Quantum Autoencoder for MNIST classification

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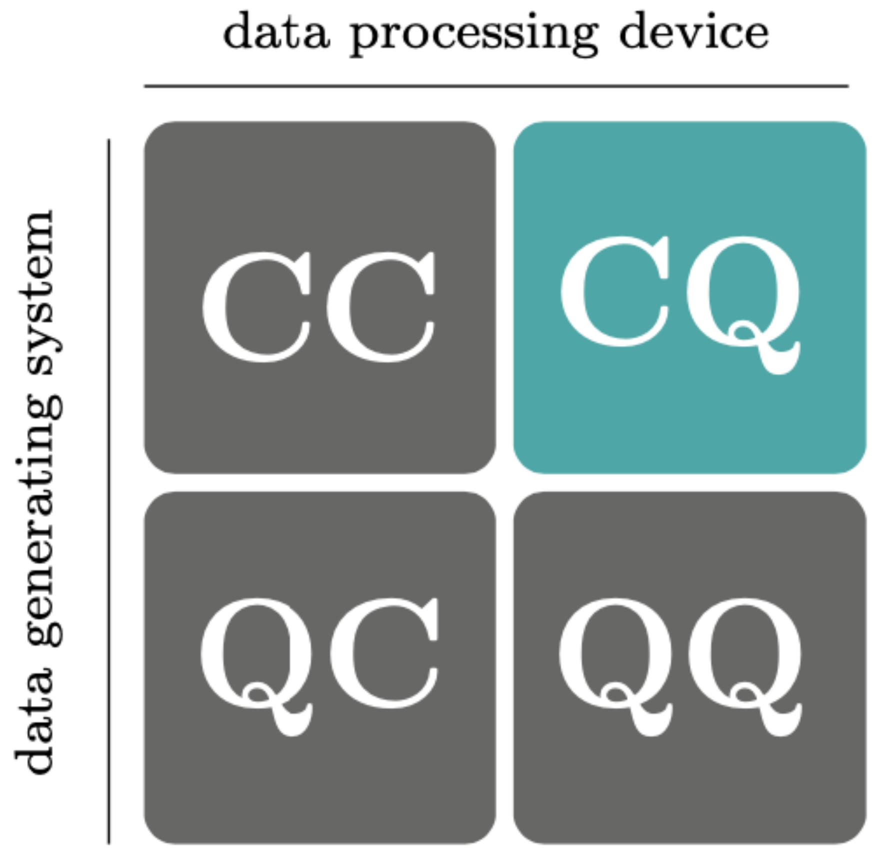
Quantum Machine Learning

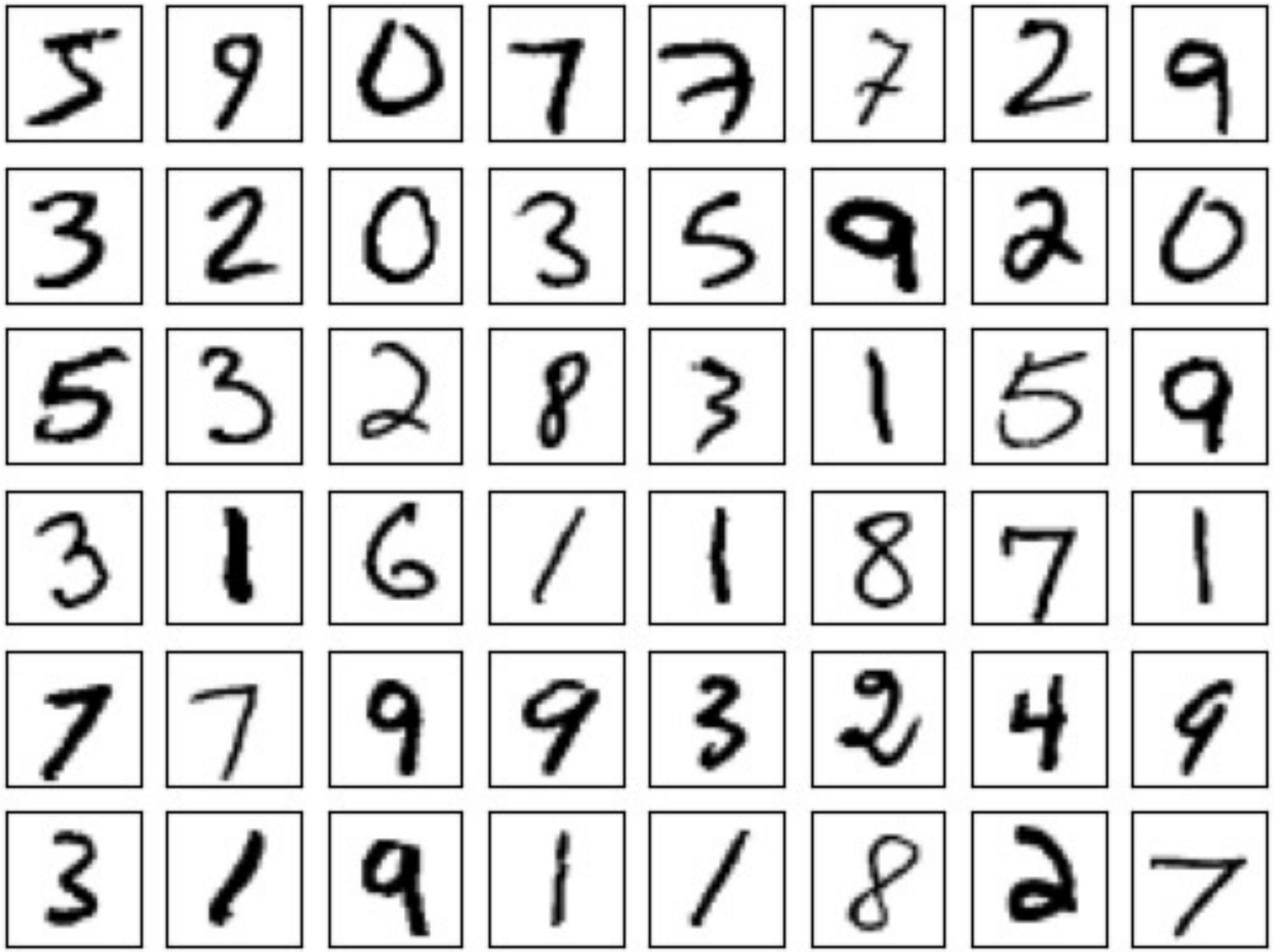
- **ML** ⟶ making computers learn from data how to solve problems
- **QC** ⟶ information processing with devices based on QM



The **Project**:

