University of Stuttgart
Institute for Computational Physics

SimTech

Topical Meeting – Machine Learning

Daniel Fink

Overview:

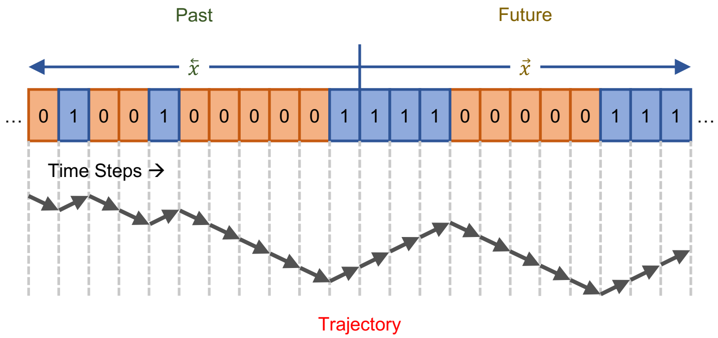
Simulating Stochastic Processes with Quantum Devices

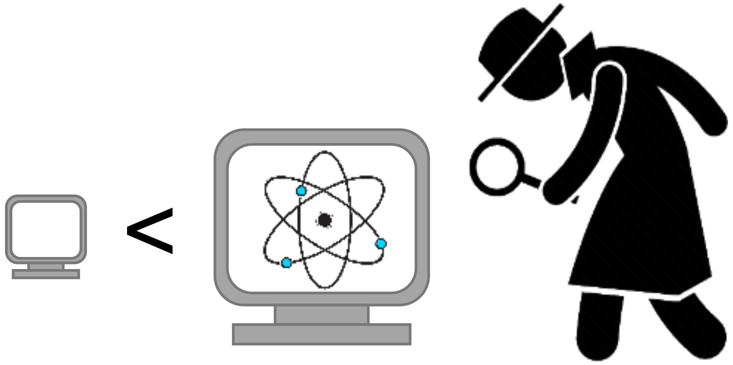
Part II

June 1st, 2022

Agenda

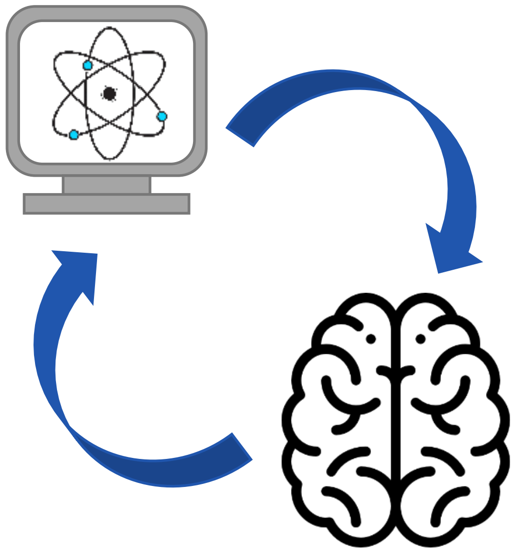
- Last time:
  - Simulation of stochastic processes
  - Why quantum computing is relevant there





Agenda

- Last time:
  - Simulation of stochastic processes
  - Why quantum computing is relevant there
- Today:
  - What is the connection to machine learning?



Agenda

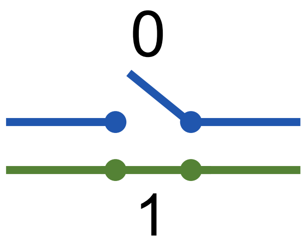
- Part 1: Qubits
- Part 2: Quantum Circuits
- Part 3: Example
- Part 4: Parameterized Quantum Circuits (PQCs)
- Part 5: Issues and open questions

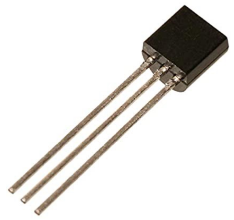
Part 1:
Qubits

Qubits

Bit

logical





physical

notation

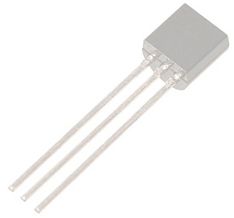
$$
\begin{aligned}
000 &\rightarrow 0\\
001 &\rightarrow 1\\
010 &\rightarrow 2\\
011 &\rightarrow 3
\end{aligned}
$$

...

Qubits

Bit

logical



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Qubit

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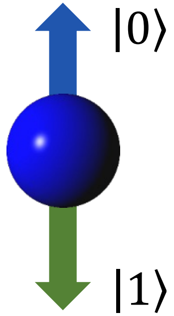

$^{171}Yb^{+1}$ γ e … physical

notation

$|000\rangle \rightarrow |0\rangle$
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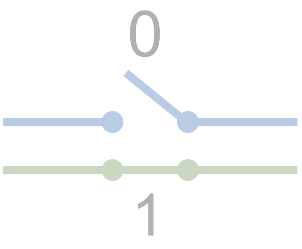
…

Qubits

Bit

logical



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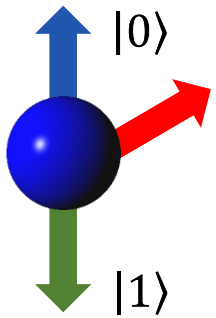

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Qubits

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Qubits

basis states

$$|0\rangle = \begin{bmatrix} 1 \\ 0 \end{bmatrix} \in \mathbb{C}^2 \qquad |1\rangle = \begin{bmatrix} 0 \\ 1 \end{bmatrix} \in \mathbb{C}^2$$

$$|2\rangle = |010\rangle = |0\rangle \otimes |1\rangle \otimes |0\rangle = \begin{bmatrix} 1 \\ 0 \end{bmatrix} \otimes \begin{bmatrix} 0 \\ 1 \end{bmatrix} \otimes \begin{bmatrix} 1 \\ 0 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 1 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{bmatrix} \in \mathbb{C}^8 = \mathbb{C}^{2^3}$$

Qubits

Single-qubit state: $|\psi_1\rangle = \alpha|0\rangle + \beta|1\rangle$

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Multi-qubit state: $|\psi_n\rangle = \sum_{i=0}^{2^n-1} \alpha_i |i\rangle \in \mathbb{C}^{2^n}$

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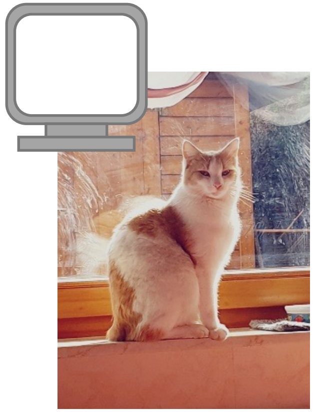
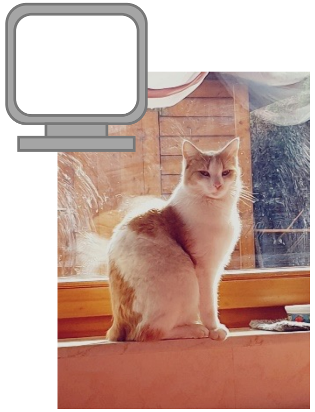
Amplitude Encoding



$$= \begin{bmatrix} x_0 \\ x_1 \\ x_2 \\ \vdots \\ x_{n-1} \end{bmatrix} \in \mathbb{R}^n$$

Amplitude Encoding



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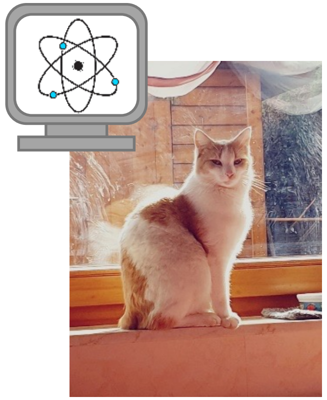
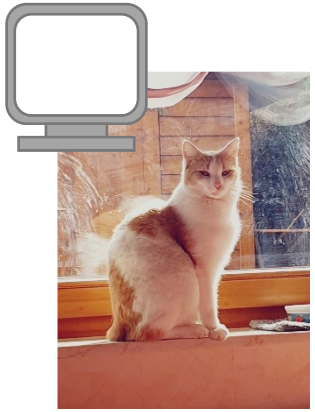


$$= |x\rangle$$

Amplitude Encoding



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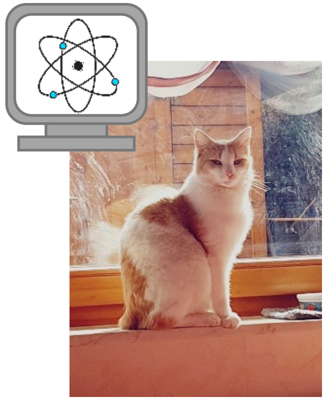

$$= |x\rangle = x_0|0\rangle + \cdots + x_{n-1}|n-1\rangle \in \mathbb{C}^{2^d}$$

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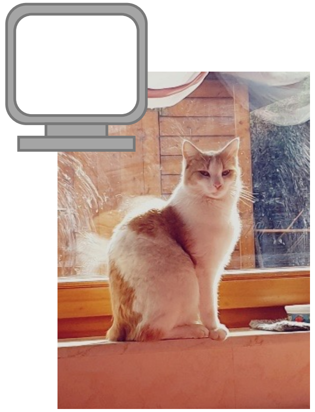

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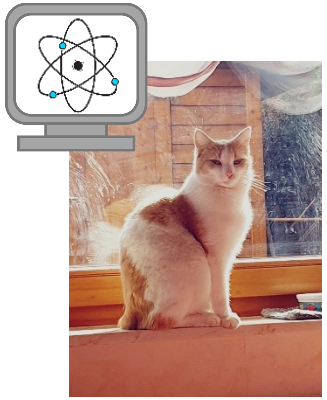

