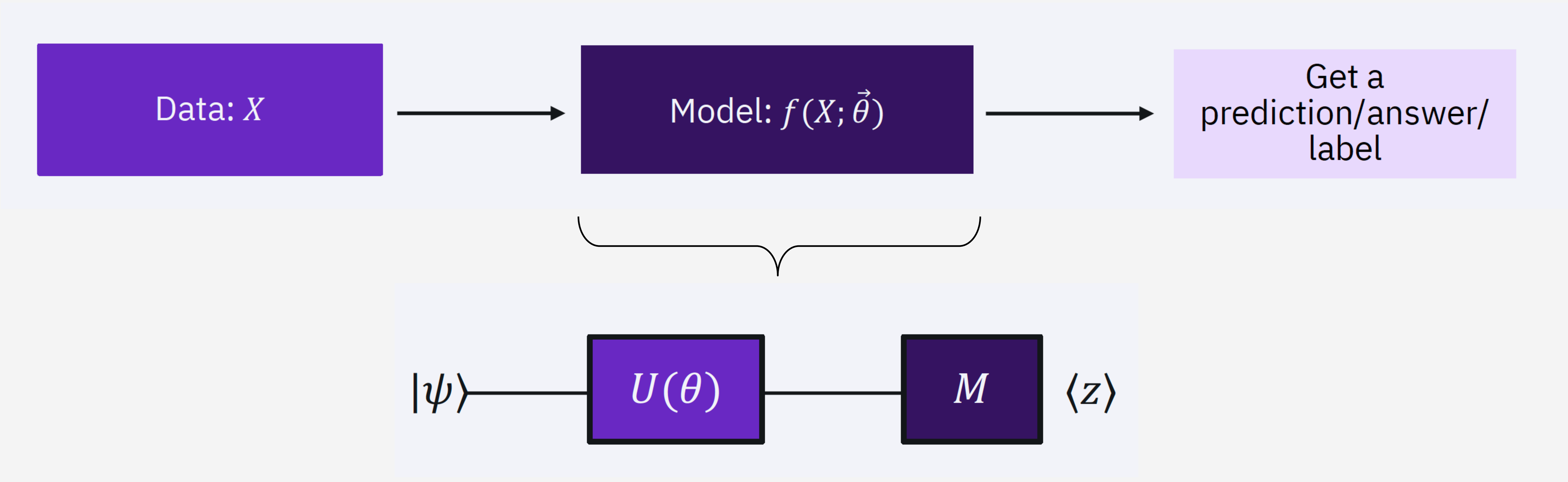



Also: **near-term** vs fault-tolerant

- Quantum SVM
- Quantum NNs
- HHL algorithm
- Quantum PCA


Harrow, Aram W., Avinatan Hassidim, and Seth Lloyd. "Quantum algorithm for linear systems of equations." Physical review letters 103.15 (2009): 150502.
Lloyd, Seth, Masoud Mohseni, and Patrick Rebentrost. "Quantum principal component analysis." Nature Physics 10.9 (2014): 631-633.

# Variational circuit as a classifier




Variational circuit

Parametrized quantum circuit (PQC)

Ansatz

# Variational circuit as a classifier

**Task:** Supervised learning (suppose binary classification, {1, -1})

**Step 1:** Encode the classical data into a quantum state

**Step 2:** Apply a parameterized model

**Step 3:** Measure the circuit to extract labels

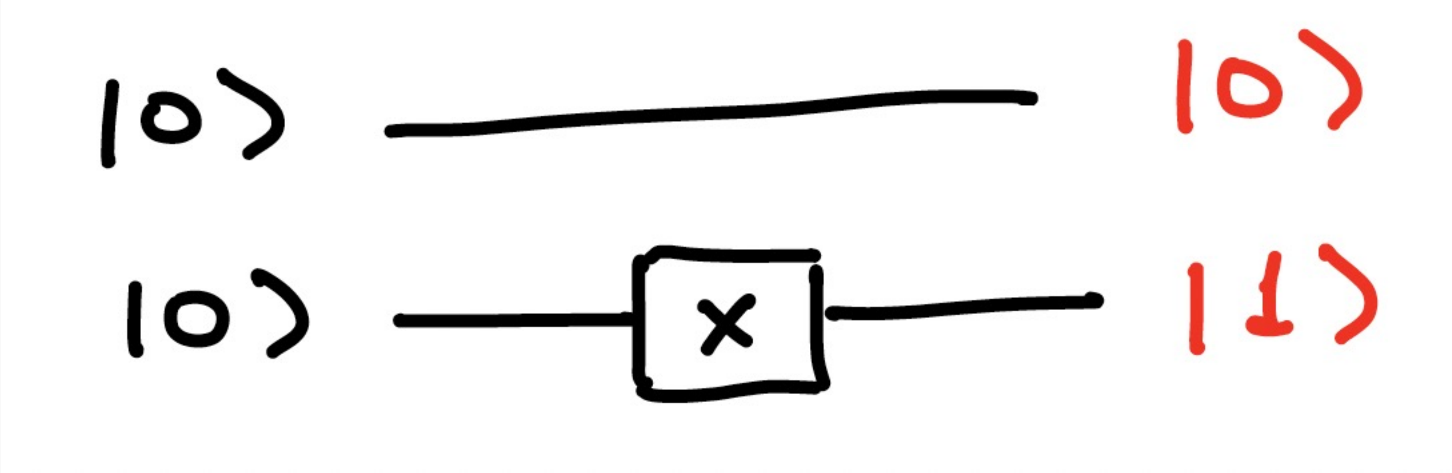
**Step 4:** Use optimization techniques (like gradient descent) to update model parameters

# Data encoding

| | |
|---|---|
| 3 | 1 |
| 0 | 3 |

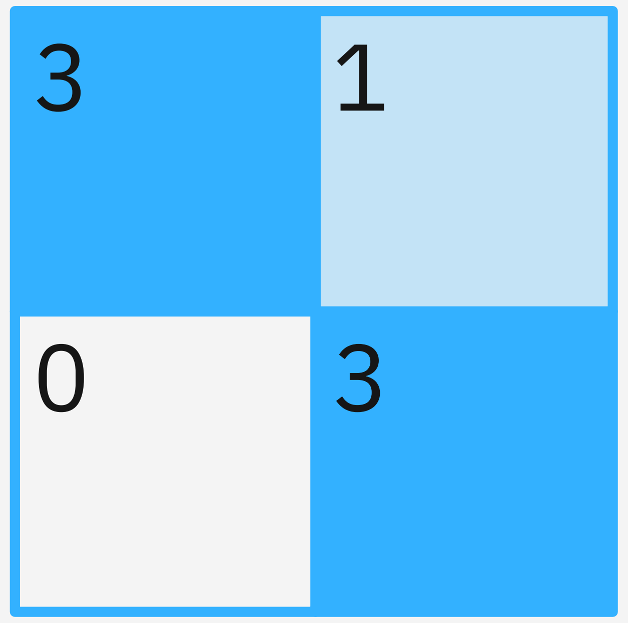
**Basis encoding:** Encode each $n$-bit feature into $n$ qubits

$$\vec{x} = \begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{bmatrix} = \begin{bmatrix} 3 \\ 1 \\ 0 \\ 3 \end{bmatrix} = \begin{bmatrix} 11 \\ 01 \\ 00 \\ 11 \end{bmatrix} = \begin{bmatrix} |11\rangle \\ |01\rangle \\ |00\rangle \\ |11\rangle \end{bmatrix}$$



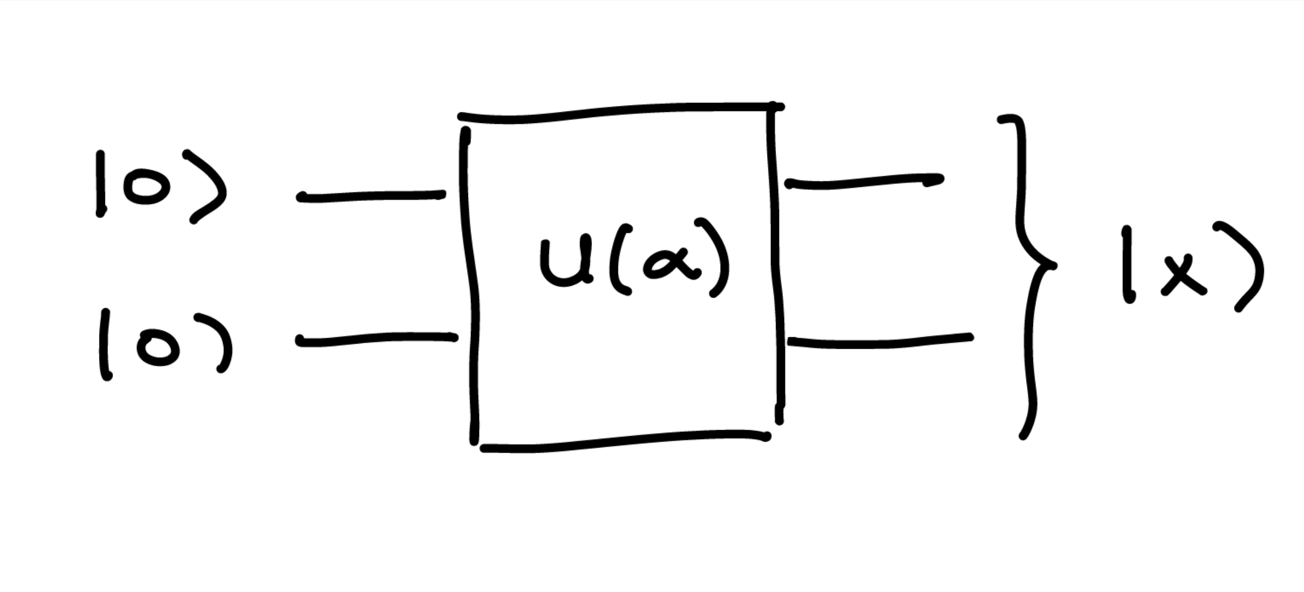

One of the computational basis states of 8 qubits

# Data encoding



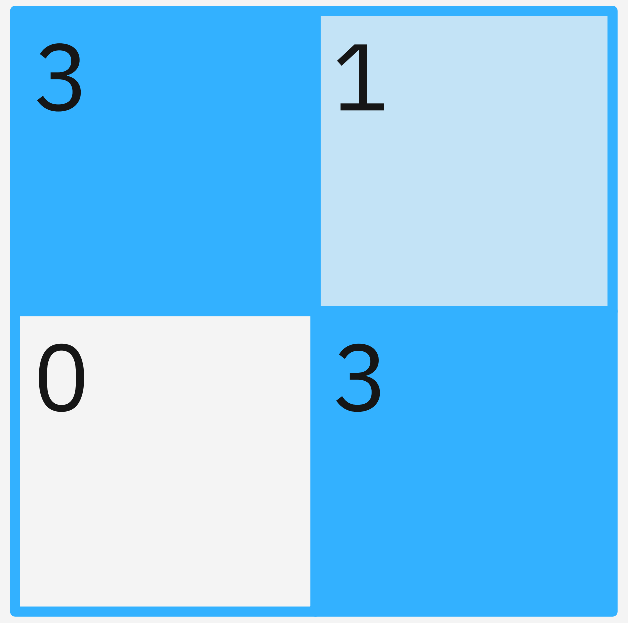

**Amplitude encoding:** Encode into quantum state amplitudes $|\psi_x\rangle = \sum_{i=1}^{N} x_i |i\rangle$

$$\vec{x} = \begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{bmatrix} = \begin{bmatrix} 3/\sqrt{19} \\ 1/\sqrt{19} \\ 0/\sqrt{19} \\ 3/\sqrt{19} \end{bmatrix}$$