1. MNIST database
2. PCA reduction
3. Quantum Autoencoder
4. Random Forest Classifier

MNIST database

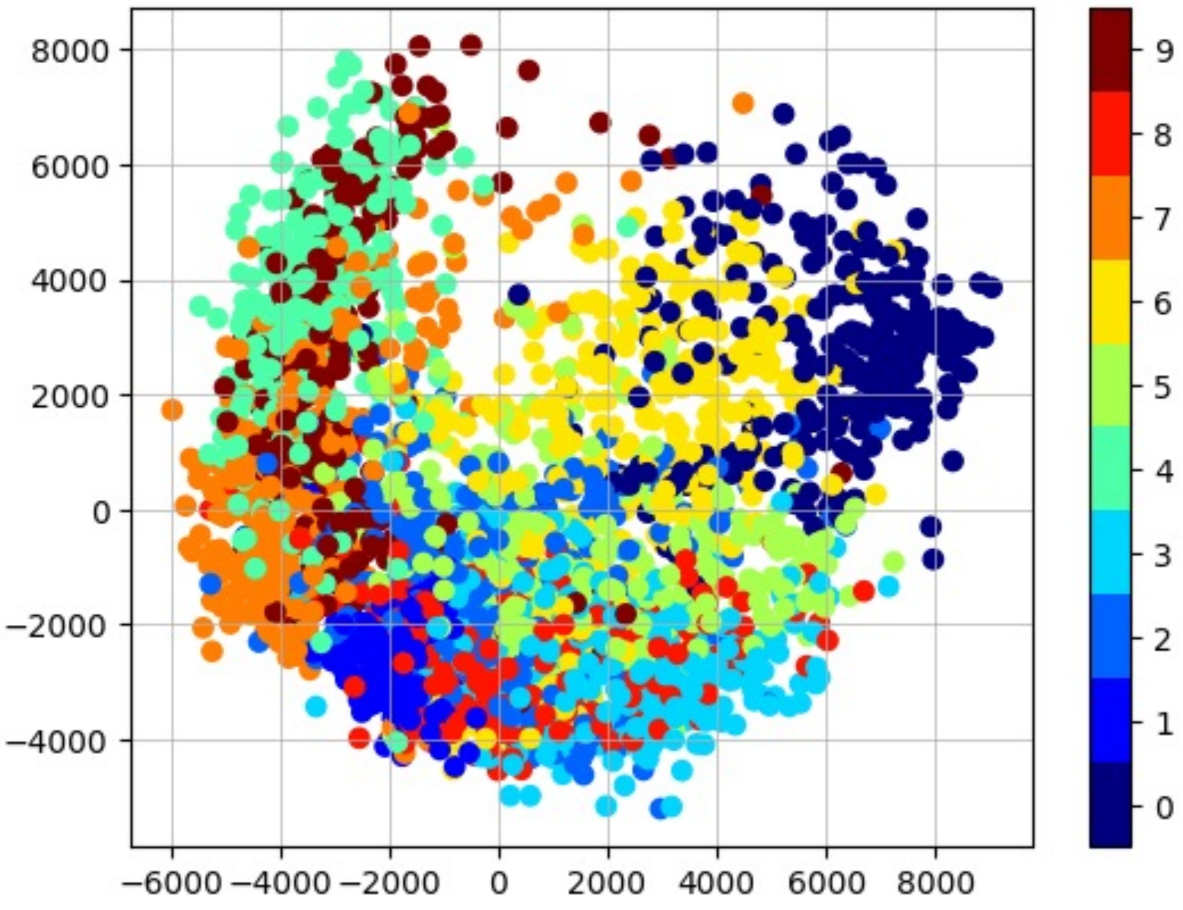


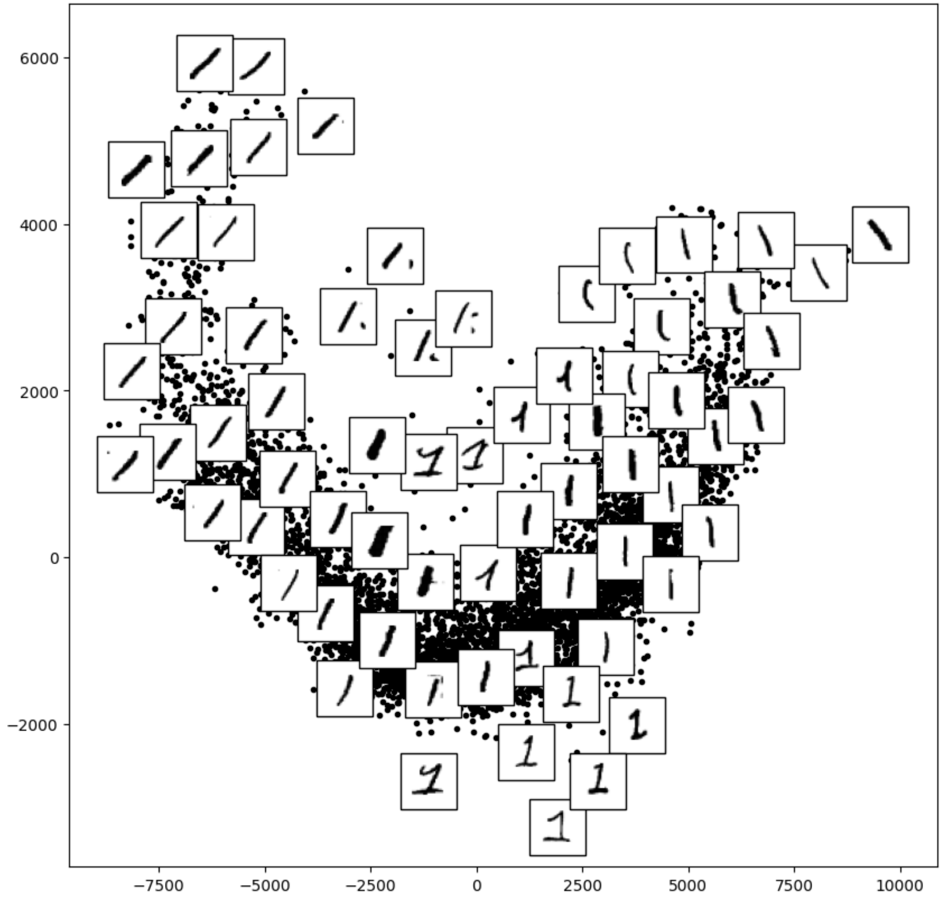
- 70.000 handwritten digits
- 10 classes
- Images 28×28 pixels

$\Longrightarrow$ **784 features**

Isomap

784-D parameter space → Projection to 2-D parameter space





Principal Component Analysis (PCA)

Pixel basis $\longrightarrow$ $\text{image}(x) = x_1 \cdot \text{pixel } 1 + x_2 \cdot \text{pixel } 2 + \cdots + x_{784} \cdot \text{pixel } 784$

PCA basis $\longrightarrow$ $\text{image}(x) = \text{mean} + x_1 \cdot \text{basis } 1 + x_2 \cdot \text{basis } 2 + \cdots + x_{784} \cdot \text{basis } 784$

