

# Machine Learning Guest Lecture

## A Glimpse of Quantum Machine Learning

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# Outline

1. Part I – Basics of Quantum Information Processing

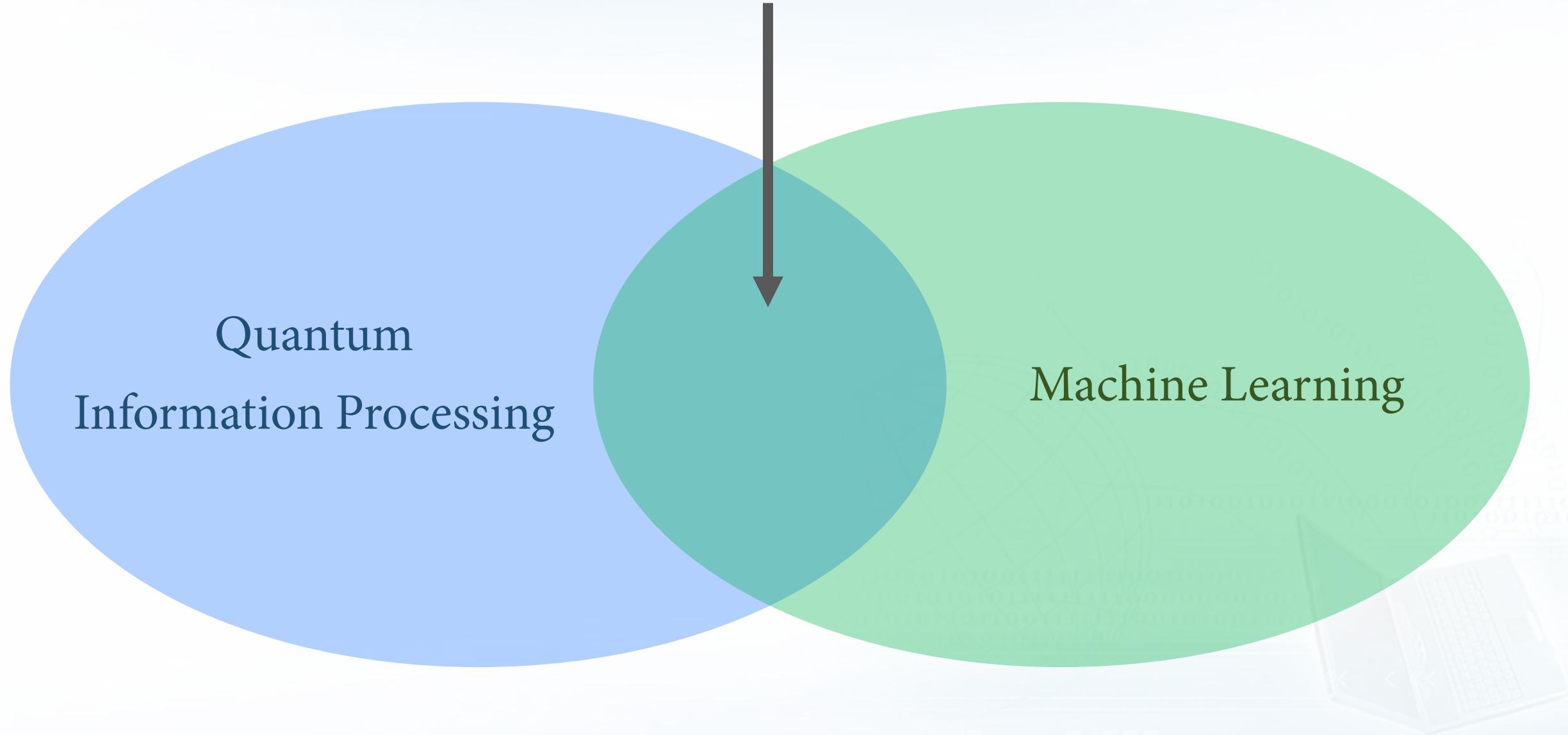
2. Part II – Various Models of Quantum ML

3. Part III – ML with Quantum Algorithmic Speed-up

4. Part IV – Learning with Quantum Machines

5. Conclusions and Outlooks

# Quantum Machine Learning?



# Prologue

- *Quantum information science* have demonstrated advantages in several fields:
  - Computing: speed-ups certain computational tasks where no classical methods can do.
  - Communication: entanglement-assisted communication increases channel capacity.
  - Cryptography: extending classical key with information-theoretic security.
  - Sensing: more accurate estimation, positioning, and synchronization.
  - Simulation: simulating complex reactions that are formidable for classical computers.
- Any other applications/advantages of quantum information technologies?
- Artificial intelligence and machine learning tasks are essentially implemented on a physical device. How about doing the job on a quantum computational device?
- Can quantum information science revolutionize the way of learning from data?

# Part I – Basics of Quantum Information Processing

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# Brief History of Quantum Computation (1/2)

- Paul Benioff (1979):  
“The computer as a physical system: A microscopic quantum mechanical Hamiltonian model of computers as represented by Turing machines.
- Feynman (1981): “Why don’t we store information on individual particles that already follow the very rules of quantum mechanics that we try to simulate?  
*“Nature Isn’t classical, dammit, and if you want to make a simulation of nature, you’d better make it quantum mechanical.”*
- David Deutsch (1985) described what a quantum algorithm would look like, and Richard Jozsa (1992) demonstrated a *deterministic* quantum advantage.
- Umesh Vazirani and Ethan Bernstein (1993) pushed it forward (bounded error).
- Daniel Simon (1994) demonstrated an exponential speedup.



Richard Feynman  
(1918-1988)

# Brief History of Quantum Computation (2/2)

- Seth Lloyd (1993) described a method of building a working quantum computer.
- Peter Shor (1994) invented a polynomial-time quantum algorithm for factoring.
- David DiVincenzo (1996) outlined the key criteria of a quantum computer.
- Isaac Chuang *et al.* (2001) implemented Shor's algorithm on a nuclear magnetic resonance (NMR) system to factor the number 15 as a demonstration.
- :
- → A variety of interdisciplinary fields such as  
Quantum Computation, Quantum Communication,  
Quantum Simulation, Quantum Sensing, Quantum Chemistry, etc.



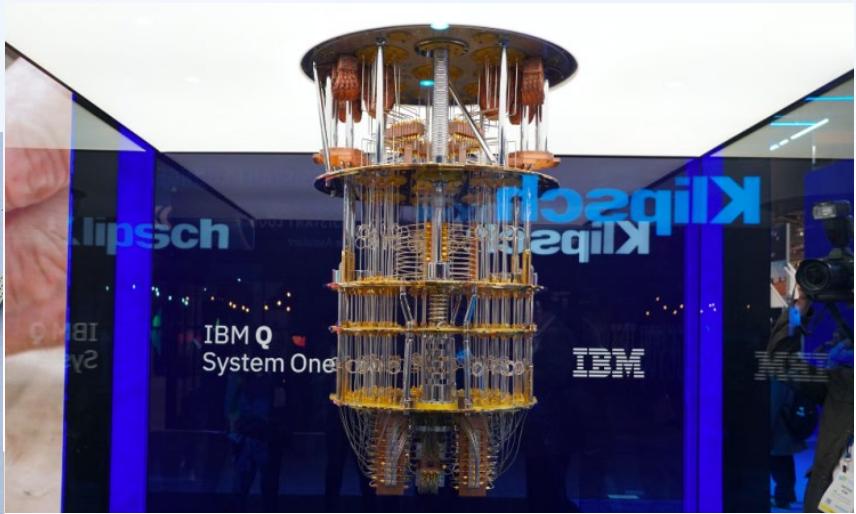
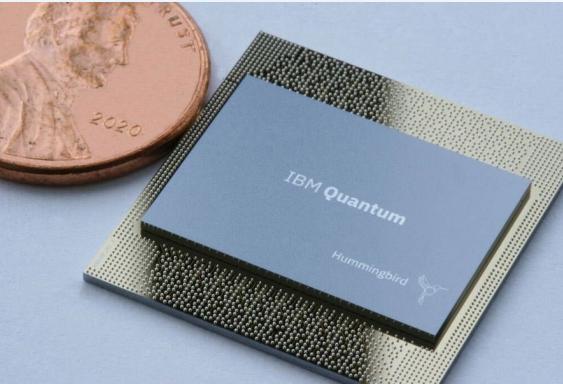
*Quantum Information Science*

Peter Shor (1959 -)

# Industry – Tech Giants



- ▶ IBM Q System One Computer Center
- ▶ 53, 65-qubit processor for IBM Q Network



- ▶ 54-qubit processor “Sycamore”
- ▶ 72-qubit processor “Bristlecone”

**nature**

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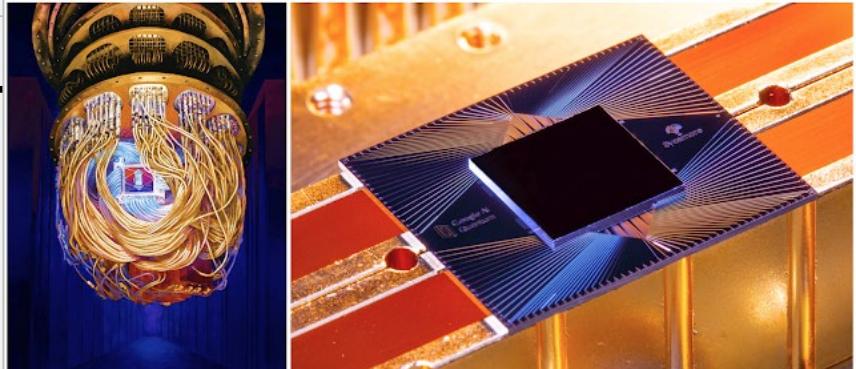
nature > articles > article

Article | Published: 23 October 2019

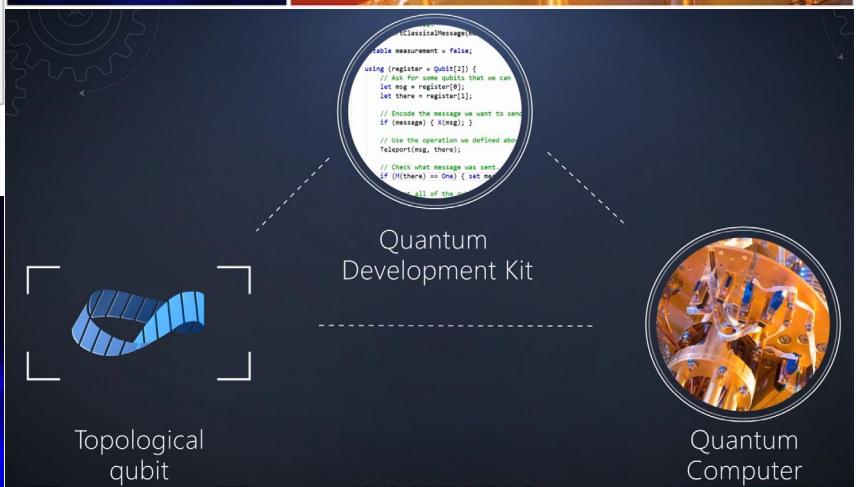
## Quantum supremacy using a programmable superconducting processor

Frank Arute, Kunal Arya, [...] John M. Martinis

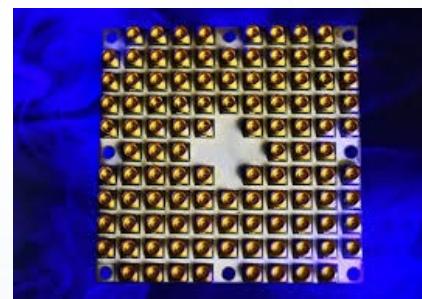
Nature 574, 505–510(2019) | Cite this article



- ▶ Quantum Development Kit
- ▶ Q# Programming Language
- ▶ Azure Quantum – cloud service

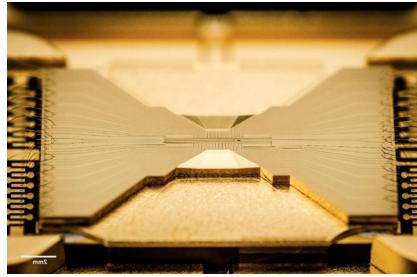
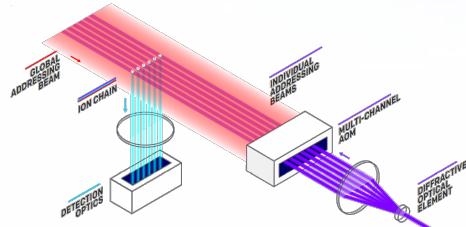


- ▶ 49-qubit processor



# Other Quantum Processors

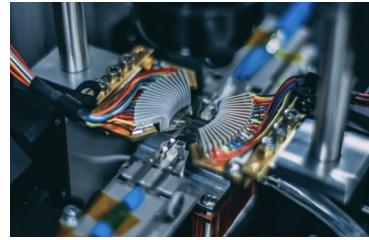
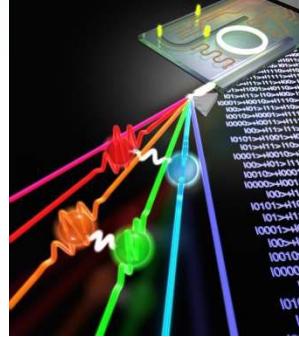
Trapped Ion



(32 qubits)

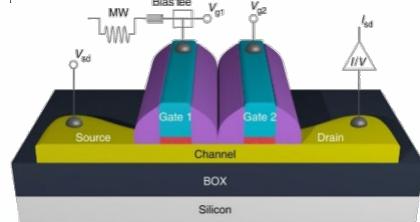
Honeywell

Photonics



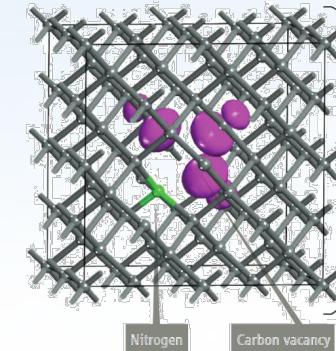
XANADU  $\Psi$  PsiQuantum

Silicon-Based Spin



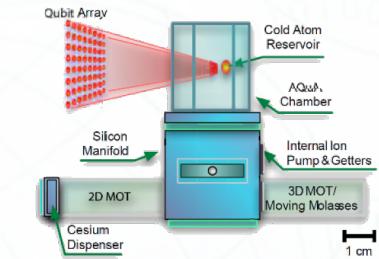
Silicon  
Quantum  
Computing

NV Center-in-Diamond

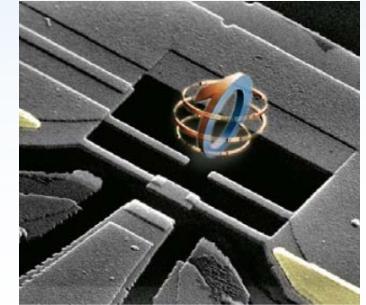


 QUANTUM  
BRILLIANCE

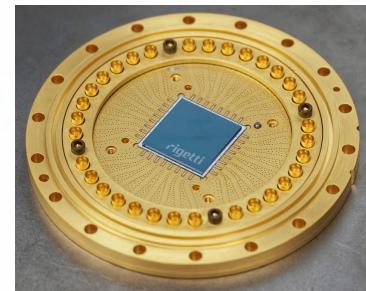
NMR



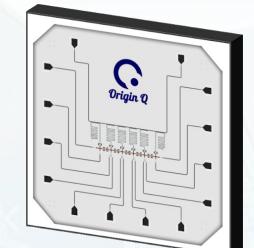
Superconducting







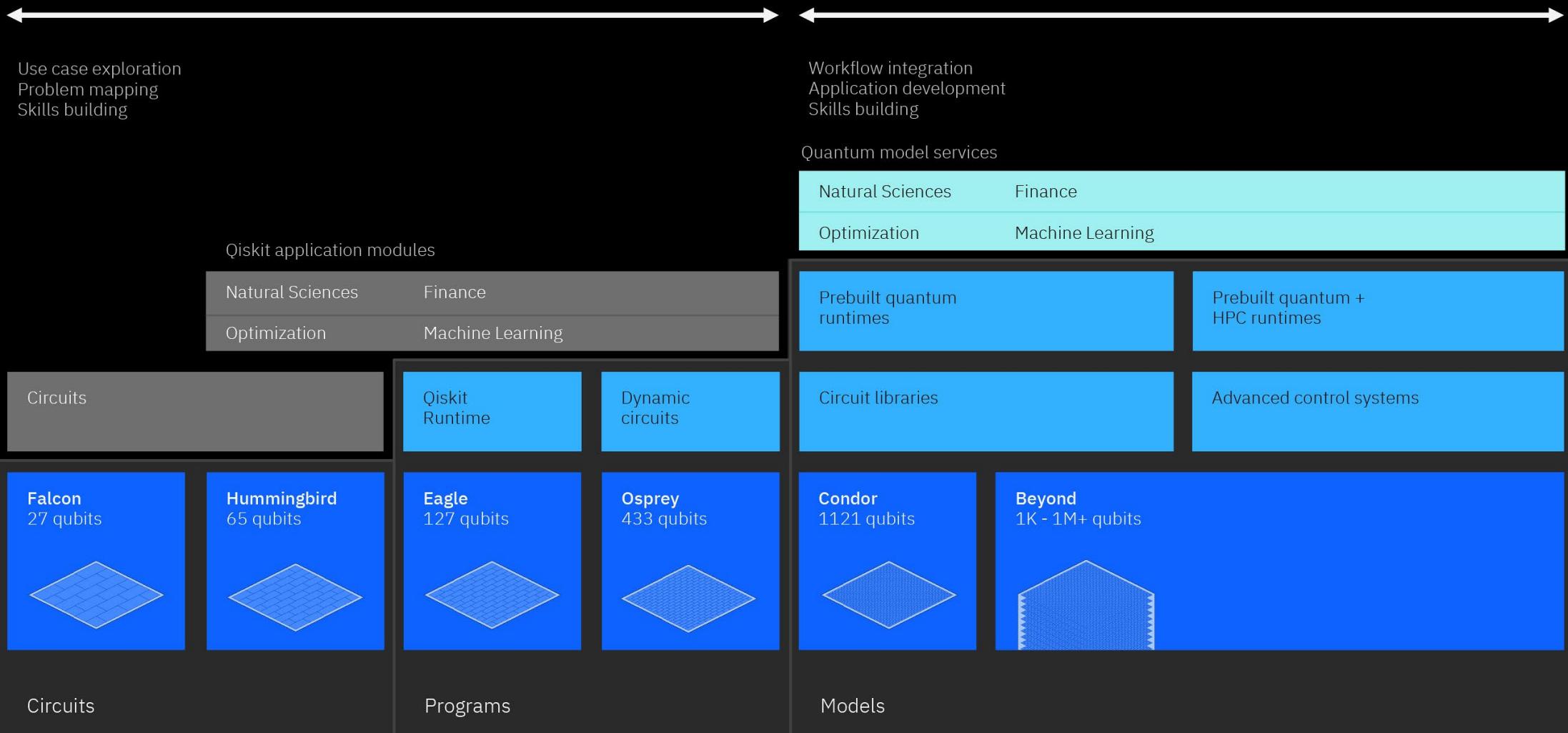
 本源量子  
Origin Quantum



# Development Roadmap

IBM Quantum

2019      2020      2021      2022      2023      2024      2025      2026+





Jeremy O'Brien

1,000,000  
qubits

Photonics is the only  
way to deliver

A useful quantum computer requires  
**at least a million qubits.**

Our quantum computer will be built using the  
**same industrial tools that produce your  
laptop.**

Error correction is at the centre of everything  
we do. It is the only known way to ensure  
that such a complex device can function  
reliably.