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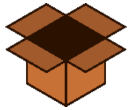
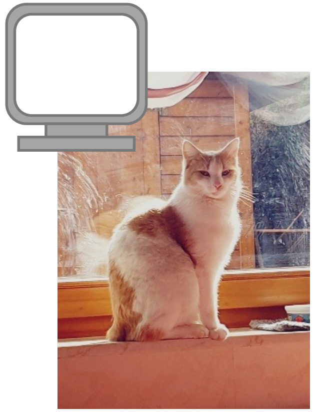
$O(d)$ qubits



Amplitude Encoding



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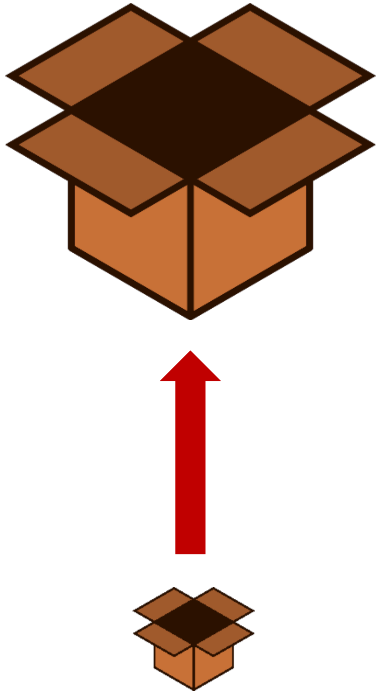
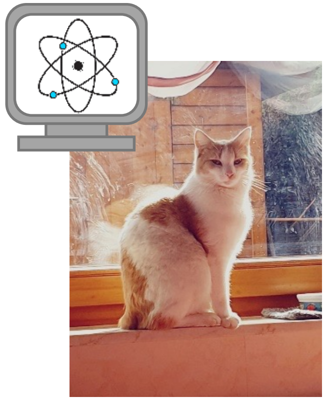
$O(n = 2^d)$ bits





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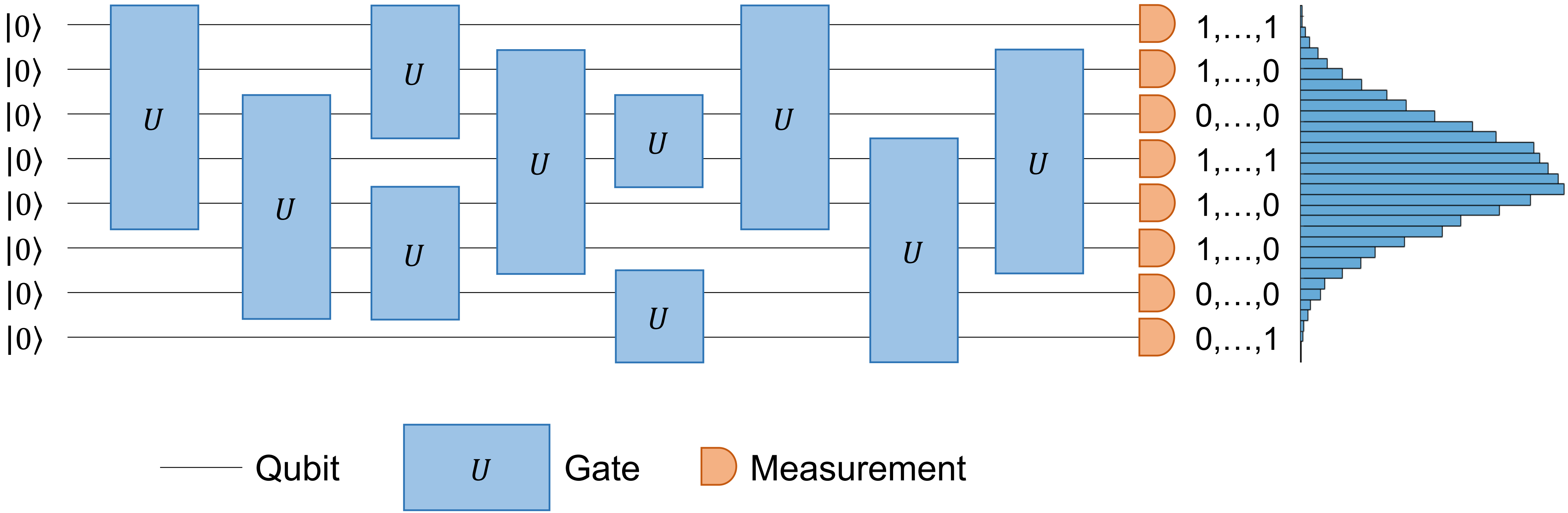
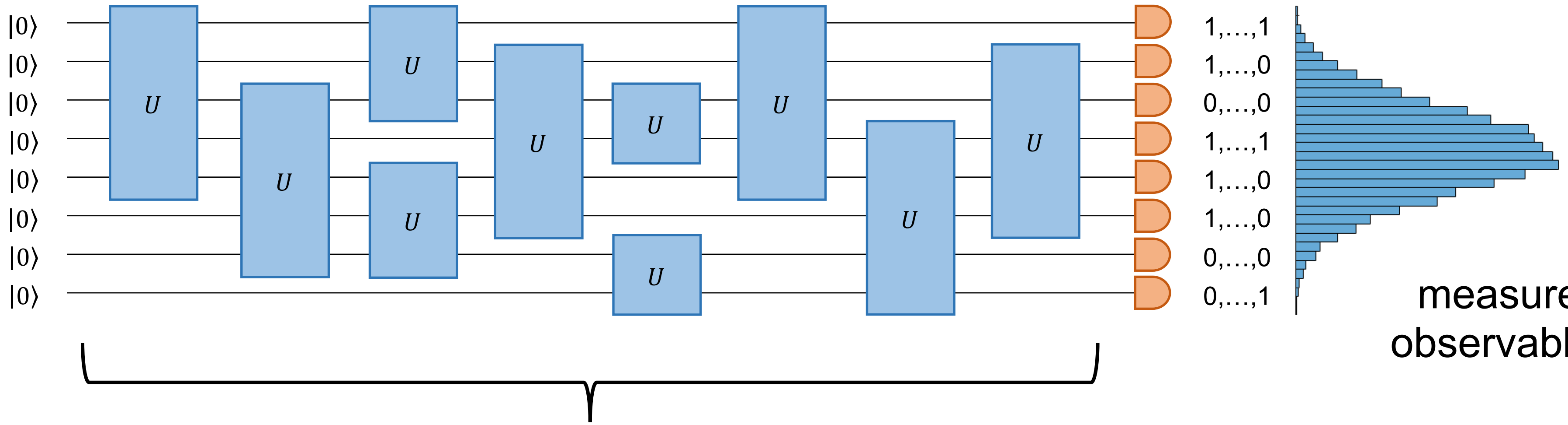
$O(d)$ qubits

Part 2:
Quantum Circuits


|0⟩
|0⟩
|0⟩
|0⟩
|0⟩
|0⟩
|0⟩
|0⟩
U
1,…,1
1,…,0
0,…,0
1,…,1
1,…,0
1,…,0
0,…,0
0,…,1
Qubit
U
Gate
Measurement