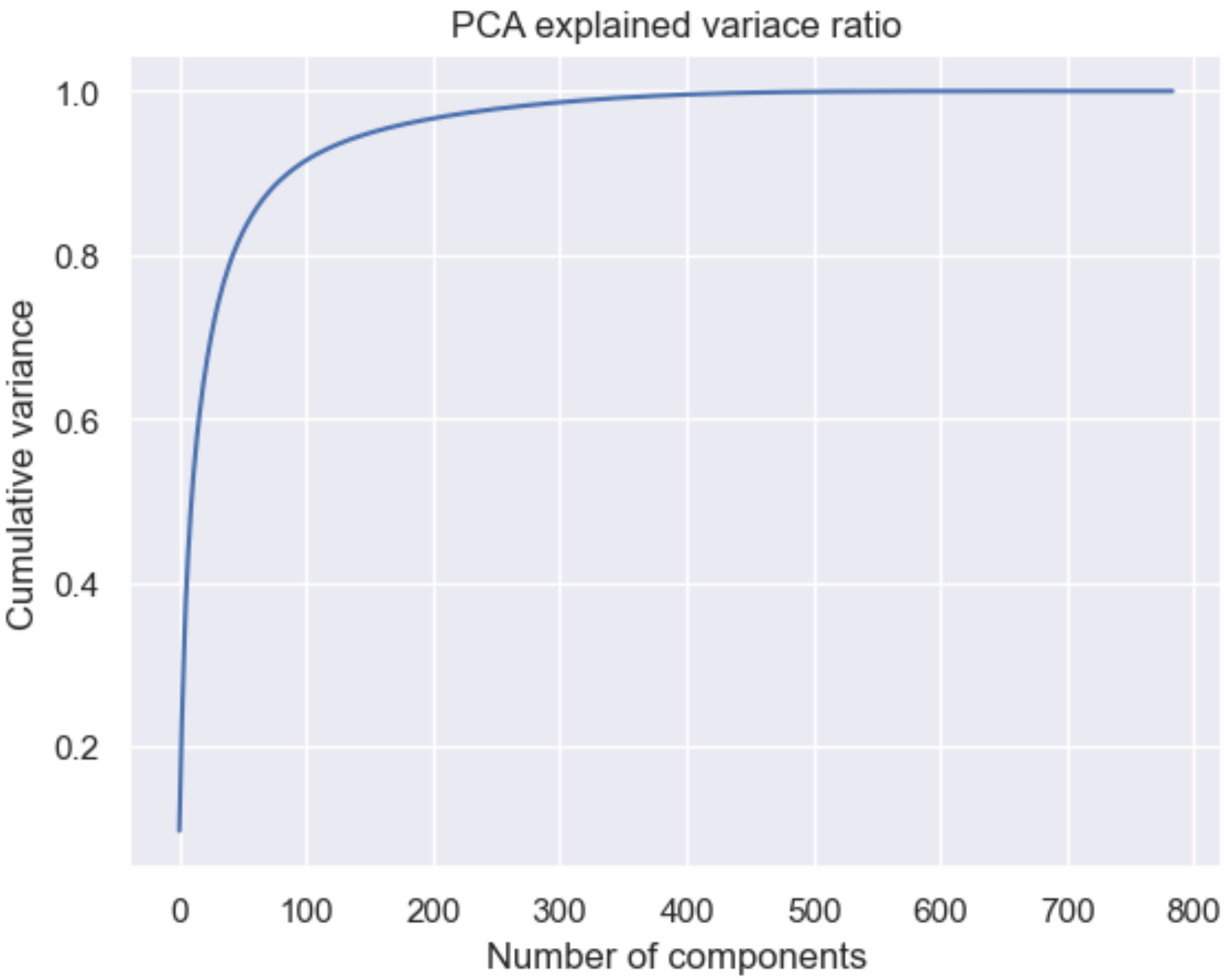
1. **Covariance matrix**: $\begin{bmatrix} Cov(x_1, x_1) & \cdots & Cov(x_1, x_{784}) \\ \vdots & \ddots & \vdots \\ Cov(x_{784}, x_1) & \cdots & Cov(x_{784}, x_{784}) \end{bmatrix}$

2. **Diagonalization:**

Eigenvectors — Direction where there is the most variance (Principal Components)

Eigenvalues λ_i — Amount of variance carried in each direction

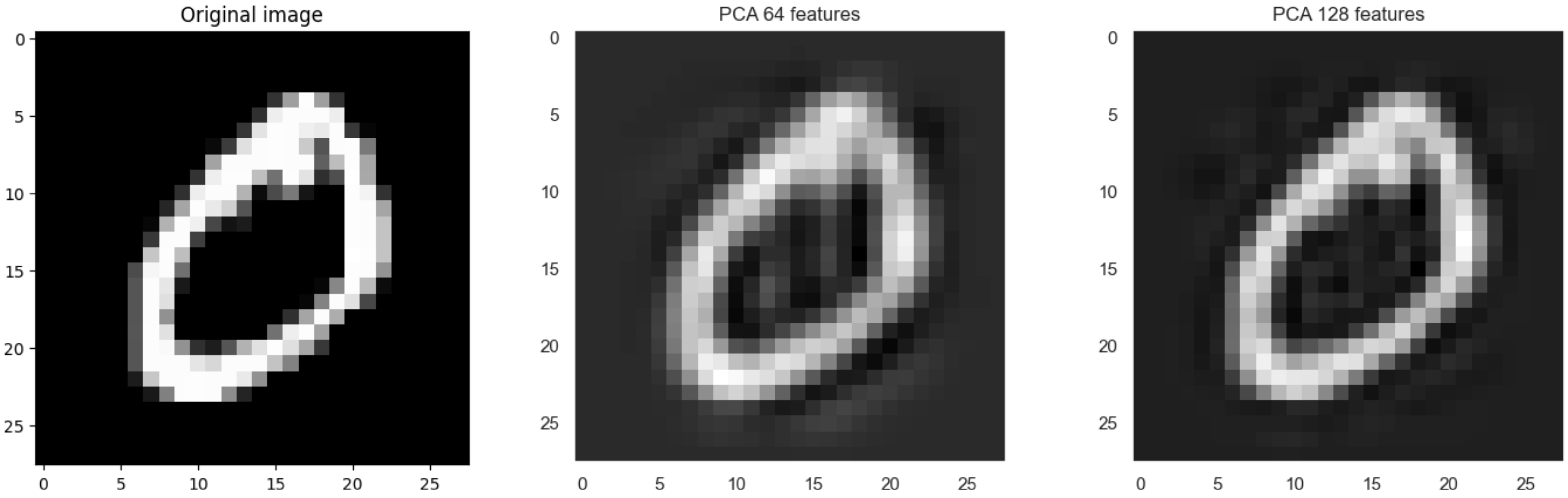
PCA explained variance ratio



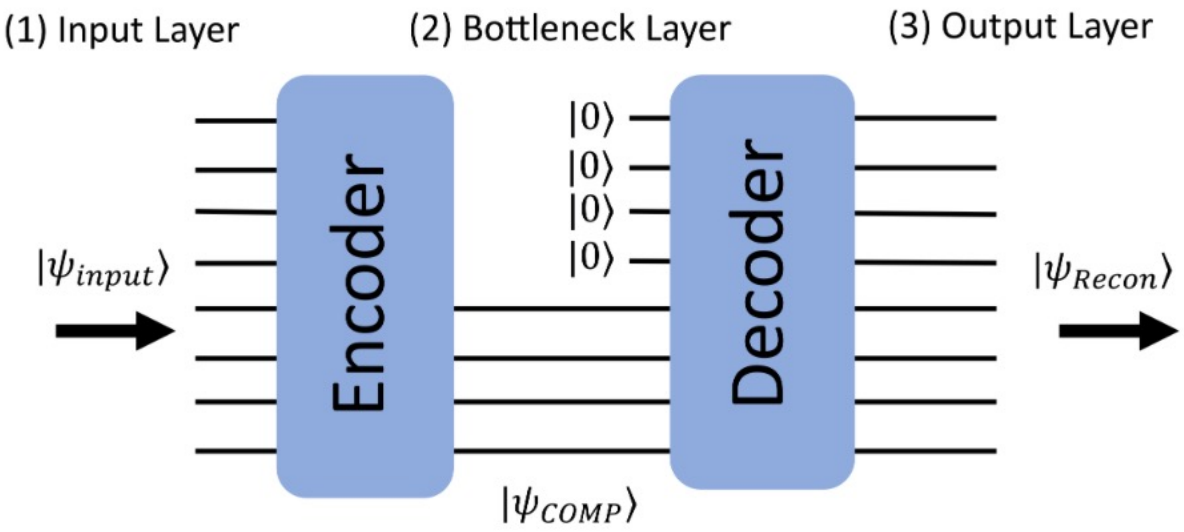
$$\text{exp. var. ratio} = \frac{\sum_1^N \lambda_i}{\sum_1^{784} \lambda_i}$$