Thirty years ago photonic quantum computing was  
believed impossible. Twenty years ago, it was proved  
possible but dismissed as impractical. Today, after  
numerous architectural breakthroughs and advances in  
silicon photonics, PsiQuantum uniquely has a clear path  
to a useful quantum computer.

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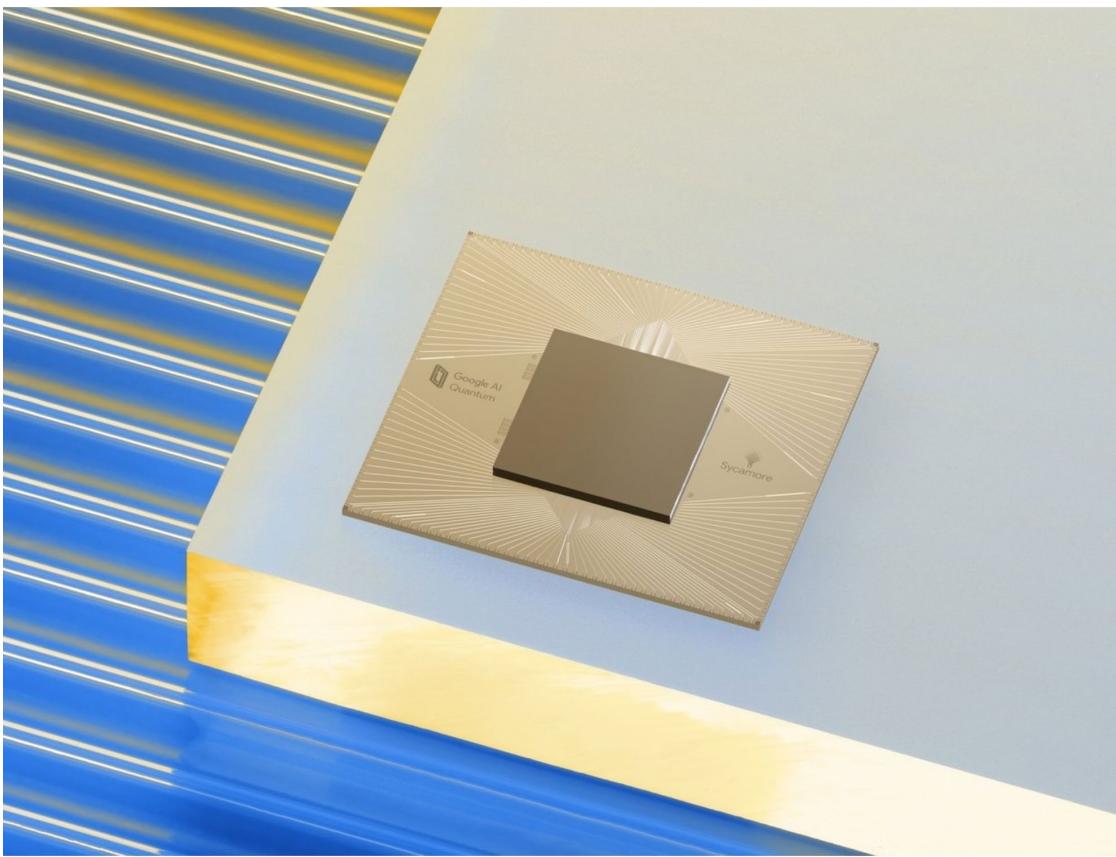
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CIO JOURNAL

## Google Aims for Commercial-Grade Quantum Computer by 2029

Tech giant is one of many companies racing to build a business around the nascent technology





QUANTUM SYSTEMS ACCELERATOR  
Catalyzing the Quantum Ecosystem



ENTROPICA  
LABS



ColdQuanta  
The Quantum Atomics Company



Alibaba Cloud Computing

riverlane

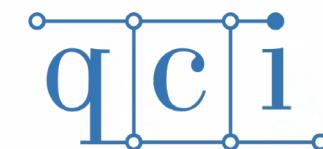
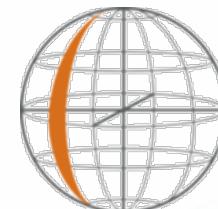


ISARA



kiutra

QUANTUM  
MOTION



PHASE CRAFT



Tencent 腾讯



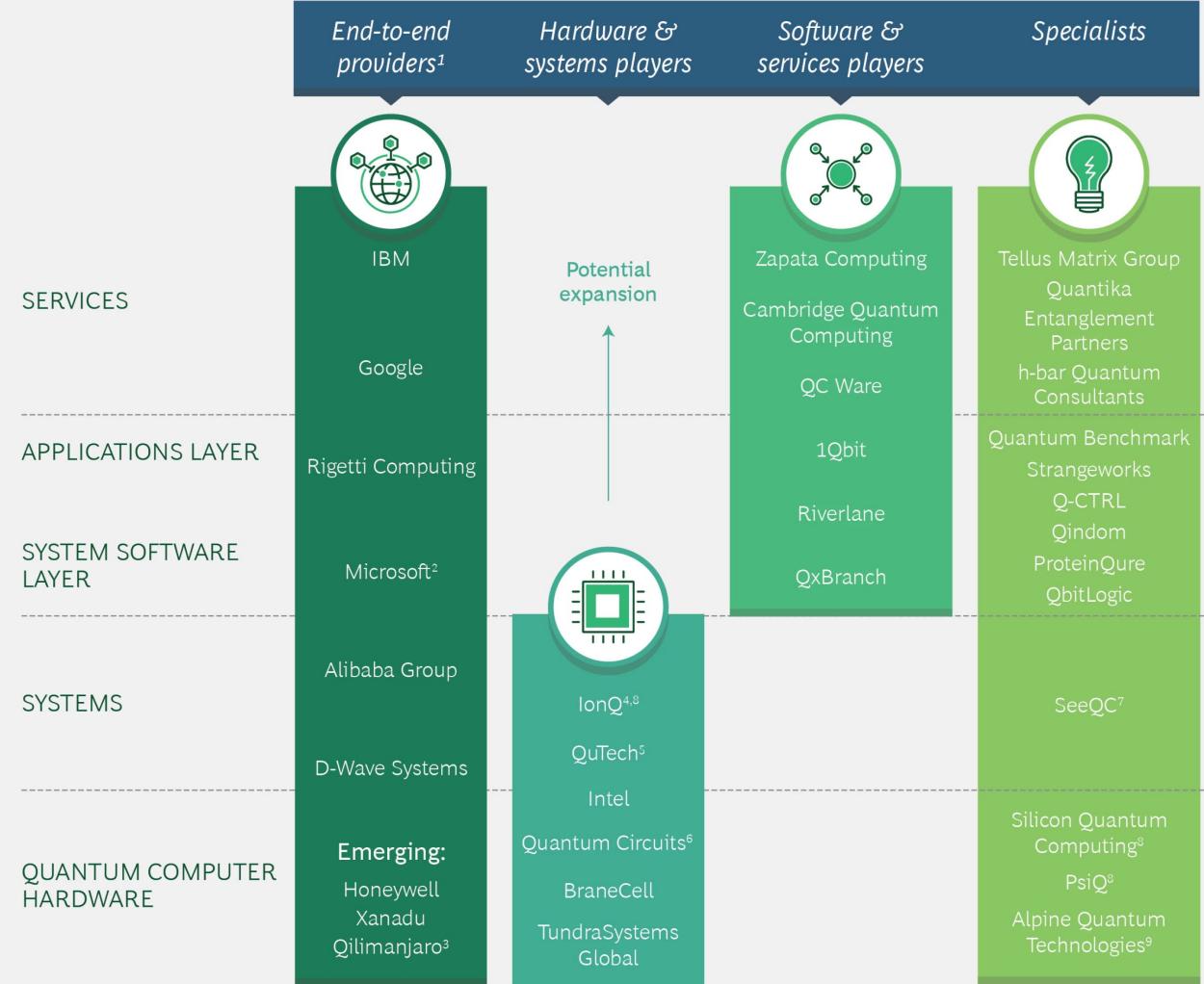
| KETS >

QUANTUM  
SECURITY

Sparrow  
Quantum



EXHIBIT 1 | Companies Assume Four Roles Across Layers of the Stack in the Quantum Computing Ecosystem



Sources: Quantum Computing Report ([quantumcomputingreport.com](http://quantumcomputingreport.com)); BCG analysis.

<sup>1</sup>Based on player's ambition with varying levels of maturity and service activities.

<sup>2</sup>Multiple technologies in the labs with focus on topological qubits.

<sup>3</sup>Qilimanjaro is a spinoff from the University of Barcelona.

<sup>4</sup>AWS is invested in IonQ.

<sup>5</sup>QuTech was founded by TU Delft and TNO, and has collaborations with Intel and Microsoft.

<sup>6</sup>Quantum Circuits (qci) is a spinoff from Yale University.

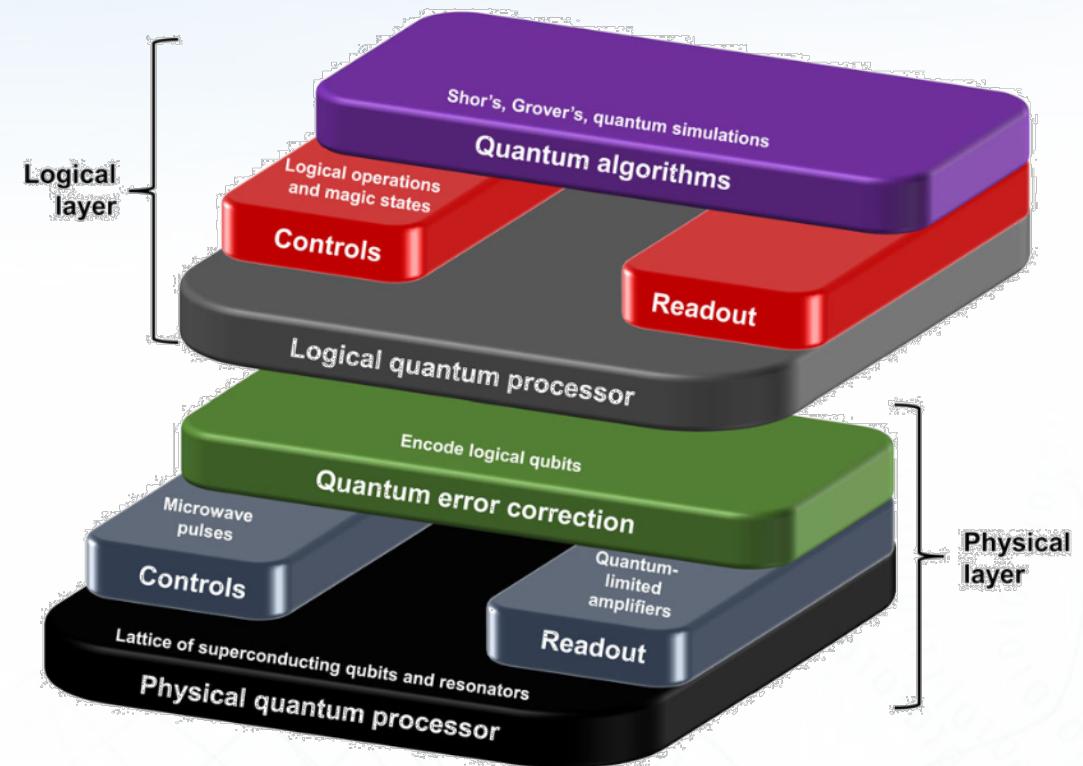
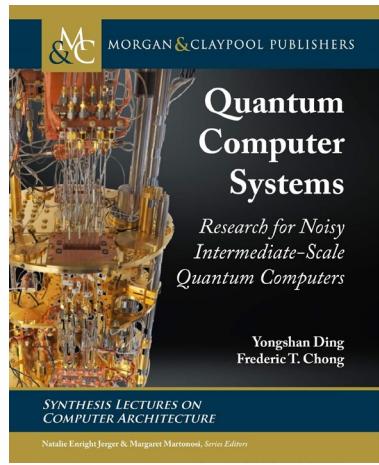
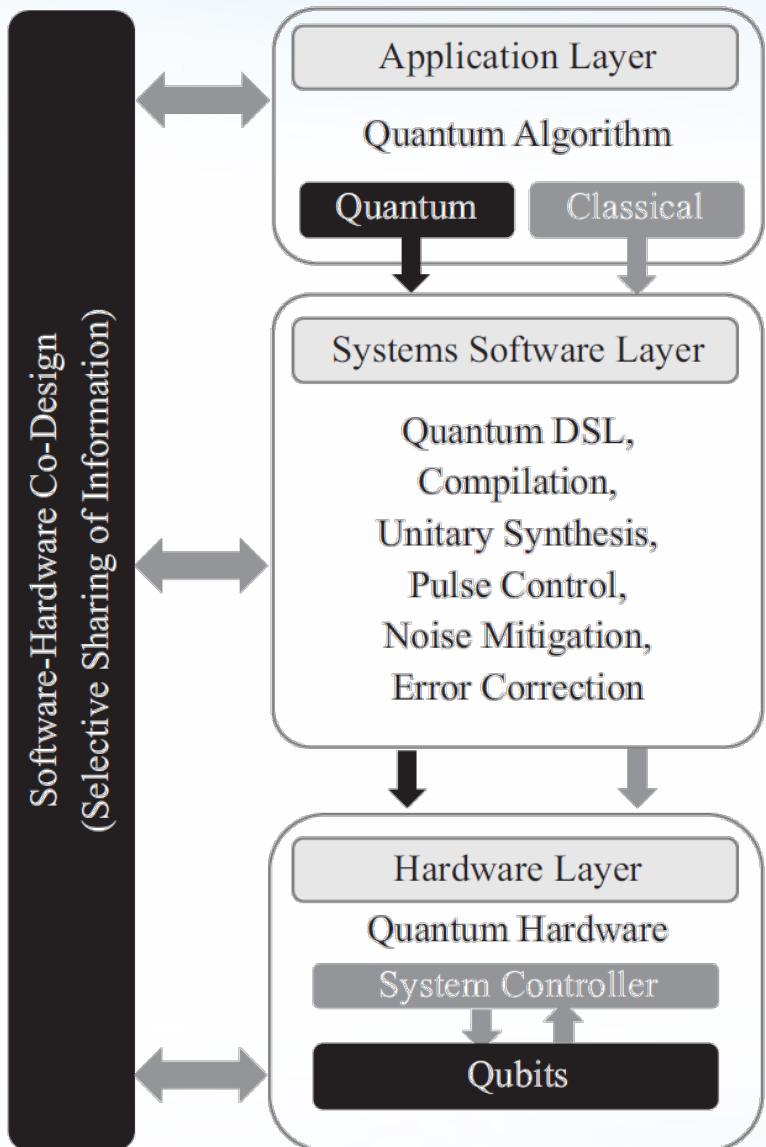
<sup>7</sup>SeeQC is a subsidiary of Hypres.

<sup>8</sup>Vision to become end-to-end provider.

<sup>9</sup>Alpine Quantum Technologies (AQT) is a spinoff from University of Innsbruck.