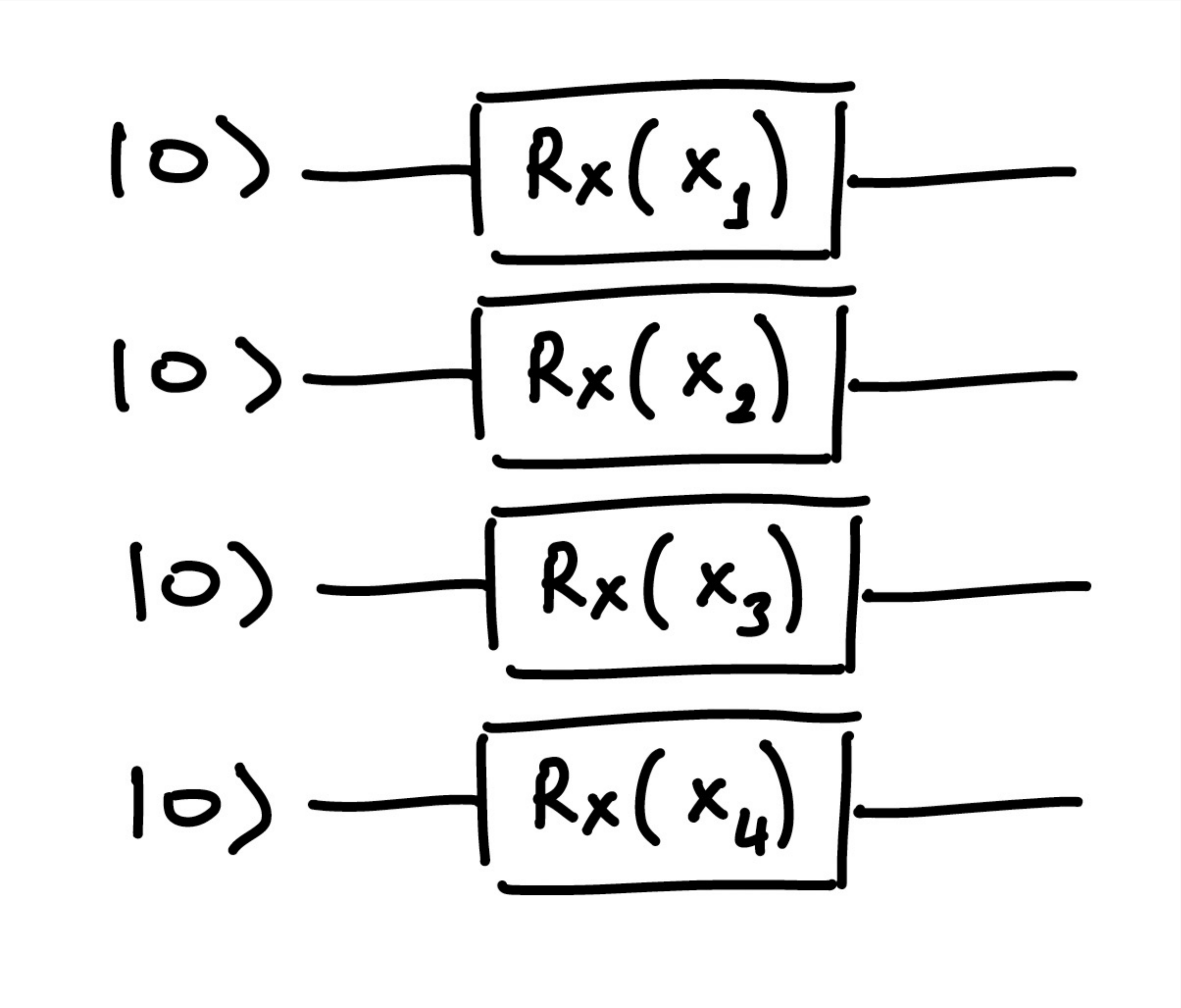

Amplitudes of 2 qubits

# Data encoding




**Angle encoding:** Encode values into qubit rotation angles

$$\vec{x} = \begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{bmatrix} = \begin{bmatrix} 3/\sqrt{19} \\ 1/\sqrt{19} \\ 0/\sqrt{19} \\ 3/\sqrt{19} \end{bmatrix}$$



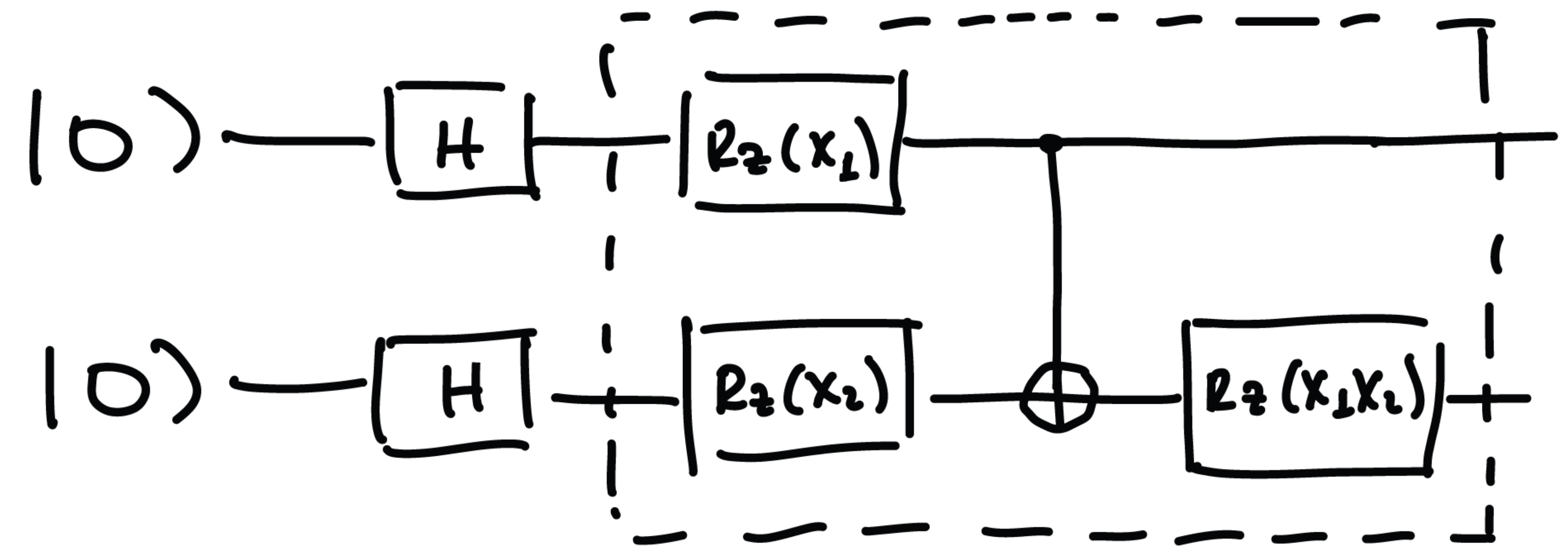

$$|x\rangle = \bigotimes_{i=1}^{N} \cos(x_i)|0\rangle + \sin(x_i)|1\rangle$$ angle encoding

$$|x\rangle = \bigotimes_{i=1}^{n} \cos(x_{2i-1})|0\rangle + e^{ix_{2i}} \sin(x_{2i-1})|1\rangle$$ dense angle encoding

# Data encoding

**Higher order encoding:** Feature maps

$$\vec{x} = \begin{bmatrix} x_1 \\ x_2 \end{bmatrix}$$




blocks can be repeated

Havlíček, Vojtěch, et al. "Supervised learning with quantum-enhanced feature spaces." Nature 567.7747 (2019): 209-212.

# Data encoding

## Basis Encoding

Encode each $n$-bit feature into $n$ qubits

$$x = (b_{n-1}, \dots, b_1, b_0) \rightarrow |x\rangle = |b_{n-1}, \dots, b, b_0\rangle$$

## Amplitude Encoding

Encode into quantum state amplitudes

$$x = \begin{bmatrix} x_0 \\ \vdots \\ x_{N-1} \end{bmatrix} \rightarrow |\psi_x\rangle = \sum_{j=0}^{N-1} x_j |j\rangle$$