Choose $N = 64$

PCA reconstruction



Autoencoder



$|\psi_{input}\rangle = n + k\ qubits$

$|\psi_{COMP}\rangle = n\ qubits$

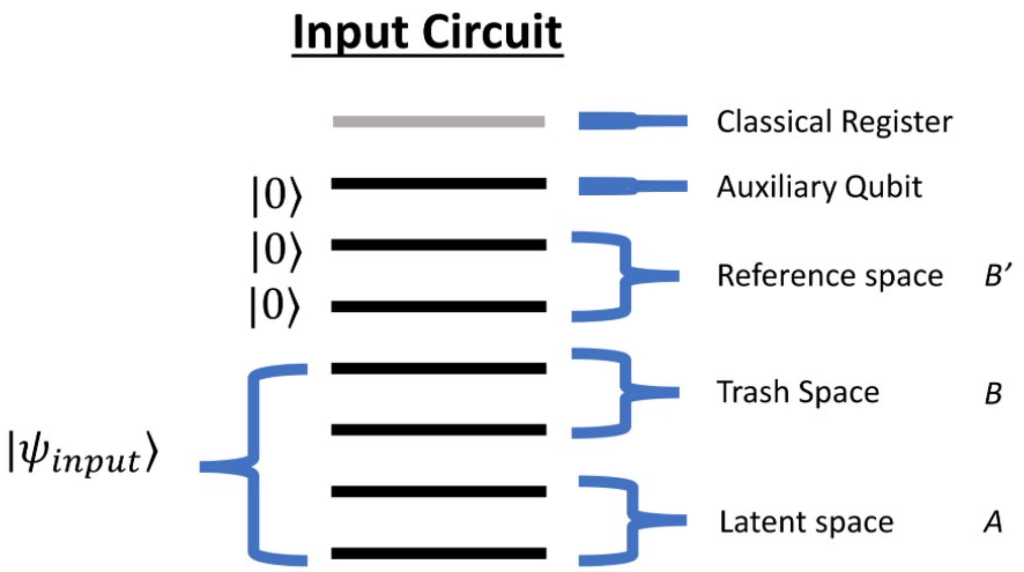
$|\psi_{Recon}\rangle = n + k\ qubits$

Encoder function $\boldsymbol{h} = f(\boldsymbol{x})$

Decoder function $\boldsymbol{r} = g(\boldsymbol{h})$

$g(f(\boldsymbol{x})) = \boldsymbol{x}$ not so useful $\Rightarrow$ learn useful properties of the dataset

Quantum Autoencoder in Qiskit



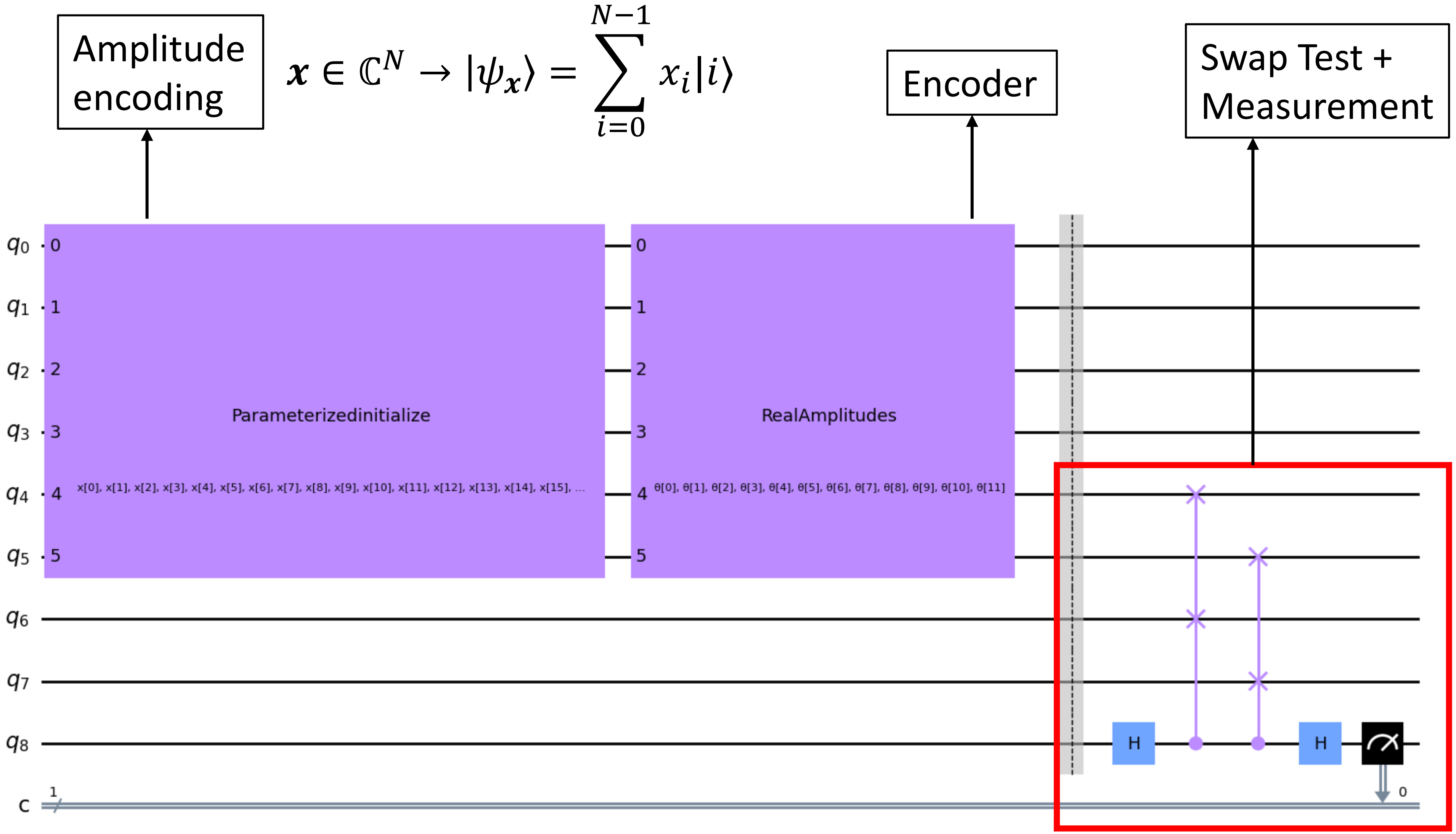
The "**algorithm**":

