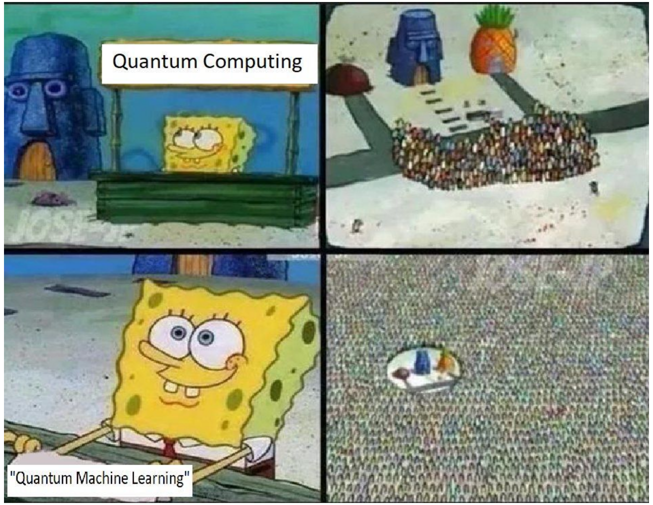
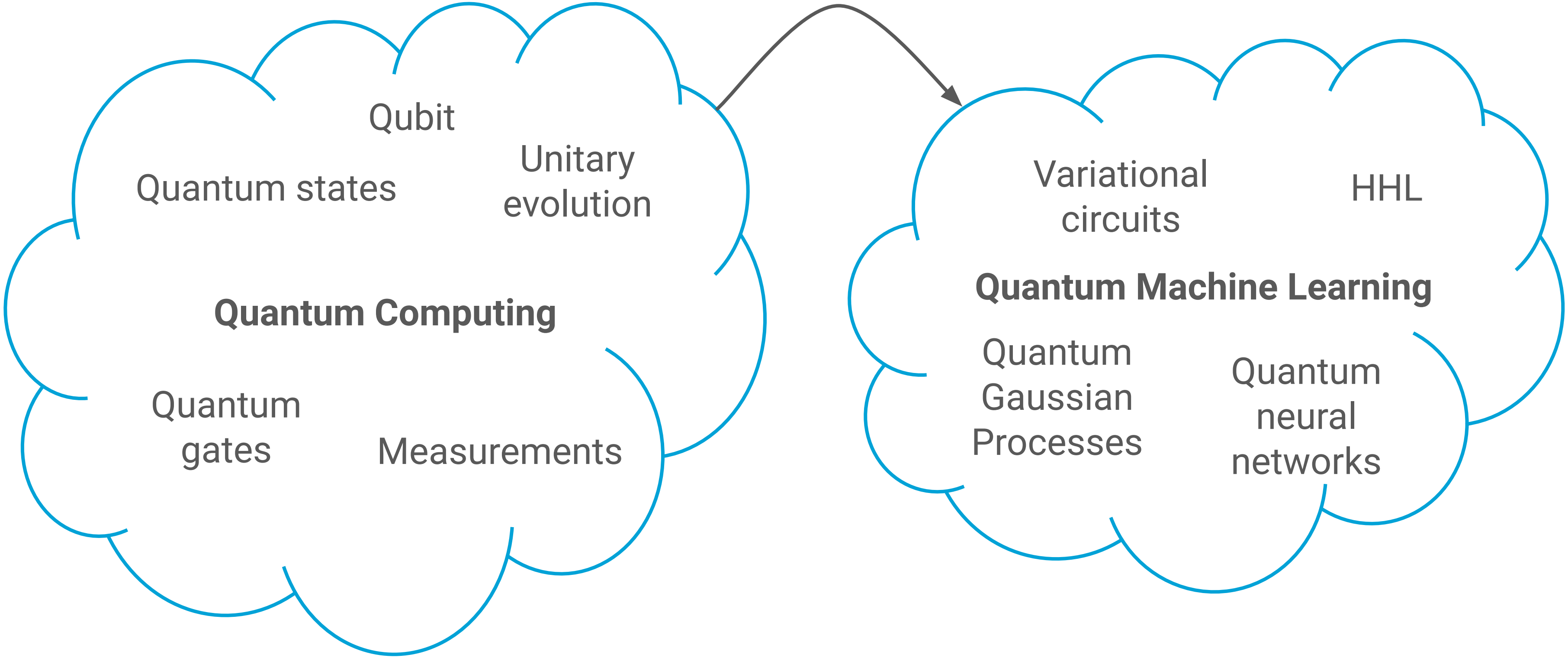
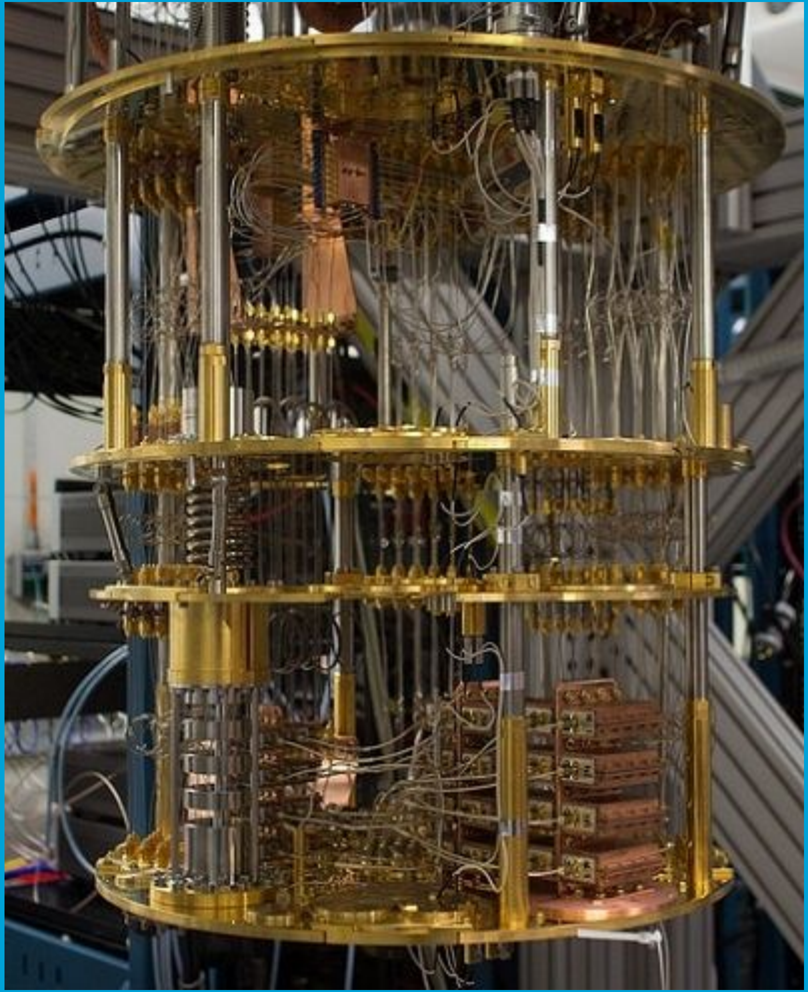
Quantum Machine Learning Beyond the Hype

Arthur Pesah
Previously 1QBit, Waterloo, Canada
KTH Royal Institute of Technology, Stockholm, Sweden



What are you going to learn?