## Angle Encoding

Encode values into qubit rotation angles

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

## Arbitrary Encoding (Feature Map)

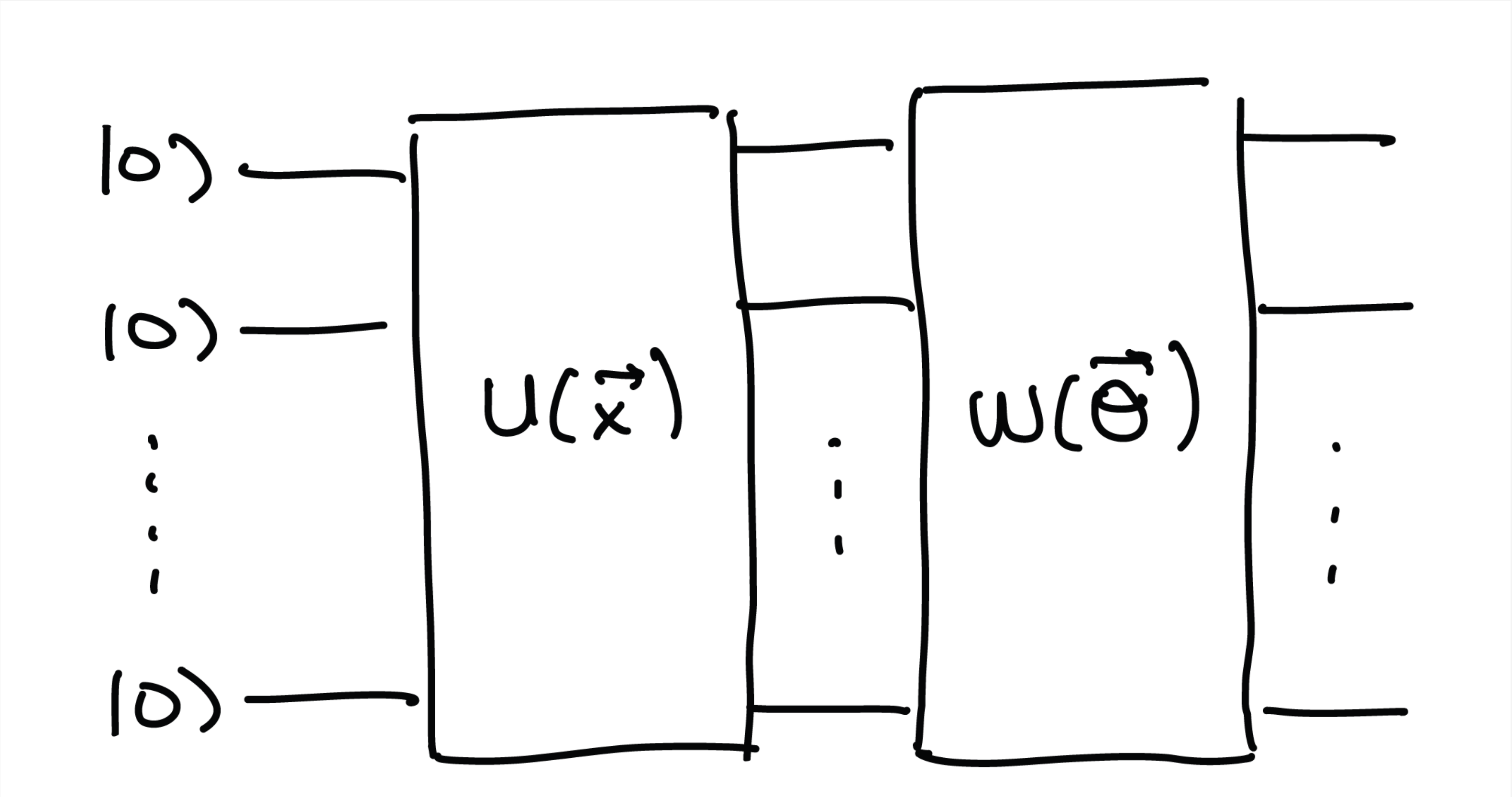
Encode $N$ features on $N$ rotation gates in constant-depth circuit with $n$ qubits

$$x = \begin{bmatrix} x_0 \\ \vdots \\ x_{N-1} \end{bmatrix} \rightarrow |\psi_x\rangle = \mathcal{U}_{\Phi(x)}|0\rangle$$

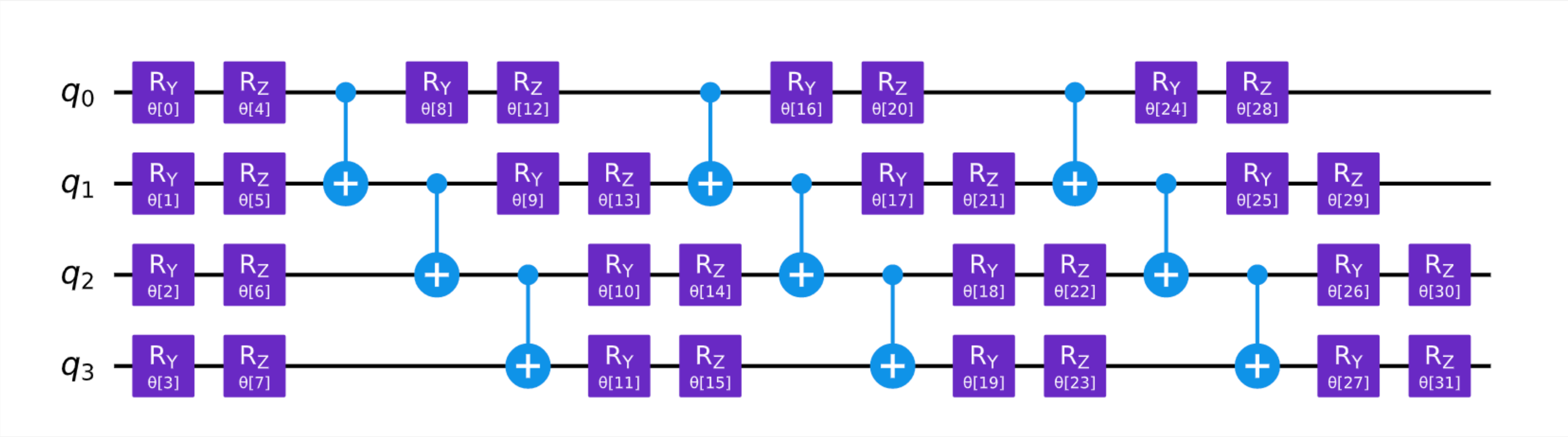
| Encoding | # Qubits | State prep runtime |
|---|---|---|
| Basis | $nN$ | $O(N)$ |
| Amplitude | $\log(N)$ | $\frac{O(N)}{O(\log(N))}$ |
| Angle | $N$ | $O(N)$ |
| Arbitrary | $n$ | $O(N)$ |

$N$ features each

# Variational model




Data encoding Ansatz

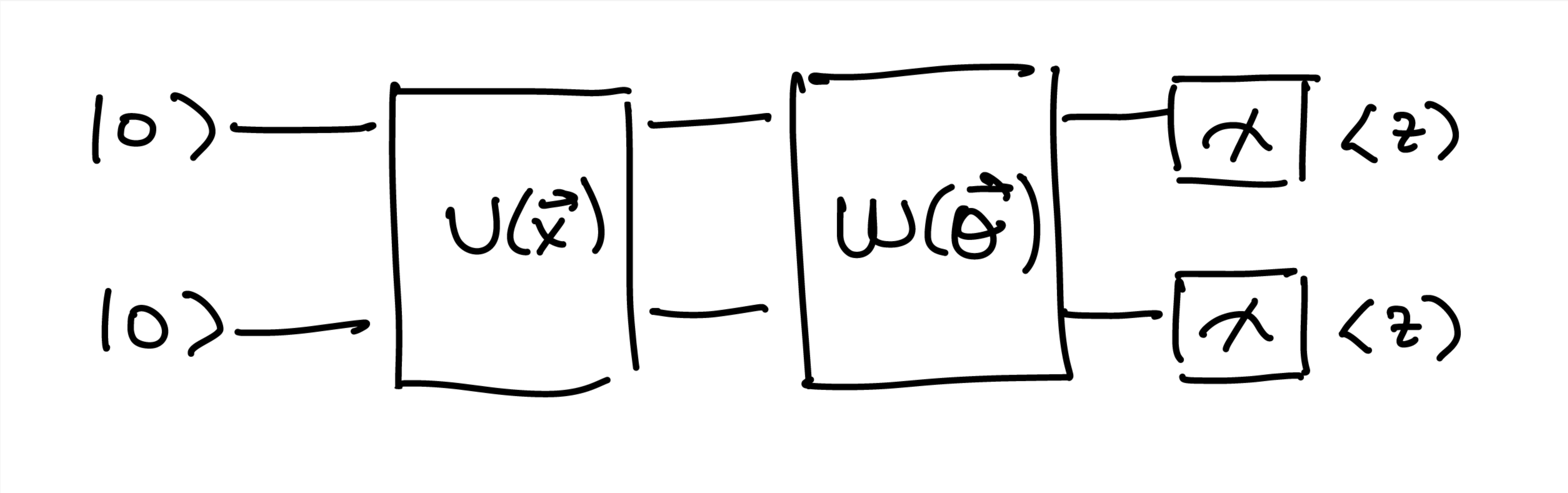



Goal: designing a **hardware-efficient** ansatz

expressivity and depth

Leone, Lorenzo, et al. "On the practical usefulness of the hardware efficient ansatz." arXiv preprint arXiv:2211.01477 (2022).

# Extracting labels




measurement outcomes → labels

↓

cost function

↓

classical optimizer

Binary classification {1,-1}:

1. Parity post-processing (00, 01, 10, 11)
2. Measure only 1 qubit (<Z> >= 0, otherwise)

**Qiskit**

*sampler*

*estimator*

# Optimization: parameter update

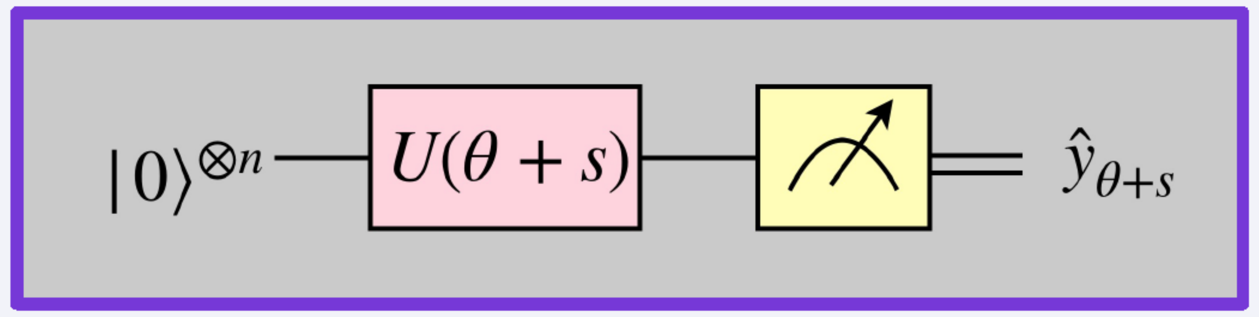
e.g. Mean squared error

Cost: $$\mathrm{MSE} = \frac{1}{n}\sum_{i=1}^{n}\left(Y_i - \hat{Y}_i\right)^2.$$

If optimizer needs: $\partial_{\theta_i} f(\boldsymbol{\theta})$

Parameter-shift rule

Gradient =

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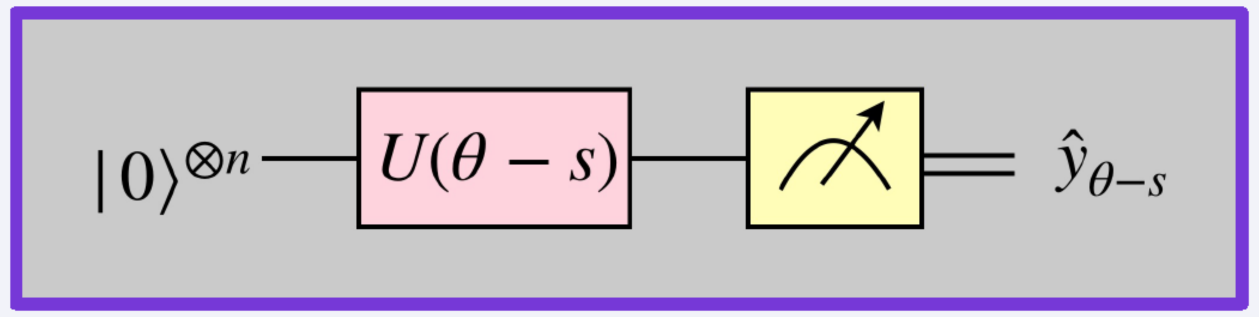