1. Amplitude encoding $\rightarrow |\psi\rangle_{AB} \otimes |a\rangle_{B'}$
2. Encoder $\rightarrow U(\theta)_{AB}\,(|\psi\rangle_{AB} \otimes |a\rangle_{B'})$
3. Swap test $\rightarrow V_{BB'}\, U(\theta)_{AB}\,(|\psi\rangle_{AB} \otimes |a\rangle_{B'})$
4. Cost function + optimization
5. Decoder $\rightarrow U^{\dagger}\,(\theta)_{AB'} V_{BB'} U(\theta)_{AB}\,(|\psi\rangle_{AB} \otimes |a\rangle_{B'}$

$$\rho_{out} = U^{\dagger}(\theta)_{AB'} Tr_B\big[V_{BB'} U(\theta)_{AB}[\psi_{AB} \otimes a_{B'}] U^{\dagger}(\theta)_{AB} V^{\dagger}_{BB'}\big] U(\theta)_{AB'}$$

Goal $\longrightarrow$ $\boxed{\max F(|\psi\rangle_{AB}, \rho_{out})}$ $\Longleftrightarrow$ $\boxed{\max F\big(Tr_A[U(\theta)_{AB}\psi_{AB}U^{\dagger}(\theta)_{AB}], a_{B'}\big)}$

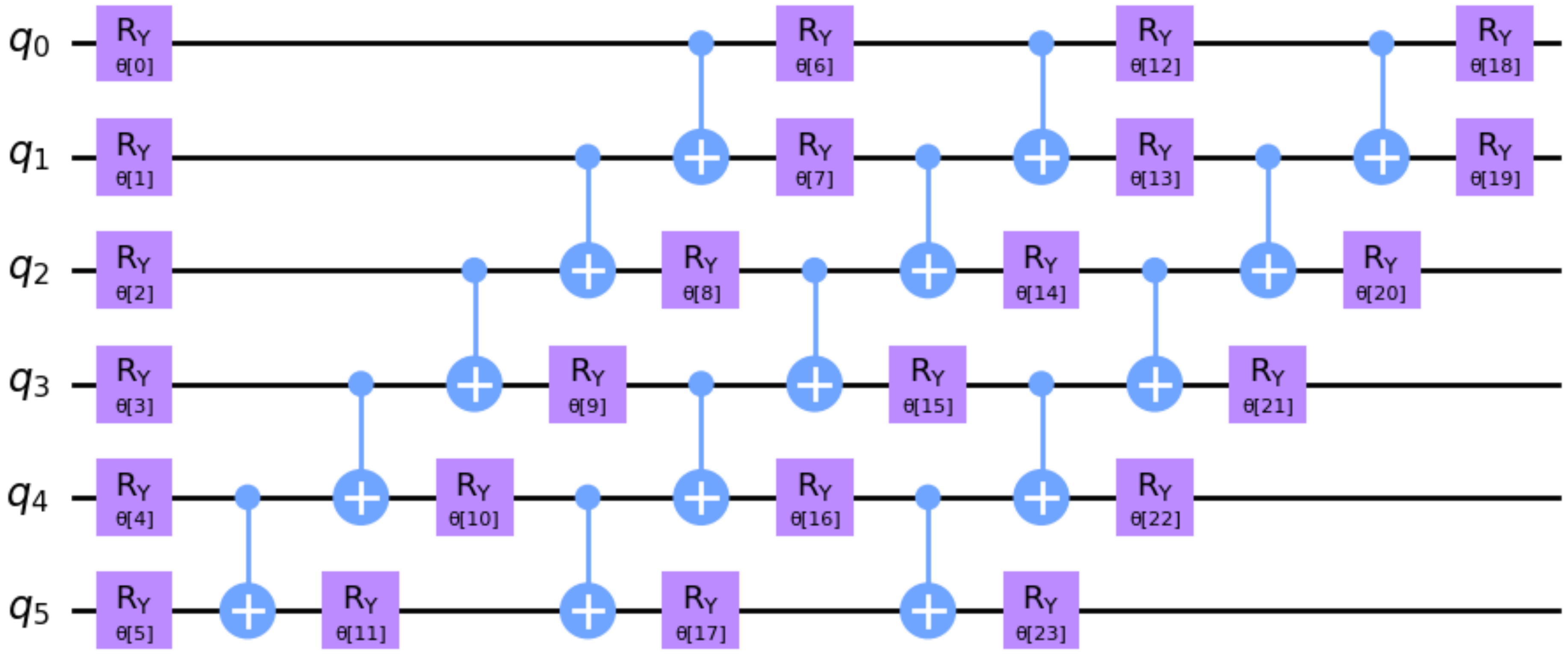
The circuit



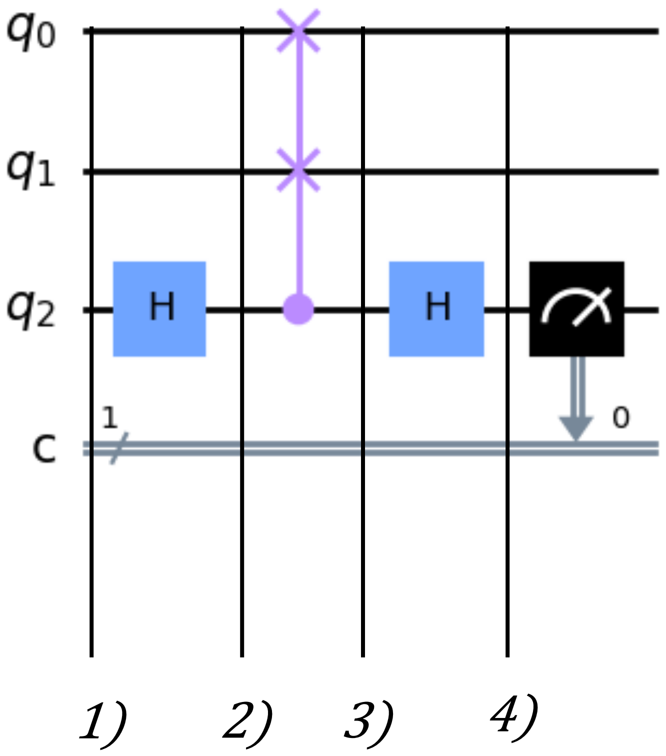
Amplitude encoding
$\boldsymbol{x} \in \mathbb{C}^N \to |\psi_{\boldsymbol{x}}\rangle = \sum_{i=0}^{N-1} x_i |i\rangle$
Encoder
Swap Test + Measurement
q_0
q_1
q_2
q_3
q_4
q_5
q_6
q_7
q_8
c
Parameterizedinitialize
x[0], x[1], x[2], x[3], x[4], x[5], x[6], x[7], x[8], x[9], x[10], x[11], x[12], x[13], x[14], x[15], ...
RealAmplitudes
θ[0], θ[1], θ[2], θ[3], θ[4], θ[5], θ[6], θ[7], θ[8], θ[9], θ[10], θ[11]
H
H

Encoder

- *RealAmplitudes* circuit → Layers of **Y** rotations + **C-X** entanglement
- Parameters → Trainable weights for QNN



Swap Test



1) $|\psi\rangle_1 = |a\rangle|b\rangle \otimes |0\rangle$

2) $|\psi\rangle_2 = |a\rangle|b\rangle \otimes \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle)$