# Quantum Computer System Stacks

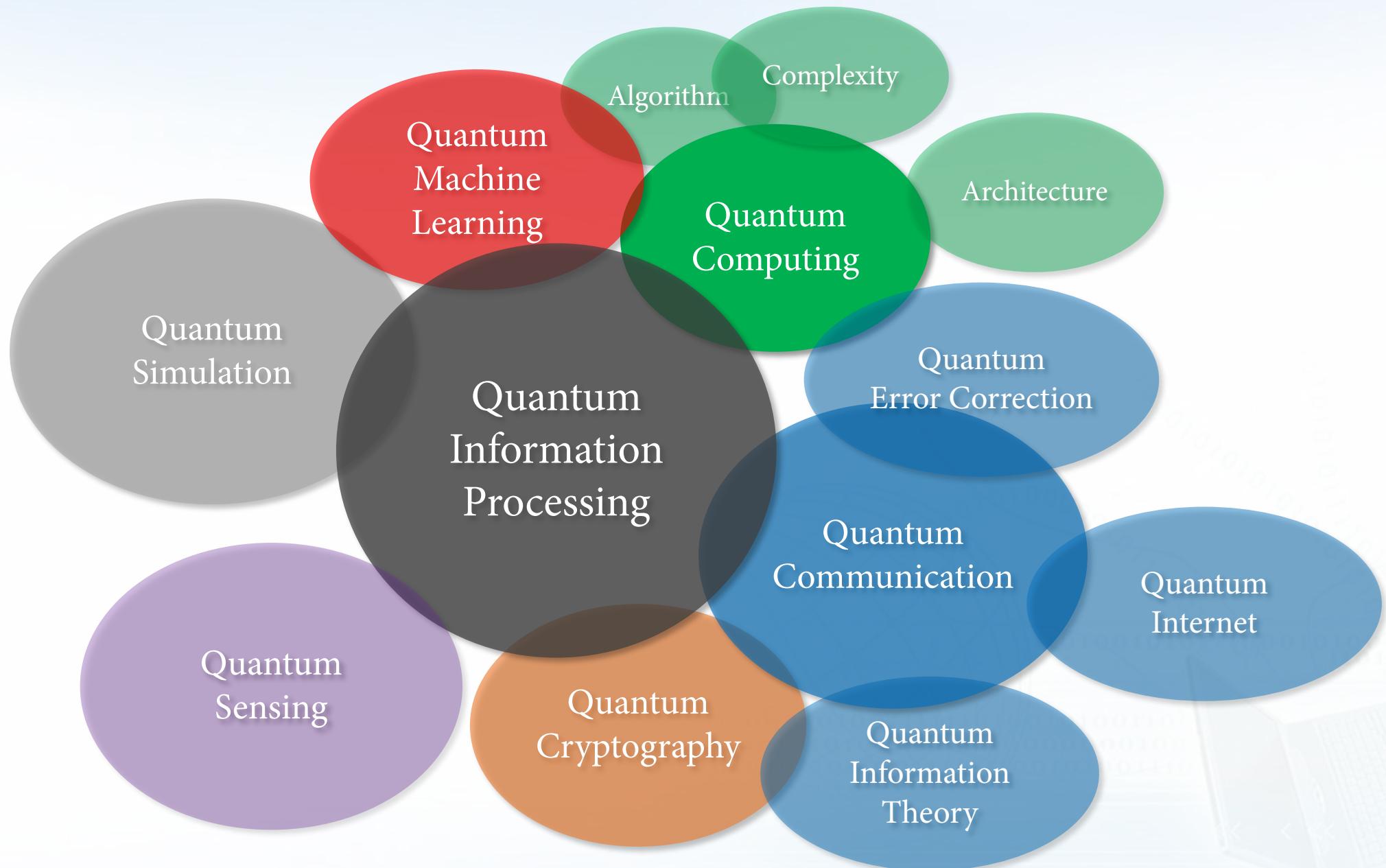


Review Article | Open Access | Published: 13 January 2017

## Building logical qubits in a superconducting quantum computing system

Jay M. Gambetta , Jerry M. Chow & Matthias Steffen

*npj Quantum Information* 3, Article number: 2 (2017) | Cite this article



# A Statistical Framework of Quantum Theory



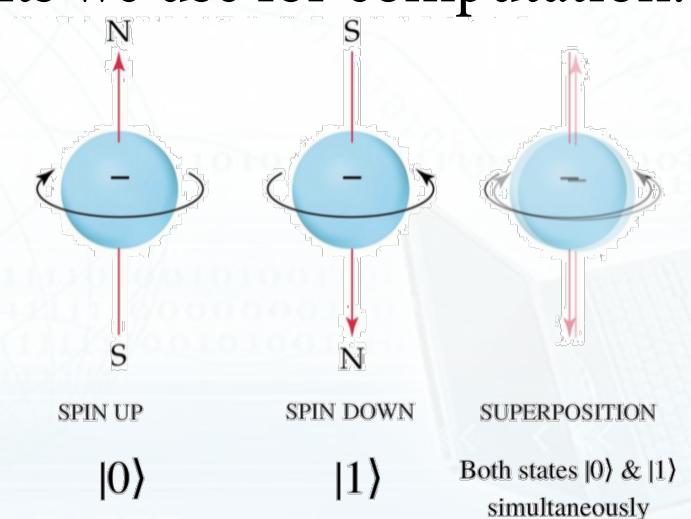
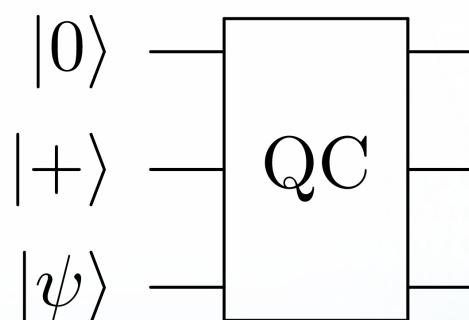
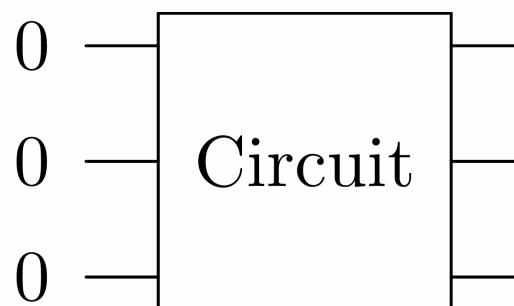
- ▶ **Preparation:** A preparation procedure determines the *state* of a system.
- ▶ **Evolution:** How is a quantum state *evolving*?
- ▶ **Measurement:** A measurement procedure produces some random outcomes.

# The Quantum Bit (Qubit)

- **Definition:** A **qubit** is the fundamental unit of quantum information.  
It is a *superposition* state represented by a linear combination of  $|0\rangle$  and  $|1\rangle$  in  $\mathbb{C}^2$ :

$$|\psi\rangle = a|0\rangle + b|1\rangle, \quad a, b \in \mathbb{C}, \quad |a|^2 + |b|^2 = 1$$

- Physically, a qubit can be realized by a two-state (two-level) quantum-mechanical system e.g. a spinning electron or polarized light.
- A *quantum register* (a quantum system) is a collection of qubits we use for computation.



# Vector Representation (Dirac Notation) for a Qubit

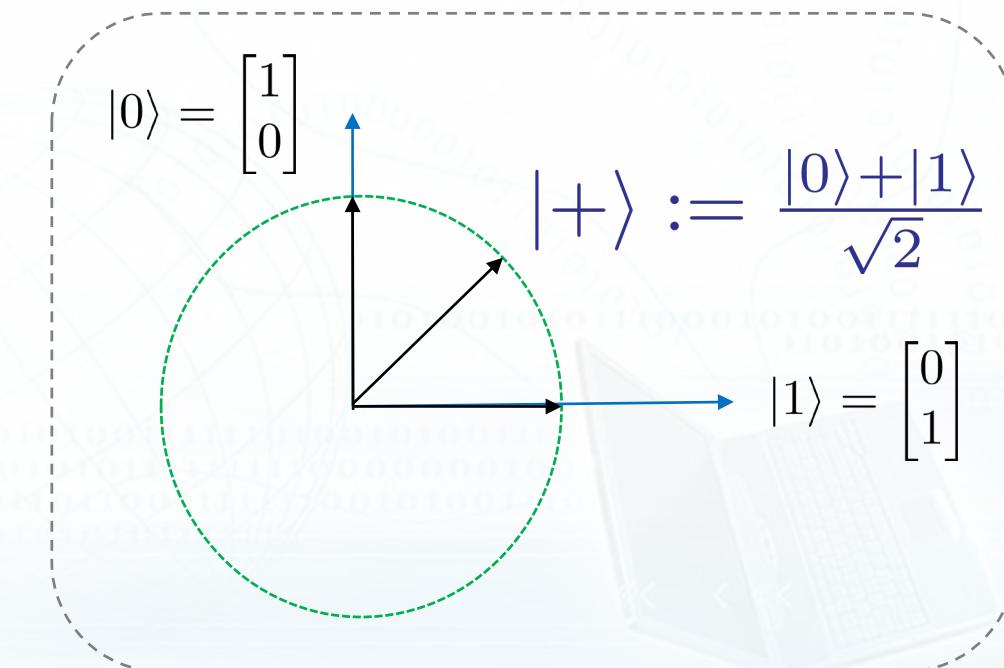
- $|0\rangle = \begin{bmatrix} 1 \\ 0 \end{bmatrix}, |1\rangle = \begin{bmatrix} 0 \\ 1 \end{bmatrix} \Rightarrow |\psi\rangle = a|0\rangle + b|1\rangle = \begin{bmatrix} a \\ b \end{bmatrix} \in \mathbb{C}^2, |a|^2 + |b|^2 = 1$

- Bra-Ket notation: the Ket vectors  $|\psi\rangle = \begin{bmatrix} a \\ b \end{bmatrix}, |\phi\rangle = \begin{bmatrix} c \\ d \end{bmatrix}$

Paul Dirac (1902-1984)

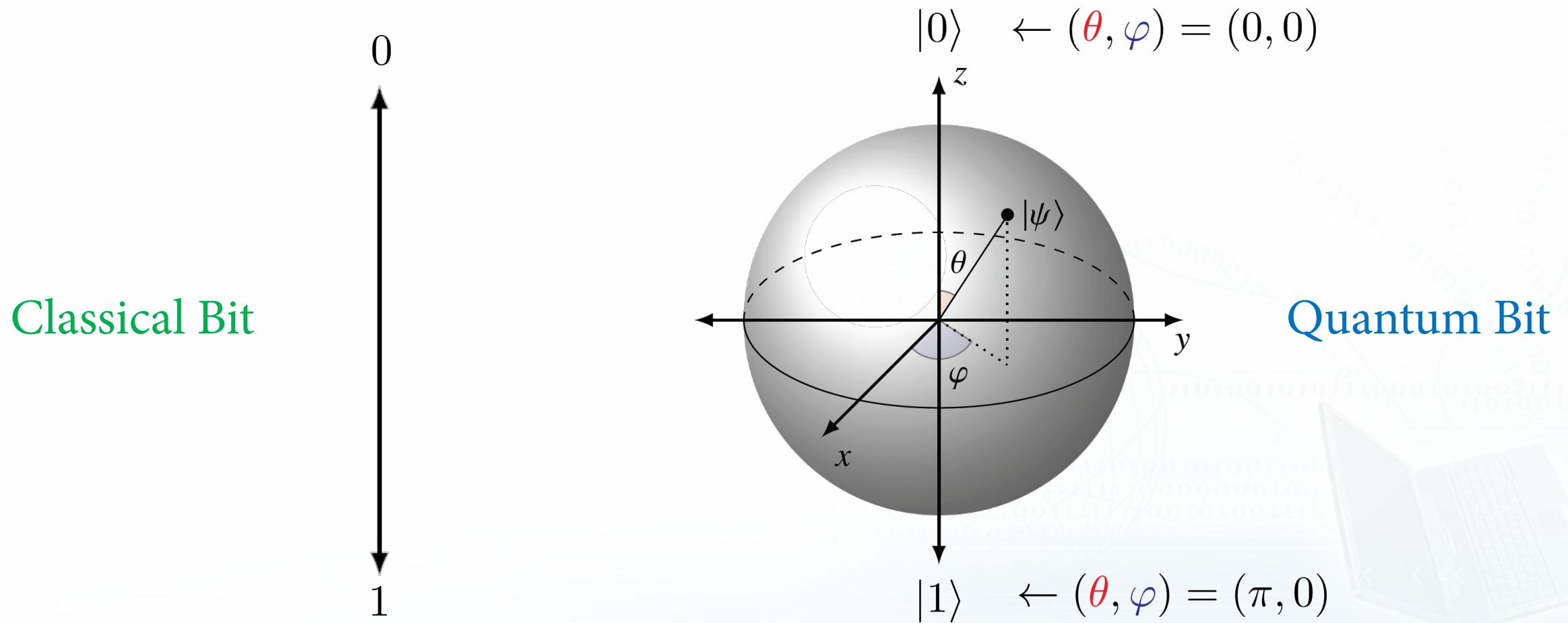
- Inner product:  $\langle\phi| := |\phi\rangle^\dagger = [c^*, d^*]$

$$\Rightarrow \langle\phi|\psi\rangle = [c^*, d^*] \begin{bmatrix} a \\ b \end{bmatrix} = c^*a + d^*b \in \mathbb{C}$$



# Bloch-Sphere Representation for a Qubit

$$\Rightarrow |\psi\rangle = \cos\left(\frac{\theta}{2}\right)|0\rangle + \sin\left(\frac{\theta}{2}\right)e^{i\varphi}|1\rangle, \quad \theta \in [0, \pi], \varphi \in [0, 2\pi]$$



# Quantum Measurement

- A **quantum measurement**  (with respect to the **computational basis**  $\{|0\rangle, |1\rangle\}$ ) gives you the readout of ‘0’ or ‘1’ with certain probability

- The Born rule:  $|\psi\rangle = a|0\rangle + b|1\rangle$  

$$\Pr(0) = |\langle 0|\psi \rangle|^2 = \left| [1 \quad 0] \begin{bmatrix} a \\ b \end{bmatrix} \right|^2 = |a|^2$$

$$\Pr(1) = |\langle 1|\psi \rangle|^2 = \left| [0 \quad 1] \begin{bmatrix} a \\ b \end{bmatrix} \right|^2 = |b|^2$$



Max Born (1882-1970)

- After measurement, a qubit is forced to **collapse** (irreversibly) through projection to one of the basis

# Single-Qubit Gates (1/2)

- In gate-based quantum computers, a quantum operation is a *unitary operation*.
- The quantum  $X$  gate is given by the Pauli  $X$  matrix
  - It is called the *NOT* gate or the “*bit flip*” gate since it rotates  $\pi$  around the  $x$ -axis.

$$X := |0\rangle\langle 1| + |1\rangle\langle 0| = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \quad \xrightarrow{\text{Matrix representation}} \quad \Rightarrow X|0\rangle = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \begin{bmatrix} 1 \\ 0 \end{bmatrix} = \begin{bmatrix} 0 \\ 1 \end{bmatrix} = |1\rangle$$

- The quantum  $Z$  gate rotates  $\pi$  around the  $z$ -axis     $Z := |0\rangle\langle 0| - |1\rangle\langle 1|$ 
  - It is called the “*phase flip*” gate     $\Rightarrow Z|\psi\rangle = r_1|0\rangle + r_2 e^{i(\pi+\psi)}|1\rangle$
- The quantum  $Y$  gate rotates  $\pi$  around the  $y$ -axis.
  - It does the bit flip and phase flip at the same time.



Wolfgang Pauli (1900-1958)

# Single-Qubit Gates (2/2)

$$H := \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}$$

- The Hadamard gate changes the basis from  $\{|0\rangle, |1\rangle\}$  to  $\{|+\rangle, |-\rangle\}$   
→ It creates *superposition*; and it is self-inverse:  $HH = I$

$$|b\rangle \xrightarrow{H} \frac{1}{\sqrt{2}} (|0\rangle + (-1)^b |1\rangle), \quad b \in \{0, 1\}$$



Jacques Hadamard (1865-1963)

- The quantum  $R_\varphi^Z$  gate rotates  $\varphi$  around the  $z$ -axis  $R_\varphi^Z := \begin{pmatrix} 1 & 0 \\ 0 & e^{i\varphi} \end{pmatrix}$
- The quantum  $R_\varphi^X$  gate rotates  $\varphi$  around the  $x$ -axis  $R_\varphi^X := \begin{pmatrix} \cos(\frac{\varphi}{2}) & -i \sin(\frac{\varphi}{2}) \\ -i \sin(\frac{\varphi}{2}) & \cos(\frac{\varphi}{2}) \end{pmatrix}$
- The quantum  $R_\varphi^Y$  gate rotates  $\varphi$  around the  $y$ -axis  $R_\varphi^Y := \begin{pmatrix} \cos(\frac{\varphi}{2}) & -\sin(\frac{\varphi}{2}) \\ \sin(\frac{\varphi}{2}) & \cos(\frac{\varphi}{2}) \end{pmatrix}$

# Just a bit math...

- Definition. *Tensor product* of matrices  $A := \begin{pmatrix} a_{1,1} & a_{1,2} \\ a_{2,1} & a_{2,2} \end{pmatrix}$ ,  $B := \begin{pmatrix} b_{1,1} & b_{1,2} \\ b_{2,1} & b_{2,2} \end{pmatrix}$

$$A \otimes B = \begin{pmatrix} a_{1,1} & a_{1,2} \\ a_{2,1} & a_{2,2} \end{pmatrix} \otimes B$$

$$:= \begin{pmatrix} a_{1,1}B & a_{1,2}B \\ a_{2,1}B & a_{2,2}B \end{pmatrix} = \begin{pmatrix} a_{1,1} \begin{pmatrix} b_{1,1} & b_{1,2} \\ b_{2,1} & b_{2,2} \end{pmatrix} & a_{1,2} \begin{pmatrix} b_{1,1} & b_{1,2} \\ b_{2,1} & b_{2,2} \end{pmatrix} \\ a_{2,1} \begin{pmatrix} b_{1,1} & b_{1,2} \\ b_{2,1} & b_{2,2} \end{pmatrix} & a_{2,2} \begin{pmatrix} b_{1,1} & b_{1,2} \\ b_{2,1} & b_{2,2} \end{pmatrix} \end{pmatrix}$$

$$= \begin{pmatrix} a_{1,1}b_{1,1} & a_{1,1}b_{1,2} & a_{1,2}b_{1,1} & a_{1,2}b_{1,2} \\ a_{1,1}b_{2,1} & a_{1,1}b_{2,2} & a_{1,2}b_{2,1} & a_{1,2}b_{2,2} \\ a_{2,1}b_{1,1} & a_{2,1}b_{1,2} & a_{2,2}b_{1,1} & a_{2,2}b_{1,2} \\ a_{2,1}b_{2,1} & a_{2,1}b_{2,2} & a_{2,2}b_{2,1} & a_{2,2}b_{2,2} \end{pmatrix}$$

# More Qubits – Quantum Entanglement (1/2)

- General 2-qubit state:

$$|\psi\rangle = a_{00}|00\rangle + a_{01}|01\rangle + a_{10}|10\rangle + a_{11}|11\rangle \in \mathbb{C}^4 \quad \sum_{i,j \in \{0,1\}} |a_{ij}|^2 = 1$$

Probability amplitude

- A two-qubit is represented by a unit vector in *four*-dimensional linear space  $\mathbb{C}^{2 \times 2}$

→ The computational basis:

$$|00\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix} \quad |01\rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix} \quad |10\rangle = \begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \end{pmatrix} \quad |11\rangle = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix}$$

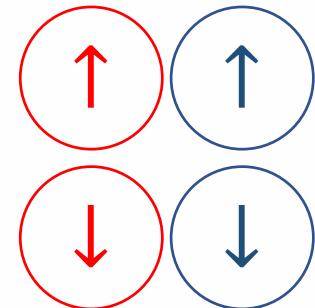
- Tensor product:  $|01\rangle \equiv |0\rangle \otimes |1\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \otimes \begin{pmatrix} 0 \\ 1 \end{pmatrix} := \begin{pmatrix} 1 & \begin{pmatrix} 0 \\ 1 \\ 0 \\ 1 \end{pmatrix} \\ 0 & \begin{pmatrix} 0 \\ 1 \end{pmatrix} \end{pmatrix} = \begin{pmatrix} 1 \times 0 \\ 1 \times 1 \\ 0 \times 0 \\ 0 \times 1 \end{pmatrix} = \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix}$

# More Qubits – Quantum Entanglement (1/2)

- **Entangled state:** there are states that cannot be expressed as the product form, i.e.