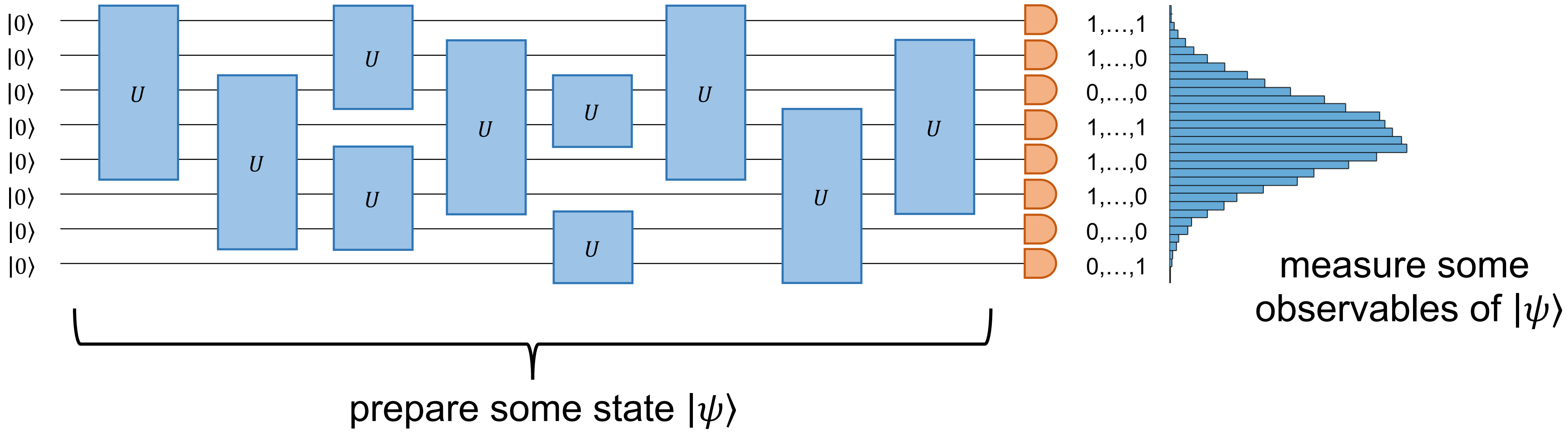
Quantum Circuits



measure some observables of $|\psi\rangle$

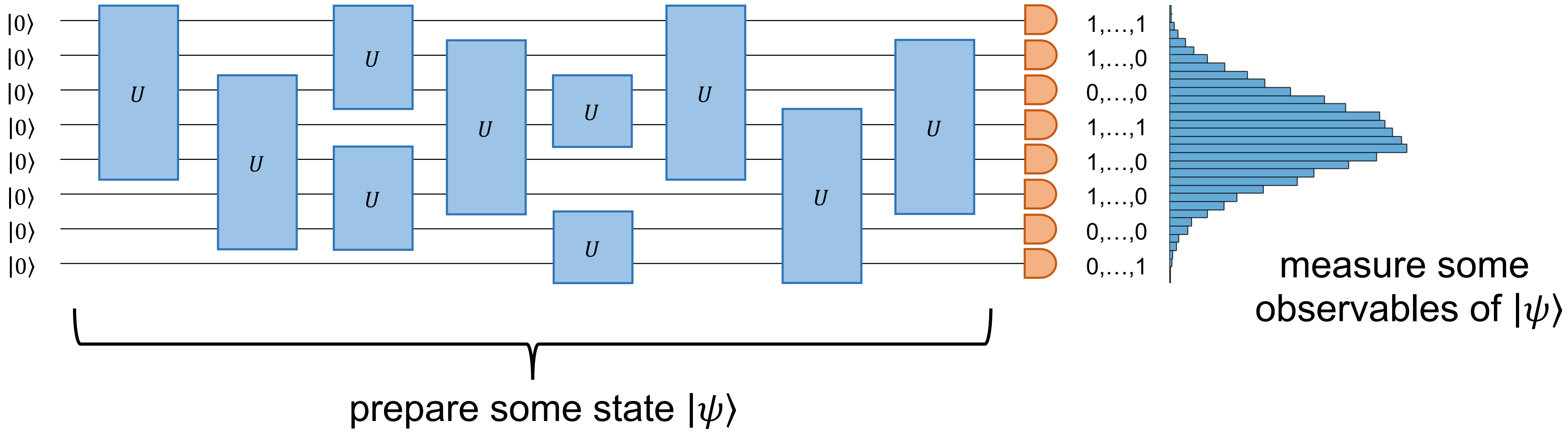
prepare some state $|\psi\rangle$

Quantum Circuits



Mathematically: Gate → $U: \mathbb{C}^n \rightarrow \mathbb{C}^n$, unitary → $U|\psi\rangle = |\psi'\rangle$

Quantum Circuits

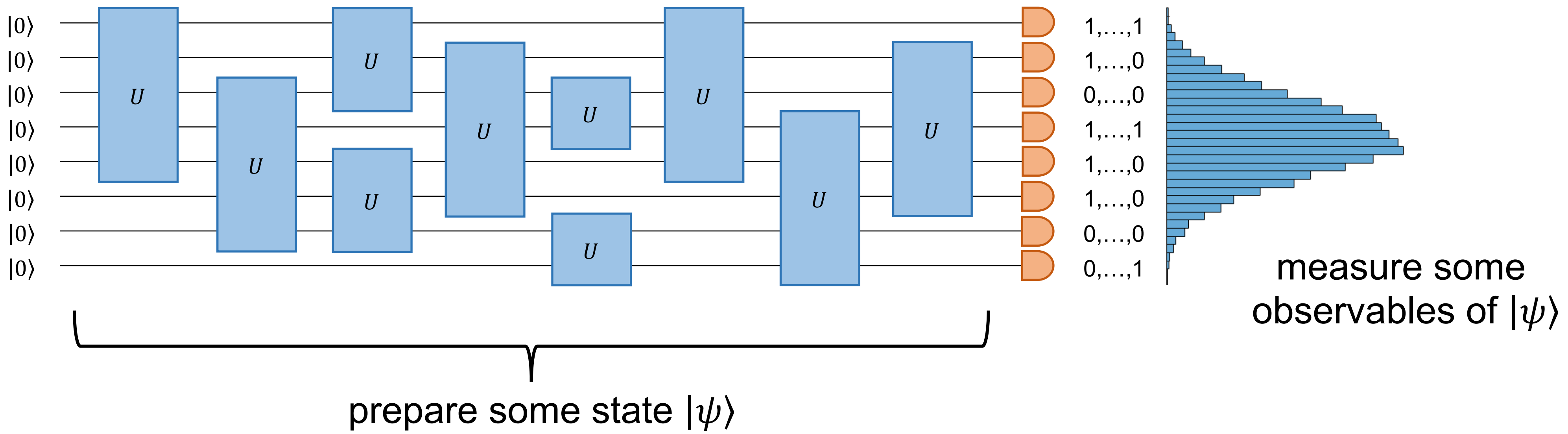


Mathematically: Gate → $U: \mathbb{C}^n \rightarrow \mathbb{C}^n$, unitary → $U|\psi\rangle = |\psi'\rangle$

Measurement → $\hat{O}: \mathbb{C}^n \rightarrow \mathbb{C}^n$, Hermitian → $\hat{O}|\psi\rangle \neq |\psi'\rangle$

instead → $|\psi\rangle \overset{\hat{O}}{\rightarrow} |\phi\rangle$

Quantum Circuits



Mathematically:

Output → $\langle \hat{O} \rangle = \langle \psi | \hat{O} | \psi \rangle = \langle 0 | U^{\dagger} \hat{O} U | 0 \rangle$

Important Gates

- Hadamard gate: $H|0\rangle = \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle) = |+\rangle$

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create superposition

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  e.g. $CNOT|1,1\rangle = |1,1 \oplus 1\rangle = |1,0\rangle$

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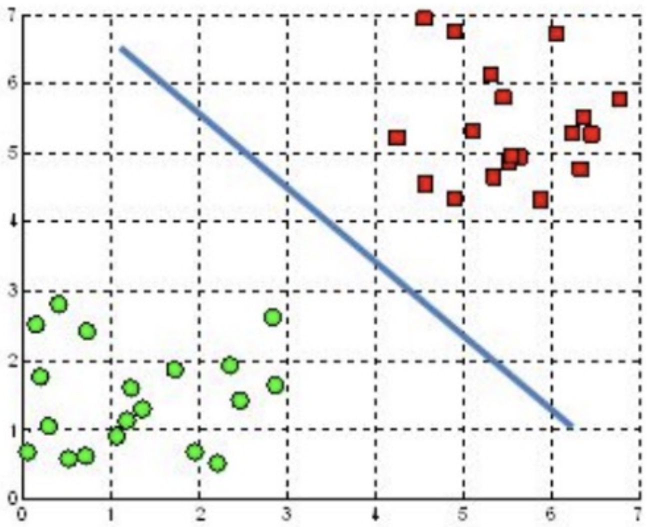
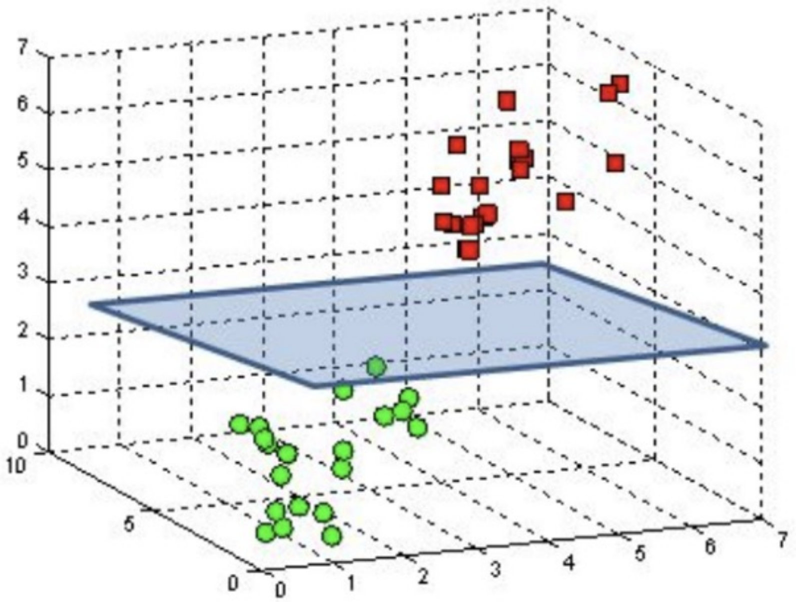
$$(H \otimes I)CNOT|00\rangle = \frac{1}{\sqrt{2}}(|00\rangle + |11\rangle)$$