/ 2

$s = \pi/2$

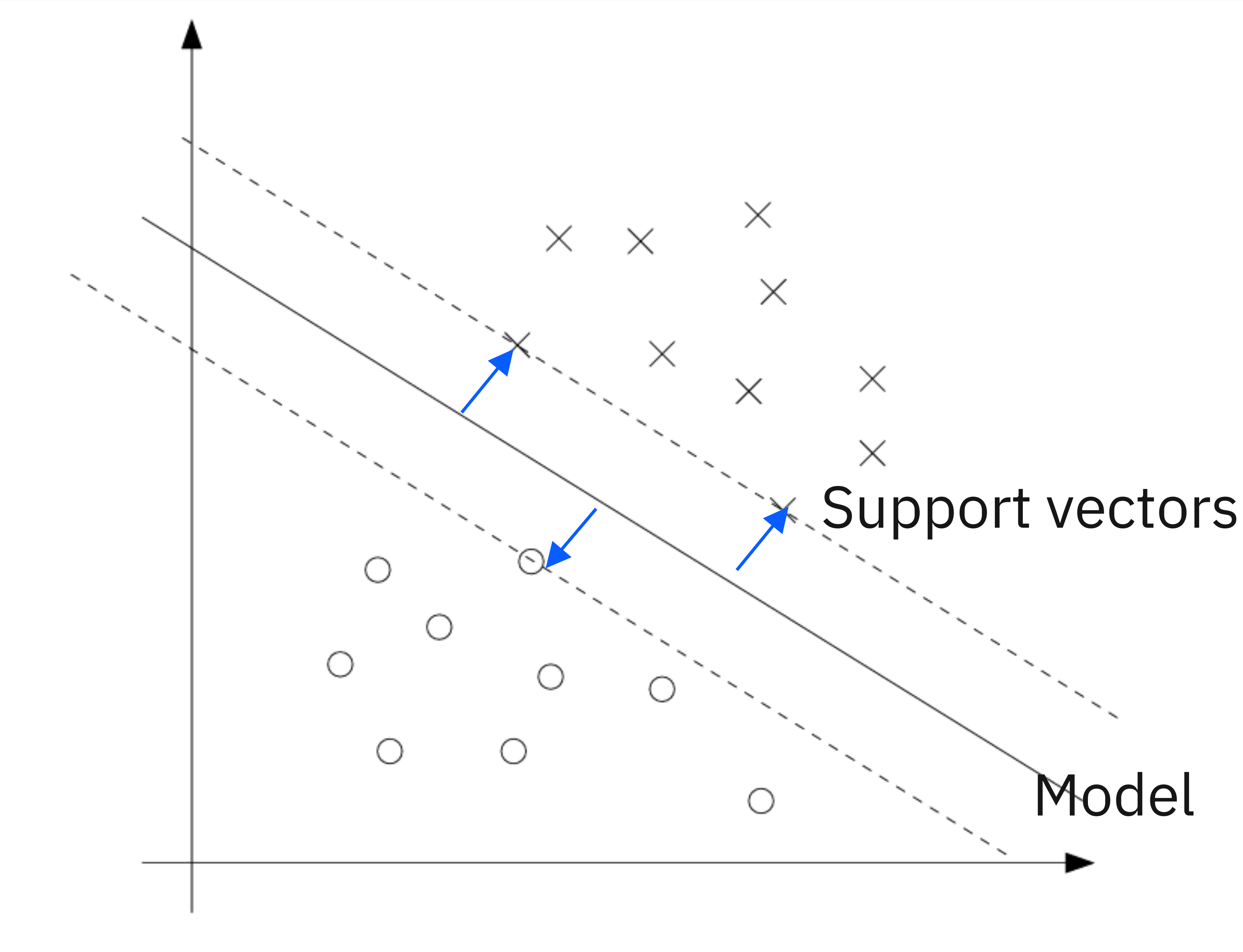
Remark: SPSA (Simultaneous Perturbation Stochastic Approximation )



Schuld, Maria, et al. "Circuit-centric quantum classifiers." Physical Review A 101.3 (2020): 032308.