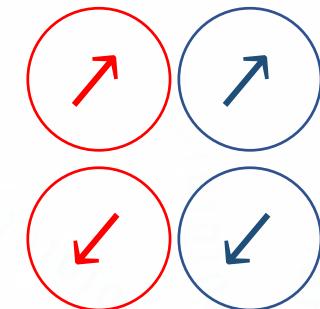
$$\nexists |q_1\rangle, |q_2\rangle \in \mathbb{C}^2, \text{ s.t. } |\psi\rangle = |q_1\rangle \otimes |q_2\rangle$$

$\begin{cases} \text{with } \frac{1}{2} \text{ probability,} \\ \text{with } \frac{1}{2} \text{ probability,} \end{cases}$



or

$\begin{cases} \text{with } \frac{1}{2} \text{ probability,} \\ \text{with } \frac{1}{2} \text{ probability,} \end{cases}$



Einstein, Podolsky, and Rosen

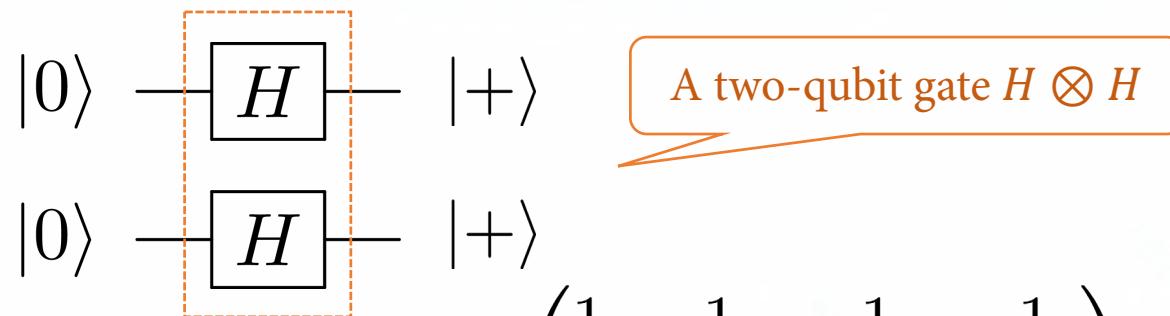
$$\begin{aligned} |\Phi^+\rangle &= \frac{|00\rangle + |11\rangle}{\sqrt{2}} \\ &= \frac{|+++ \rangle + |---\rangle}{\sqrt{2}} \end{aligned}$$



John S. Bell (1928-1990)

# Multi-Qubit Gates (1/3)

- A qubit gate has a 2 by 2 unitary matrix in a given basis.  
→ For an  $n$ -qubit gate, the matrix is  $2^n$  by  $2^n$  (tensor product of matrices).



$$H^{\otimes 2} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} \otimes \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} = \frac{1}{2} \begin{pmatrix} 1 & 1 & 1 & 1 \\ 1 & -1 & 1 & -1 \\ 1 & 1 & -1 & -1 \\ 1 & -1 & -1 & 1 \end{pmatrix}$$

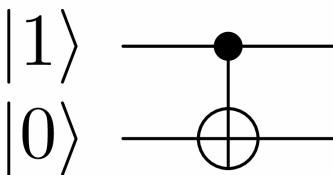
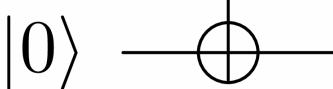
$$\Rightarrow H^{\otimes 2}|00\rangle = \frac{1}{2} \begin{pmatrix} 1 \\ 1 \\ 1 \\ 1 \end{pmatrix} = |+\rangle \otimes |+\rangle$$

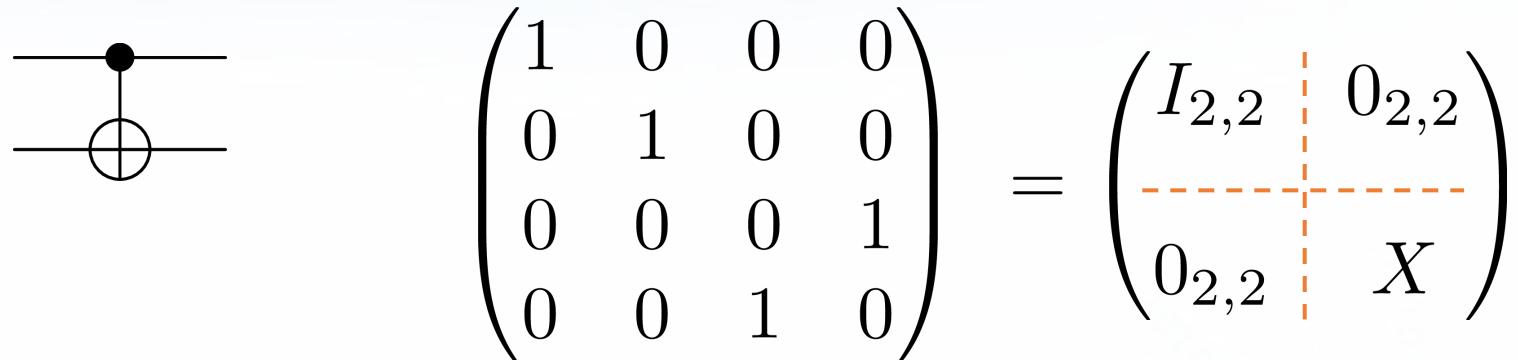
$$(A \otimes B)\mathbf{a} \otimes \mathbf{b} = (A\mathbf{a}) \otimes (B\mathbf{b})$$

## Multi-Qubit Gates (2/3)

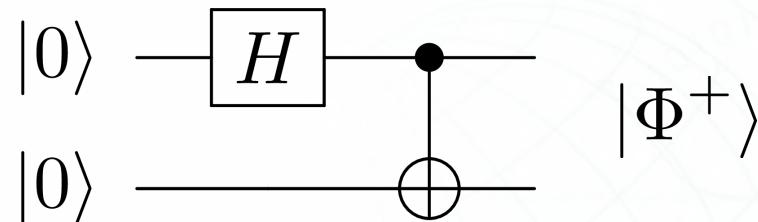
- The previous example is a 2-qubit gate of the *product form*.

- Controlled-NOT gate:

Ex.  $|1\rangle$    $|1\rangle$   
 $|0\rangle$    $|1\rangle$


$$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix} = \begin{pmatrix} I_{2,2} & & & 0_{2,2} \\ & X & & \\ 0_{2,2} & & & \\ & & & \end{pmatrix}$$

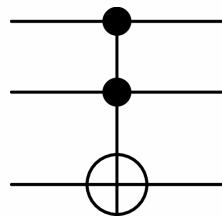
- Used to prepare the Bell state:



$$|00\rangle \xrightarrow{H \otimes I} \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle) \otimes |0\rangle = \frac{1}{\sqrt{2}}(|00\rangle + |10\rangle) \xrightarrow{CNOT} \frac{1}{\sqrt{2}}(|00\rangle + |11\rangle)$$

# Multi-Qubit Gates (3/3)

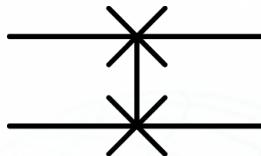
- Toffoli gate (CCNOT gate)  
→ *universal* classically



Truth Table

$ 000\rangle$	$\mapsto  000\rangle$
$ 001\rangle$	$\mapsto  001\rangle$
$ 010\rangle$	$\mapsto  010\rangle$
$ 011\rangle$	$\mapsto  011\rangle$
$ 100\rangle$	$\mapsto  100\rangle$
$ 101\rangle$	$\mapsto  101\rangle$
$ 110\rangle$	$\mapsto  111\rangle$
$ 111\rangle$	$\mapsto  110\rangle$

- Swap gate



$$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

- *Universal* quantum gates sets:  $\{CNOT, T, H\}$  or  $\{CCNOT, H\}$

# Elementary Quantum Gates

- Pauli gates  $X := \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$   $Y := \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$   $Z := \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$

- Rotation gates

$$R_x(\phi) := e^{-i\frac{\phi}{2}X} = \begin{pmatrix} \cos(\frac{\phi}{2}) & -i\sin(\frac{\phi}{2}) \\ -i\sin(\frac{\phi}{2}) & \cos(\frac{\phi}{2}) \end{pmatrix}$$

$$R_y(\phi) := e^{-i\frac{\phi}{2}Y} = \begin{pmatrix} \cos(\frac{\phi}{2}) & -\sin(\frac{\phi}{2}) \\ \sin(\frac{\phi}{2}) & \cos(\frac{\phi}{2}) \end{pmatrix}$$

Phase gate

$$R_z(\phi) := e^{-i\frac{\phi}{2}Z} = \begin{pmatrix} 1 & 0 \\ 0 & e^{i\phi} \end{pmatrix} \quad S := R_z(\frac{\pi}{2}) \quad T := R_z(\frac{\pi}{4})$$

- CNOT gate

$$\begin{array}{c} |c\rangle \xrightarrow{\text{---}} |c\rangle \\ |t\rangle \xrightarrow{\text{---}} |c \oplus t\rangle \end{array} \quad \begin{pmatrix} I_2 & 0 \\ 0 & X \end{pmatrix}$$

- Hadamard gates

$$H := \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}$$

- Controlled-Z gates

$$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix}$$

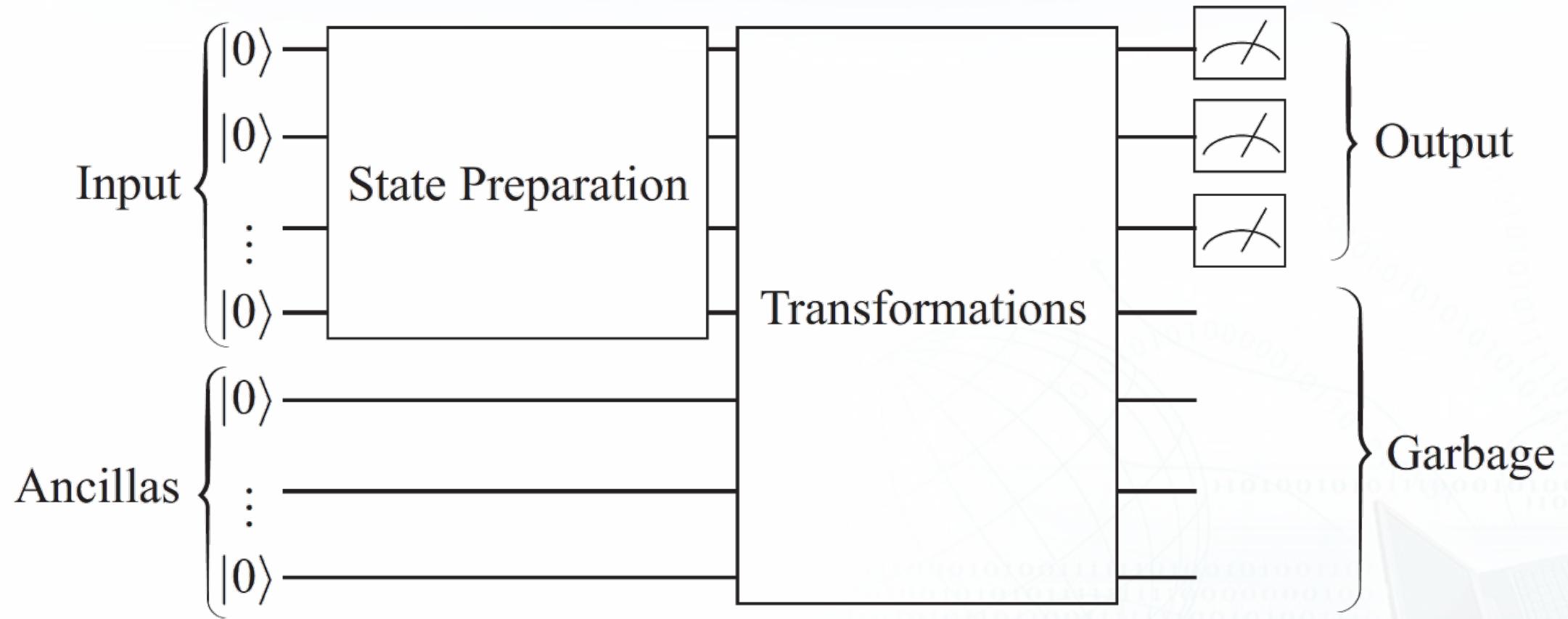
- Swap gate  $|\psi\rangle|\phi\rangle \mapsto |\phi\rangle|\psi\rangle$

- Toffoli (CCNOT) gate

$$\begin{array}{ccccc} |c_1\rangle & \xrightarrow{\text{---}} & |c_1\rangle & & \begin{pmatrix} I_3 & 0 & 0 \\ 0 & I_3 & 0 \\ 0 & 0 & X \end{pmatrix} \\ |c_2\rangle & \xrightarrow{\text{---}} & |c_2\rangle & & \xrightarrow{\text{---}} \\ |t\rangle & \xrightarrow{\text{---}} & |(c_1 \wedge c_2) \oplus t\rangle & & \xrightarrow{\text{---}} \end{array}$$

$$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

# Gate-Based Quantum Computation



# Efficiently Preparing Superposition States

- We can create a superposition of *exponentially many* terms with only a *linear* number of the Hadamard gates.

The diagram illustrates a quantum circuit with three parallel horizontal lines representing qubits. Each qubit starts in the  $|0\rangle$  state. A Hadamard gate ( $H$ ) is applied to each qubit. The resulting state for each qubit is  $|+\rangle$ . A large curly brace on the right side of the circuit groups all three qubits together, indicating that the final state is a multi-qubit superposition. To the right of the brace, the expression  $\left(\frac{1}{\sqrt{2}}(|0\rangle + |1\rangle)\right)^{\otimes n}$  is shown, where  $n$  represents the number of qubits (in this case, 3).

$$\left( \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle) \right)^{\otimes n}$$

$$H^{\otimes n} |0\rangle^{\otimes n} = |+\rangle^{\otimes n} = \frac{1}{\sqrt{2^n}} \sum_{x \in \{0,1\}^n} |x\rangle$$

# The Quantum Oracle & Quantum Parallelism

- The *quantum oracle* for any Boolean function  $f: \{0,1\}^n \rightarrow \{0,1\}^m$  is given by the quantum gate  $U_f: |x\rangle|y\rangle \mapsto |x\rangle|y \oplus f(x)\rangle$ ,  $\forall x \in \{0,1\}^n$ ,  $\forall y \in \{0,1\}^m$ .
- We set the input register to an equal superposition of all  $2^n$  possible  $n$ -bit strings:

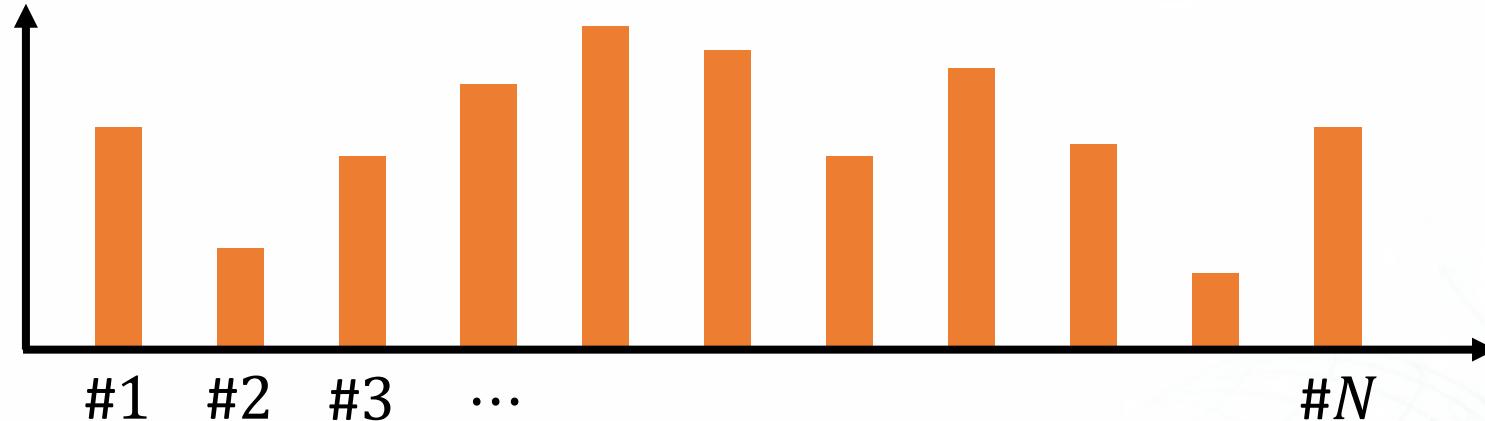
$$U_f : \frac{1}{\sqrt{2^n}} \sum_{x \in \{0,1\}^n} |x\rangle|0\rangle \mapsto \frac{1}{\sqrt{2^n}} \sum_{x \in \{0,1\}^n} |x\rangle|f(x)\rangle$$

- In *one* run of the protocol, we obtain a final state which depends on all of the function values. On the other hand, we would need *exponentially* many queries to have full access to the function  $f$ .

# Quantum Computing – Unstructured Search



- ▶ Searching in an unstructured list with size  $N$



Lov Grover (1961 –)

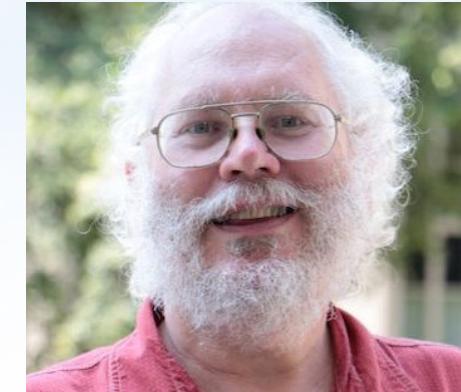
The best classical algorithm requires number of queries proportional to  $N$

→ Lov Grover (1996) proposed a quantum algorithm requires  $\approx \sqrt{N}$  queries

# Quantum Computing – Factorization

- Integer Factorization used in the RSA cryptography system

Example:  $\underbrace{463570199875051}_{\approx 2^{49}} = 27644437 \times 16769023$



Peter Shor (1959 -)

The computational complexity of the best known classical algorithm scales *exponentially* in the number of bits of the integer.

→ Peter Shor (1994) invented a *polynomial-time* quantum algorithm

- Other cryptosystem such as the *Diffie–Hellman key exchange security* (based on the hardness of the *discrete logarithm problem*) and the *Elliptic curve cryptography* can be broke in polytime by applying Shor's idea.