create entanglement

Part 3: Example



0
1
2
3
4
5
6
7

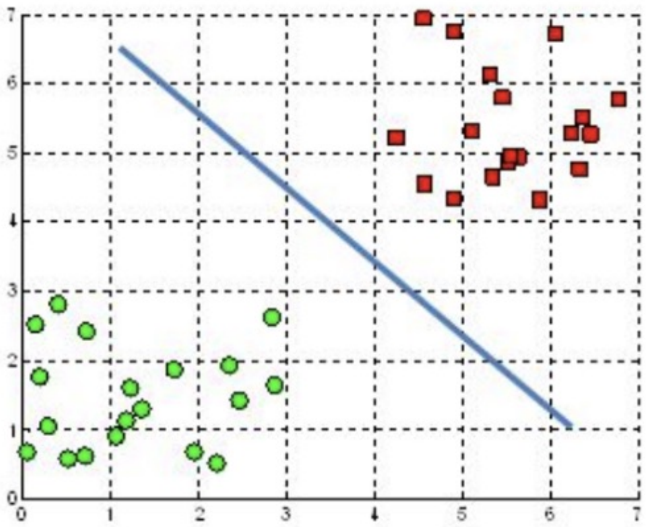


0
1
2
3
4
5
6
7
10
5

Simple Quantum Classifier

- Given training data set: $T = \{(\boldsymbol{x}^p, c^p)\}_{p=1,\ldots,N}$

$c = 1$



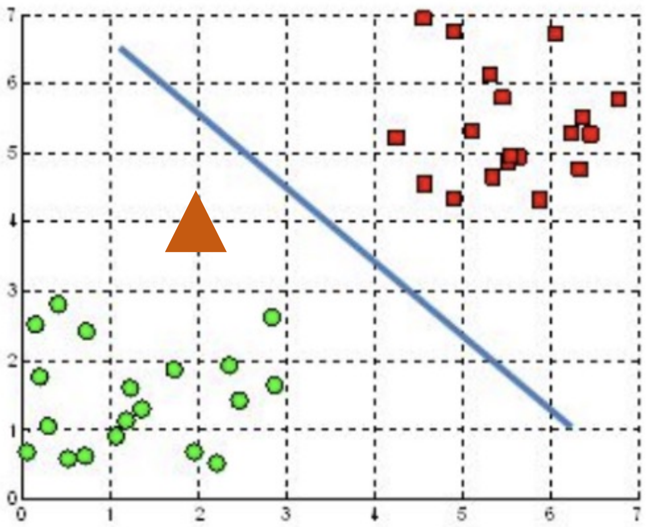
$c = 0$

Simple Quantum Classifier

- Given training data set: $T = \{(\boldsymbol{x}^p, c^p)\}_{p=1,\ldots,N}$

- Given new data point: $\boldsymbol{x}' \in \mathbb{R}^n$

$\boldsymbol{c = 1}$

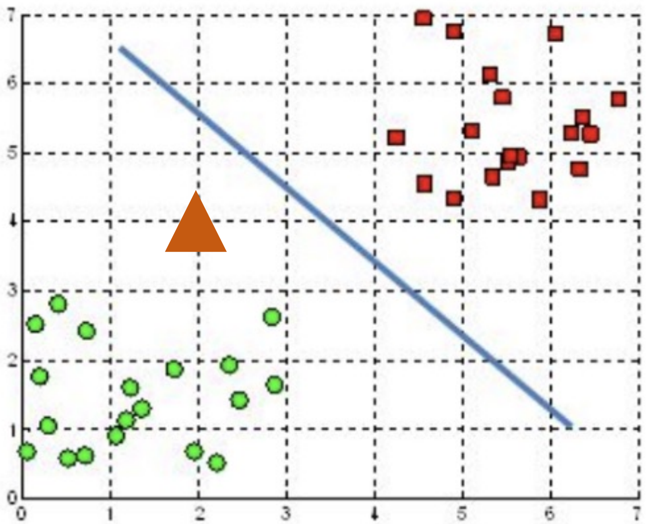


$\boldsymbol{c = 0}$

Simple Quantum Classifier

- Given training data set: $T = \{(\boldsymbol{x}^p, c^p)\}_{p=1,\ldots,N}$
- Given new data point: $\boldsymbol{x}' \in \mathbb{R}^n$
- Goal: Find class c' of $\boldsymbol{x}'$

$\boldsymbol{c = 1}$



$\boldsymbol{c = 0}$

Simple Quantum Classifier

1. Step: Construct $|\phi_0\rangle = \sum_p |p\rangle(|0\rangle|\psi_{\boldsymbol{x}'}\rangle + |1\rangle|\psi_{\boldsymbol{x}^p}\rangle)\,|c^p\rangle$

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$|0\rangle$ —

$|0\rangle$ —

$|0\rangle$ —

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Simple Quantum Classifier

marker

1. Step: Construct $|\phi_0\rangle = \sum_p |p\rangle (|0\rangle|\psi_{\boldsymbol{x}'}\rangle + |1\rangle|\psi_{\boldsymbol{x}^p}\rangle)\, |c^p\rangle$

$|0\rangle$ —

$|0\rangle$ —

$|0\rangle$ —

$|0\rangle$ —

Simple Quantum Classifier

marker

1. Step: Construct $|\phi_0\rangle = \sum_p |p\rangle(|0\rangle|\psi_{\boldsymbol{x}'}\rangle + |1\rangle|\psi_{\boldsymbol{x}^p}\rangle)\,|c^p\rangle$

ancilla

$|0\rangle$ —

$|0\rangle$ —

$|0\rangle$ —

$|0\rangle$ —

Simple Quantum Classifier

marker input training

1. Step: Construct $|\phi_0\rangle = \sum_p |p\rangle(|0\rangle|\psi_{x'}\rangle + |1\rangle|\psi_{x^p}\rangle)\,|c^p\rangle$

ancilla

$|0\rangle$ —

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$|0\rangle$ —

$|0\rangle$ —

Simple Quantum Classifier

marker — input — training

1. Step: Construct $|\phi_0\rangle = \sum_p |p\rangle \big(|0\rangle|\psi_{\boldsymbol{x}'}\rangle + |1\rangle|\psi_{\boldsymbol{x}^p}\rangle\big)\,|c^p\rangle$

ancilla — class

$|0\rangle$ —

$|0\rangle$ —

$|0\rangle$ —

$|0\rangle$ —

Simple Quantum Classifier

1. Step: Construct $|\phi_0\rangle = \sum_p \underbrace{|p\rangle}_{\text{marker}} (\underbrace{|0\rangle}_{\text{ancilla}} \underbrace{|\psi_{x'}\rangle}_{\text{input}} + \underbrace{|1\rangle}_{\text{ancilla}} \underbrace{|\psi_{x^p}\rangle}_{\text{training}}) \underbrace{|c^p\rangle}_{\text{class}}$

2. Step: Applying one gate and one partial measurement…

Simple Quantum Classifier

marker input training

1. Step: Construct $|\phi_0\rangle = \sum_p |p\rangle(|0\rangle|\psi_{x'}\rangle + |1\rangle|\psi_{x^p}\rangle)\,|c^p\rangle$

ancilla class

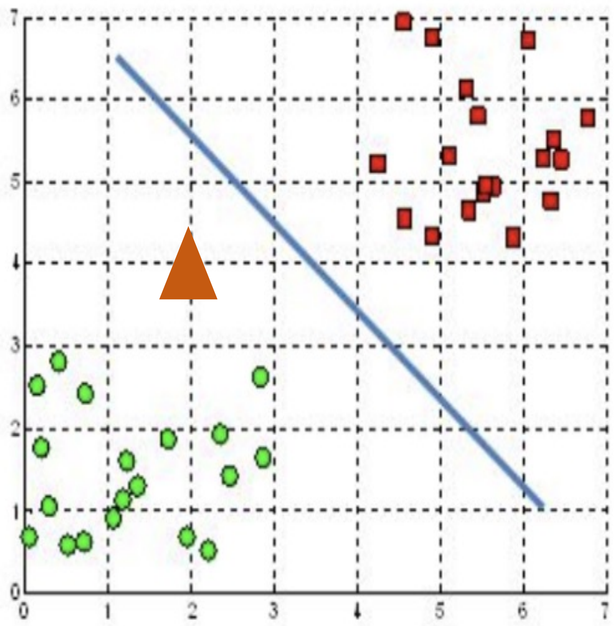
2. Step: Applying one gate and one partial measurement…

3. Step: Measure class qubit $P(|c\rangle = 0) = \sum_{p|c^p=0} d(x', x^p)^{-1}$

Simple Quantum Classifier

$$P(|c\rangle = 0) = \sum_{p|c^p=0} d(x', x^p)^{-1}$$

$c = 1$



$c = 0$

Simple Quantum Classifier

1. Step: Construct $|\phi_0\rangle = \sum_p \underbrace{|p\rangle}_{\text{marker}} (\underbrace{|0\rangle}_{\text{ancilla}} \underbrace{|\psi_{x'}\rangle}_{\text{input}} + \underbrace{|1\rangle}_{\text{ancilla}} \underbrace{|\psi_{x^p}\rangle}_{\text{training}}) \underbrace{|c^p\rangle}_{\text{class}}$

2. Step: Applying one gate and one partial measurement…

3. Step: Measure class qubit $P(|c\rangle = 0) = \sum_{p|c^p=0} d(x', x^p)^{-1}$

4. Step: Take c with higher probability

Simple Quantum Classifier

1. Step: Construct $|\phi_0\rangle = \sum_p |p\rangle(|0\rangle|\psi_{x'}\rangle + |1\rangle|\psi_{x^p}\rangle)\,|c^p\rangle$

2. Step: Applying one gate and one partial measurement…

3. Step: Measure class qubit $O(1)$ ☺

4. Step: Take c with higher probability

Simple Quantum Classifier

1. Step: Construct $|\phi_0\rangle = \sum_p |p\rangle(|0\rangle|\psi_{x'}\rangle + |1\rangle|\psi_{x^p}\rangle)\,|c^p\rangle$

2. Step: Applying one gate and one partial measurement… $O(1)$ ☺

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Simple Quantum Classifier

1. Step: Construct $|\phi_0\rangle = \sum_p |p\rangle(|0\rangle|\psi_{x'}\rangle + |1\rangle|\psi_{x^p}\rangle)\,|c^p\rangle$ $O(2^N)$ ☹