Quantum Computing Overview

Quantum computing: overview

Do we have quantum computers?

Yes!

Google AI
53 qubits

rigetti
32 qubits

XANADU
8 qubits

IONQ
55 qubits

IBM Q
53 qubits

D-Wave
The Quantum Computing Company™
3,000 (non-universal) qubits

Cloud access!

But...

...no quantum advantage has been shown on a practical application yet!

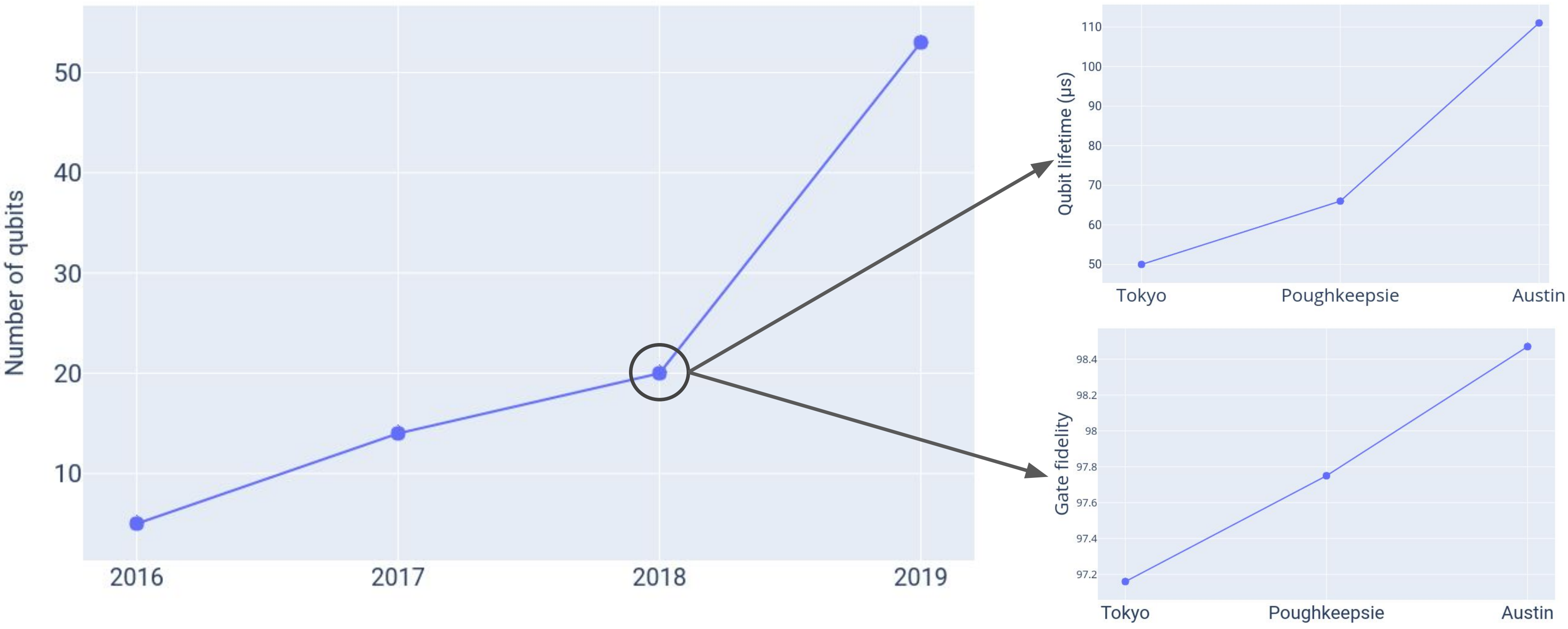
Why?

1. Not enough qubits
2. Qubits too noisy

Quantum computing: overview

Do we have quantum computers?

However, huge progress recently (e.g. IBM quantum computers)

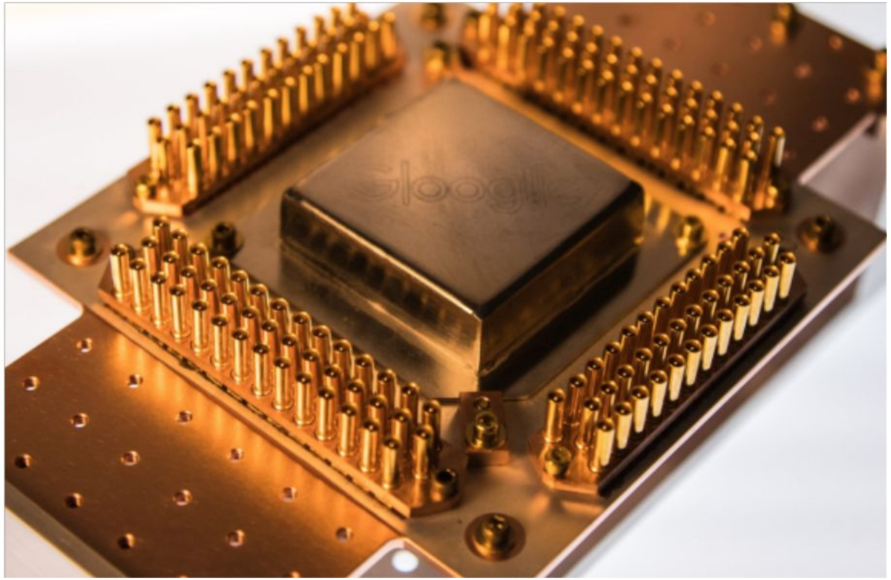


Source: https://quantumcomputingreport.com/scorecards/qubit-quality/

Quantum computing: overview

Do we have quantum computers?

However, huge progress recently (e.g. quantum supremacy)



- [x] Quantum supremacy
- [ ] Practical quantum advantage

Source: Google AI, *Supplementary information for “Quantum supremacy using a programmable superconducting processor”*, arxiv.org/abs/1910.11333

Quantum computing: overview

How can we achieve a practical quantum advantage?

Long-term

Traditional quantum algorithms

- Factoring algorithm (Shor)
- Search in unstructured database (Grover)
- Quantum machine learning (QSVM, QPCA...)