# Quantum kernels and support vector machines

# Support vector machines (SVMs)




Classification problem, e.g. binary classification

– Primal formulation

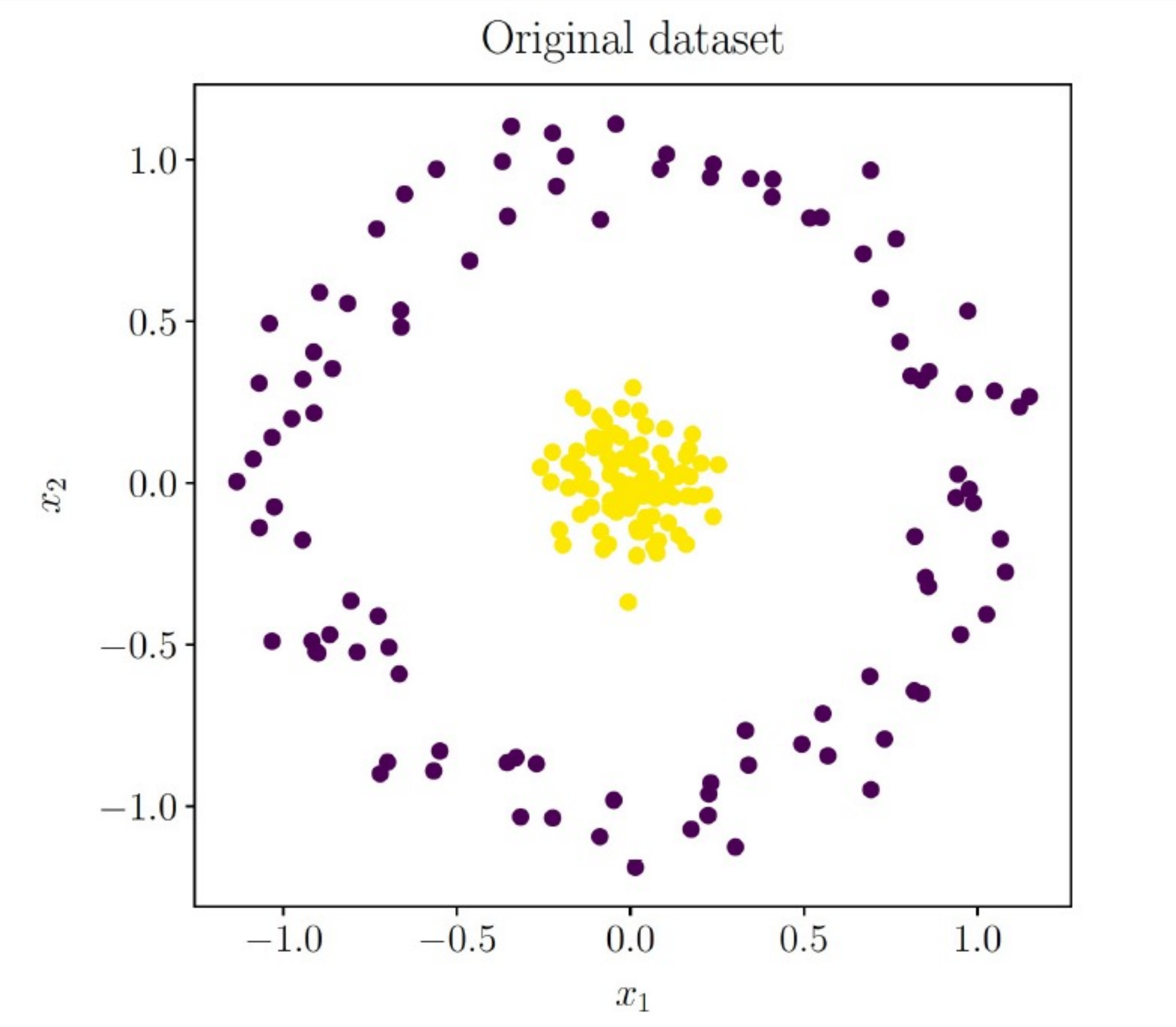
$$f(x) = \vec{\theta}^T \vec{x} + b$$

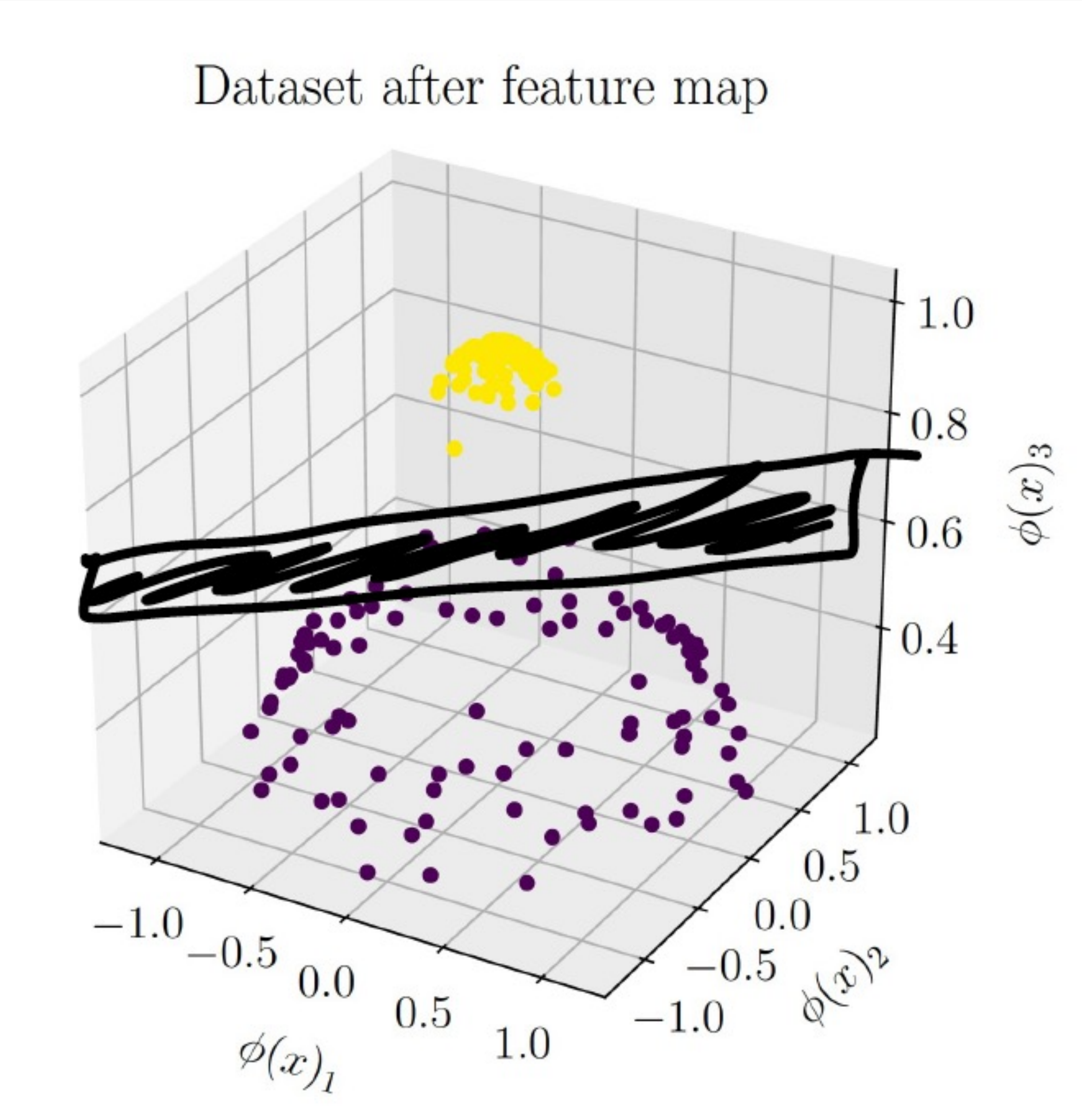
– Dual formulation

$$f(x) = \sum_{i=1}^{n} \alpha_i y_i \left( \vec{x}_i^T \vec{x} \right) + b$$

# Support vector machines

When data is not linearly separable




$$\vec{x} = \begin{bmatrix} x_1 \\ x_2 \end{bmatrix}$$

$$\phi(\vec{x}) = \begin{bmatrix} x_1 \\ x_2 \\ x_1 x_2 \end{bmatrix}$$

feature map

# Support vector machines

Primal formulation

$$f(x) = \vec{\theta}^T \vec{x} + b$$

$$f(x) = \theta^T \phi(x) + b$$

Dual formulation

$$f(x) = \sum_{i=1}^{n} \alpha_i y_i \left( \vec{x}_i^T \vec{x} \right) + b$$

$$f(x) = \sum_{i=1}^{n} \alpha_i y_i \left( \phi(x_i)^T \phi(x) \right) + b$$

inner product
"kernel"

# Quantum kernels

- Interpreting data encoding to a quantum state as a feature map $x \rightarrow |\phi(x)\rangle$

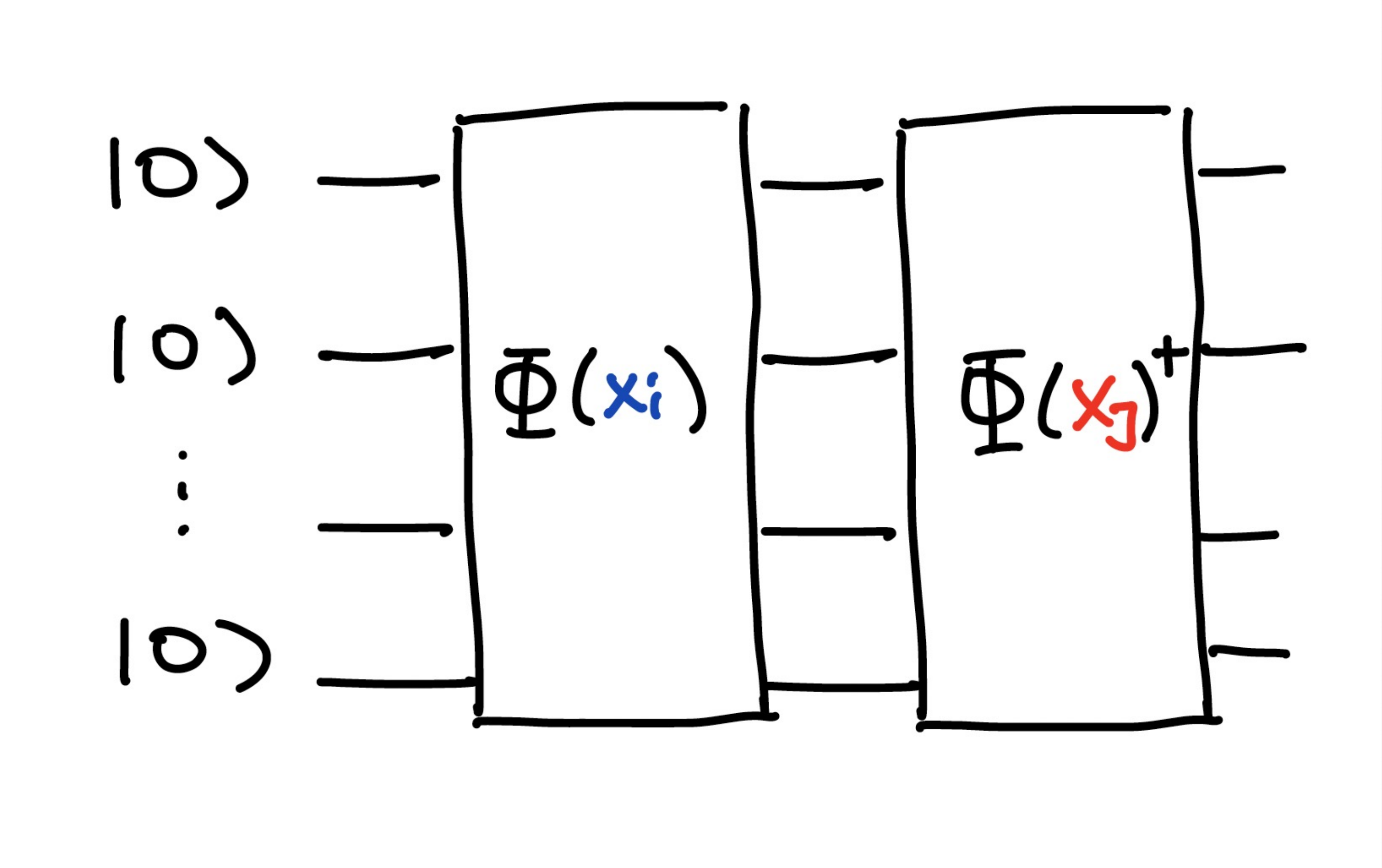
- Quantum kernels can only be expected to do better than classical kernels if they are **hard to estimate classically.**
  - necessary but not sufficient

- It was shown that learning problems **exist**, for which learners with access to quantum kernel methods have a quantum advantage over all classical learners.

Havlíček, Vojtěch, et al. "Supervised learning with quantum-enhanced feature spaces." Nature 567.7747 (2019): 209-212.

Glick, Jennifer R., et al. "Covariant quantum kernels for data with group structure." Nature Physics (2024): 1-5.

# Quantum SVM




quantum kernel estimator

$$K_{i,j} = |\langle \Phi(x_j) | \Phi(x_i) \rangle|^2$$

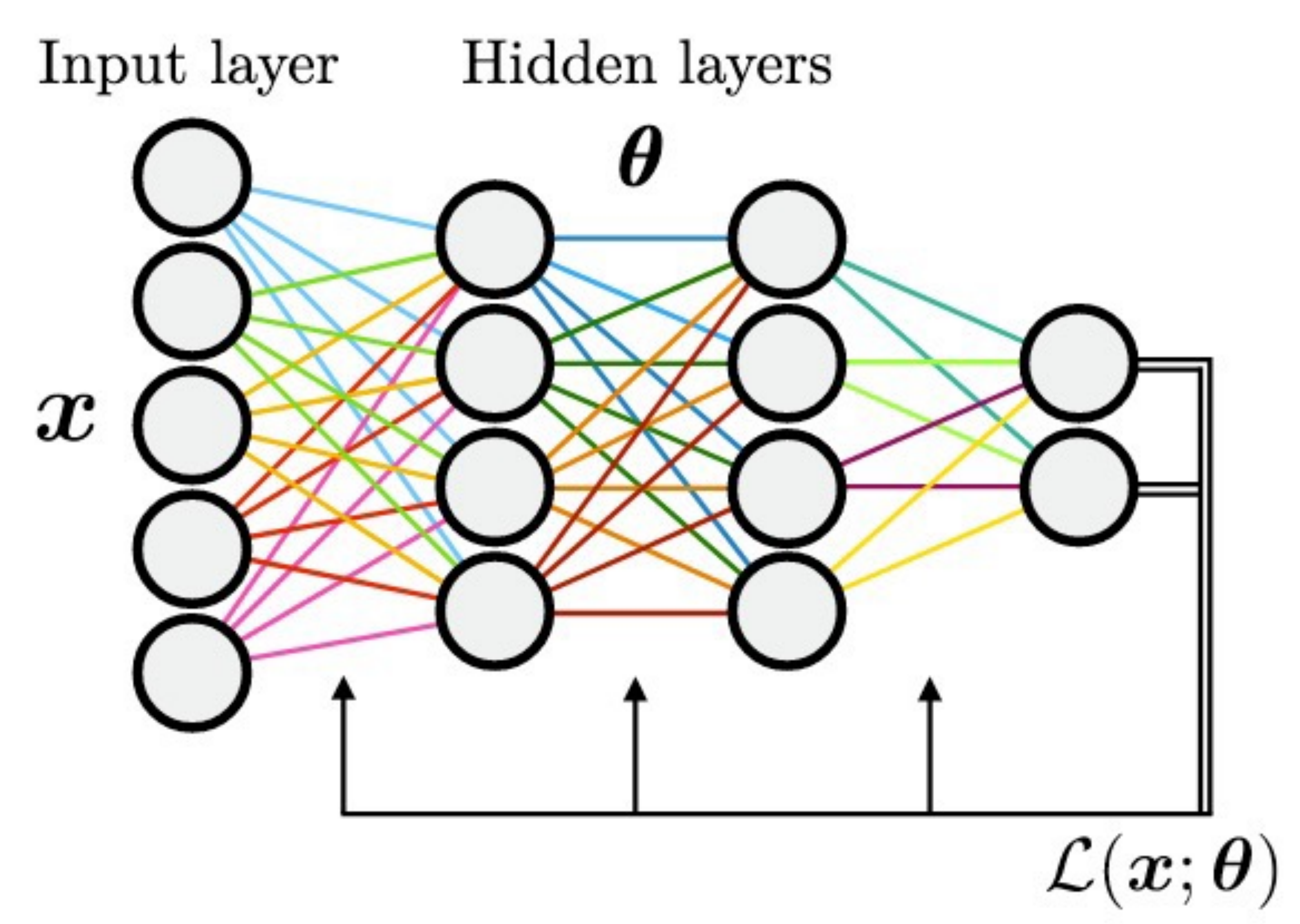
$$\Pr[\text{measure } |0\rangle] = |\langle 0| \Phi(x_j)^\dagger \Phi(x_i) |0\rangle)|^2$$