2. Step: Applying one gate and one partial measurement… $O(1)$ ☺

3. Step: Measure class qubit $O(1)$ ☺

4. Step: Take c with higher probability

1. Generation QML Algorithms

- Promised exponential speed-up
- Need "Quantum Random Access Memory" (QRAM)
- QRAM needs exponentially many steps
- No physical implementation so far

$$|\psi_x\rangle = \sum_{i=0}^{2^n-1} x_i |i\rangle$$

1. Generation QML Algorithms

- Promised exponential speed-up
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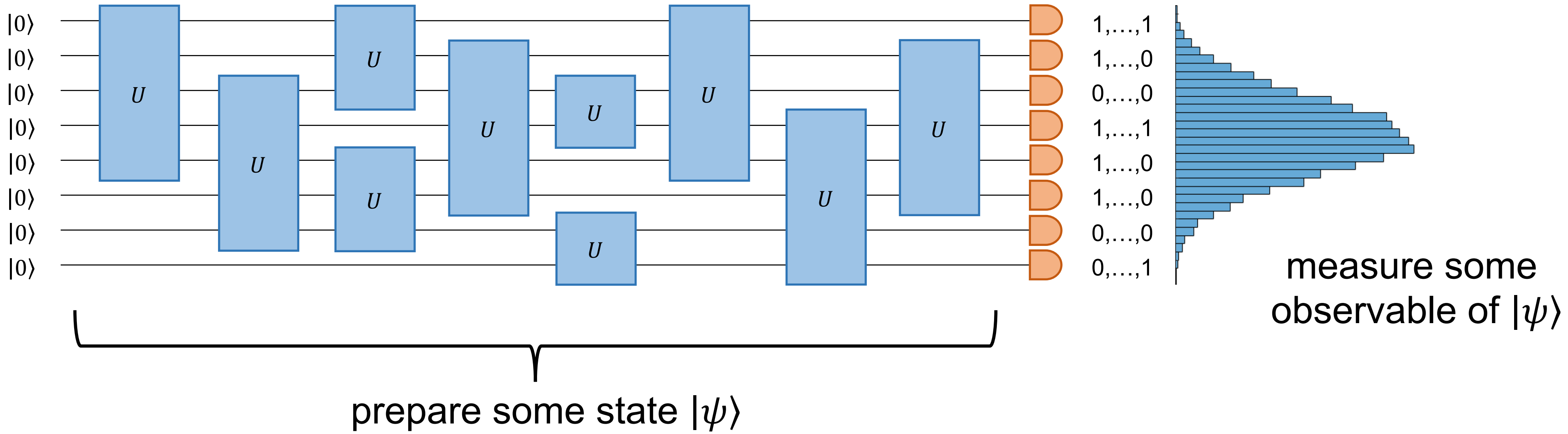
→ "Learn" the quantum states

$$|\psi_x\rangle = \sum_{i=0}^{2^n-1} x_i |i\rangle$$

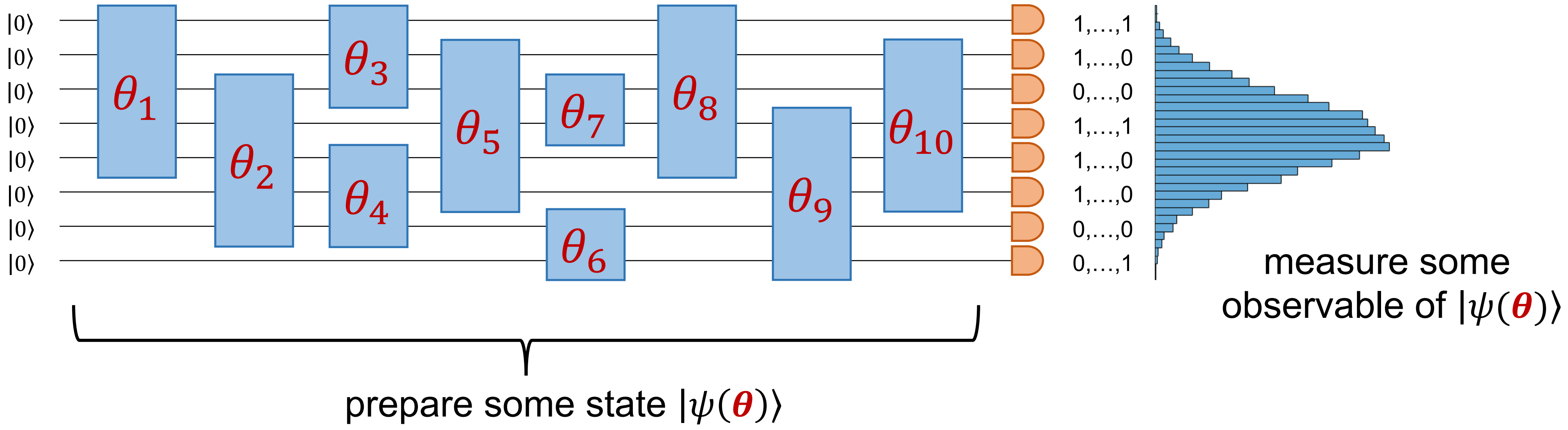
$$|\tilde{\psi}_x\rangle = \sum_{i=0}^{2^n-1} \tilde{x}_i |i\rangle$$

Part 4:
PQCs

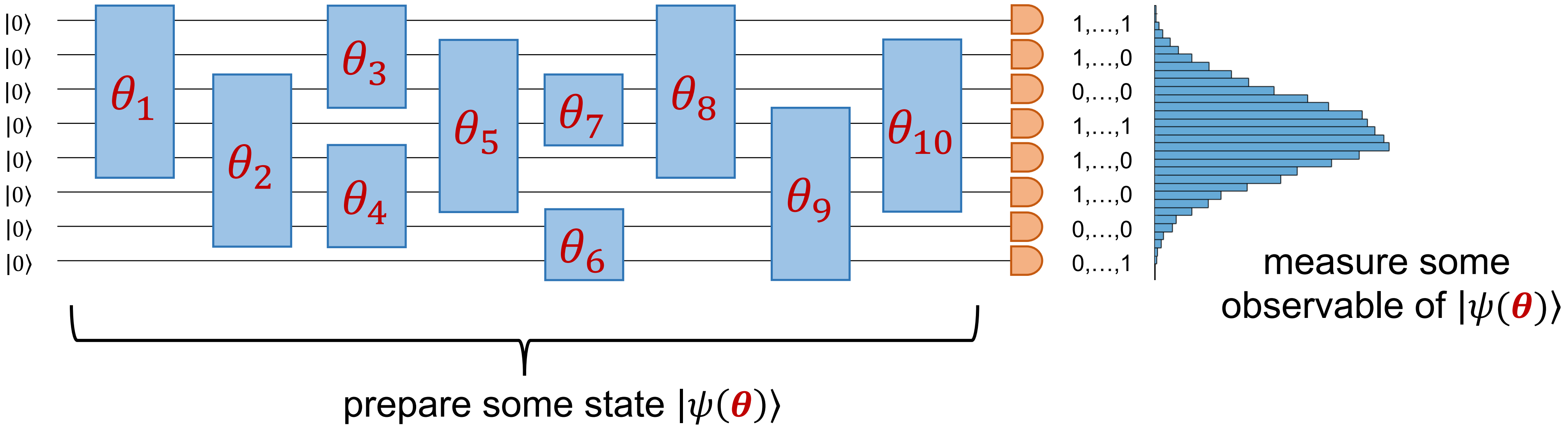
Parameterized Quantum Circuits



Parameterized Quantum Circuits



Parameterized Quantum Circuits



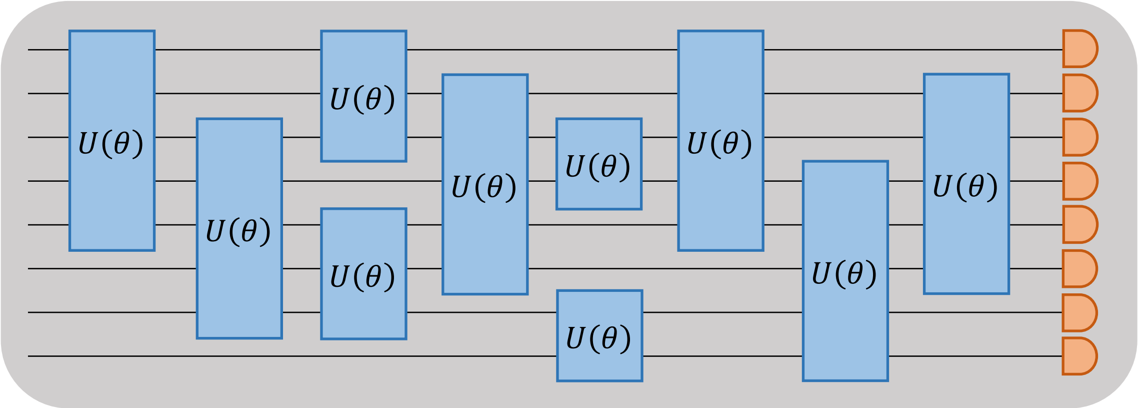
Output:

$$f(\boldsymbol{\theta}) = \langle\psi(\boldsymbol{\theta})|\hat{O}|\psi(\boldsymbol{\theta})\rangle = \langle 0|U(\boldsymbol{\theta})^{\dagger}\hat{O}U(\boldsymbol{\theta})|0\rangle$$