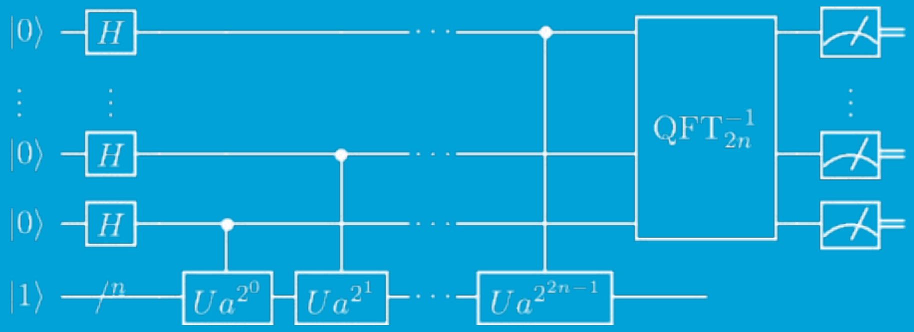
Very well understood algorithms, with precise bounds and complexity-theoretic advantage

Intermediate-term

Noisy Intermediate-term Quantum era (NISQ)

- Quantum simulation (chemistry, material...)
- Optimization problems
- Quantum “neural networks”

Very recent heuristics (>2014), as complicated to analyse as regular neural networks

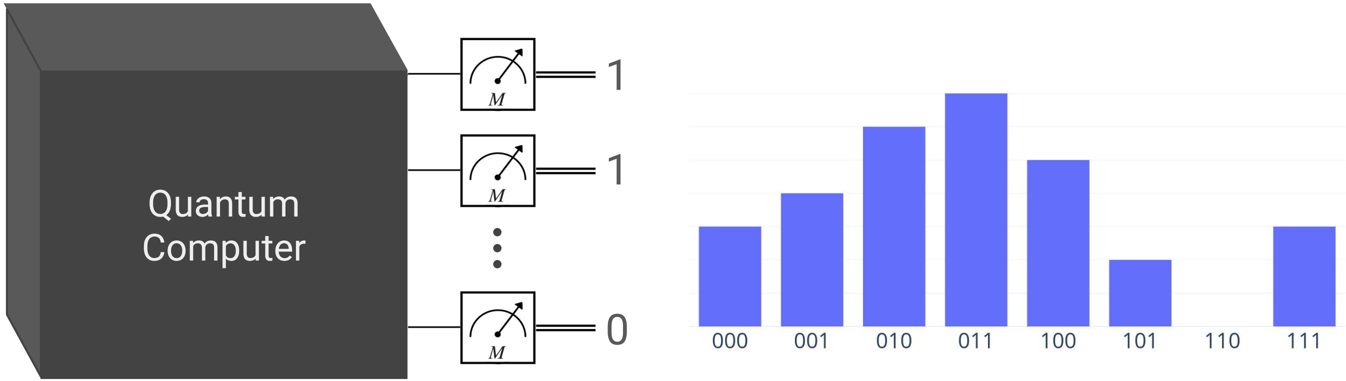


Quantum Computing Formalism

Quantum computing: formalism

What is a quantum computer?

A quantum computer is a **generative model...**



...that can be **stochastic**

Quantum computing: formalism

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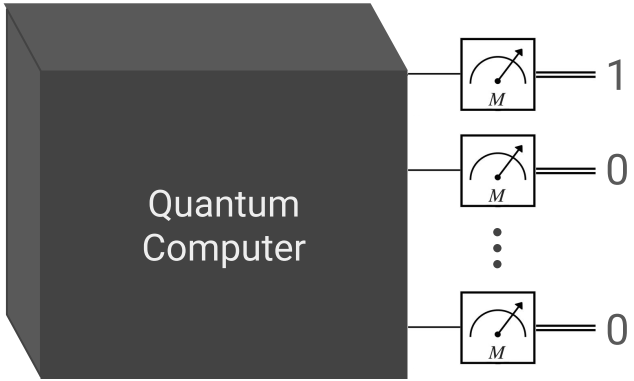
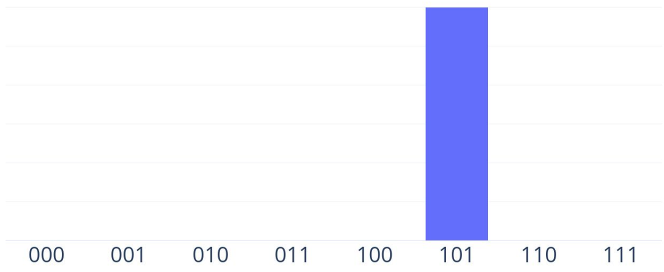


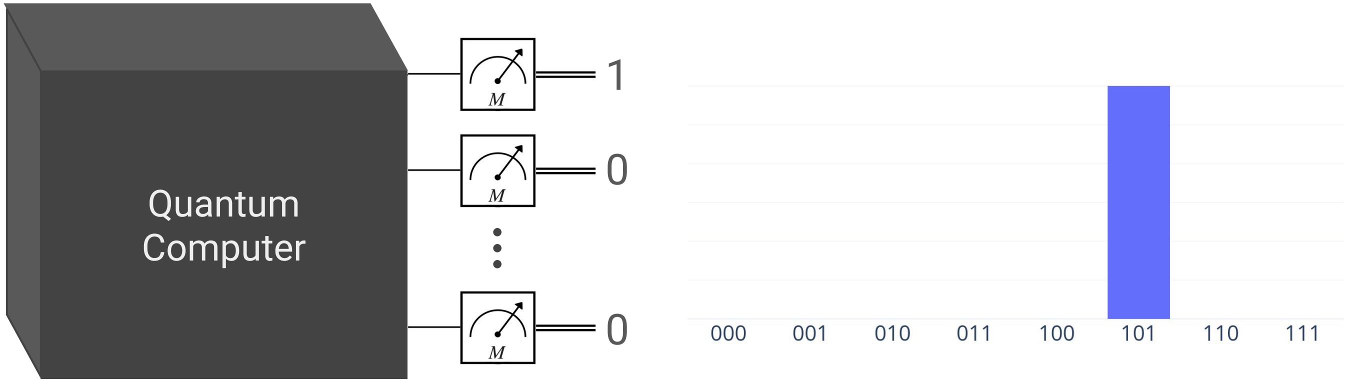


...that can be **deterministic**

Quantum computing: formalism

What is a quantum computer?