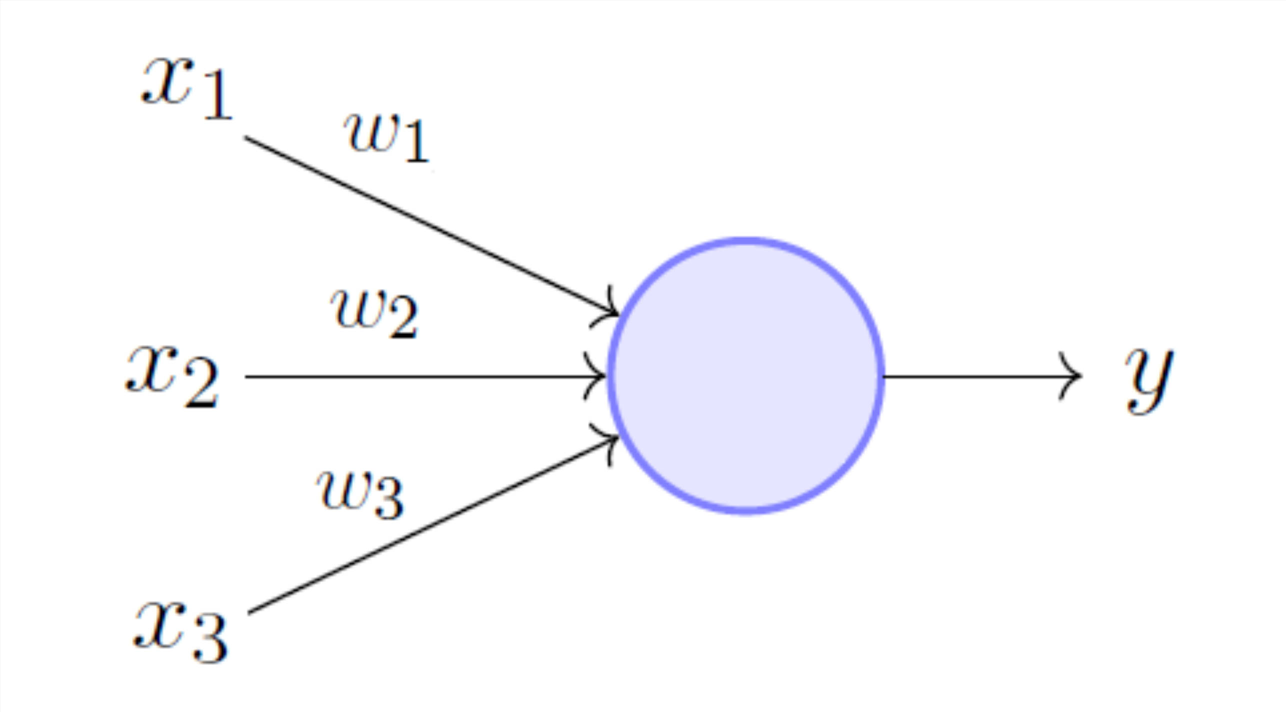
For i,j in the training set:

- Prepare $\Phi(x_j)^\dagger \Phi(x_i) |0\rangle$
- Let $K_{i,j} = \Pr[\text{measure } |0\rangle]$
- Plug $K_{i,j}$ into the dual form and solve
- Return $\{\alpha_i\}$
- Label $\text{label}(s) = \text{sign}\left(\sum_i \alpha_i K(x_i, s) + b\right)$