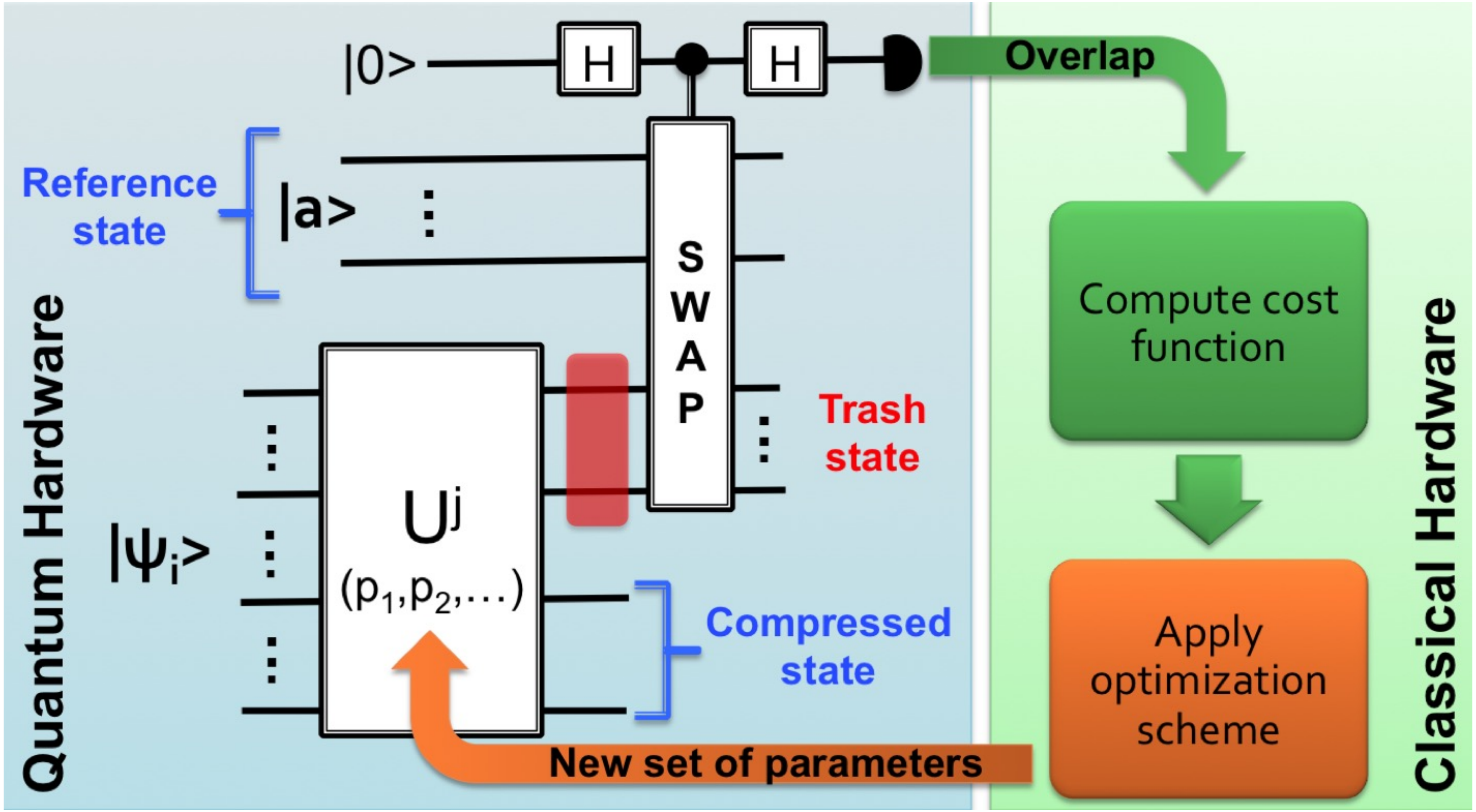
3) $|\psi\rangle_3 = \frac{1}{\sqrt{2}}(|a\rangle|b\rangle \otimes |0\rangle + |b\rangle|a\rangle \otimes |1\rangle)$

4) $|\psi\rangle_4 = \frac{1}{2}(|a\rangle|b\rangle + |b\rangle|a\rangle) \otimes |0\rangle + \frac{1}{2}(|a\rangle|b\rangle - |b\rangle|a\rangle) \otimes |1\rangle$

Measurement: $p(0) = |(\mathbb{I} \otimes \langle 0|)|\psi\rangle_4|^2 = \frac{1}{2} + \frac{1}{2}|\langle a|b\rangle|^2$

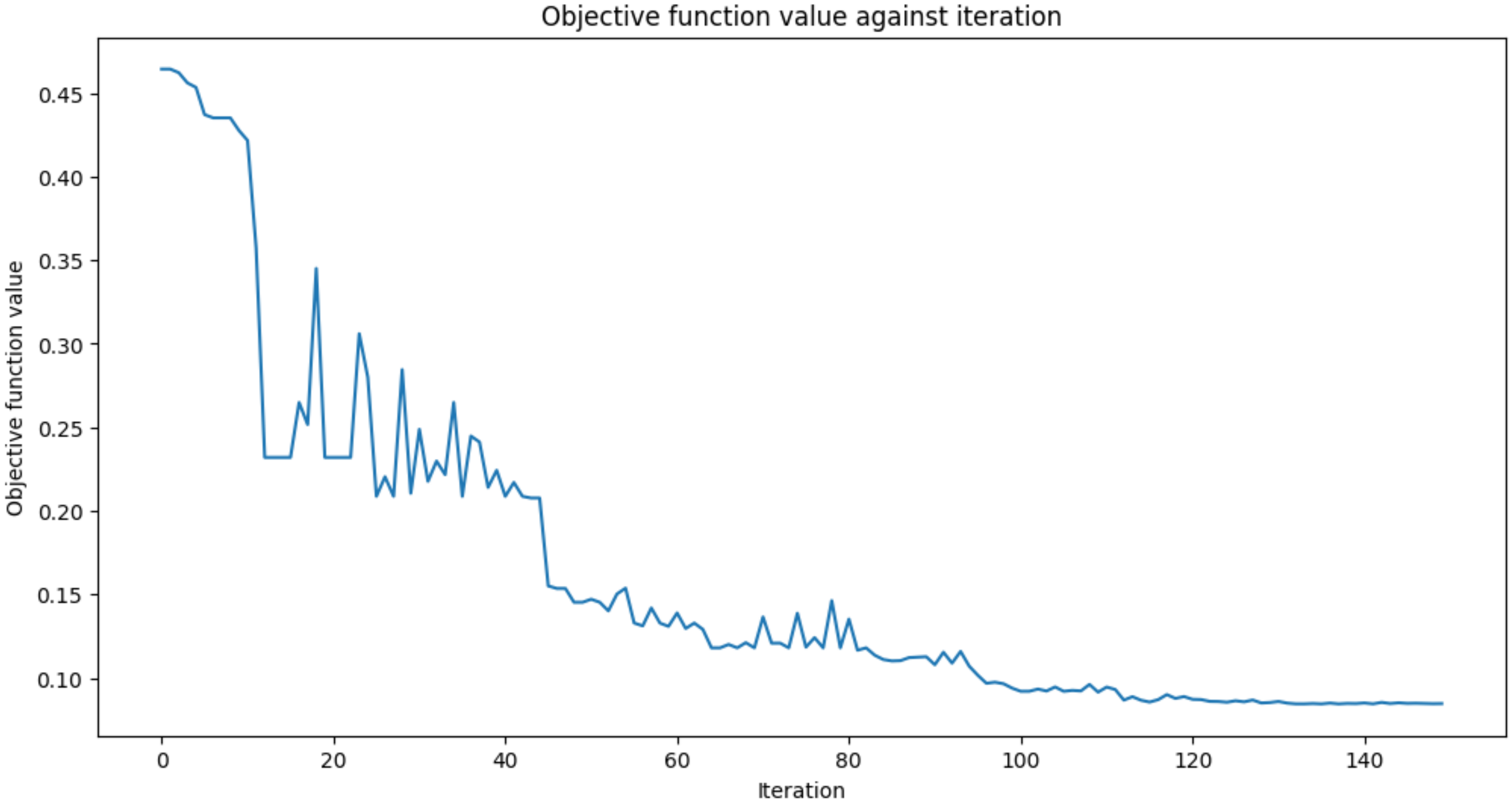
$\boxed{|\langle a|b\rangle|^2 = 2p(0) - 1 = 1 - 2p(1)}$ $\Rightarrow$ Cost function