# Relations – A Glimpse of The Complexity Zoo

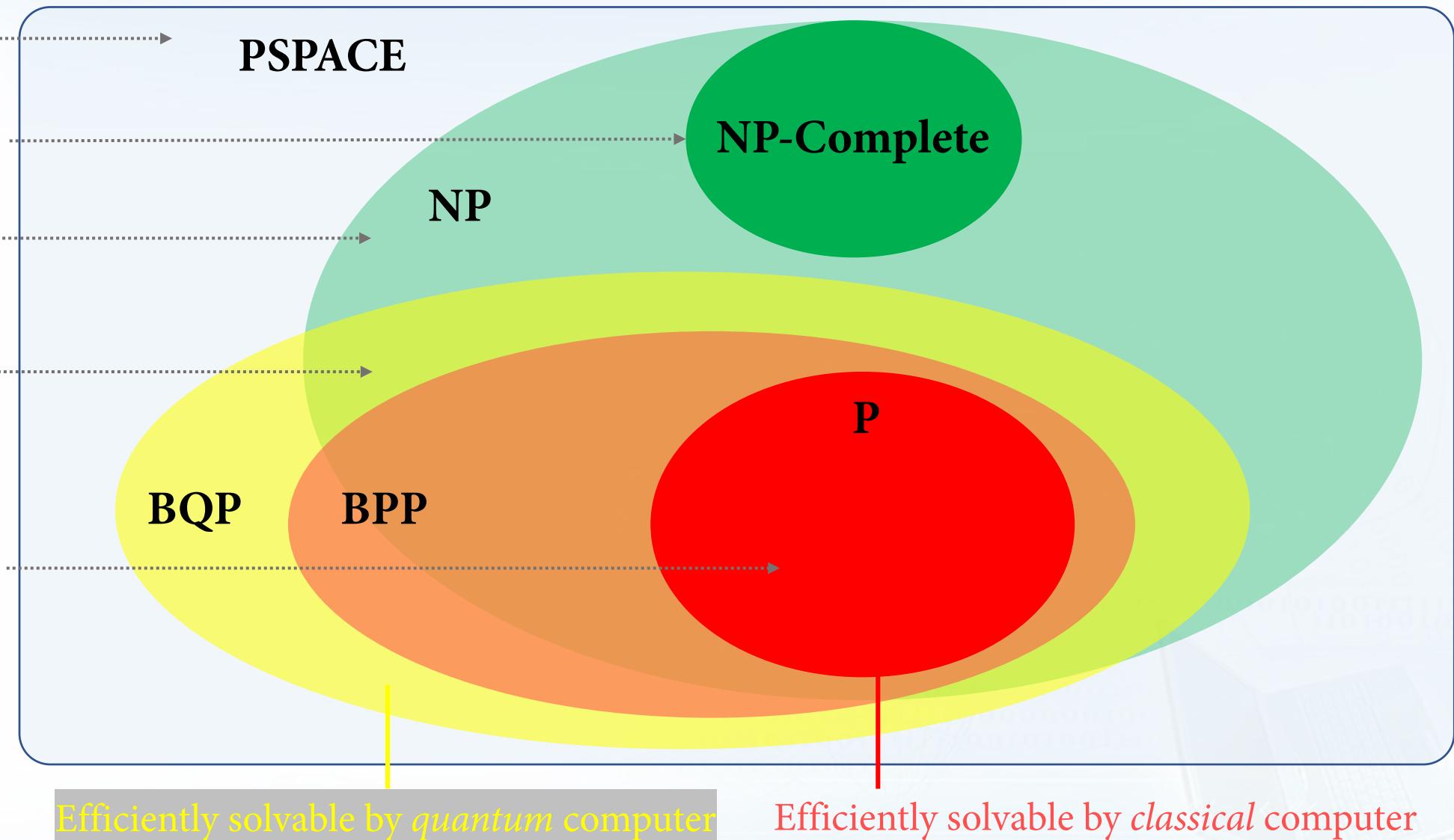
$n \times n$  Chess/Go

SAT,  $n \times n$  Sudoku  
Travelling salesman

Graph Isomorphism

Integer factorization,  
Discrete logarithm

Multiplication,  
Primality, etc.



nature &gt; letters &gt; article

Published: 09 August 2017

## Ground-to-satellite quantum teleportation

Ji-Gang Ren, Ping Xu, [...] Jian-Wei Pan *Nature* 549, 70–73(2017) | Cite this article**SHARE**

RESEARCH ARTICLES | PHYSICS



## Satellite-based entanglement distribution over 1200 kilometers

 Juan Yin<sup>1,2</sup>, Yuan Cao<sup>1,2</sup>, Yu-Huai Li<sup>1,2</sup>, Sheng-Kai Liao<sup>1,2</sup>,  Liang Zhang<sup>2,3</sup>, Ji-Gang Ren<sup>1,2</sup>, Wen-Qi Cai<sup>1,2</sup>, Wei-Yue Liu<sup>1</sup>...

+ See all authors and affiliations

Science 16 Jun 2017:  
Vol. 356, Issue 6343, pp. 1140-1144  
DOI: 10.1126/science.aan3211

PHYSICAL REVIEW LETTERS 120, 030501 (2018)

Editors' Suggestion

Featured in Physics

## Satellite-Relayed Intercontinental Quantum Network

Sheng-Kai Liao,<sup>1,2</sup> Wen-Qi Cai,<sup>1,2</sup> Johannes Handsteiner,<sup>3,4</sup> Bo Liu,<sup>4,5</sup> Juan Yin,<sup>1,2</sup> Liang Zhang,<sup>2,6</sup> Dominik Rauch,<sup>3,4</sup> Matthias Fink,<sup>4</sup> Ji-Gang Ren,<sup>1,2</sup> Wei-Yue Liu,<sup>1,2</sup> Yang Li,<sup>1,2</sup> Qi Shen,<sup>1,2</sup> Yuan Cao,<sup>1,2</sup> Feng-Zhi Li,<sup>1,2</sup> Jian-Feng Wang,<sup>7</sup> Yong-Mei Huang,<sup>8</sup> Lei Deng,<sup>9</sup> Tao Xi,<sup>10</sup> Lu Ma,<sup>11</sup> Tai Hu,<sup>12</sup> Li Li,<sup>1,2</sup> Nai-Le Liu,<sup>1,2</sup> Franz Koidl,<sup>13</sup> Peiyuan Wang,<sup>13</sup> Yu-Ao Chen,<sup>1,2</sup> Xiang-Bin Wang,<sup>2</sup> Michael Steindorfer,<sup>13</sup> Georg Kirchner,<sup>13</sup> Chao-Yang Lu,<sup>1,2</sup> Rong Shu,<sup>2,6</sup> Rupert Ursin,<sup>3,4</sup> Thomas Scheidl,<sup>3,4</sup> Cheng-Zhi Peng,<sup>1,2</sup> Jian-Yu Wang,<sup>2,6</sup> Anton Zeilinger,<sup>3,4</sup> and Jian-Wei Pan<sup>1,2</sup>

nature &gt; articles &gt; article

Published: 09 August 2017

## Satellite-to-ground quantum key distribution

Sheng-Kai Liao, Wen-Qi Cai, [...] Jian-Wei Pan *Nature* 549, 43–47(2017) | Cite this article

nature &gt; articles &gt; article

Article | Published: 15 June 2020

## Entanglement-based secure quantum cryptography over 1,120 kilometres

Juan Yin, Yu-Huai Li, Sheng-Kai Liao, Meng Yang, Yuan Cao, Liang Zhang, Ji-Gang Ren, Wen-Qi Cai, Wei-Yue Liu, Shuang-Lin Li, Rong Shu, Yong-Mei Huang, Lei Deng, Li Li, Qiang Zhang, Nai-Le Liu, Yu-Ao Chen, Chao-Yang Lu, Xiang-Bin Wang, Feihu Xu, Jian-Yu Wang, Cheng-Zhi Peng , Artur K. Ekert & Jian-Wei Pan 

*Nature* 582, 501–505(2020) | Cite this article

**SHARE****REPORT**

# Quantum computational advantage using photons

Han-Sen Zhong<sup>1,2,\*</sup>, Hui Wang<sup>1,2,\*</sup>, Yu-Hao Deng<sup>1,2,\*</sup>, Ming-Cheng Chen<sup>1,2,\*</sup>, Li-Chao Peng<sup>1,2</sup>, Yi-Han Luo<sup>1,2</sup>, Jian Qin<sup>1,2</sup>, Dian Wu<sup>1,2</sup>, Xing Ding<sup>1,2</sup>, Yi Hu<sup>1,2</sup>, Peng Hu<sup>3</sup>, Xiao-Yan Yang<sup>3</sup>, Wei-Jun Zhang<sup>3</sup>, Hao Li<sup>3</sup>, Yuxuan Li<sup>4</sup>, Xiao Jiang<sup>1,2</sup>, Lin Gan<sup>4</sup>, Guangwen Yang<sup>4</sup>, Lixing You<sup>3</sup>, Zhen Wang<sup>3</sup>, Li Li<sup>1,2</sup>, Nai-Le Liu<sup>1,2</sup>, Chao-Yang Lu<sup>1,2</sup>, Jian-Wei Pan<sup>1,2,†</sup>

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† Corresponding author. Email: [pan@ustc.edu.cn](mailto:pan@ustc.edu.cn)

\* These authors contributed equally to this work.

- Hide authors and affiliations

## Part II – Various Models of Quantum ML

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# Brief History of Quantum Machine Learning (1/4)

- In 2000's – early explorations; mostly on detection & estimation instead of learning.
- The term 'quantum machine learning' was coined around 2013 (arXiv:1307.0411).  
→ *HHL algorithm* for approximately solve linear equations with a *quantum RAM*.

PHYSICAL REVIEW LETTERS

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Featured in Physics Editors' Suggestion

Quantum Algorithm for Linear Systems of Equations

Aram W. Harrow, Avinatan Hassidim, and Seth Lloyd  
Phys. Rev. Lett. **103**, 150502 – Published 7 October 2009

nature  
International journal of science

Review Article | Published: 13 September 2017

Quantum machine learning

Jacob Biamonte  , Peter Wittek, Nicola Pancotti, Patrick Rebentrost, Nathan Wiebe & Seth Lloyd

Nature **549**, 195–202 (14 September 2017) | Download Citation 

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Quantum Support Vector Machine for Big Data Classification

Patrick Rebentrost, Masoud Mohseni, and Seth Lloyd  
Phys. Rev. Lett. **113**, 130503 – Published 25 September 2014

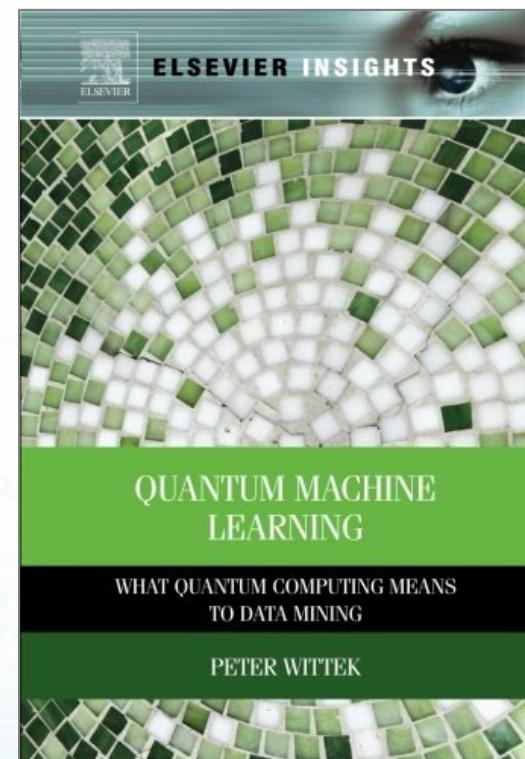
nature physics

Letter | Published: 27 July 2014

Quantum principal component analysis

Seth Lloyd  , Masoud Mohseni & Patrick Rebentrost

Nature Physics **10**, 631–633 (2014) | Download Citation 



# Brief History of Quantum Machine Learning (2/4)

- Some critiques about quantum speeding-up ML since 2015.  
→ Not just about practically building a quantum compute but caveats of using it.

The screenshot shows a news article from **naturephysics**. The title is **Published: 02 April 2015**. The main headline is **Read the fine print**, written by **Scott Aaronson**. Below the headline, there is a link to **Nature Physics 11, 291–293 (2015)** and a link to **Cite this article**.

The screenshot shows a news article from **PROCEEDINGS OF THE ROYAL SOCIETY A**. The title is **Quantum machine learning: a classical perspective**, written by **Carlo Ciliberto, Mark Herbster, Alessandro Davide Ialongo, Massimiliano Pontil, Andrea Rocchetto, Simone Severini, Leonard Wossnig**. The article was published on **17 January 2018** with DOI **10.1098/rspa.2017.0551**.

- Two types of quantum neural networks (QNNs) in 2018.
  - Unitary feed-forward network and Quantum Boltzmann machine

The screenshot shows a paper titled **Quantum Boltzmann Machine** published in **PHYSICAL REVIEW X**. The authors are **Mohammad H. Amin, Evgeny Andriyash, Jason Rolfe, Bohdan Kulchytskyy, and Roger Melko**. The paper was published in **Phys. Rev. X 8, 021050 – Published 23 May 2018**.

The screenshot shows a paper titled **Quantum circuit learning** published in **PHYSICAL REVIEW A**. The authors are **K. Mitarai, M. Negoro, M. Kitagawa, and K. Fujii**. The paper was published in **Phys. Rev. A 98, 032309 – Published 10 September 2018**.

# Brief History of Quantum Machine Learning (3/4)

- Finding applications, advantages, and preliminary analysis of QNNs.

**nature**

Letter | Published: 13 March 2019

## Supervised learning with quantum-enhanced feature spaces

Vojtěch Havlíček, Antonio D. Córcoles , Kristan Temme , Aram W. Harrow, Abhinav Kandala, Jerry M. Chow & Jay M. Gambetta

Nature **567**, 209–212 (2019) | Cite this article

**nature communications**

Article | Open Access | Published: 11 May 2021

## Power of data in quantum machine learning

Hsin-Yuan Huang, Michael Broughton, Masoud Mohseni, Ryan Babbush, Sergio Boixo, Hartmut Neven & Jarrod R. McClean 

Nature Communications **12**, Article number: 2631 (2021) | Cite this article

COLUMN

## Guest Column: A Survey of Quantum Learning Theory



Authors:  Srinivasan Arunachalam,  Ronald de Wolf [Authors Info & Affiliations](#)

Publication: ACM SIGACT News • June 2017 • <https://doi.org/10.1145/3106700.3106710>

## ADVANCED QUANTUM TECHNOLOGIES

Full Paper |  Token Access

### Expressibility and Entangling Capability of Parameterized Quantum Circuits for Hybrid Quantum-Classical Algorithms

Sukin Sim , Peter D. Johnson, Alán Aspuru-Guzik 

First published: 14 October 2019 | <https://doi.org/10.1002/qute.201900070> | Citations: 24

**PHYSICAL REVIEW LETTERS**

Editors' Suggestion

Access by

### Information-Theoretic Bounds on Quantum Advantage in Machine Learning

Hsin-Yuan Huang, Richard Kueng, and John Preskill  
Phys. Rev. Lett. **126**, 190505 – Published 14 May 2021

# Brief History of Quantum Machine Learning (4/4)

- Barren plateaus (vanishing gradients), quantum No-Free-Lunch theorem, etc...

**nature communications**

Article | Open Access | Published: 16 November 2018

## Barren plateaus in quantum neural network training landscapes

Jarrod R. McClean , Sergio Boixo , Vadim N. Smelyanskiy , Ryan Babbush & Hartmut Neven

*Nature Communications* **9**, Article number: 4812 (2018) | [Cite this article](#)

arXiv.org > quant-ph > arXiv:2010.15968

## Quantum Physics

[Submitted on 29 Oct 2020 ([v1](#)), last revised 10 Mar 2021 (this version, v2)]

## Entanglement Induced Barren Plateaus

[Carlos Ortiz Marrero](#), [Mária Kieferová](#), [Nathan Wiebe](#)

**nature communications**

Article | Open Access | Published: 19 March 2021

## Cost function dependent barren plateaus in shallow parametrized quantum circuits

M. Cerezo , Akira Sone, Tyler Volkoff, Lukasz Cincio & Patrick J. Coles 

*Nature Communications* **12**, Article number: 1791 (2021) | [Cite this article](#)

arXiv.org > quant-ph > arXiv:2007.04900

## Quantum Physics

[Submitted on 9 Jul 2020]

## Reformulation of the No-Free-Lunch Theorem for Entangled Data Sets

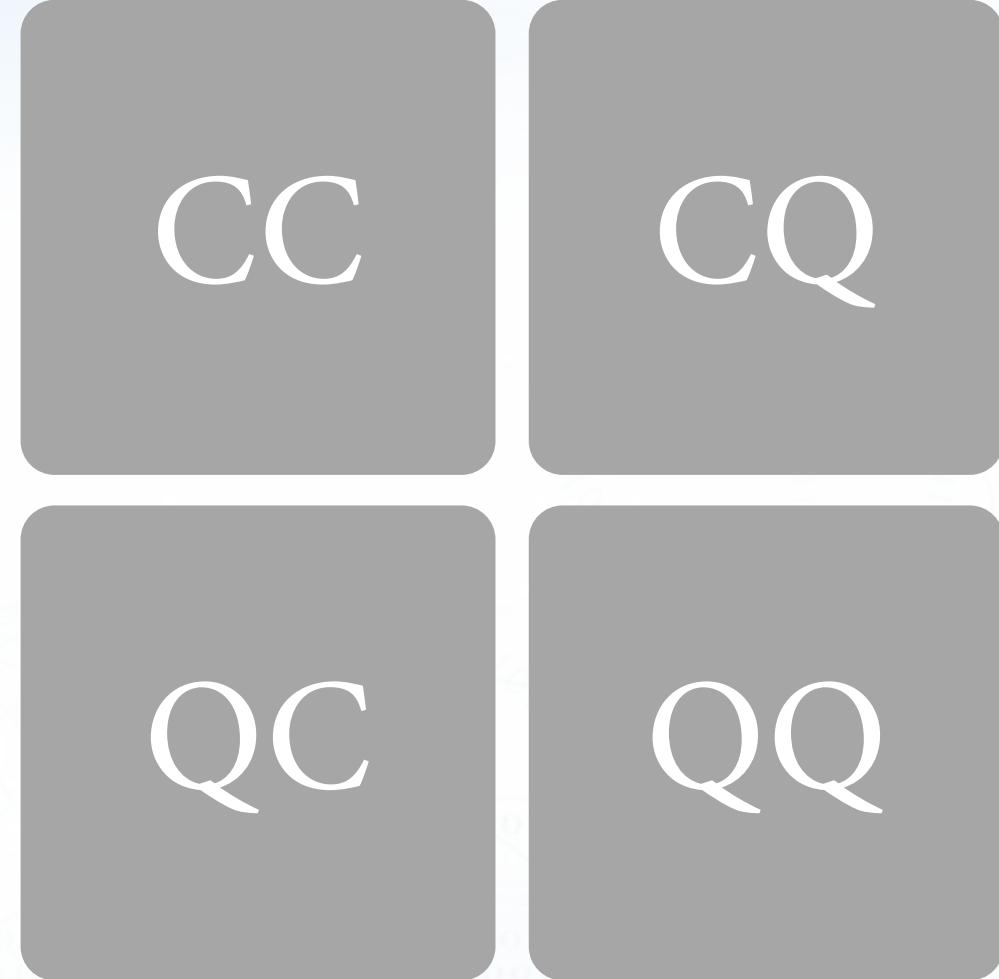
[Kunal Sharma](#), M. Cerezo, Zoë Holmes, Lukasz Cincio, Andrew Sornborger, Patrick J. Coles