# Quantum neural networks

# Classical feed-forward neural networks



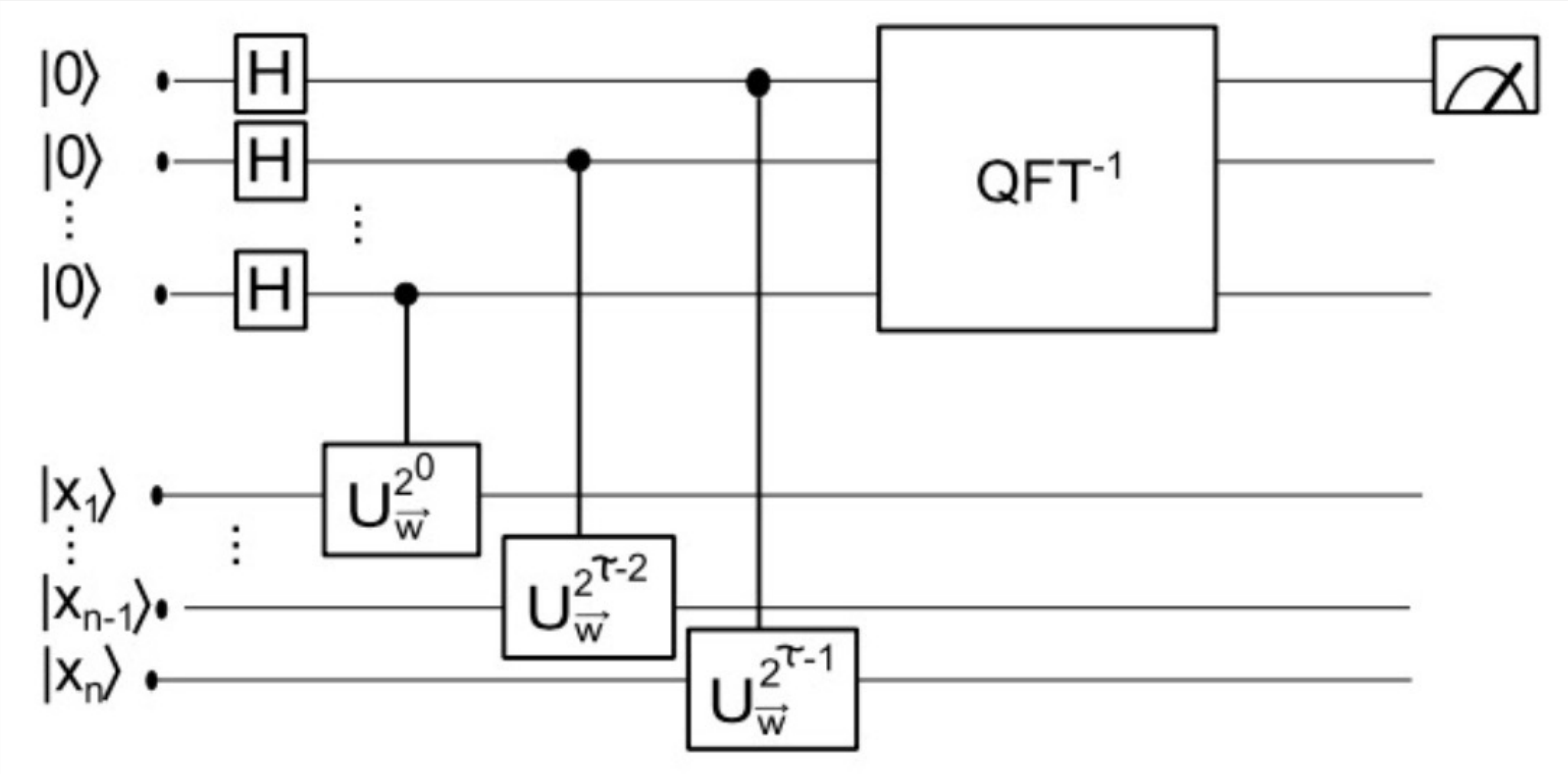

perceptron

$$f(\vec{x}) = \sigma(\vec{w} \cdot \vec{x} + b)$$

non-linear activation function

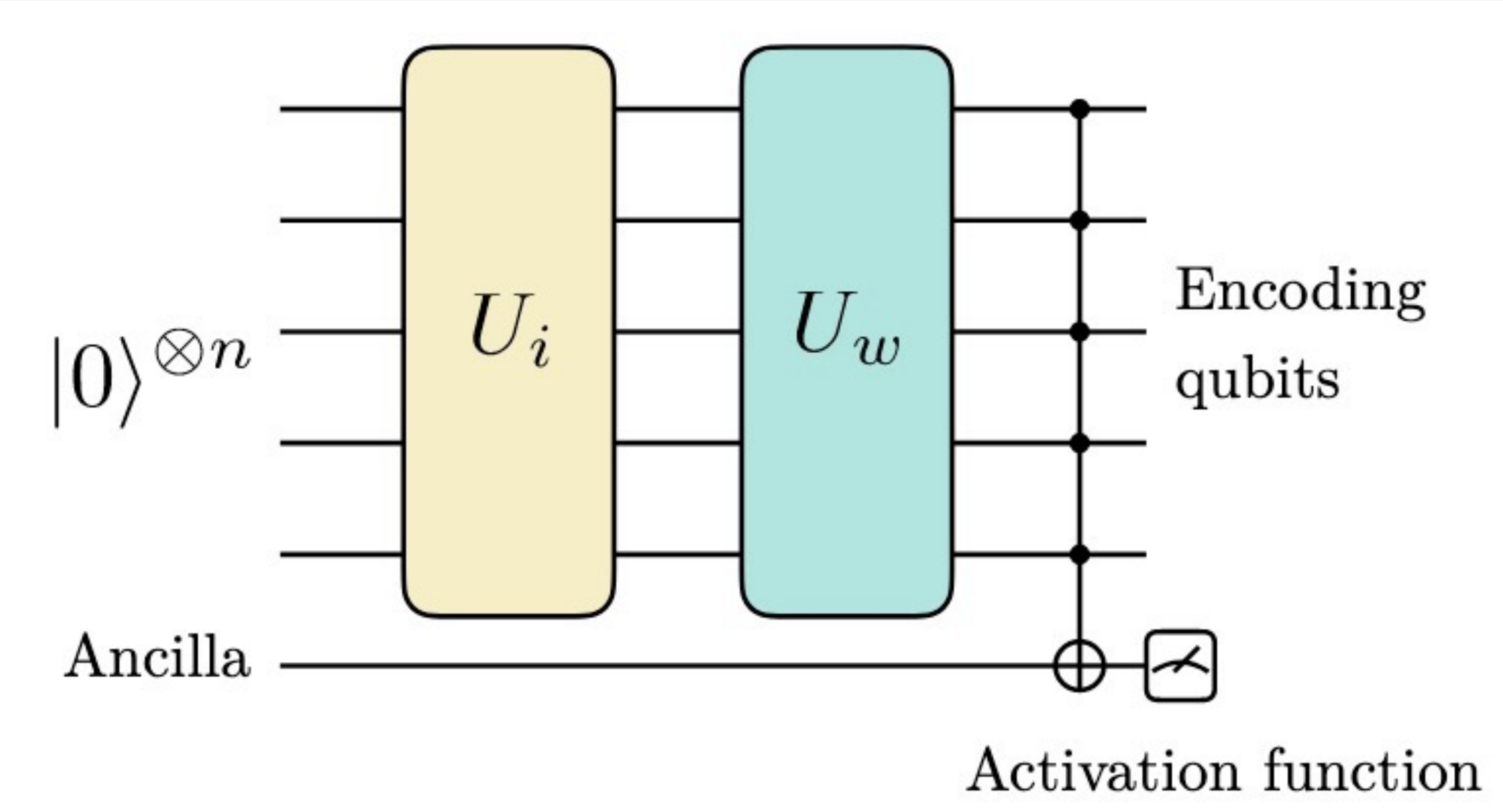
# Quantum perceptron

Need to implement non-linearity with quantum circuits




## QFT based perceptron

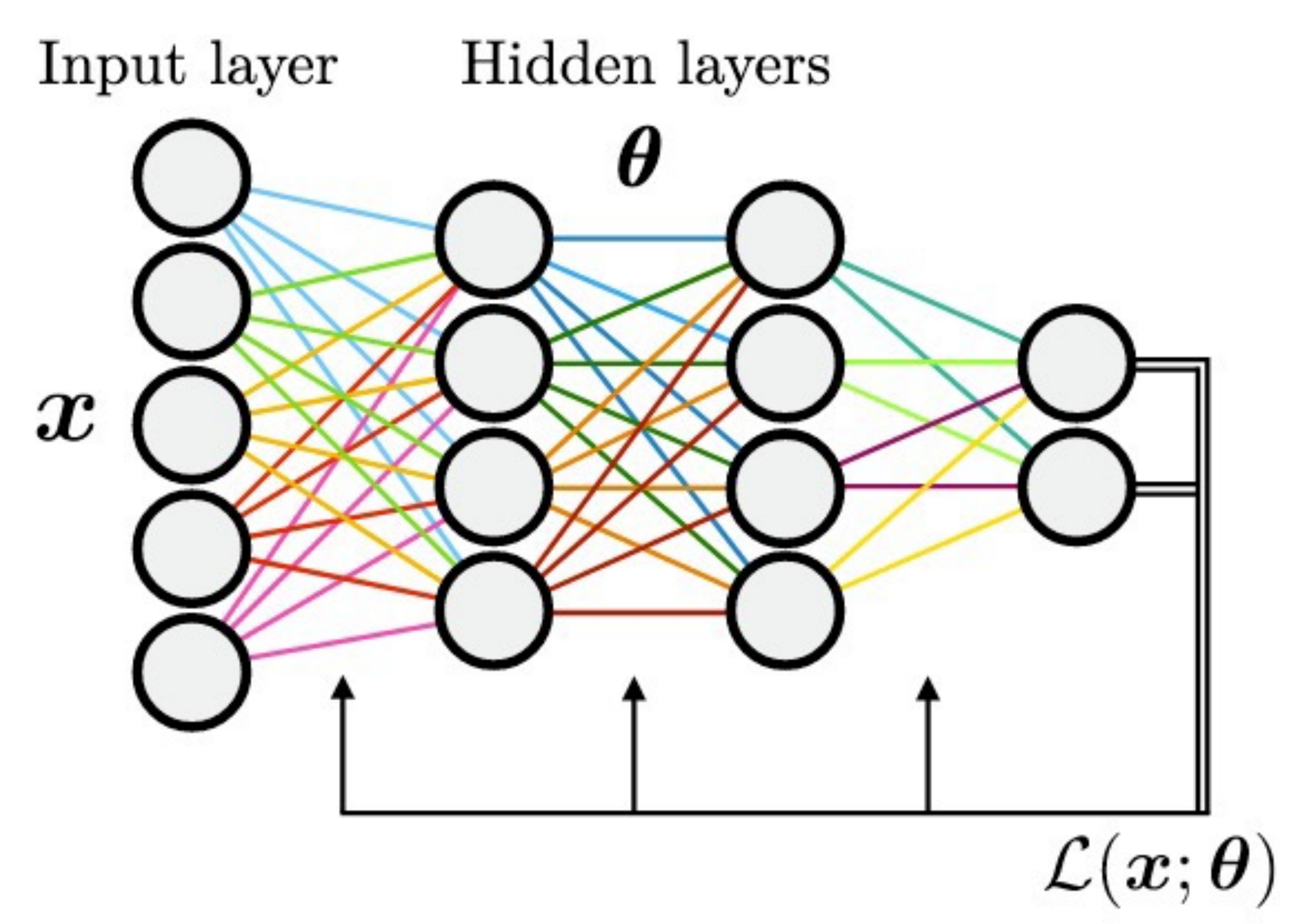
M. Schuld et al., Phys. Lett. A 379, 660 (2015)