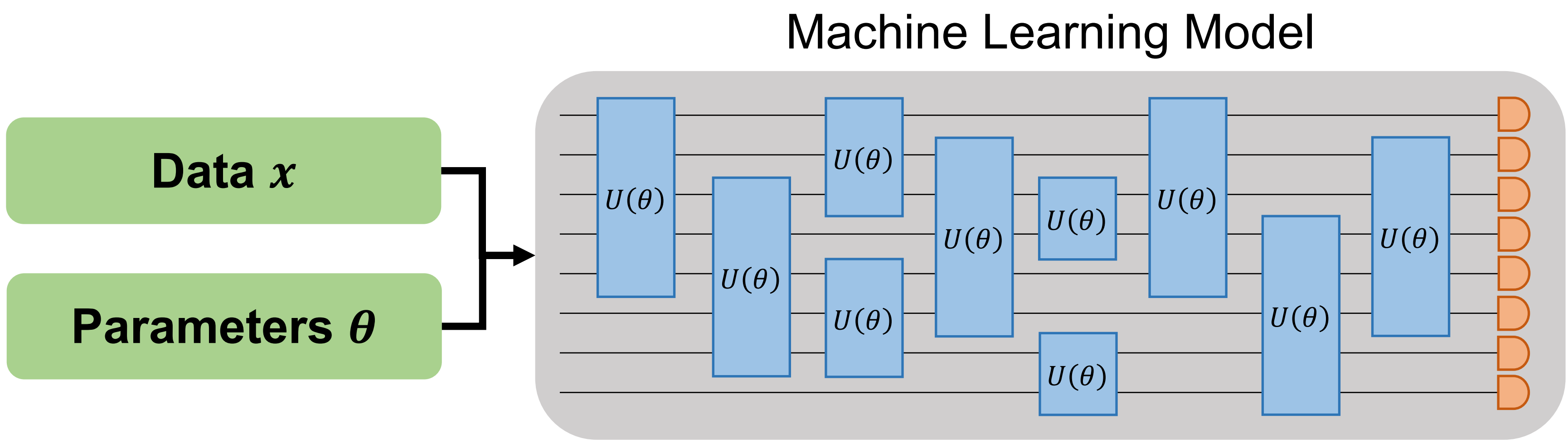
can be used within a cost function

Parameterized Quantum Circuits

Machine Learning Model

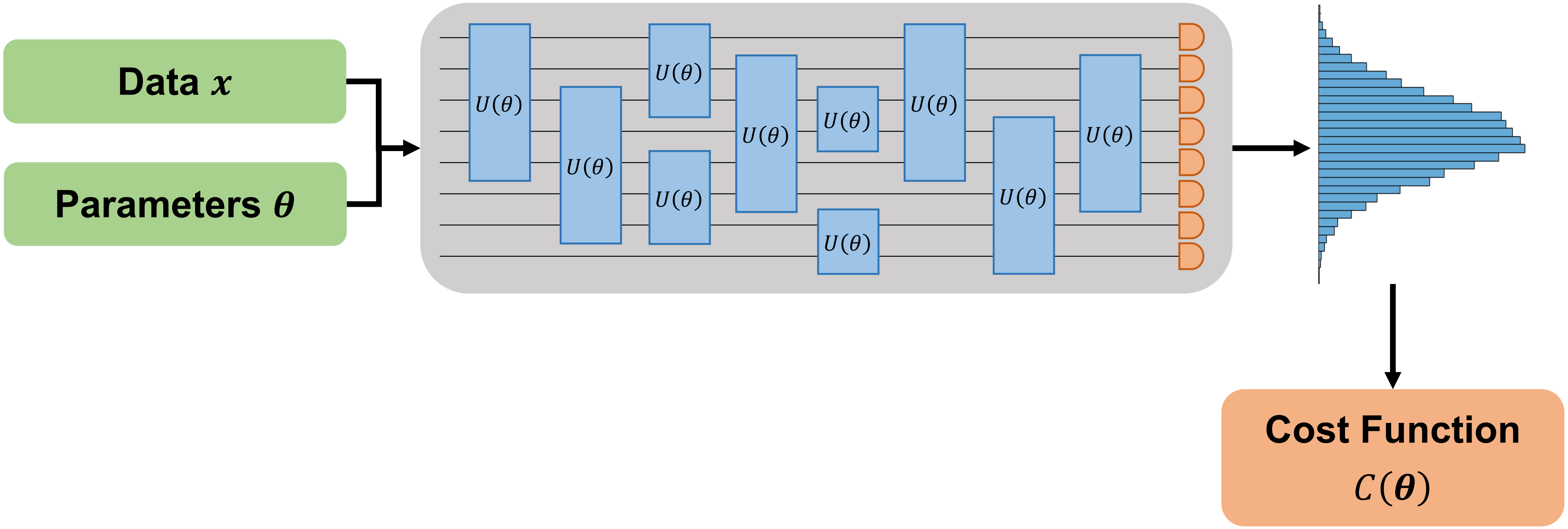


Parameterized Quantum Circuits

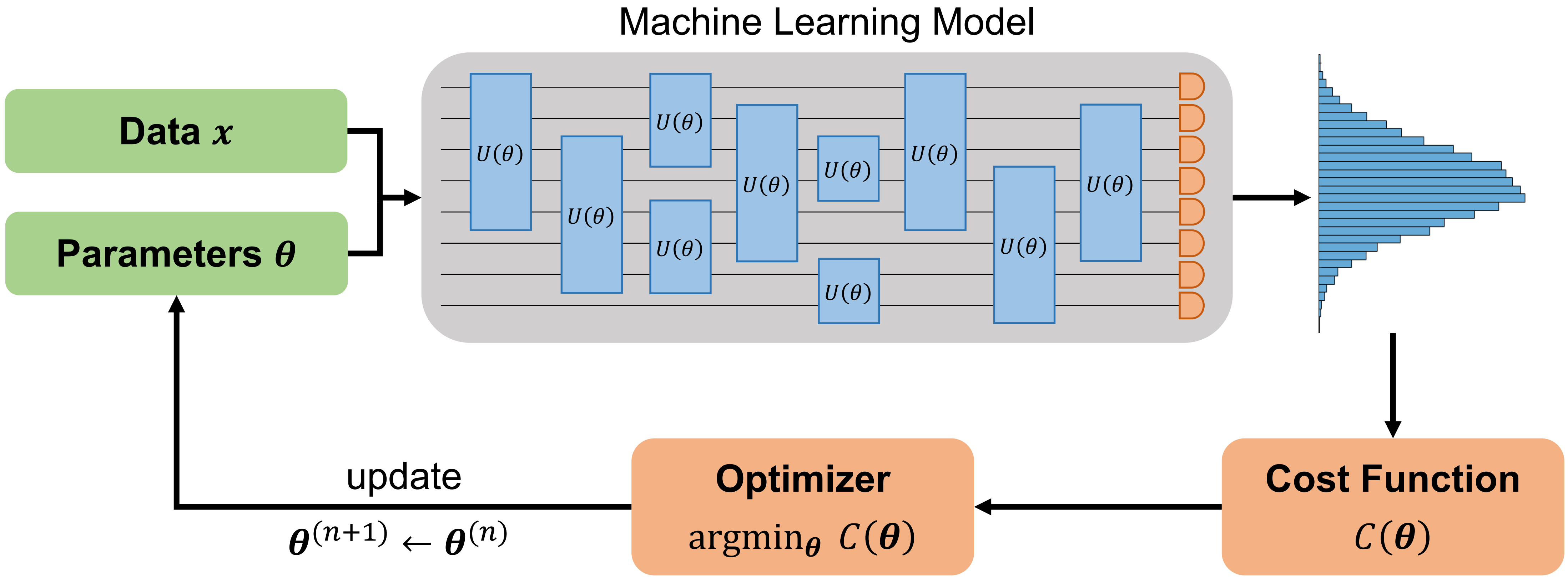


Parameterized Quantum Circuits