A quantum computer is a **generative model...**

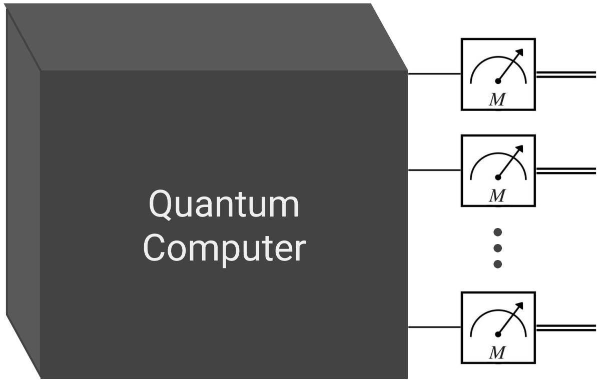


...that is very **efficient** on **specific problems**

Quantum computing: formalism

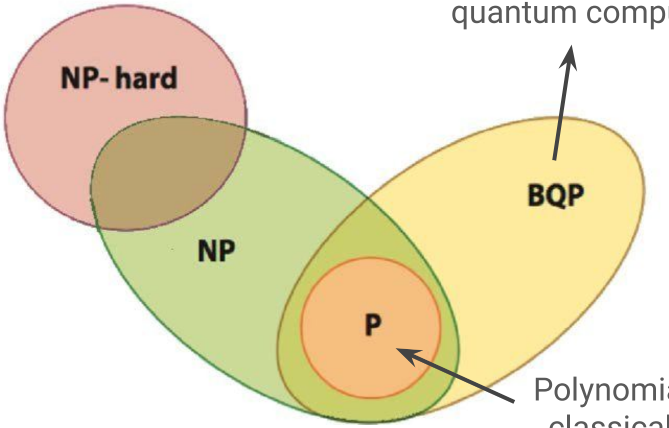
What is a quantum computer?

A quantum computer is **not** equivalent to a Turing machine:



It **cannot** be efficiently simulated by a classical computer...

Polynomial-time on a quantum computer



Polynomial-time on a classical computer

...and has different **complexity classes**

Quantum computing: formalism

Quantum physics as a generalized probability theory

	Probabilistic bit	Quantum bit (Qubit)
State	$\mathbf{p} = \begin{pmatrix} p_0 \\ p_1 \end{pmatrix} \in \mathbb{R}^2,\ \mathbf{p} \geq 0,\ \|\|\mathbf{p}\|\|_1 = 1$	$\psi = \begin{pmatrix} a_0 \\ a_1 \end{pmatrix} \in \mathbb{C}^2,\ \|\|\psi\|\|_2 = 1$

Quantum computing: formalism

Quantum physics as a generalized probability theory

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Probability of event i	p_i	$\|a_i\|^2$

Quantum computing: formalism

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Probability of event i	p_i	$\lvert a_i\rvert^2$
Evolution	**Stochastic matrix** $\lVert S\mathbf{p}\rVert_1 = \lVert\mathbf{p}\rVert_1$	**Unitary matrix** $\lVert U\psi\rVert_2 = \lVert\psi\rVert_2$

Notation: $|0\rangle := e_0 = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$

$$|1\rangle := e_1 = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

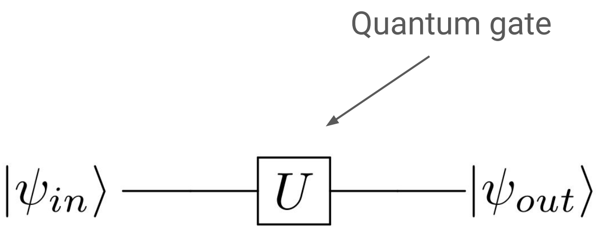
$$|\psi\rangle := \begin{pmatrix} a_0 \\ a_1 \end{pmatrix} = a_0|0\rangle + a_1|1\rangle$$

Quantum computing: formalism

Quantum circuits

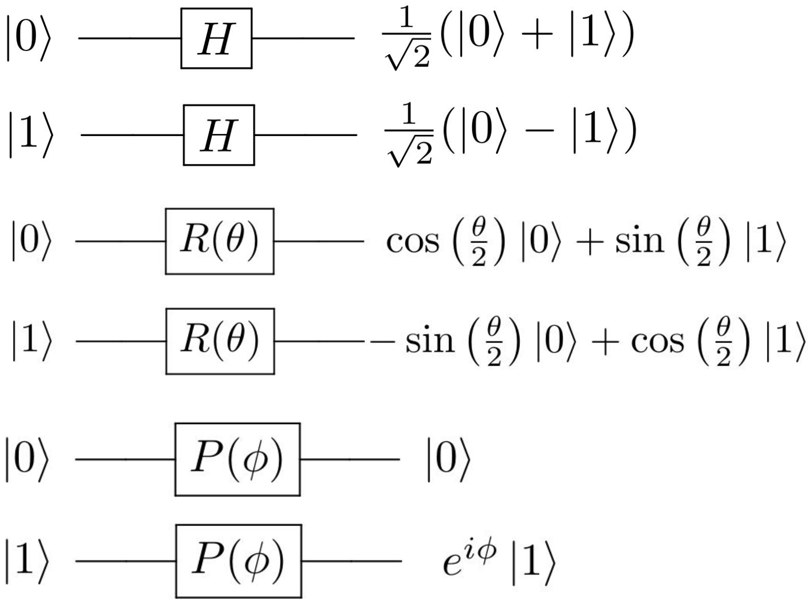
Notation:

$$|\psi_{out}\rangle = U|\psi_{in}\rangle \;:$$



Examples:

- Hadamard Gate $H = \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}$
- Rotation Gate $R(\theta) = \begin{pmatrix} \cos\left(\frac{\theta}{2}\right) & -\sin\left(\frac{\theta}{2}\right) \\ \sin\left(\frac{\theta}{2}\right) & \cos\left(\frac{\theta}{2}\right) \end{pmatrix}$
- Phase Gate $P(\phi) = \begin{pmatrix} 1 & 0 \\ 0 & e^{i\phi} \end{pmatrix}$



Quantum computing: formalism

Multiple qubits

2-qubit state: $|\psi\rangle = \begin{pmatrix} a_{00} \\ a_{01} \\ a_{10} \\ a_{11} \end{pmatrix} = a_{00}|00\rangle + a_{01}|01\rangle + a_{10}|10\rangle + a_{11}|11\rangle \in \mathbb{C}^4$

3-qubit state: $|\psi\rangle = a_{000}|000\rangle + a_{001}|001\rangle + \ldots + a_{111}|111\rangle \in \mathbb{C}^8$

⋮

n-qubit state: $|\psi\rangle = \sum_{i=1}^{2^n} a_i|i\rangle \in \mathbb{C}^{2^n}$ ⟶ Exponentially-large storage

Could we use qubits as a memory for classical data?

Not simple: it can be exponentially-hard to retrieve those amplitudes!

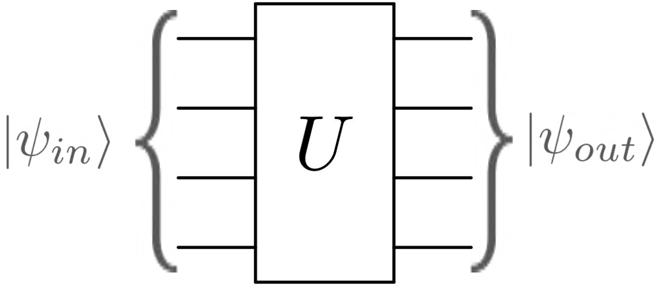
↳ **Quantum state tomography**

Quantum computing: formalism

Multiple qubits

What about the **gates**?

$$U \in \mathcal{U}(2^n)$$



Physically **efficient** operations...