# Four Categories

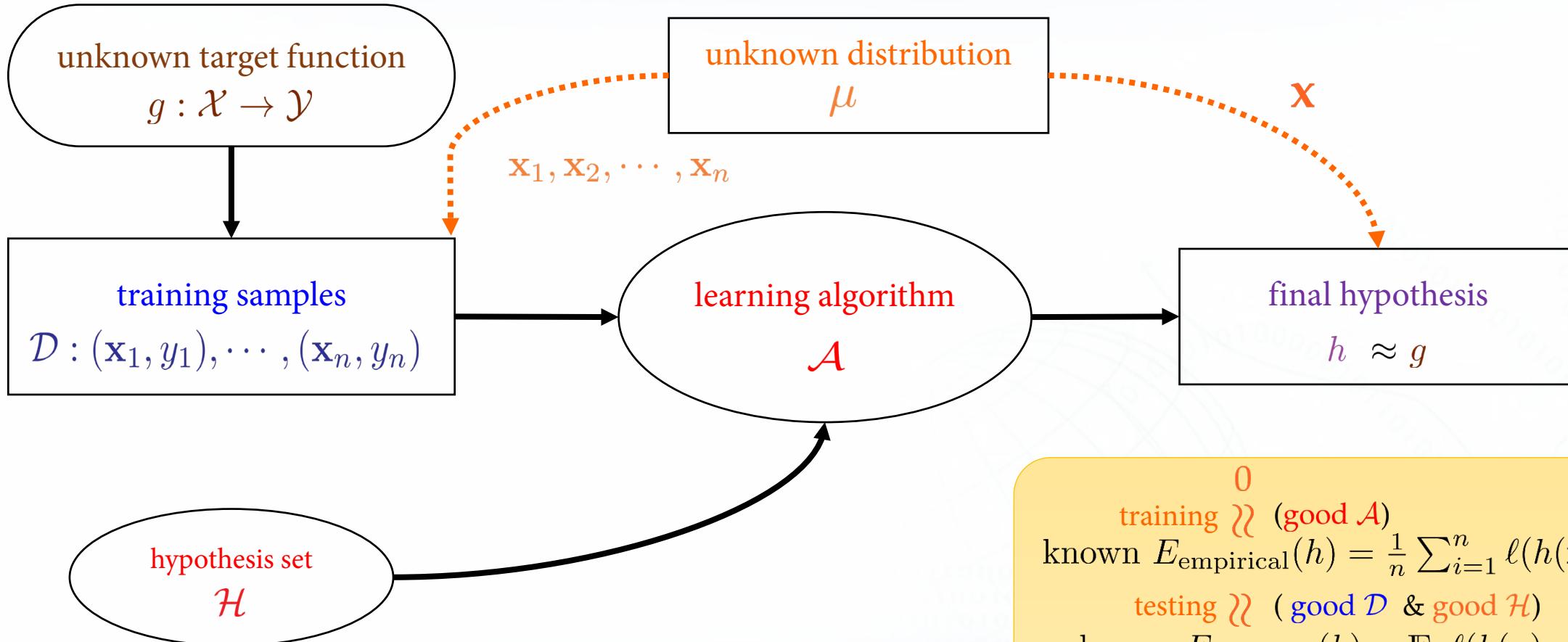
- CC: Learning **classical data** with **classical machine** – Classical ML.
- QC: Learning **quantum objects** with **classical ML** (e.g. matrix concentrations).
  - S. Aaronson'07 – Learning quantum states.
  - H.-C. Cheng, M.-H. Hsieh, P.-C. Yeh'15 – Learning quantum measurements.
- CQ: Processing **classical datasets** using **quantum computing** – Lloyd *et al.*
- QQ: Processing “**quantum data**” using **quantum machine** – largely open.

data generating system (left)

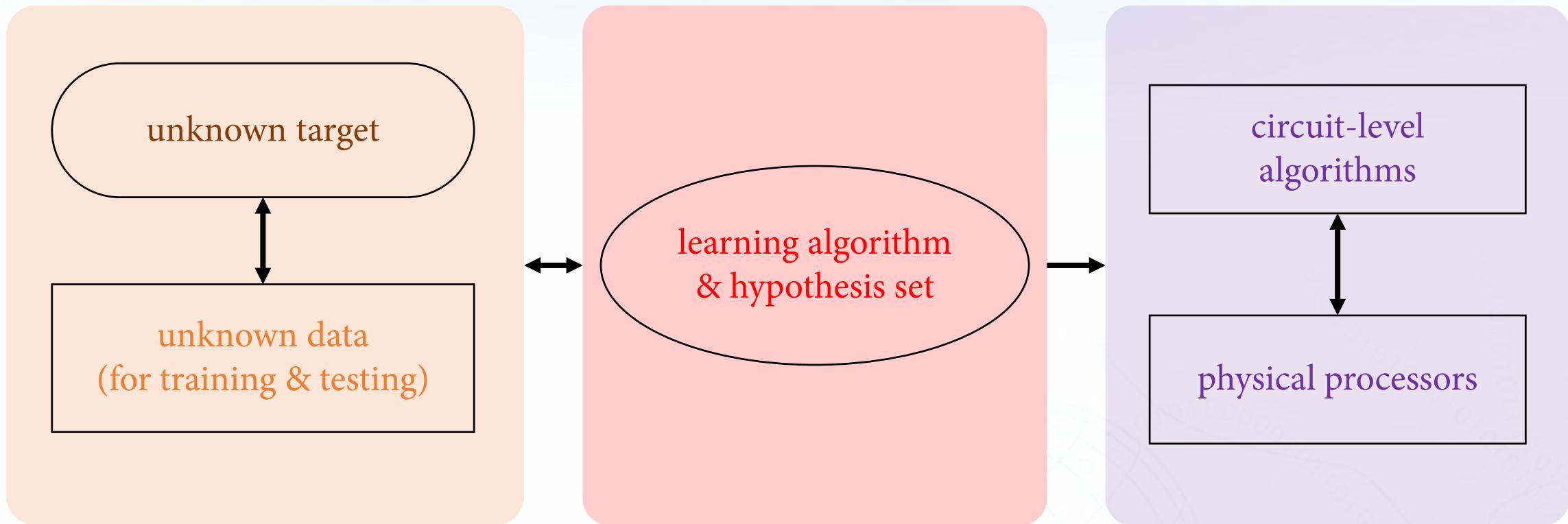
data processing device (right)



# Statistical Learning Framework



# Categories from The Learning Framework (1/2)



- ▶ **Data & Goal**
  - ▶ classical or quantum
  - ▶ hybrid

- ▶ **Learning Mechanism**
  - ▶ classical ML algorithms
  - ▶ quantum variational circuits

- ▶ **Physical device for implementation**
  - ▶ classical CPU/GPU/TPU
  - ▶ quantum processors

# Categories from The Learning Framework (2/2)

Data & goal	Learning mechanism	Physical device	Examples
classical	classical	classical	classical ML
classical	classical	quantum	speedup running time
classical	quantum	classical	VQC & simulator
classical	quantum	quantum	VQC & QPU
quantum	classical	classical	tomography & simulator
quantum	classical	quantum	tomography & QPU
quantum	quantum	classical	quantum simulation VQC? & simulator
quantum	quantum	quantum	quantum Boltzmann machine?

Today →

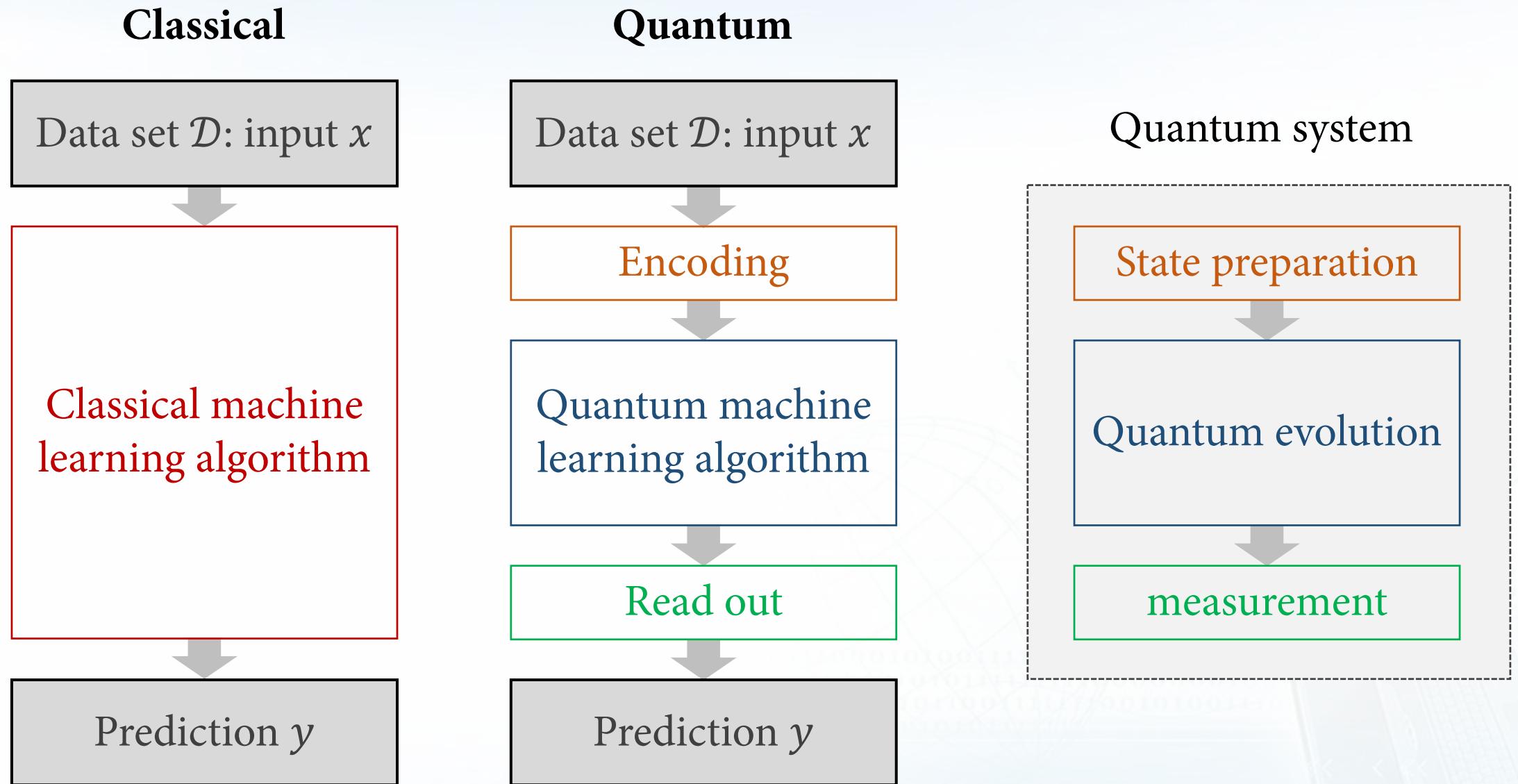
Today →

## Part III – ML with Quantum Algorithmic Speeding-up

---

Data & goal	Learning mechanism	Physical device
classical	classical	quantum

# Flowchart of Classical ML with Quantum Algorithm



# Information Encoding

- To learn from classical data, we need to load data from classical memory into the quantum computer; this process is called *state preparation* in QML.
- In the training phase, we consider data set  $\mathcal{D} = \{x_1, \dots, x_m\}$  of  $N$ -dimensional real feature vectors.

Encoding	Number of qubits	Runtime of state preparation	Input feature
Basis	$N$	$O(MN)$	Binary
Amplitude	$\log N$	$O(MN)/O(\log MN)$	Continuous
Qsample	$N$	$O(MN)/O(\log MN)$	Binary
Hamiltonian	$\log N$	$O(MN)/O(\log MN)$	Continuous

# Basis Encoding (1/2)

- Assume each data is  $N$ -dimensional bit string, i.e.  $x_m \in \{0,1\}^N$  for  $x_m \in \mathcal{D}$ :

$$x_m \mapsto |x_m\rangle \quad \mathcal{D} \mapsto |\mathcal{D}\rangle := \frac{1}{\sqrt{M}} \sum_{m=1}^M |x_m\rangle$$

- For example, given  $\mathcal{D} = \{x_1, x_2\} = \{0101, 1110\}$ , then  $|\mathcal{D}\rangle = \frac{1}{\sqrt{2}}(|0101\rangle + |1110\rangle)$ .

$$|0101\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \otimes \begin{pmatrix} 0 \\ 1 \end{pmatrix} \otimes \begin{pmatrix} 1 \\ 0 \end{pmatrix} \otimes \begin{pmatrix} 0 \\ 1 \end{pmatrix} = (0, 0, 0, 0, 0, 1, 0, 0, 0, 0, 0, 0, 0, 0, 0)^T$$

$$|1110\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix} \otimes \begin{pmatrix} 0 \\ 1 \end{pmatrix} \otimes \begin{pmatrix} 0 \\ 1 \end{pmatrix} \otimes \begin{pmatrix} 1 \\ 0 \end{pmatrix} = (0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 1, 0)^T$$

$$\Rightarrow |\mathcal{D}\rangle = \left(0, 0, 0, 0, 0, 1/\sqrt{2}, 0, 0, 0, 0, 0, 0, 0, 0, 1/\sqrt{2}, 0\right)^T$$

# Basis Encoding (2/2)

- Preparation in time  $O(MN)$  by Ventura–Martinez, and Trugenberger.
- Approach by the Quantum random access memory, in time  $O(\log N)$ .

$$\text{QRAM: } \frac{1}{\sqrt{M}} \sum_{m=1}^M |m\rangle |0 \cdots 0\rangle \mapsto \frac{1}{\sqrt{M}} \sum_{m=1}^M |m\rangle |x_m\rangle$$



- However, an efficient hardware implementation is still an open challenge.

# Computing in Basis Encoding

- Suppose we have a Boolean logic gate  $f: \{0,1\}^N \rightarrow \{0,1\}$  giving binary label to each data  $x_m$ . Then, this can be implemented by (universal) quantum Toffoli gates. This is called a *quantum oracle*  $U_f: |x\rangle|0\rangle \mapsto |x\rangle|f(x)\rangle$ .
- *Quantum parallelism*:

$$U_f: \frac{1}{\sqrt{M}} \sum_{m=1}^M |x_m\rangle|0\dots0\rangle \mapsto \frac{1}{\sqrt{M}} \sum_{m=1}^M |x_m\rangle|f(x_m)\rangle$$

- To read-out the state of the qubits, we have to measure it (quantum tomography).  
→ *Frequentist estimator* via multiple shots of measurements.
- **Caveats:** (i) large amounts of qubits needed; (ii) realizing a quantum RAM.

# Amplitude Encoding

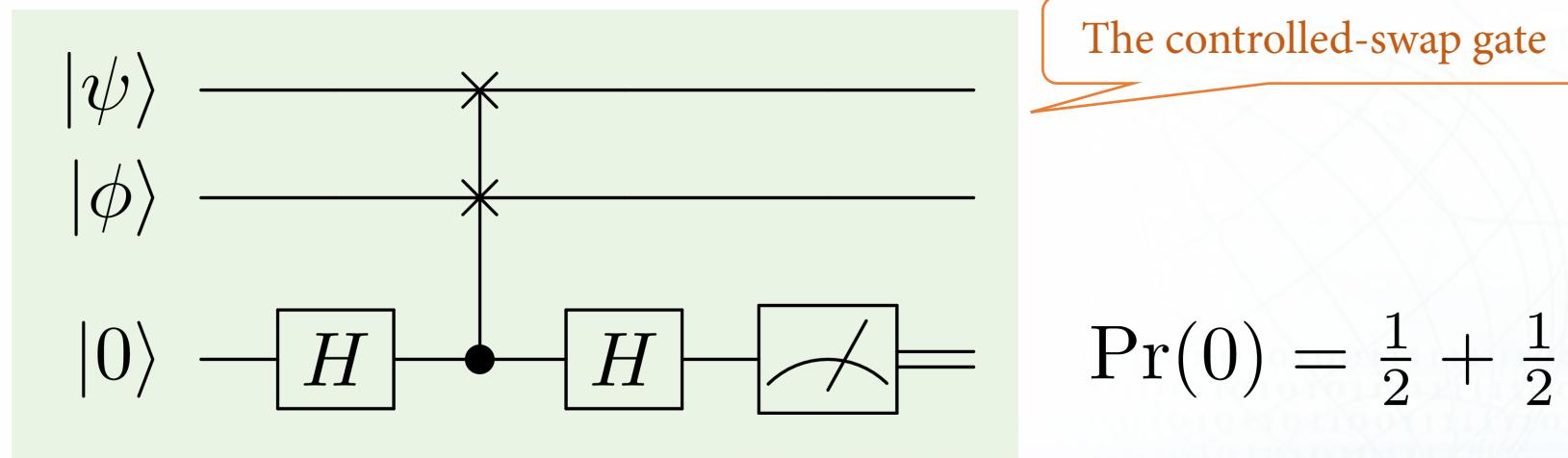
- For simplicity, suppose each feature vector  $x_m = (x_{m,1}, \dots, x_{m,N})$  is normalized, i.e.  $\sum_{i=1}^N x_{m,i}^2 = 1$ . (This condition can be removed by non-expansive manipulations.)
- Then, we can prepare the quantum state  $|x_m\rangle$  by using  $n = \log N$  quantum bits:

$$x_m \mapsto |x_m\rangle := \sum_{i=1}^N x_{m,i} |i\rangle \quad \mathcal{D} \mapsto |\mathcal{D}\rangle := \frac{1}{\sqrt{M}} \sum_{m=1}^M \sum_{i=1}^N x_{m,i} |m\rangle |i\rangle$$

- State preparation in linear time:  $O(MN)/O(\log MN)$ .
- For sufficiently *uniform* vectors, the preparation may be efficiently done via qRAM.