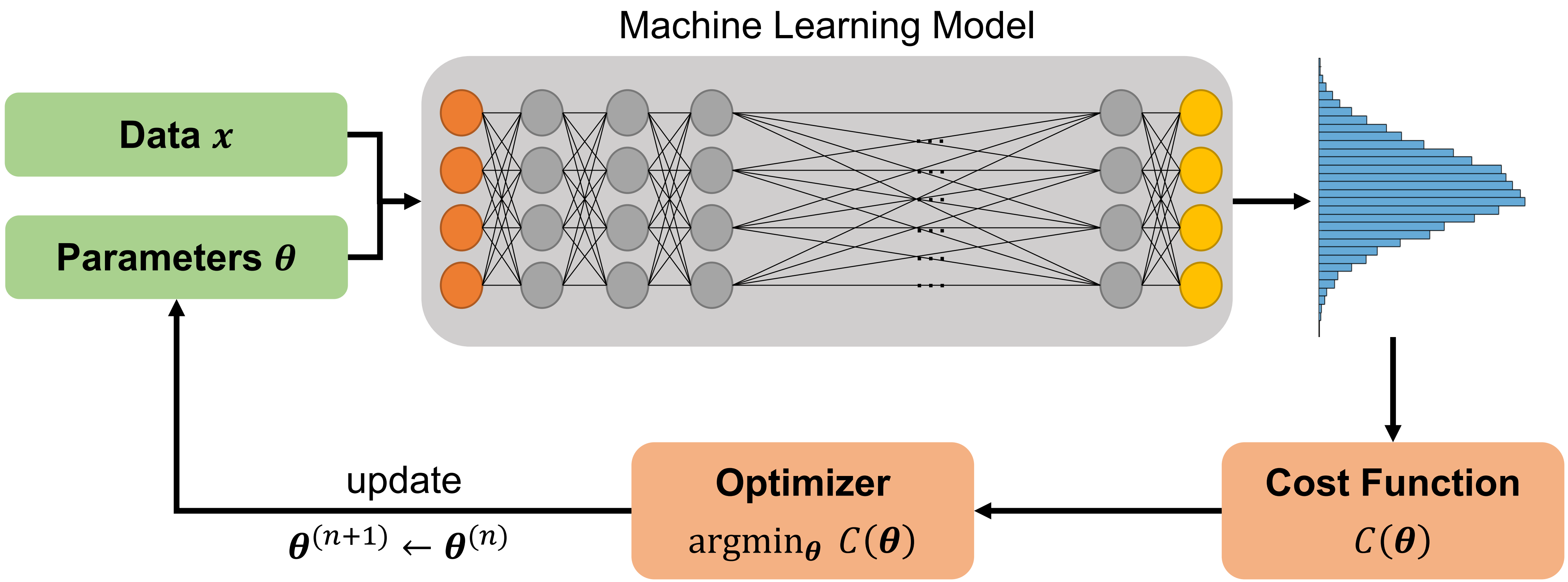
Machine Learning Model



Parameterized Quantum Circuits

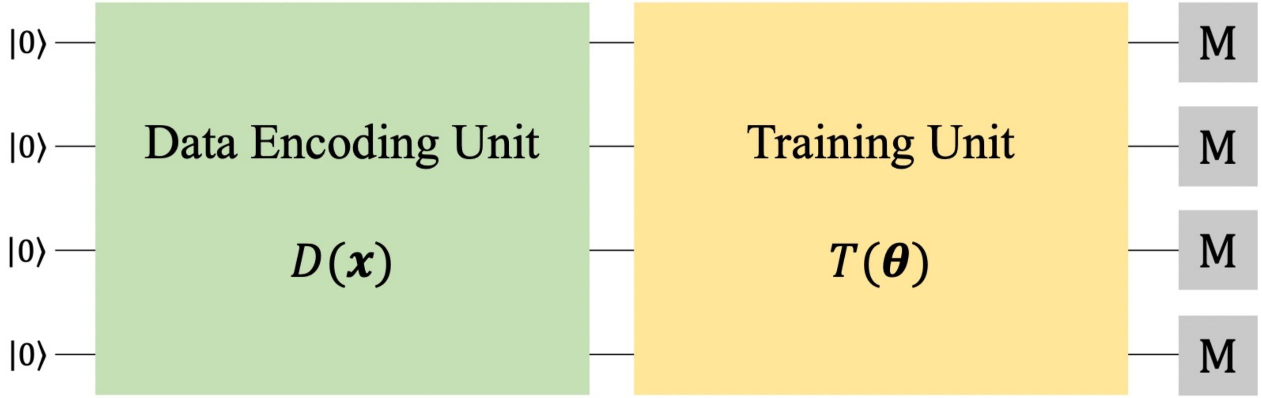


Parameterized Quantum Circuits

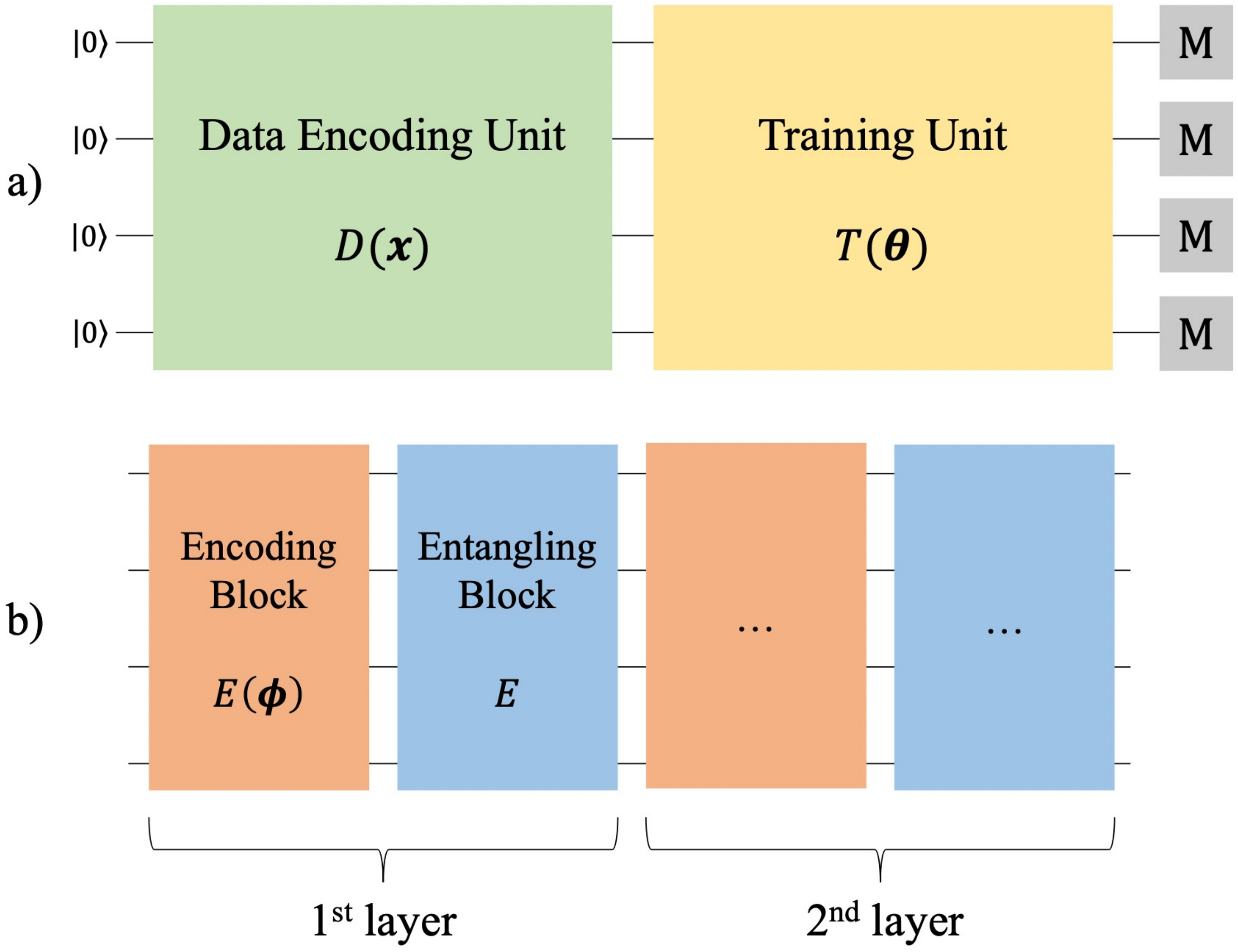


Parameterized Quantum Circuits

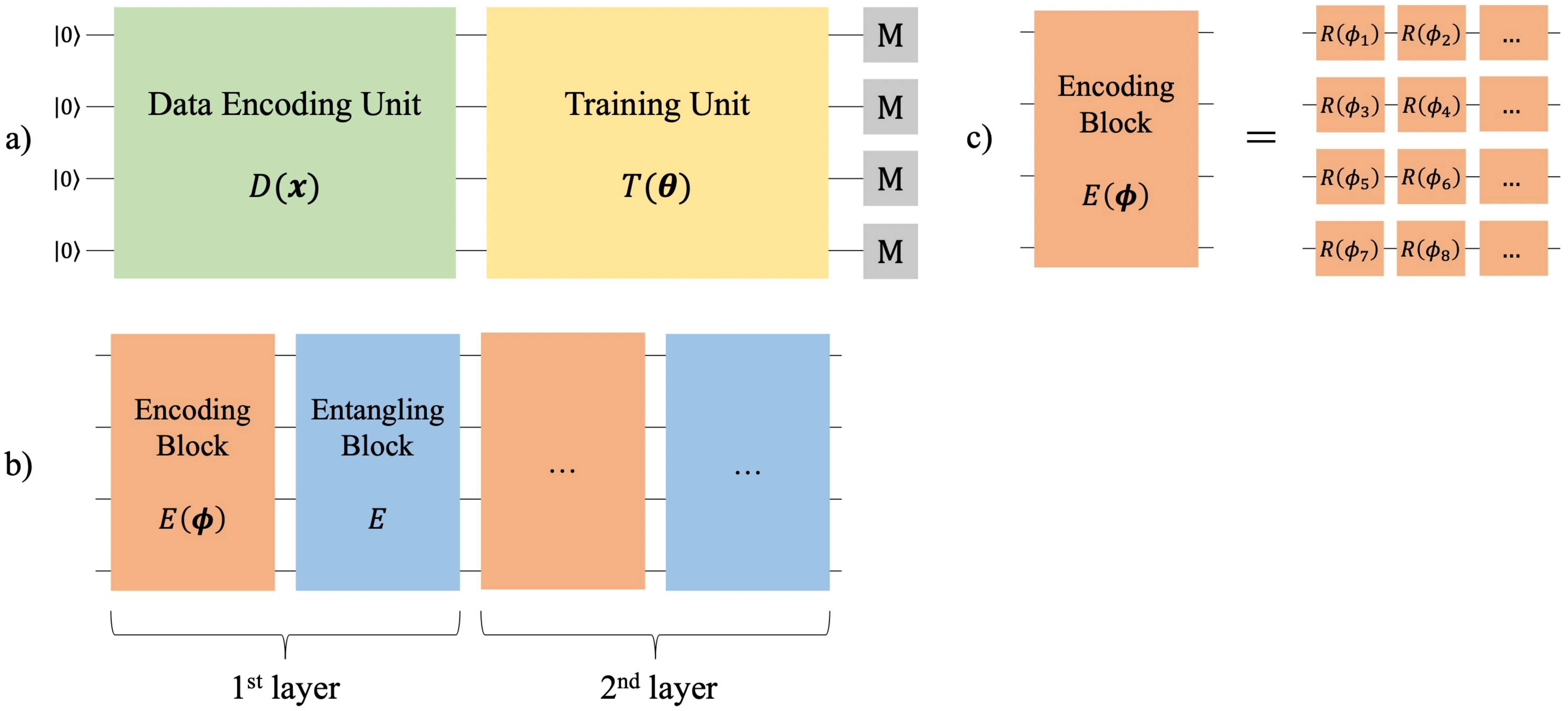
a)