...that can perform **exponentially-large** matrix multiplications

Quantum "parallelism"? **Yes** and **No**

It's what makes quantum computers powerful

You can only retrieve the result efficiently in very specific cases

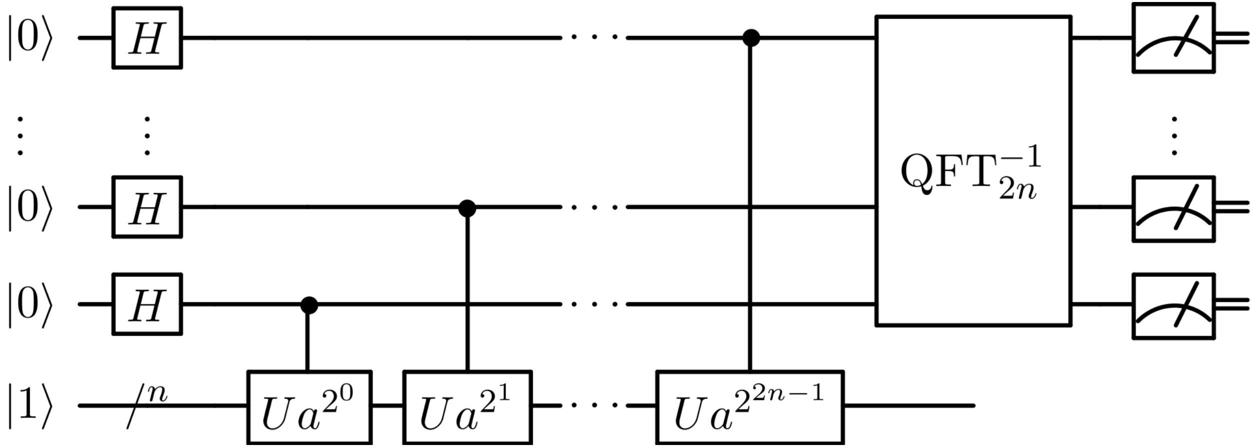
Quantum computing: formalism

Quantum Algorithms

Shor's Algorithm

Goal: Factor a number N into its prime factors

Speed-up: exponential



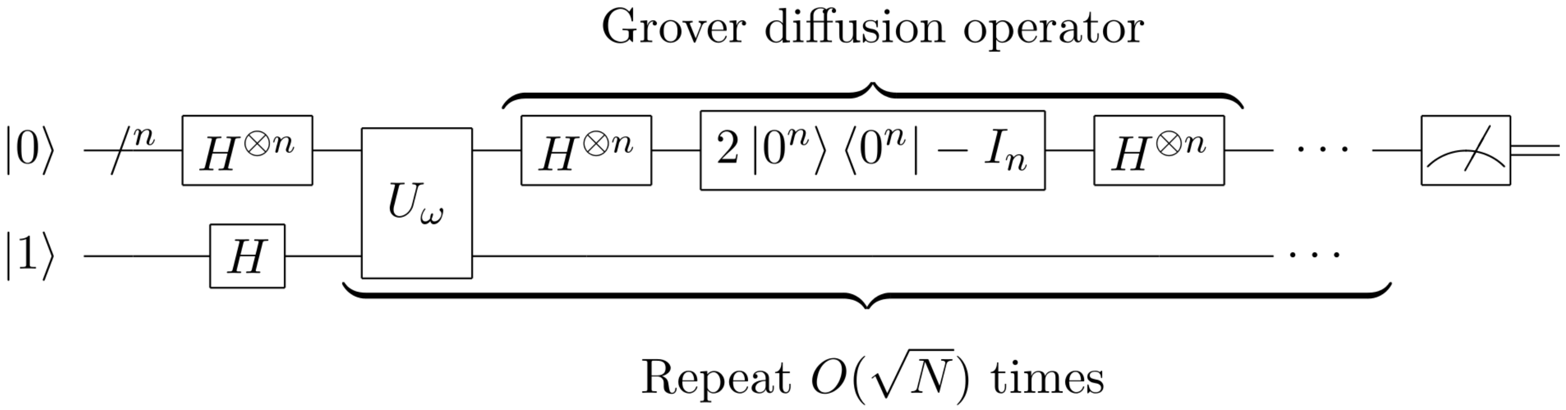
Quantum computing: formalism

Quantum Algorithms

Grover Algorithm

Goal: Search an element in an unstructured list

Speed-up: quadratic



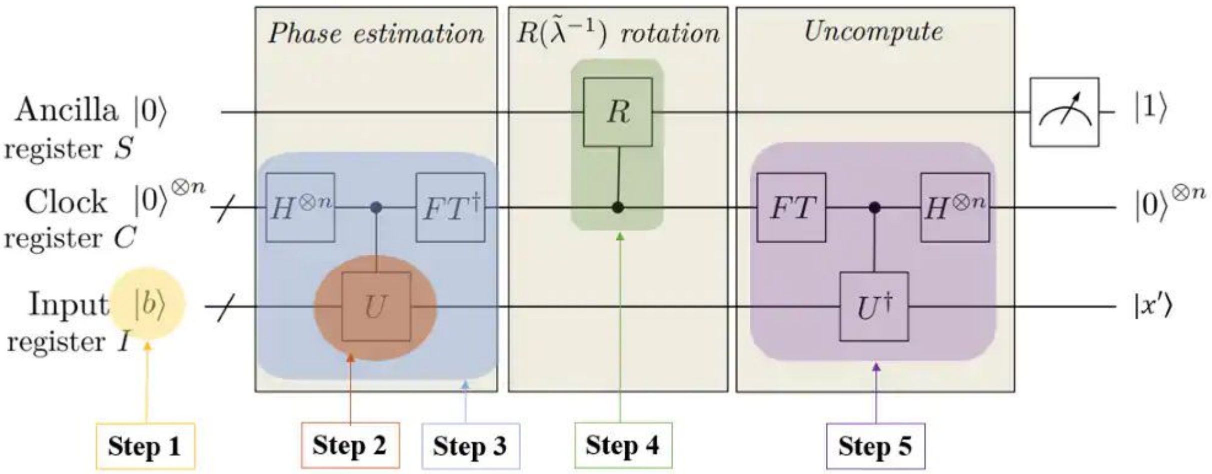
Quantum computing: formalism

Quantum Algorithms

HHL Algorithm

Goal: Solve well-conditioned linear system of equations $A\mathbf{x} = b$

Speed-up: exponential (with some major caveats)



Source: Dervovic et al., *Quantum linear systems algorithms: a primer*, arxiv.org/abs/1802.08227