# Computing in Amplitude Encoding (1/2)

- Clustering: Assigning a vector  $\vec{u} \in \mathbb{C}^N$  to two groups:  $\{\vec{v}_m\}_{m=1}^M$  and  $\{\vec{w}_m\}_{m=1}^M$ .
- Classical approach: to compare the distance  $\left| \vec{u} - \frac{1}{M} \sum_m \vec{v}_m \right|^2$ .  
Takes time  $O(\text{poly}(MN))$ . ← involving evaluating inner product  $\langle \vec{u}, \vec{v}_m \rangle$
- The *swap test* for computing the inner product.



$$\Pr(0) = \frac{1}{2} + \frac{1}{2} |\langle \psi | \phi \rangle|^2$$

# Computing in Amplitude Encoding (2/2)

- The clustering can be done in  $O(\log MN)$  in a quantum computer.

- Caveats:**

Exponential speed-up!

- If wanted to read-out the value of any specific entry  $x_i$  of  $|x\rangle = \sum_{i=1}^N x_i |i\rangle$ , then in general would require repeating the algorithm roughly  $O(N)$  times, this then kills the exponential speed-up.  
← measurement outcome  $x_i$  with  $\Pr(x_i^2)$
- Once again, if preparing the amplitude encoding in  $|x\rangle$  requires super-logarithmic time, then the speed-up unfortunately vanishes.

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**Quantum machine learning: a classical perspective**

Carlo Ciliberto, Mark Herbster, Alessandro Davide Ialongo, Massimiliano Pontil, Andrea Rocchetto, Simone Severini, Leonard Wossnig

Published 17 January 2018. DOI: 10.1098/rspa.2017.0551

**nature physics**

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Published: 02 April 2015

**Read the fine print**

Scott Aaronson 

*Nature Physics* 11, 291–293 (2015) | Cite this article

# Support Vector Machine with Quantum RAM

- The Support Vector Machine (SVM) can be formulated as a quadratic programming problem, which can be solved in time  $O(\text{poly}(M, N))$ , i.e.

$$\max_{\vec{\alpha}} \left\{ L(\vec{\alpha}) = \langle \vec{\alpha}, \vec{y} \rangle - \frac{1}{2} \langle \vec{\alpha}, K \vec{\alpha} \rangle : \sum_{j=1}^M \alpha_j = 0, y_j \alpha_j \geq 0 \right\}, [K]_{ij} := k(\vec{x}_i, \vec{x}_j).$$

- Efficient inner product evaluation via quantum algorithm takes  $O(\text{poly}(M) \log N)$ .
- Using a non-sparse matrix exponentiation technique for approximating the kernel matrix inverse requires  $O(\log MN)$ .

← Exponential speed-up!

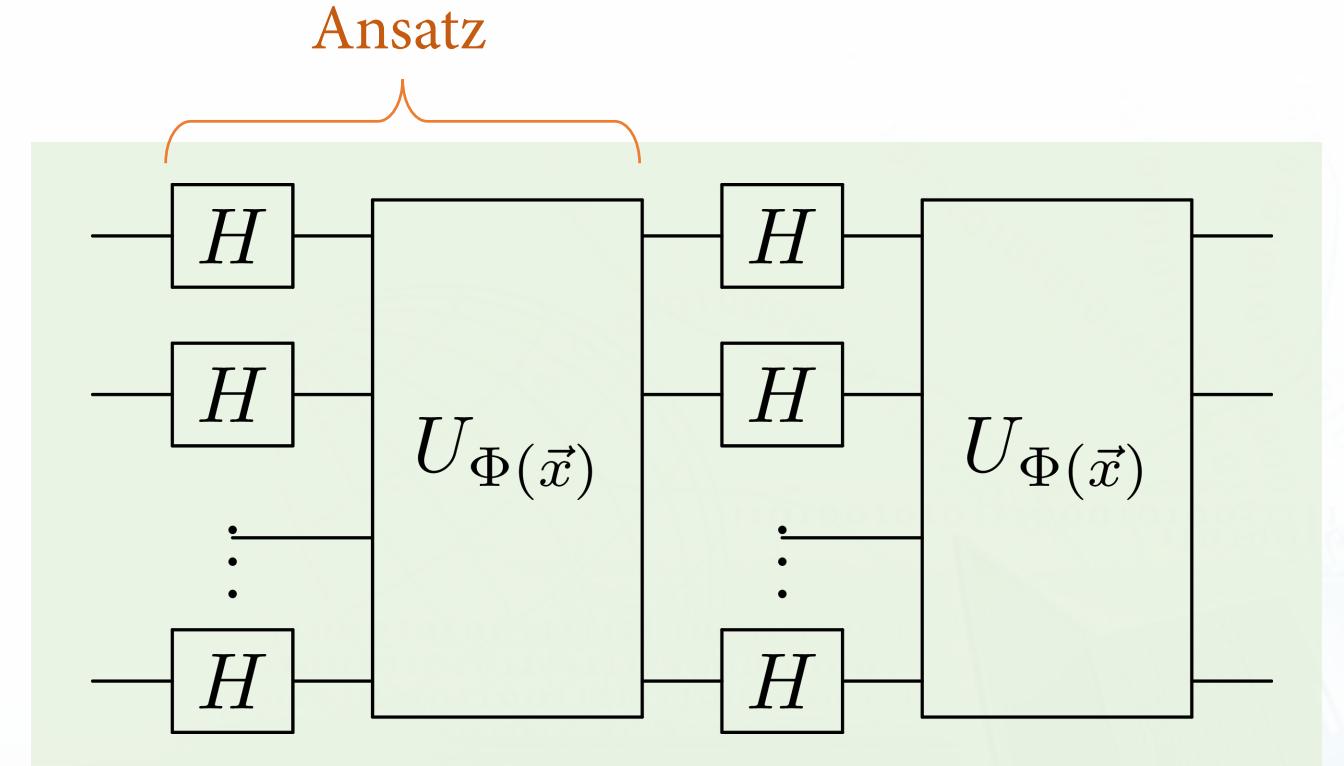
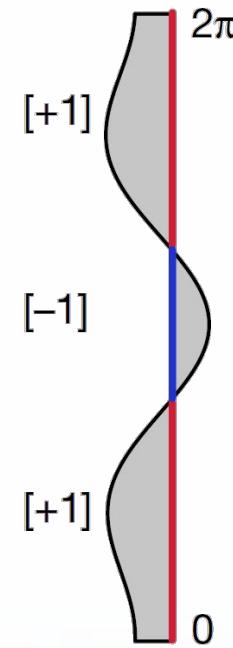
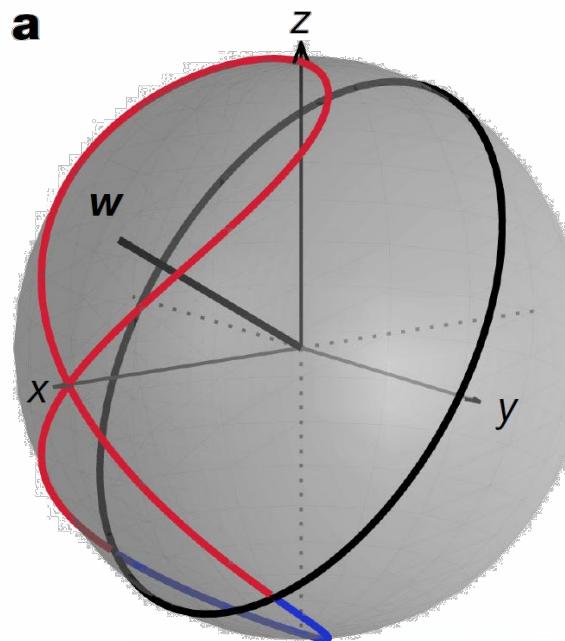
## Caveats:

- Works with non-sparse kernel matrix, which has a small *condition number* (as in the HHL).
- Again, the quantum RAM is indispensable.



# Support Vector Machine without Quantum RAM (1/3)

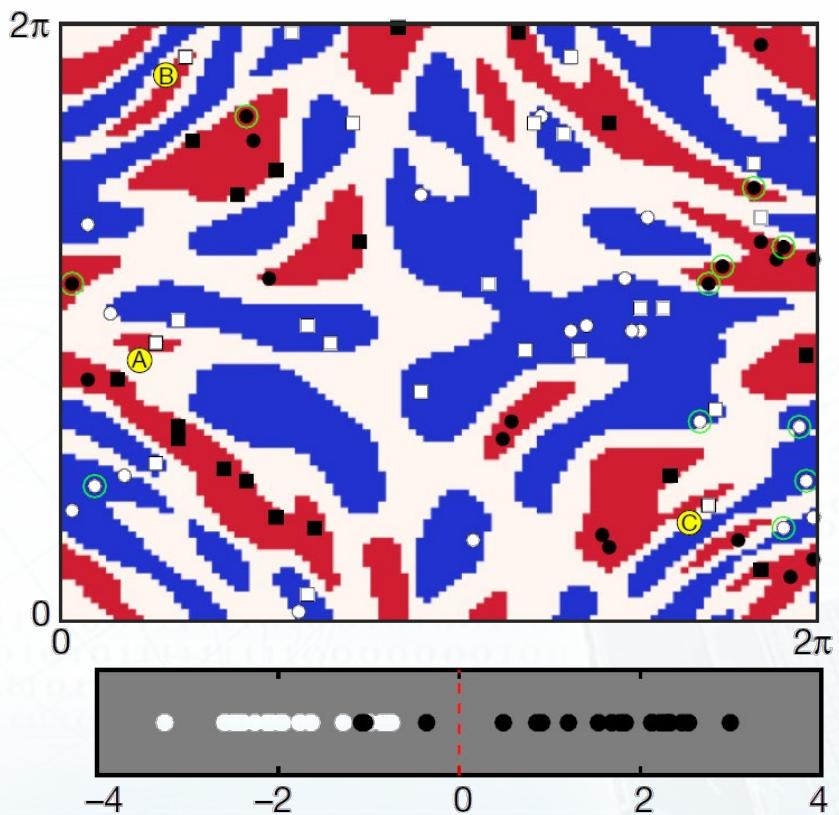
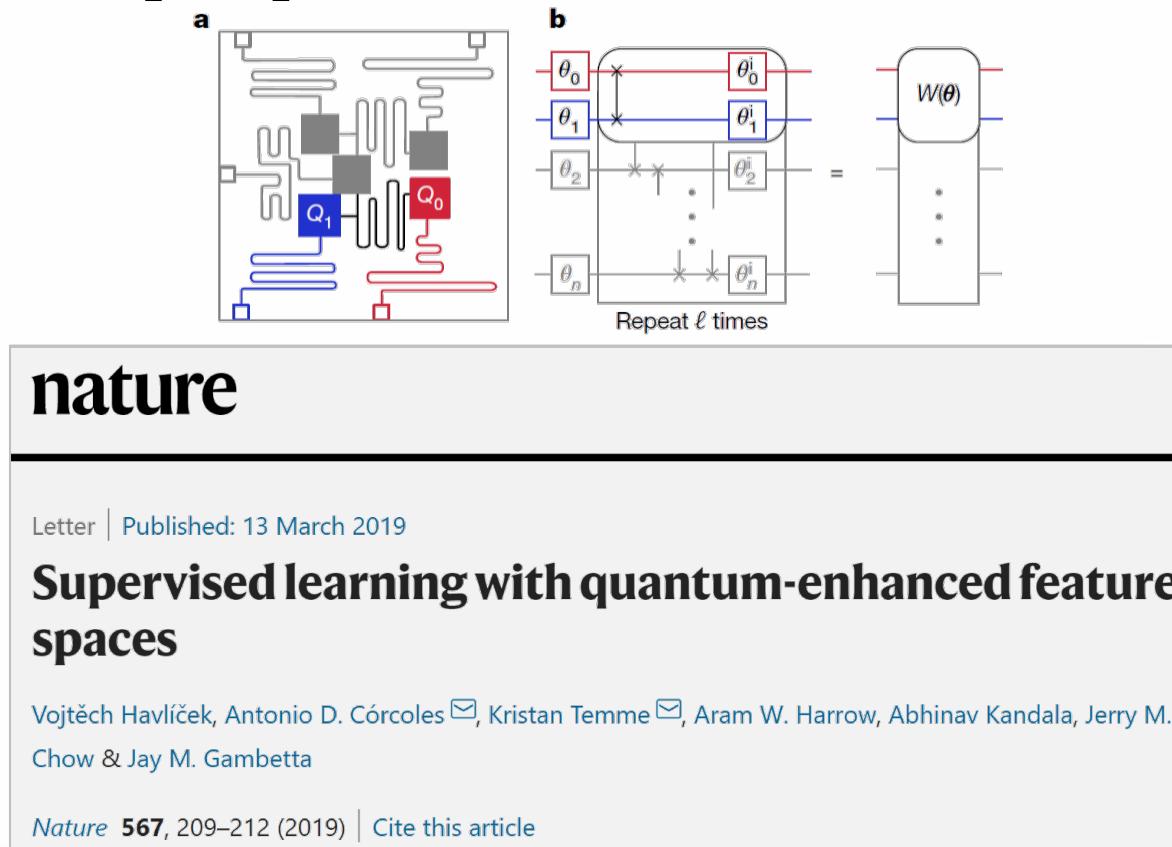
- *Rotation encoding*:  $\Phi: \vec{x} \mapsto |\Phi(\vec{x})\rangle$  mapping the data to the *quantum feature space*.
- To implement the feature map, a rotation Z gate  $U_{\Phi(\vec{x})}$  is used in the *ansatz*  $U_{\Phi(\vec{x})}H$   
e.g.  $U_{\Phi(x)} = e^{-ixZ}$  for 1-bit  $x$ ;  $U_{\Phi(\vec{x})} = e^{i(x_1Z_1+x_2Z_2+(\pi-x_1)(\pi-x_2)Z_1Z_2)}$  for 2-bit  $\vec{x}$ .



[Havlicek *et al.*, “Supervised learning with quantum enhanced feature spaces,” *Nature*, 2018 ]

# Support Vector Machine without Quantum RAM (2/3)

- With the quantum feature map, the classical kernel is  $k(\vec{x}_i, \vec{x}_j) = |\langle \Phi(\vec{x}_i) | \Phi(\vec{x}_j) \rangle|^2$ .
- Such a kernel (constructed from the above ansatz) is efficiently implementable via short-depth quantum circuits, but believed *classically hard*.



# Support Vector Machine without Quantum RAM (3/3)

← → ⌂ qiskit.org/documentation/stubs/qiskit.aqua.algorithms.QSVM.html

 Qiskit

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Docs > Qiskit Aqua API Reference > Aqua (Algorithms for QUantum Applications) (qiskit.aqua) > Algorithms (qiskit.aqua.algorithms) > qiskit.aqua.algorithms.QSVM

qiskit.aqua.algorithms.QSVM 

CLASS `QSVM(feature_map, training_dataset=None, test_dataset=None, datapoints=None, multiclass_extension=None, Lambda2=0.001, quantum_instance=None)`

Quantum SVM algorithm.



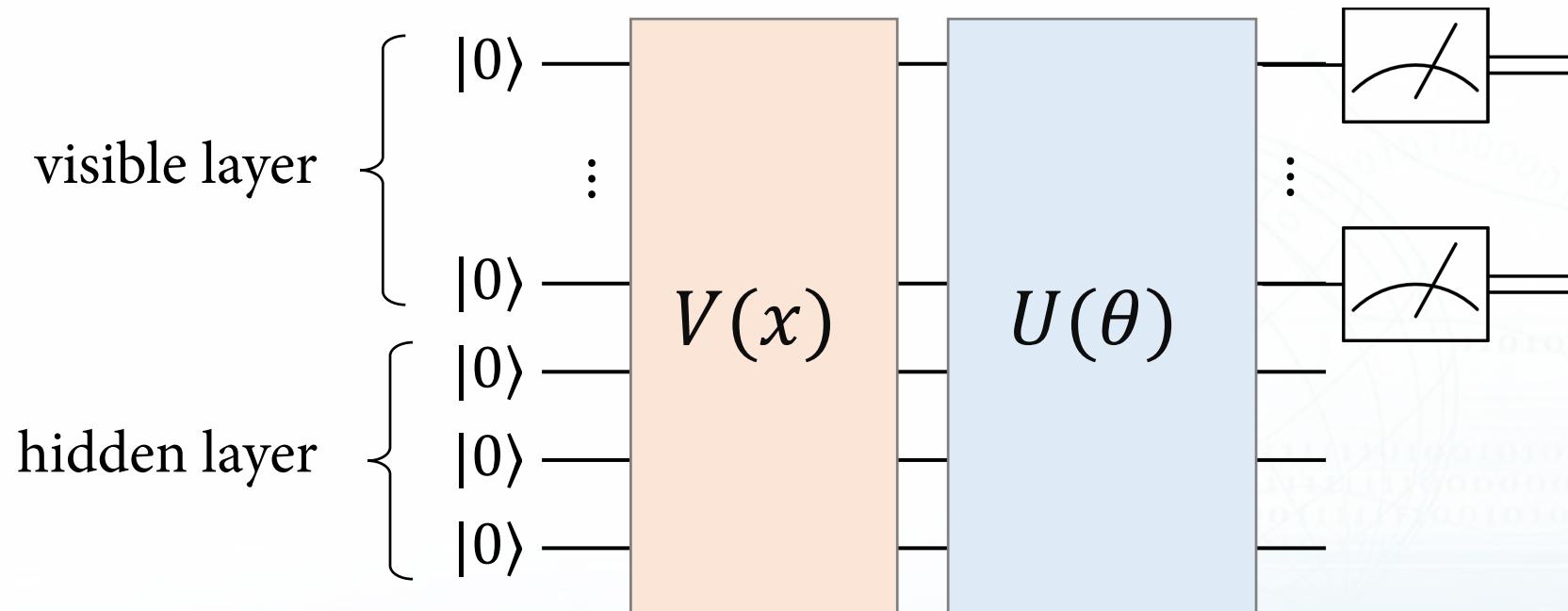
## Part IV – Learning with Quantum Machines

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Data & goal	Learning mechanism	Physical device
classical	quantum	classical/quantum