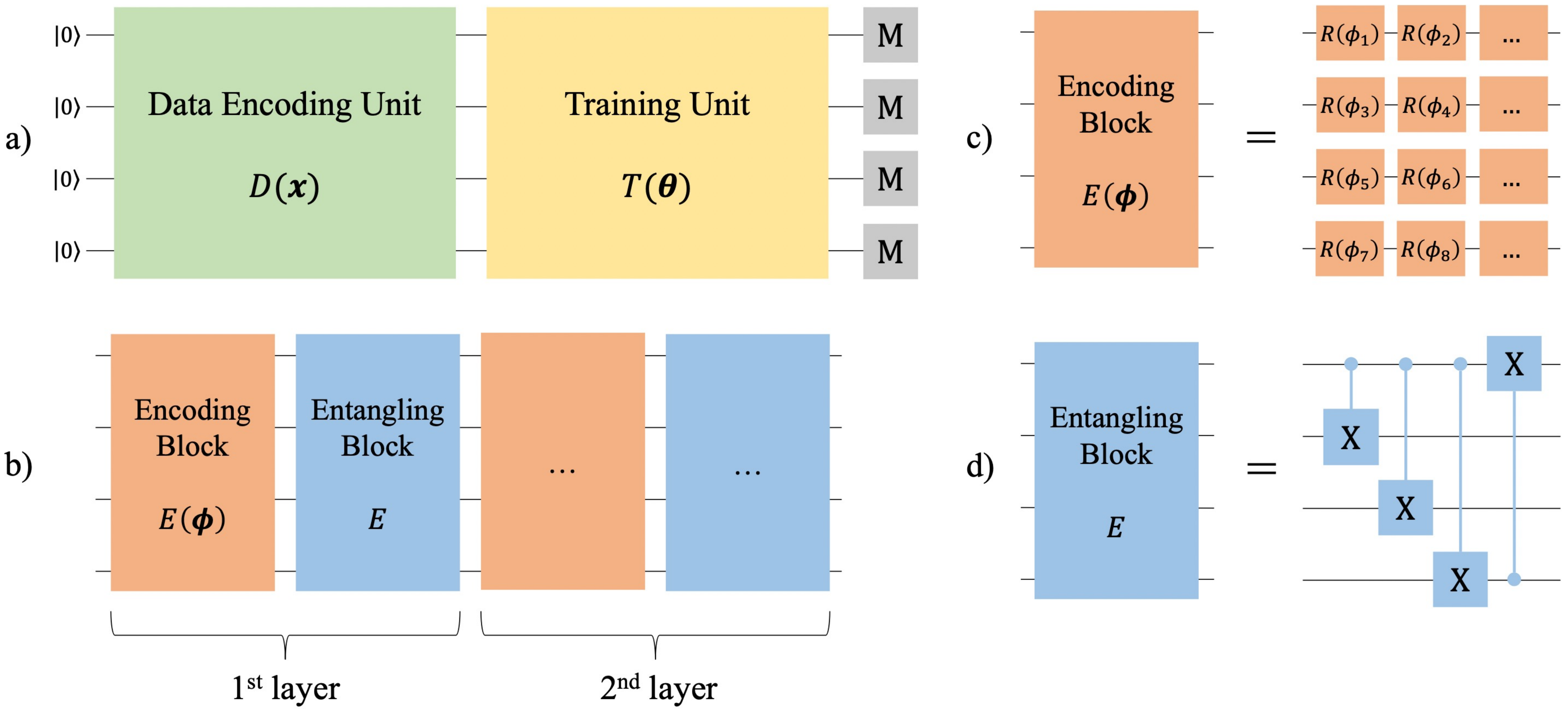
Parameterized Quantum Circuits



Parameterized Quantum Circuits



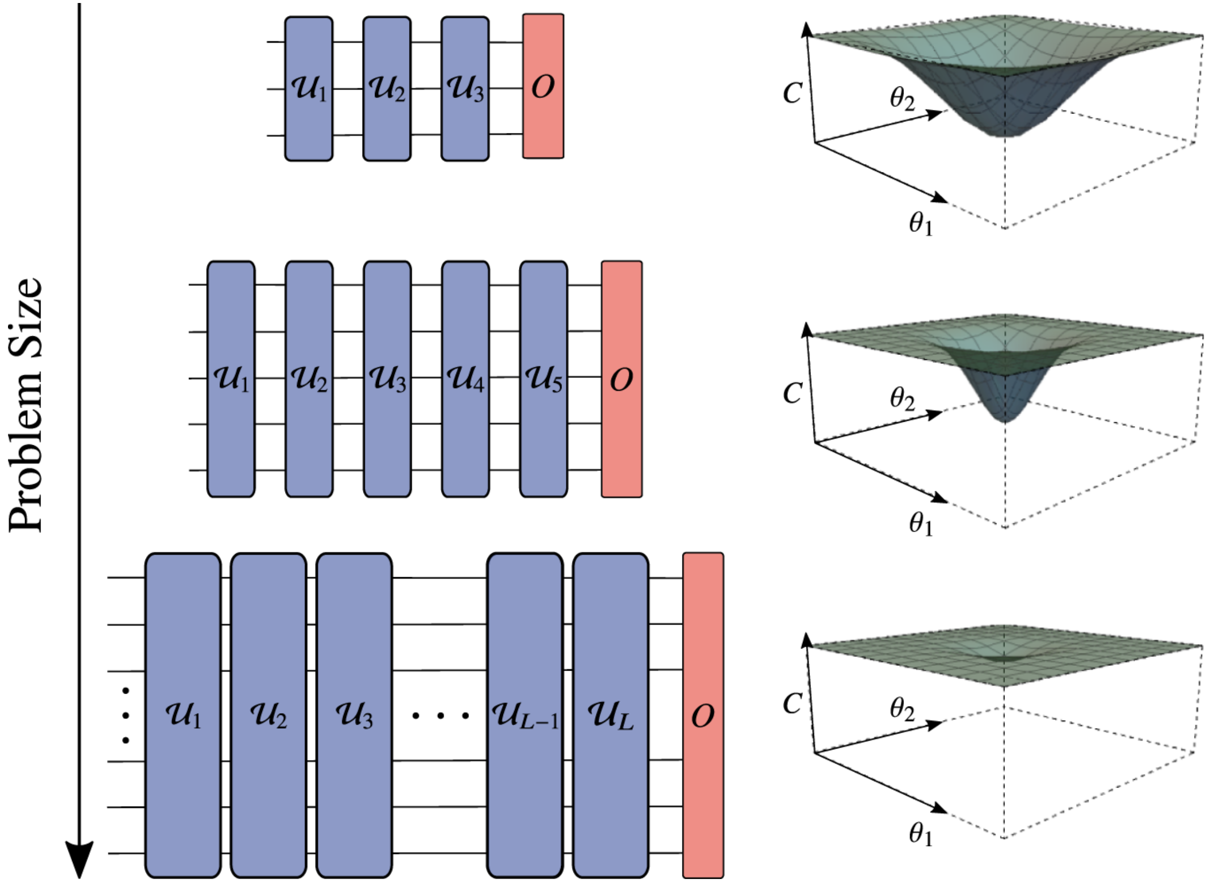
Parameterized Quantum Circuits



Part 5:
Open Questions

Open Questions

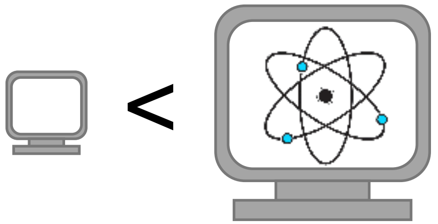
- How to avoid Barren Plateaus?



Open Questions

- How to avoid Barren Plateaus?

- Is there a Quantum Advantage?



Open Questions

- How to avoid Barren Plateaus?
- Is there a Quantum Advantage?
- How to define cost functions?

$$C(\boldsymbol{\theta}) = \langle \psi(\boldsymbol{\theta}) | \hat{O} | \psi(\boldsymbol{\theta}) \rangle + \cdots \ ?$$

Open Questions

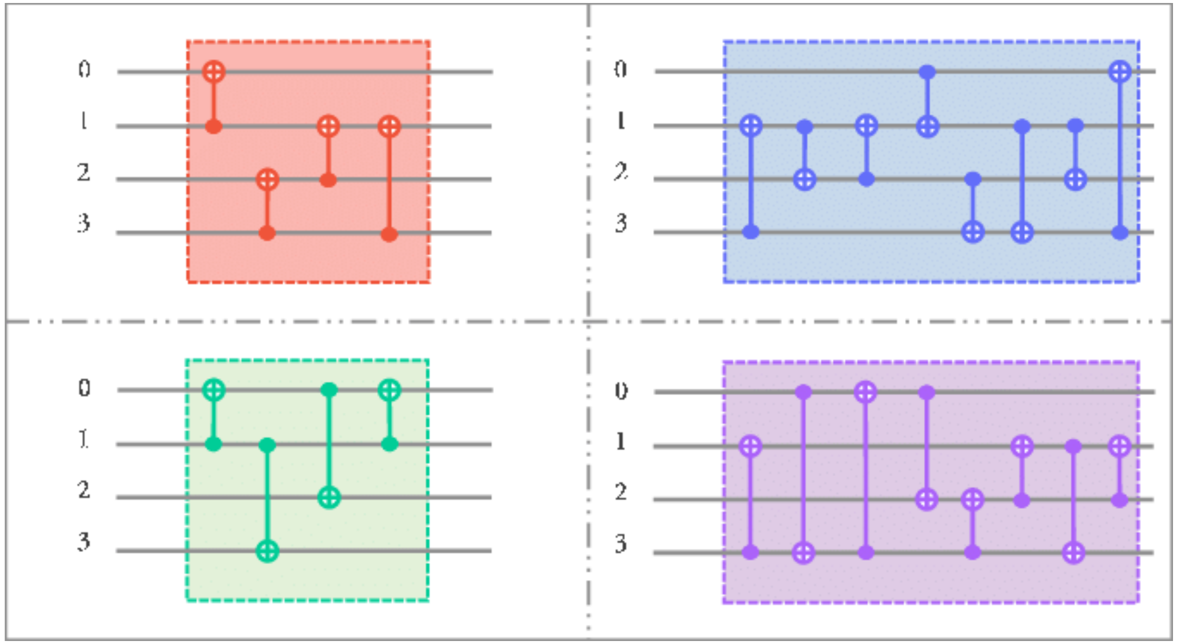
- How to avoid Barren Plateaus?
- Is there a Quantum Advantage?
- How to define cost functions?
- How to implement constraints?

minimize $C(\boldsymbol{\theta})$

subject to $???$

Open Questions

- How to avoid Barren Plateaus?
- Is there a Quantum Advantage?
- How to define cost functions?
- How to implement constraints?
- Which architecture is useful for which problems?



Thanks!

A discussion
is highly
welcome.