Optimization Routine



Optimization Routine

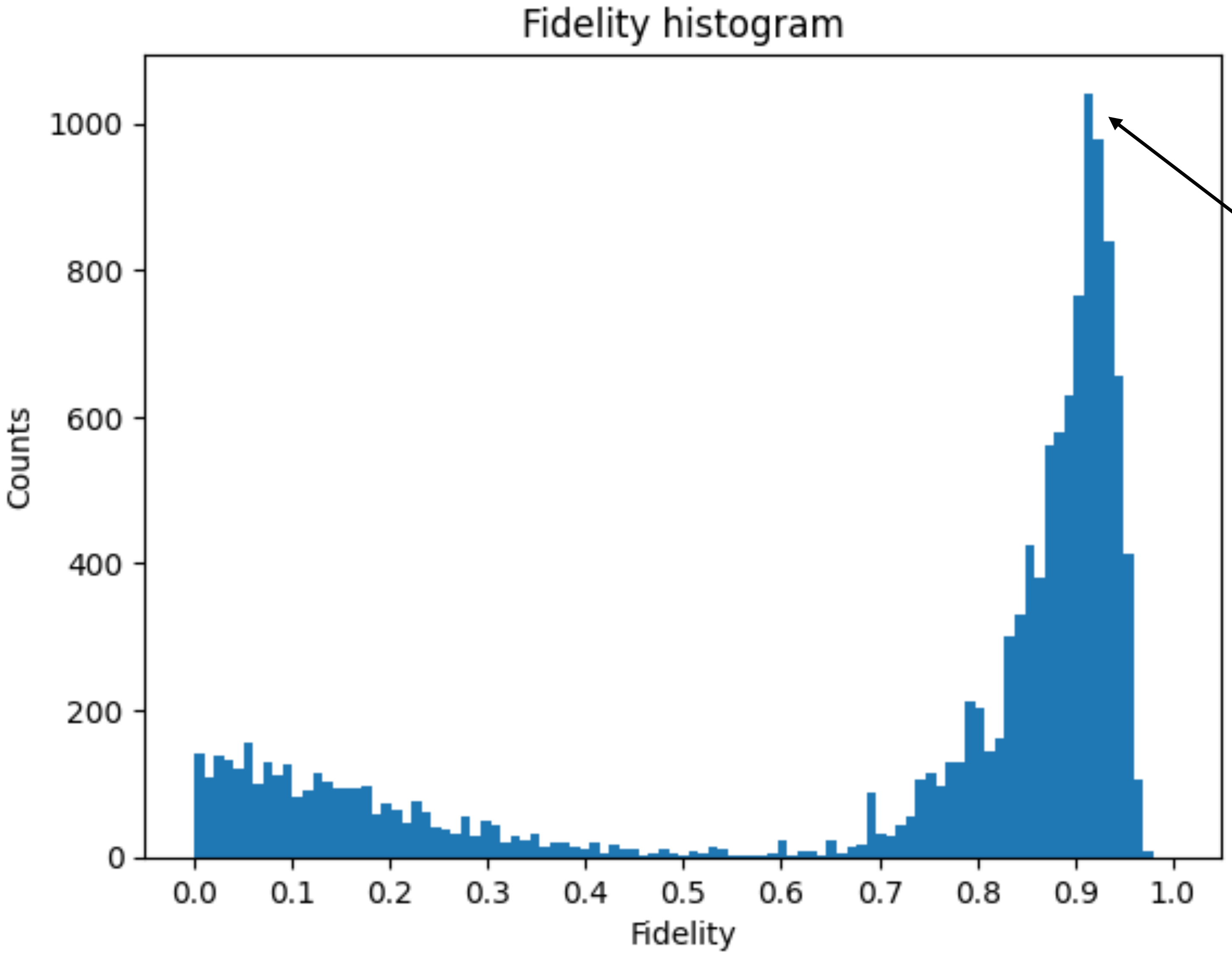
Time consuming $\Longrightarrow$ only $1/10$ of $0'$s and $1'$s $\begin{cases} \simeq 1200 \text{ train} \\ \simeq 250 \text{ test} \end{cases}$



Result:
Optimal parameters for $U(\theta)$

- RealAmplitudes, 3 repetitions
- Time $\simeq$ 40 min.