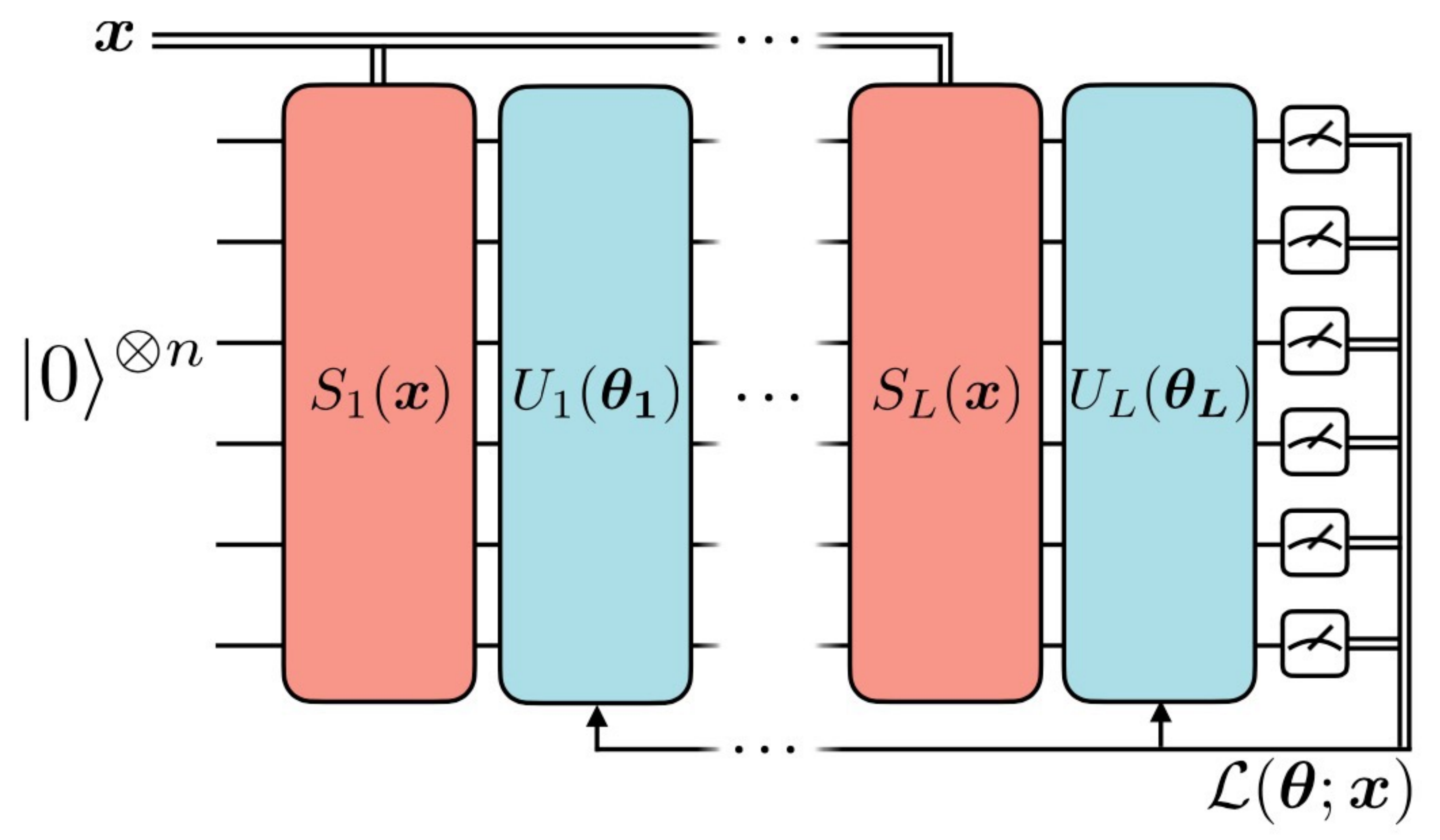

## Non-linearity from measurement

F. Tacchino et al., npj Quantum Inf. 5, 26 (2019)

# Quantum neural networks




classical feed-forward neural network



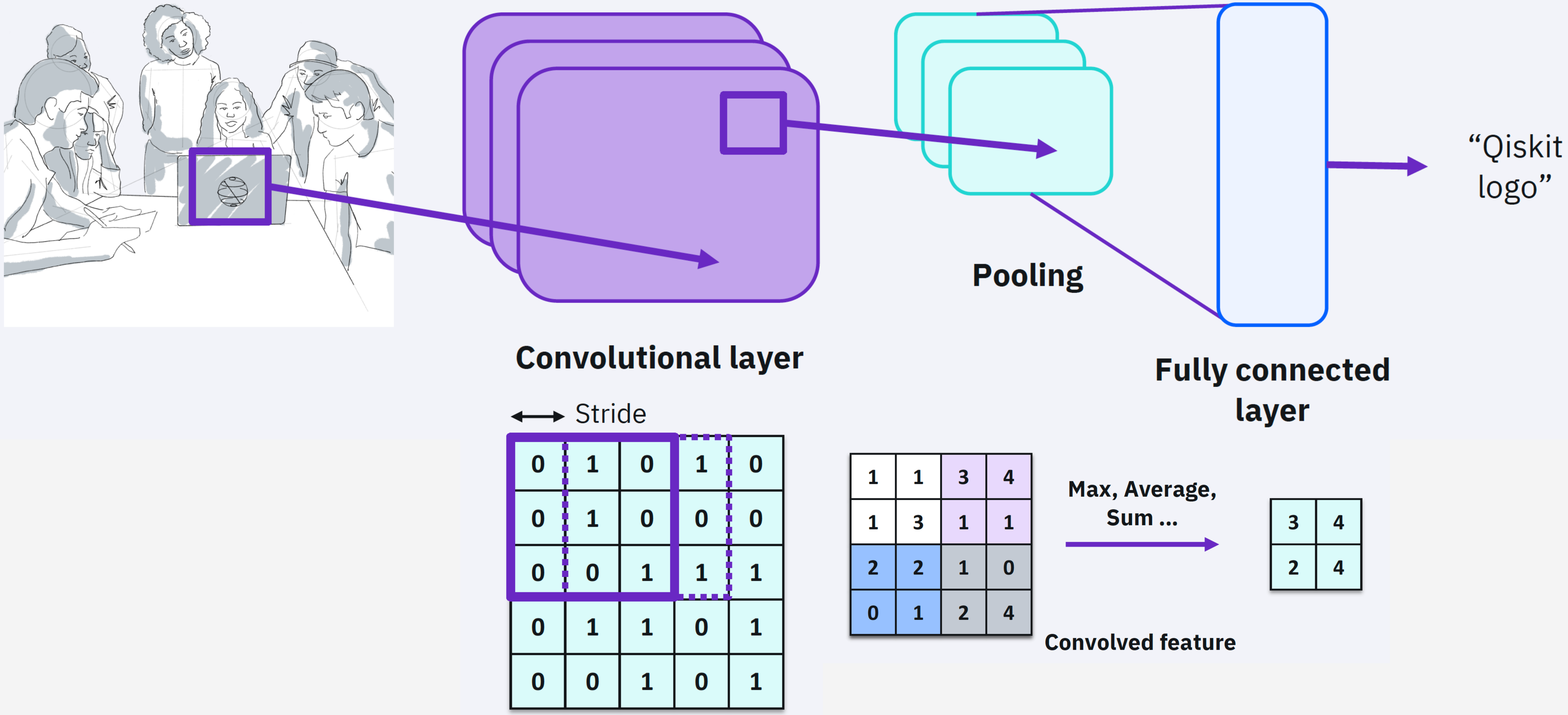

quantum neural networks

**difference:** data reuploading

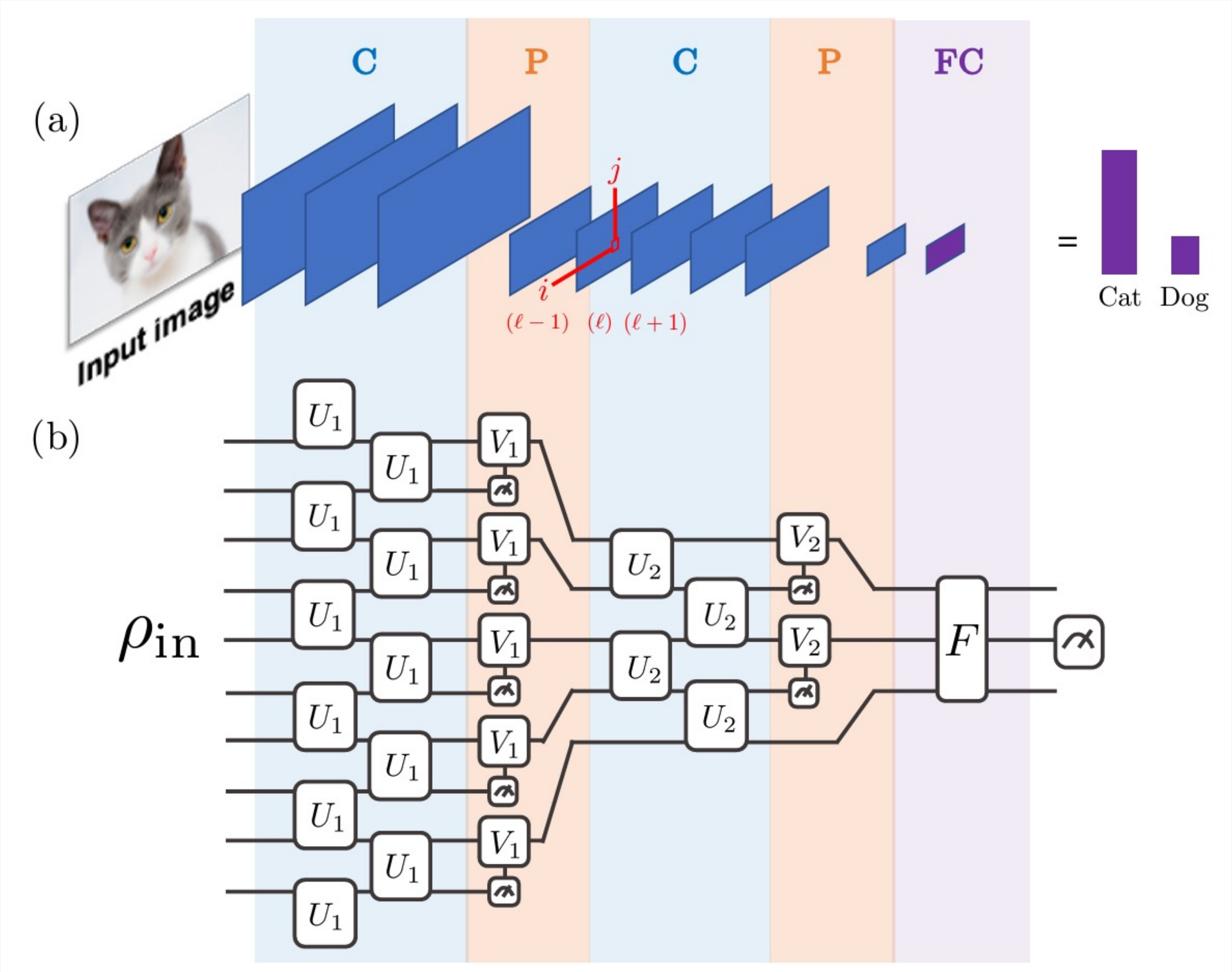
universal function approximators

Pérez-Salinas, Adrián, et al. "Data re-uploading for a universal quantum classifier." Quantum 4 (2020): 226.

# Convolutional neural networks (CNNs)



# Quantum convolutional neural networks (QCNNs)




Properties:

- QCNNs have *O(logN)* layers and parameters
- They don't suffer from the problem of barren plateaus

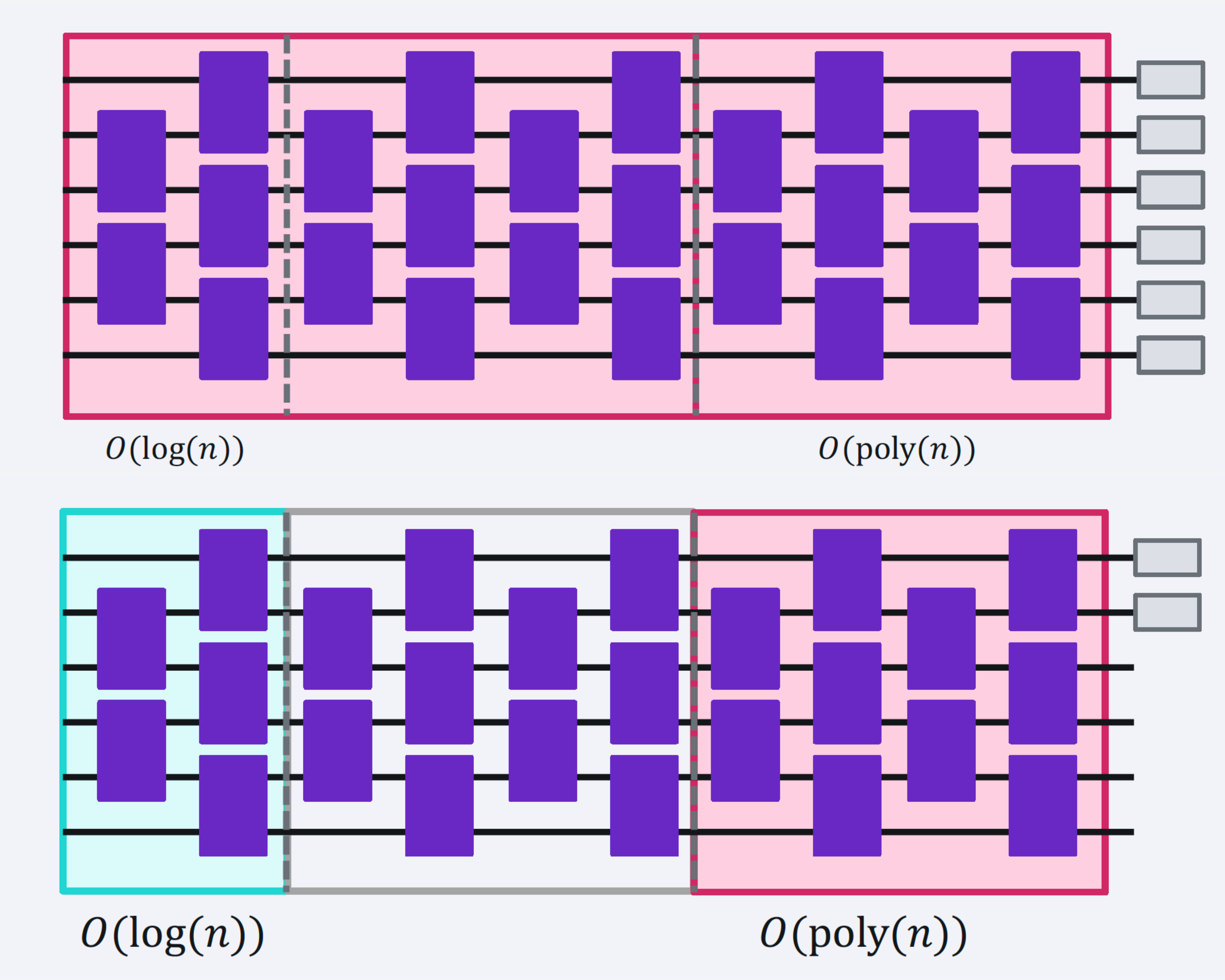
Pesah, Arthur, et al. "Absence of barren plateaus in quantum convolutional neural networks." Physical Review X 11.4 (2021): 041011.

Cong, Iris, Soonwon Choi, and Mikhail D. Lukin. "Quantum convolutional neural networks." Nature Physics 15.12 (2019): 1273-1278.

# Barren plateaus

Random initialization of parameters in deep circuits:

**Gradients** of the cost function **vanish** exponentially with the number of qubits




Mitigating barren plateaus:

Initialization strategies

For an alternating layered ansatz:

shallow circuits

local cost functions


McClean, Jarrod R., et al. "Barren plateaus in quantum neural network training landscapes." Nature communications 9.1 (2018): 4812
Cerezo, Marco, et al. "Cost function dependent barren plateaus in shallow parametrized quantum circuits." Nature communications 12.1 (2021): 1791..

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