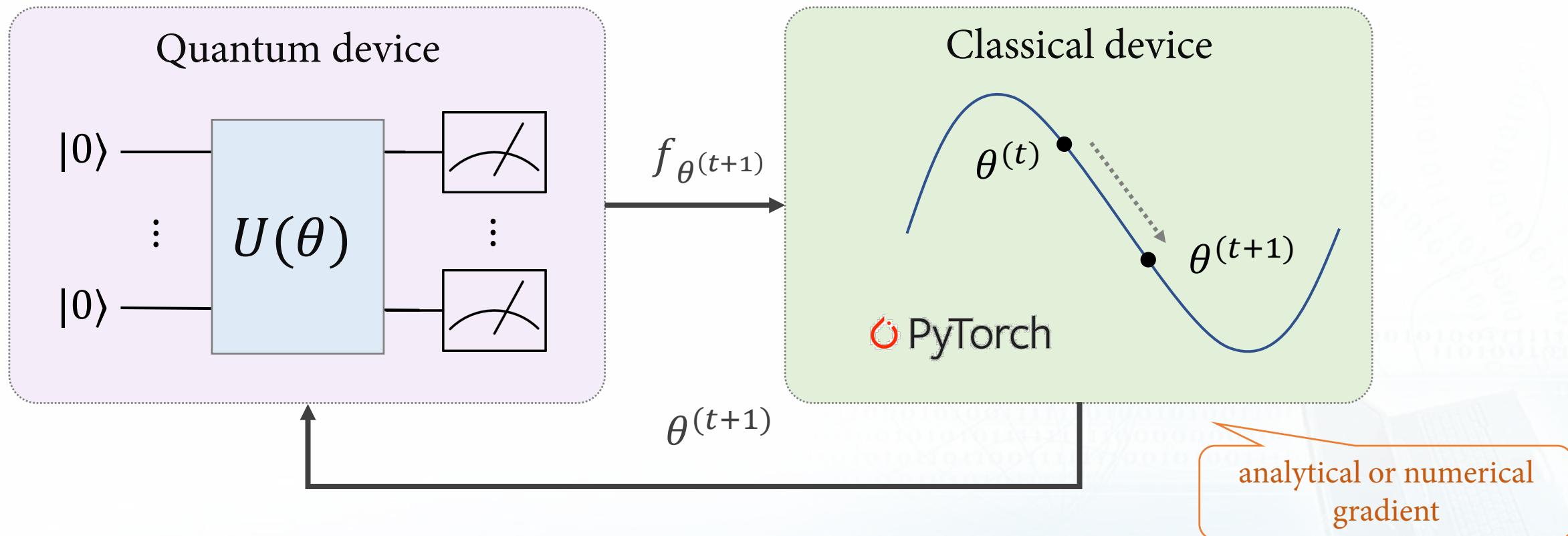
# Variational (Parametric) Quantum Circuits

- The QNN is characterized by a unitary ansatz  $U(\theta) := e^{-iH_n\theta_n} \dots e^{-iH_n\theta_n}$ , where  $\theta = \{\theta_1, \dots, \theta_n\}$  are the parameters we aim to learn and  $H_i$  are Hermitian operators.
- Goal: find a good assignment of parameters (e.g. via gradient descent) in terms of an objective function  $f_\theta(x) := \langle \psi_{\theta,x} | \Pi \otimes I | \psi_{\theta,x} \rangle$ , where  $|\psi_{\theta,x}\rangle := U(\theta)V(x)|0\rangle$ .



# Hybrid Training for Variational Algorithms

- Idea: Use the quantum machine to compute the objective function  $f(\theta^{(t)})$ , and then use a classical device to compute better circuit parameters  $\theta^{(t+1)}$  with respect to the objective. Iterate the routine until the objective is optimized.



# Optimization Methods (1/2)

- Quantum Approximate Optimization Algorithm (QAOA) for the MaxCut Problem.  
→ heuristic, highly problem-specific, could be computationally expensive.
- Iterative derivative-free methods (e.g. the PSO).
- Numerical gradient (finite difference).
- Analytical gradient (**parameter shift rule**).
  - In general,  $\partial U(\theta)$  might not be unitary.
  - By rotation gate,  $\partial U(\theta)$  can be expressed as linear combinations of unitaries; hence computable by circuits.
  - Other gradient methods.

arXiv.org > quant-ph > arXiv:1411.4028

Quantum Physics

[Submitted on 14 Nov 2014]

**A Quantum Approximate Optimization Algorithm**

Edward Farhi, Jeffrey Goldstone, Sam Gutmann

arXiv.org > quant-ph > arXiv:1701.01450

Quantum Physics

[Submitted on 5 Jan 2017]

**Practical optimization for hybrid quantum-classical algorithms**

Gian Giacomo Guerreschi, Mikhail Smelyanskiy



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Quantum circuit learning

K. Mitarai, M. Negoro, M. Kitagawa, and K. Fujii  
Phys. Rev. A **98**, 032309 – Published 10 September 2018

# Optimization Methods (2/2)

← → ⌂ qiskit.org/textbook/ch-applications/qaoa.html

 Qiskit

Learn Quantum Computation using Qiskit

What is Quantum?

0. Prerequisites

1. Quantum States and Qubits

1.1 Introduction

1.2 The Atoms of Computation

1.3 Representing Qubit States

1.4 Single Qubit Gates

←

## Solving combinatorial optimization problems using QAOA

In this tutorial, we introduce combinatorial optimization problems, explain approximate optimization algorithms, explain how the Quantum Approximate Optimization Algorithm (QAOA) works and present the implementation of an example that can be run on a simulator or on a 5 qubit quantum chip

← → ⌂ qiskit.org/textbook/ch-machine-learning/machine-learning-qiskit-pytorch.html

 Qiskit

Learn Quantum Computation using Qiskit

What is Quantum?

0. Prerequisites

1. Quantum States and Qubits

1.1 Introduction

←

## Hybrid quantum-classical Neural Networks with PyTorch and Qiskit

← → ⌂ pennylane.ai/qml/index.html

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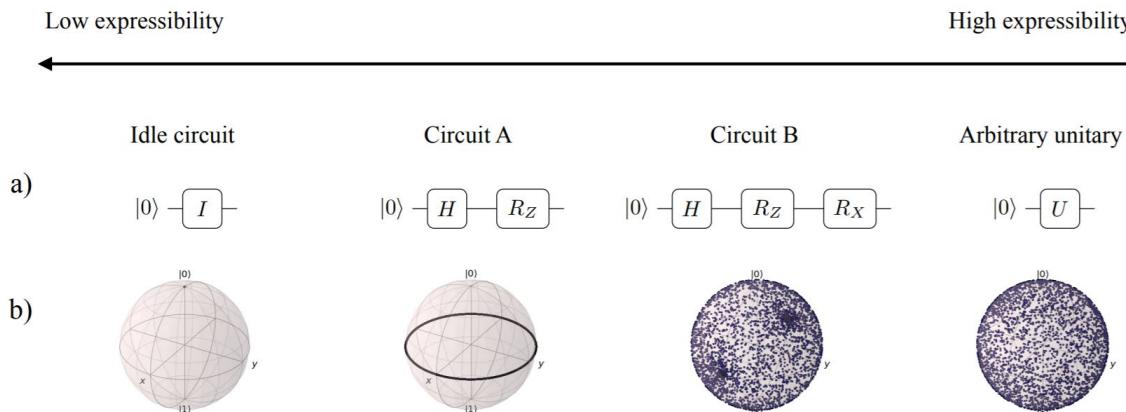
## Quantum machine learning

We're entering an exciting time in quantum physics and quantum computation: [near-term quantum devices](#) are rapidly becoming a reality, accessible to everyone over the internet.

This, in turn, is driving the development of quantum machine learning and variational quantum circuits.

# Various Ansatzs for QNNs (1/2)

- The dimension of the parameter space is typically much smaller than the space of all unitary operators (e.g.  $O(2^{2n})$  for  $n$ -qubits).
  - *Goal:* designing an ansatz for the QNN such that it is rich enough to allow the parameterized circuit to approximate the solution with as few parameters as possible.
  - It is desirable that the qubit-efficient circuits are hard for classical simulation – the objective function cannot be efficiently computed on a classical computer.  
(But it does not rule out the possibility that there are other efficient classical ways.)



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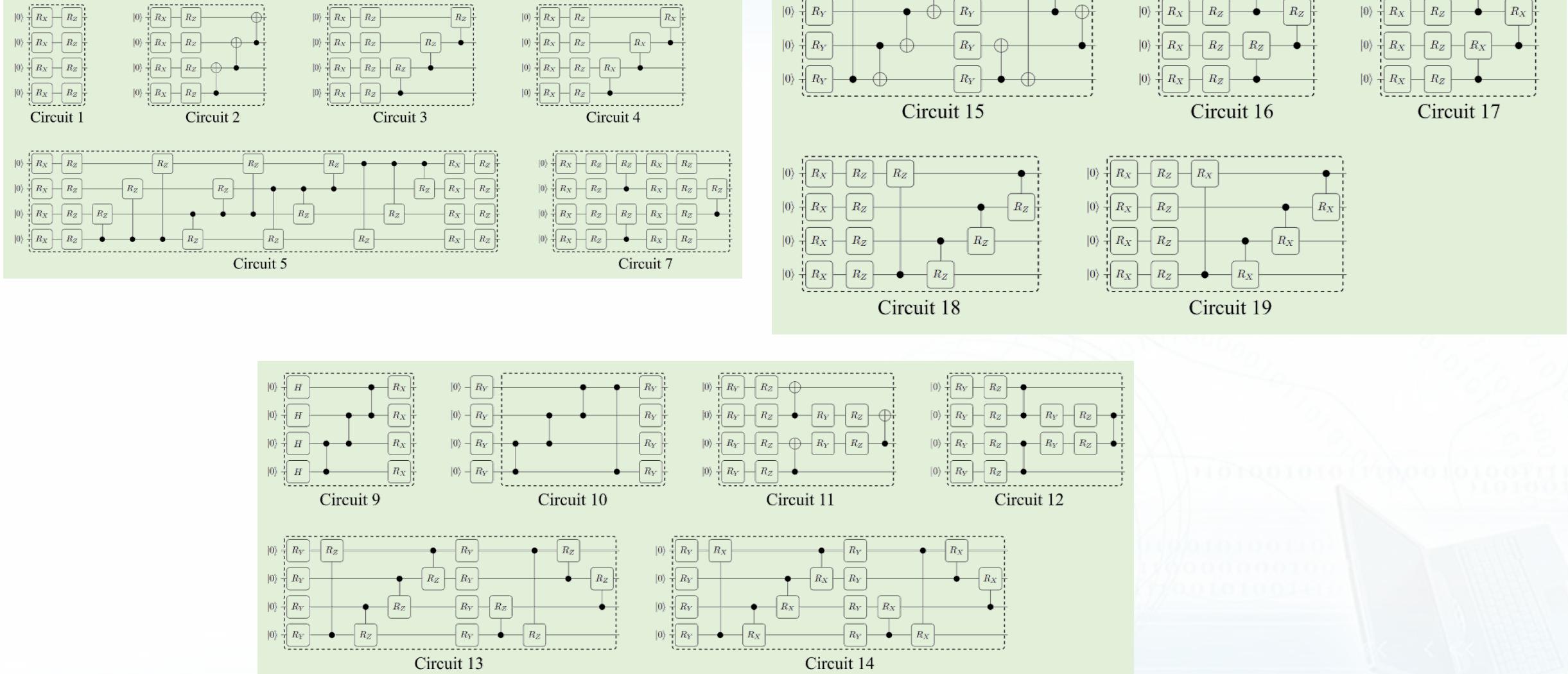
Full Paper |  Token Access

# Expressibility and Entangling Capability of Parameterized Quantum Circuits for Hybrid Quantum-Classical Algorithms

Sukin Sim ✉, Peter D. Johnson, Alán Aspuru-Guzik ✉

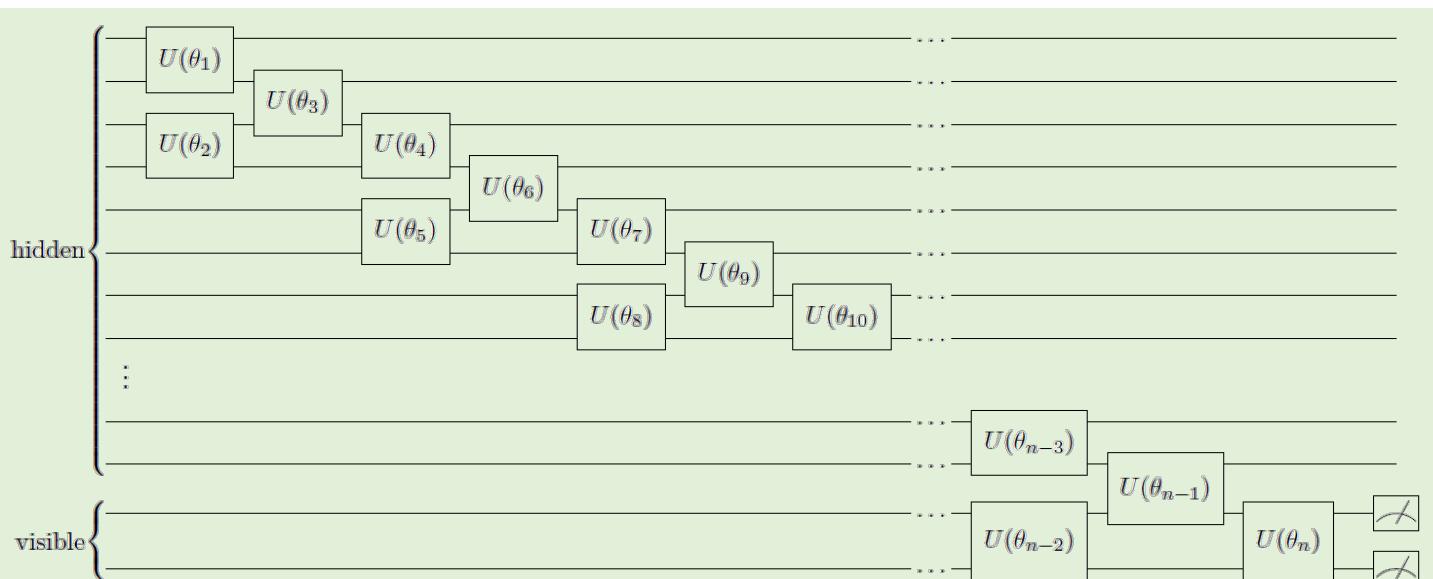
First published: 14 October 2019 | <https://doi.org/10.1002/quate.201900070> | Citations: 24

# Various Ansatzs for QNNs (2/2)



# Caveat: Barren Plateaus

- On one hand, we desire *entanglement* between qubits to exploit full *quantumness*.
- On the other hand, excess of entanglement between visible and hidden layers may cause barren plateaus; hence both gradient descent and gradient methods fail.
- Any trade-off? How to quantify/characterize them?



arXiv.org > quant-ph > arXiv:2010.15968

Quantum Physics

[Submitted on 29 Oct 2020 (v1), last revised 10 Mar 2021 (this version, v2)]

**Entanglement Induced Barren Plateaus**

Carlos Ortiz Marrero, Mária Kieferová, Nathan Wiebe

# Various Quantum Software Packages

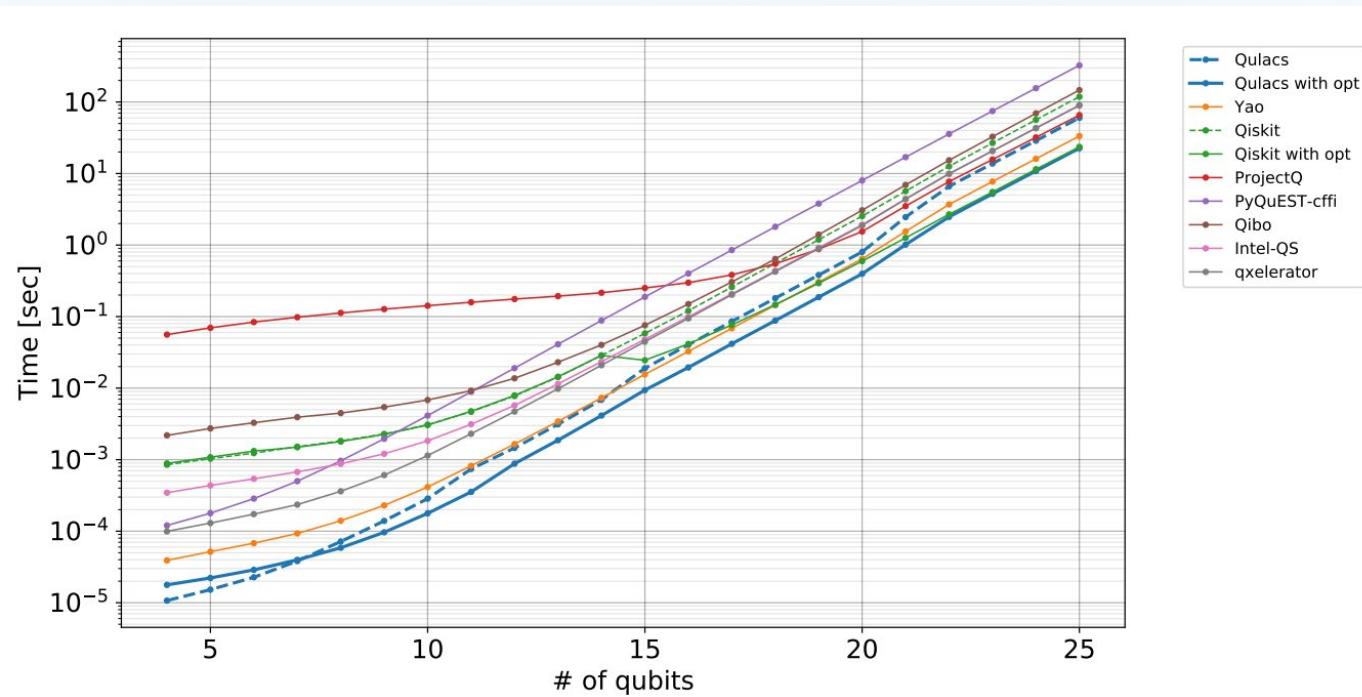


FIG. 8. Times for simulating random quantum circuits with a single thread using several libraries.

# Epilogue





# Conclusions and Outlooks

- There are other QML models that we haven't discussed in the lecture:
  - Quantum Boltzmann machines  $e^{-\sum_i \theta_i H_i} / Z(\theta)$ .
  - Quantum example oracle  $|0^n\rangle \mapsto \sum_x \sqrt{p(x)}|x\rangle|f(x)\rangle$ .
  - Quantum PAC-learning model.
- QML is still at its very early stage of research. How to demonstrate quantum advantages, to provide theoretical evidence, and to identify the field it can apply? On the other hand, can one prove that the quantum circuit learning is just a lure?
- Conversely, existing ML techniques could help quantum information development.
- Even if QML does not help classical problems, it might help quantum problems.
- My ultimate goal: to invent a truly quantumly-meaning learning paradigm.