Fidelity

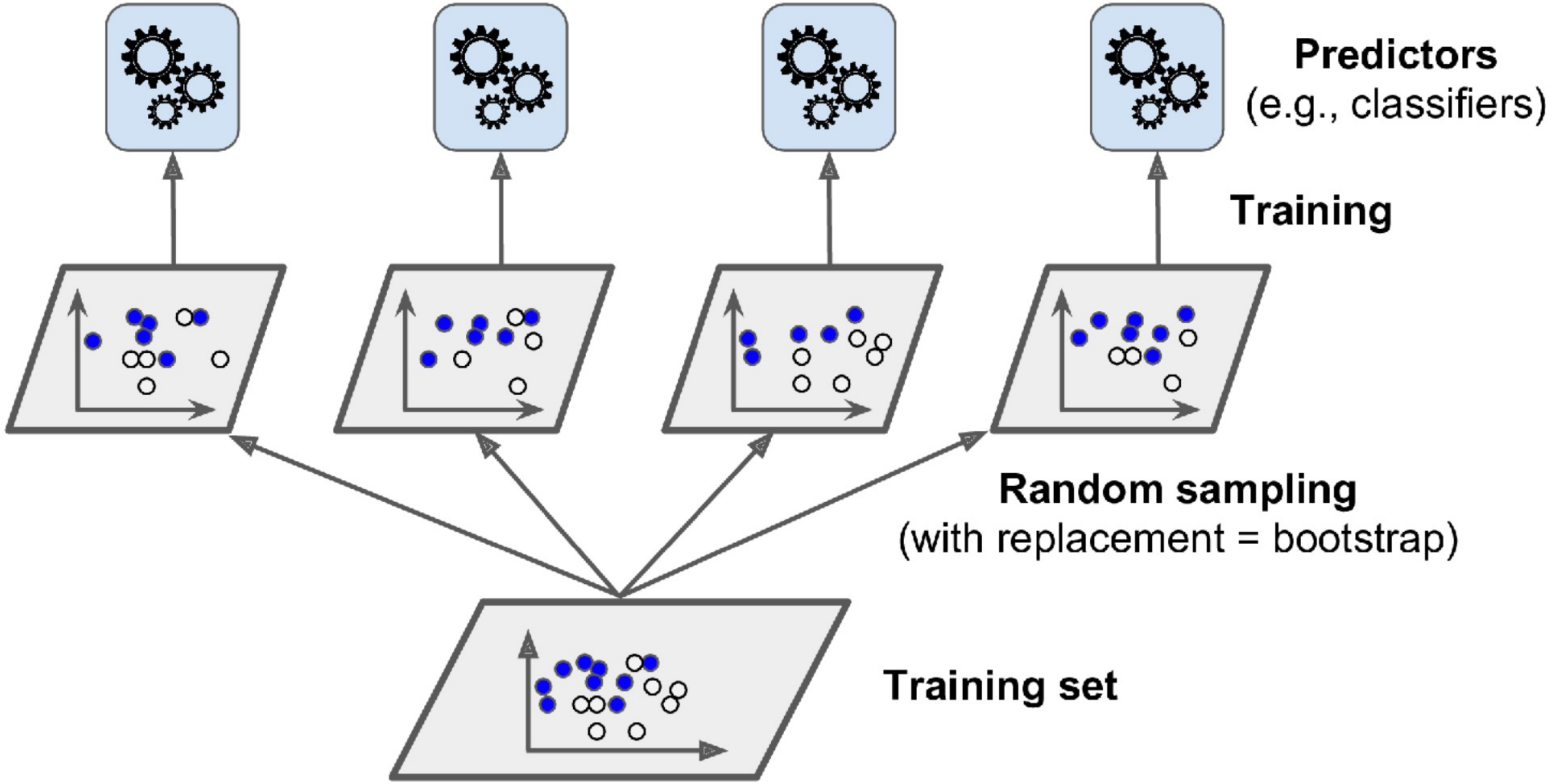


$$F = |\langle \psi_{decoder} | \psi_{initialized} \rangle|^2$$

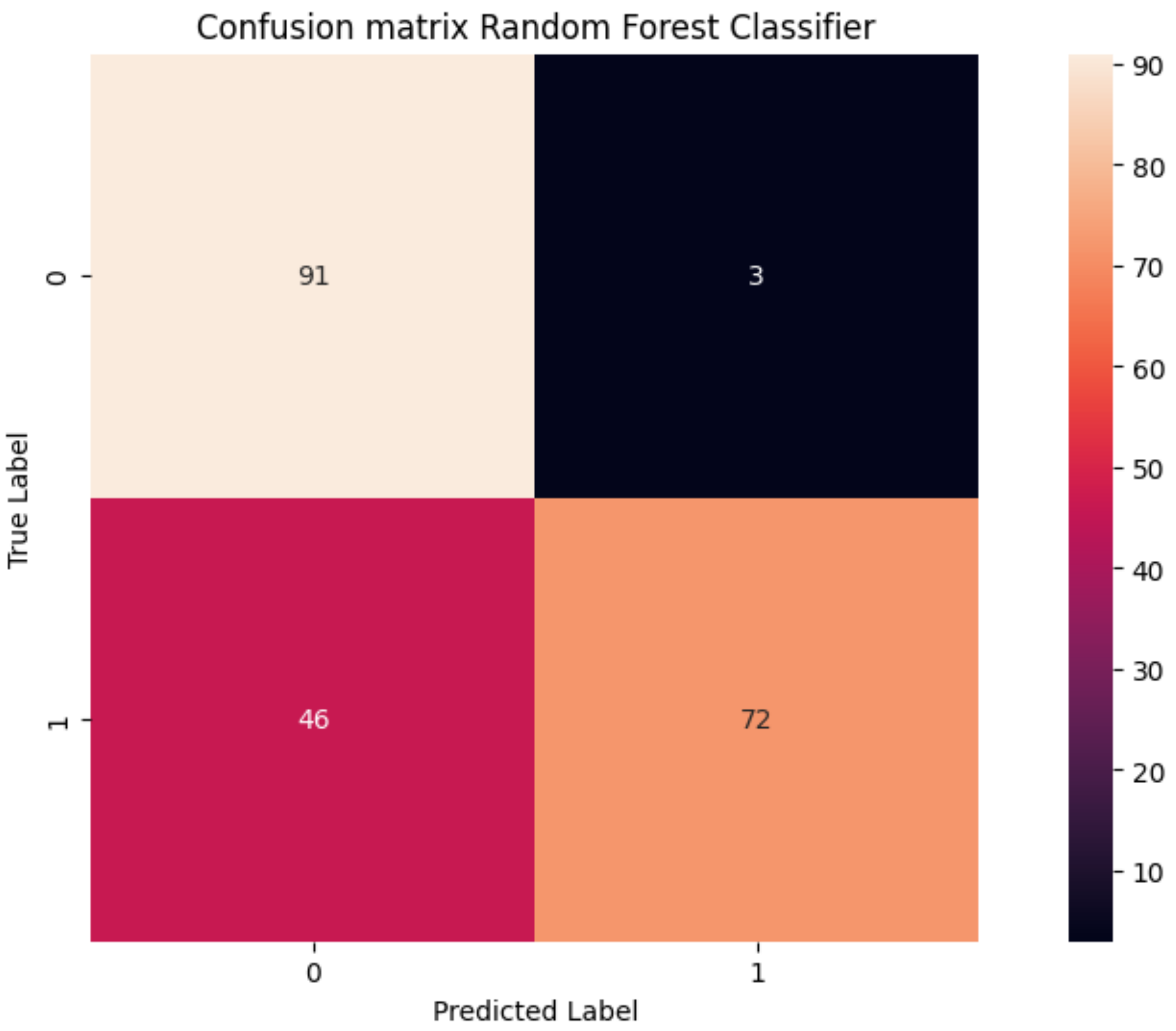
Peak at $F \simeq 0.9$

Random Forest Classifier

- *Ensemble learner* built on **decision trees**
- Decision tree ⟶ Binary splitting



Results 784 → 16 features



Class	Precision	Recall	f1-score	Support
0	0.66	0.97	0.79	94
1	0.96	0.61	0.75	118

Tp = True positive

Fp = False positive

Fn = False negative

$$\text{Precision} = \frac{\text{Tp}}{\text{Tp} + \text{Fp}} \qquad \text{Recall} = \frac{\text{Tp}}{\text{Tp} + \text{Fn}}$$

Results $784 \rightarrow 16$ features

RA, 1 rep

Class	Precision	Recall	f1-score	Support
0	0.69	0.93	0.79	94
1	0.92	0.66	0.77	118

RA, 2 rep

Class	Precision	Recall	f1-score	Support
0	0.73	0.94	0.82	94
1	0.93	0.72	0.81	118

PCA

Class	Precision	Recall	f1-score	Support
0	1.00	1.00	1.00	94
1	1.00	1.00	1.00	118

References

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2. Deep Learning, Ian Goodfellow and Yoshua Bengio and Aaron Courville, MIT Press, 2016.
3. Romero, Jonathan, Jonathan P. Olson, and Alan Aspuru-Guzik. “Quantum autoencoders for efficient compression of quantum data.” Quantum Science and Technology 2.4 (2017): 045001.
4. Qiskit Textbook Machine Learning, https://qiskit-community.github.io/qiskit-machine-learning/tutorials/12_quantum_autoencoder.html