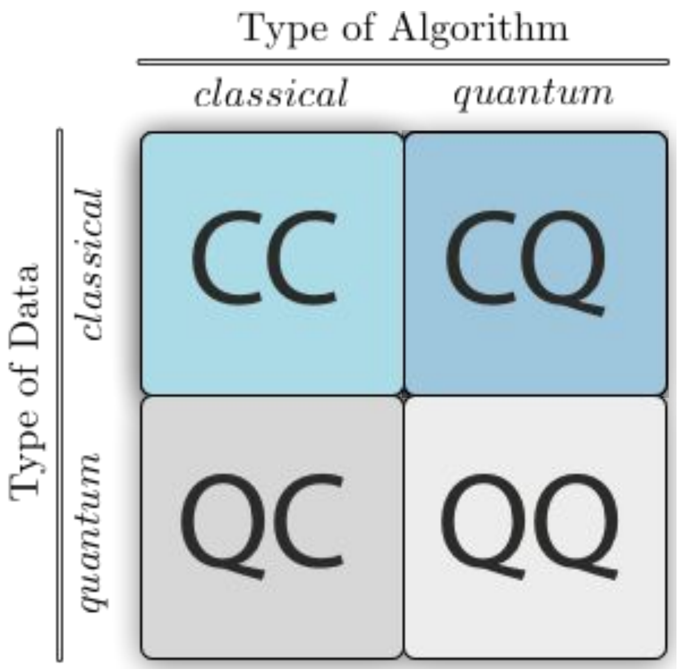
“Most **overhyped** and **underestimated** field in quantum computing”,

Iordanis Kerenidis (Paris Diderot)

Quantum Machine Learning

Quantum machine learning: overview

What is quantum machine learning?



Quantum machine learning: overview

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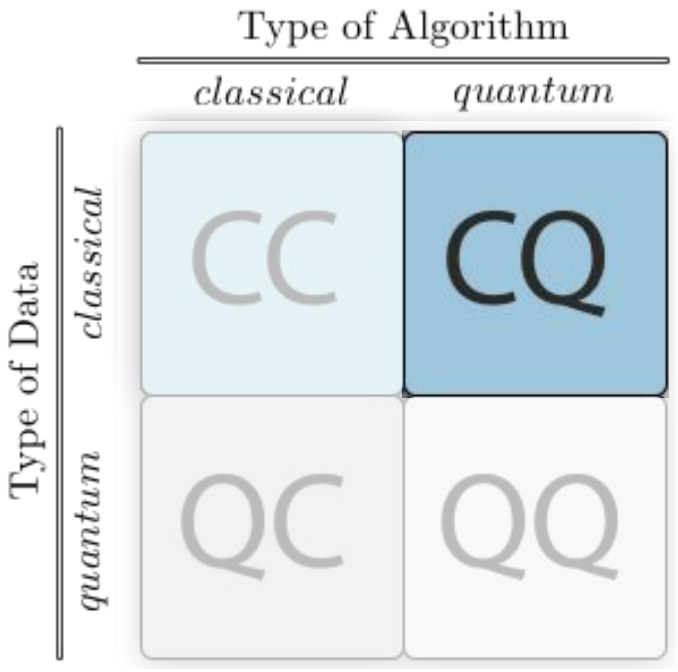
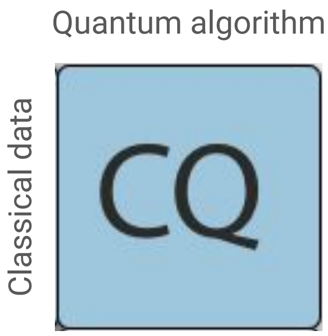


Quantum machine learning: overview

What is quantum machine learning?



First-wave QML
(from ~2010)

Fault-tolerance devices

Theoretical guarantees

Requires QRAM

QSVM, QPCA, QBoost, Q-Means, etc.

Second-wave QML
(from ~2016)

Noisy devices

Heuristics

No QRAM

Quantum NN, Quantum Kernels

Quantum machine learning: first-wave

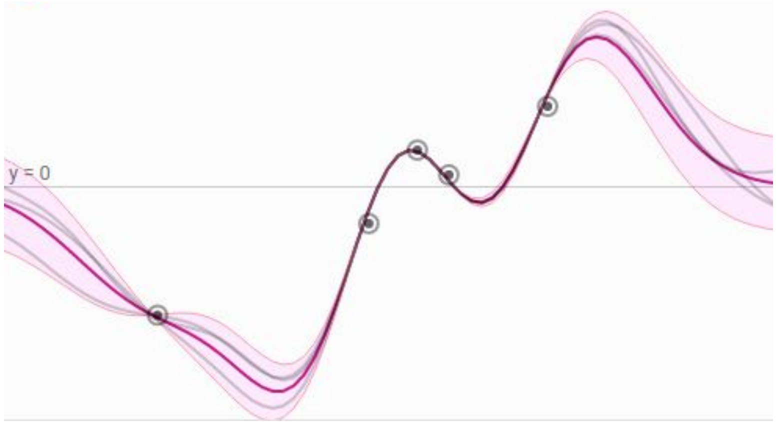
Example: Quantum Gaussian Processes (GP)

Classical GP:

The mean and std of a GP with kernel K is given by:

$$\mu_* = \mathbf{k}_*^T (K + \sigma^2 I_n)^{-1} \mathbf{y}$$

$$\sigma_* = k(\mathbf{x}_*, \mathbf{x}_*) - \mathbf{k}_*^T (K + \sigma^2 I_n)^{-1} \mathbf{k}_*$$



Source: distill.pub/2019/visual-exploration-gaussian-processes/

Quantum GP:

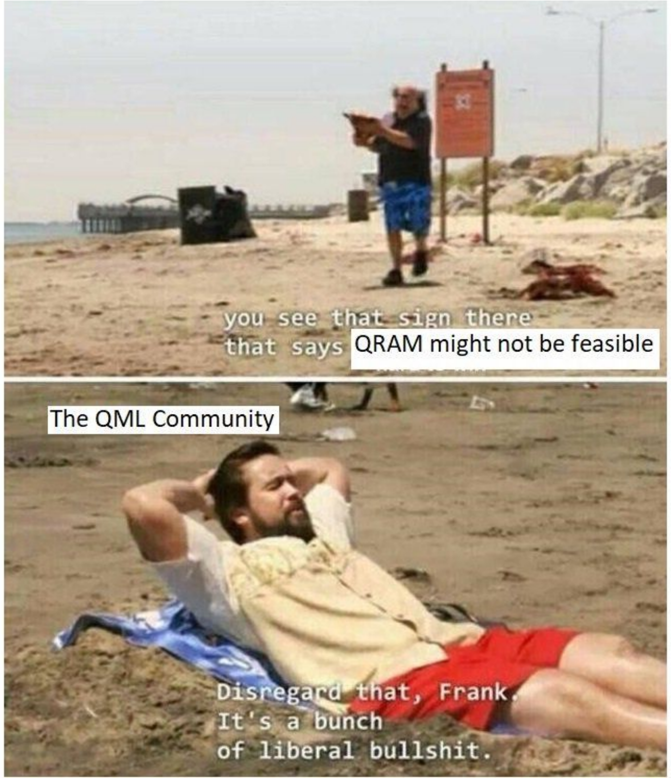
To calculate the mean:

1. Prepare states $|\mathbf{k}_*\rangle$ and $|\mathbf{y}\rangle$ on a quantum RAM
2. Calculate $|\mathbf{b}\rangle = (K + \sigma^2 I_n)^{-1} |\mathbf{y}\rangle$ using HHL
3. Calculate the inner product $\langle \mathbf{b} | \mathbf{y} \rangle$

Source: Zhao et al., *Quantum assisted Gaussian process regression*, arxiv.org/abs/1512.03929

Quantum machine learning: first-wave

Caveat 1: QRAM might not be feasible



1. It might be too slow to have any advantage
2. Requires too many qubits for short-term applications

Source: Quantum computing Memes for QMA-complete teens, Twitter

Quantum machine learning: first-wave

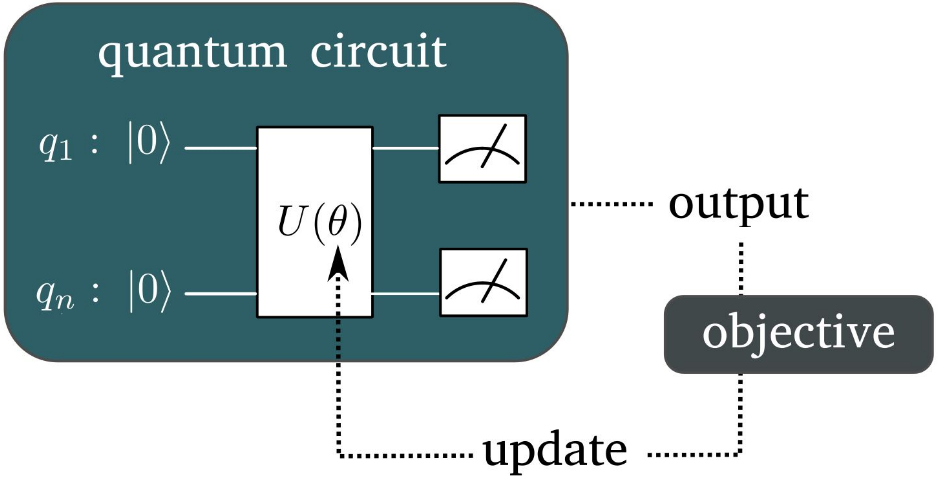
Caveat 2: Beware dequantization!

1. Quantum-inspired algorithms with same performance as purely quantum can be constructed
2. Dequantized algorithms: recommendation systems, low-rank HHL, PCA...
3. But constant factors matter!

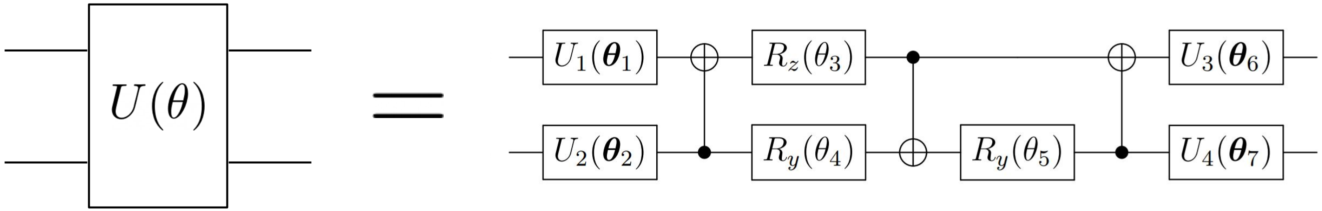
Source: Quantum computing Memes for QMA-complete teens, Twitter

Quantum machine learning: second-wave

Variational circuits

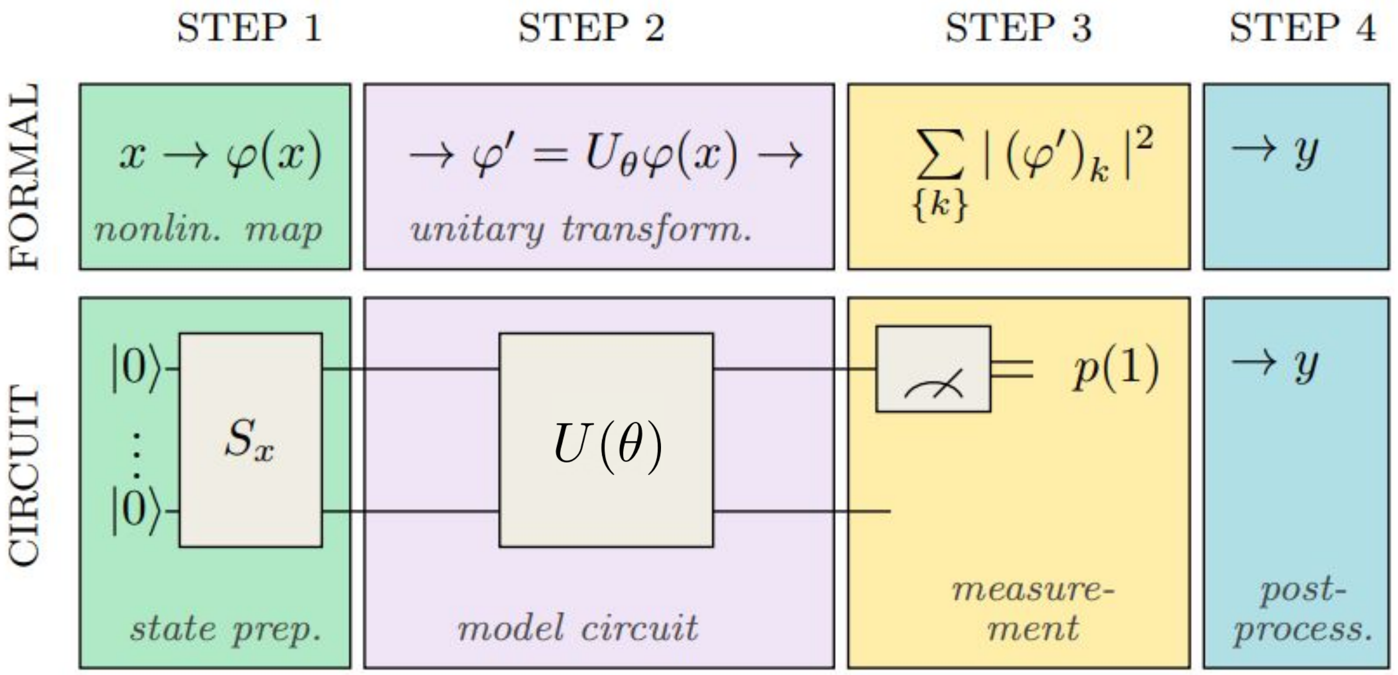


Example of **ansatz**:



Quantum machine learning: second-wave

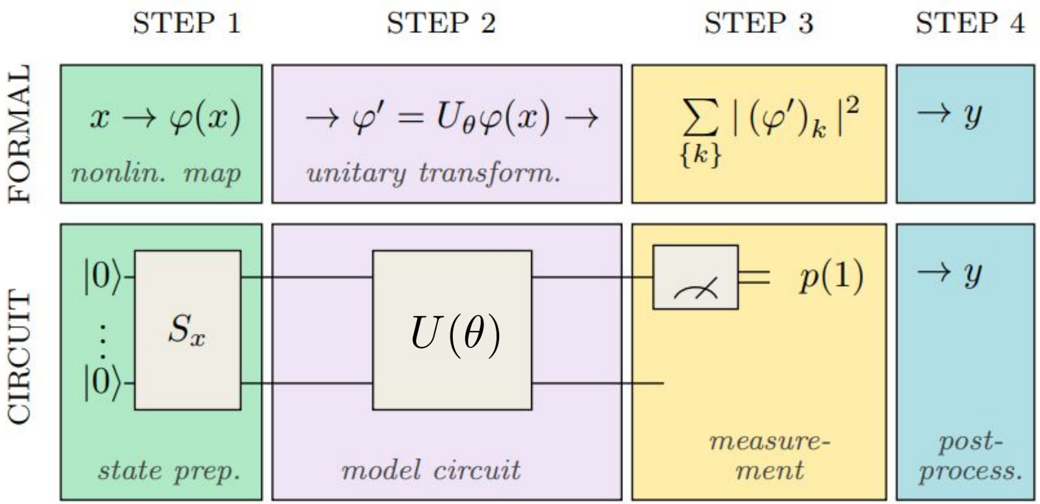
Variational quantum classifier



Source: Schuld et al., *Circuit-centric quantum classifiers*, arxiv.org/abs/1804.00633

Quantum machine learning: second-wave

Variational quantum classifier



Optimization
Quantum stochastic gradient descent

Potential advantage
Better inference time for some problems

Caveat
No proof of advantage, empirical demonstration on toy models

Source: Schuld et al., *Circuit-centric quantum classifiers*, arxiv.org/abs/1804.00633

Quantum machine learning: second-wave

How can I try it myself?

My favorite libraries for quantum ML

Pennylane (Python):

- Easy to use
- Can compute quantum and classical gradients
- Interface with PyTorch and Tensorflow
- Can connect to other simulators and real devices

Yao (Julia):

- Very modular and flexible
- Fastest simulator currently available
- Automatic differentiation as well

```python
import pennylane as qml
from pennylane import numpy as np

# create a quantum device
dev1 = qml.device('default.qubit', wires=1)

@qml.qnode(dev1)
def circuit(phi1, phi2):
  # a quantum node
  qml.RX(phi1, wires=0)
  qml.RY(phi2, wires=0)
  return qml.expval(qml.PauliZ(0))

def cost(x, y):
  # classical processing
  return np.sin(np.abs(circuit(x, y))) - 1

# calculate the gradient
dcost = qml.grad(cost, argnum=[0, 1])
```

Source: Pennylane website (pennylane.ai), Yao website (https://yaoquantum.org/)

Discussion

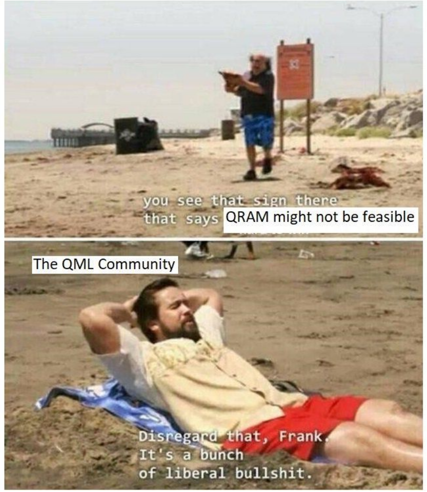
QML is the "most **overhyped** and **underestimated** field in quantum computing" (Iordanis Kerenidis)

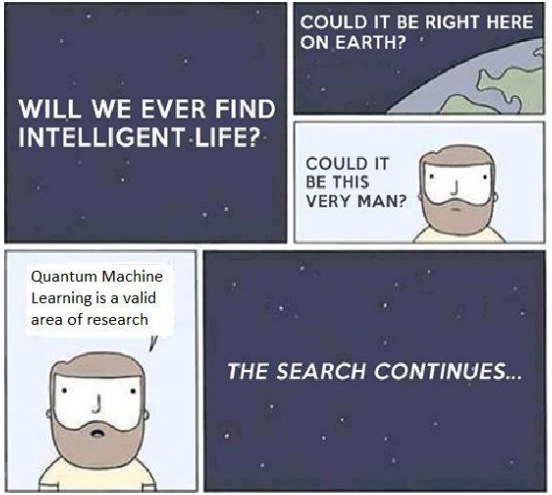
Overhyped: lot of fuss, but too early to predict if QML will ever be useful: no perfect QML algorithm has been found so far

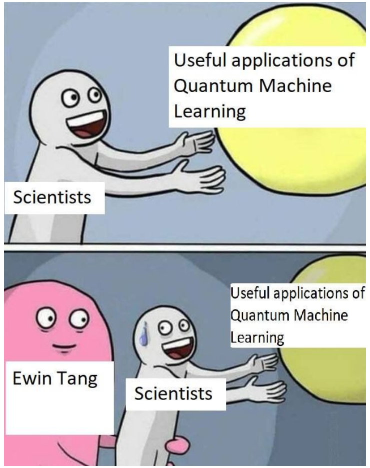
Underestimated:

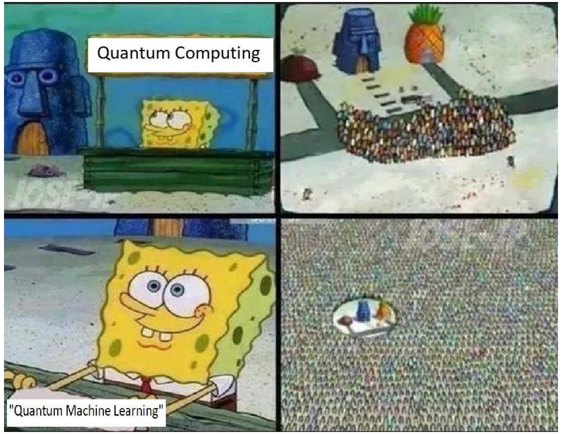
- Research in this field ⇒ new classical algorithms discovered!
- Dequantization only discovered in 2018 ⇒ non-dequantizable algorithms might still be found!
- Second-wave QML very similar to early deep learning research!
- Only a small community actively working on QML!

Source: Pennylane website (pennylane.ai), Yao website (https://yaoquantum.org/)









When someone tries to show you a Quantum Machine Learning paper