Quantum Machine Learning

Maria Schuld

Xanadu and University of KwaZulu-Natal

SMILES, August 2020

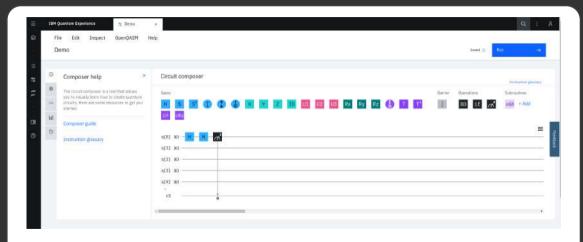




Quantum computing is an emerging technology.



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An emerging technology needs applications.

WANTED

Application which

- doesn't care about noise
- gives us access to multi-billion \$ markets
- attracts young researchers

An emerging technology needs applications.

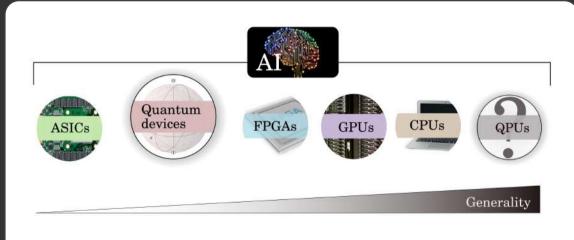
WANTED

Application which

- doesn't care about noise
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Machine Learning!

Quantum computing could potentially enrich ML.

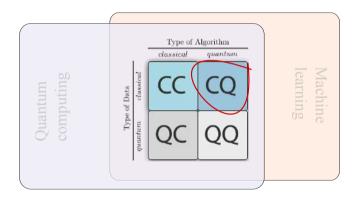


Quantum computing could potentially enrich ML.

machine intelligence = data/distributions + algorithm/hardware + models



Quantum computing could potentially enrich ML.



Agenda

- Quantum computing
- Models
- Algorithms
- Data

QUANTUM COMPUTING

- ► A quantum state $|\psi\rangle$ lives in a **Hilbert space** \mathcal{H} with scalar product $\langle\psi|\psi\rangle$.
- ▶ An **observable** is represented by a Hermitian operator O on \mathcal{H} . The eigenvectors of O form an orthonormal basis of \mathcal{H} with real eigenvalues. Every $|\psi\rangle \in \mathbb{C}^N$ can hence be expressed in O's eigenbasis $\{|\psi_i\rangle\}_{i=1...N}$, $|\psi\rangle = \sum_{i=1}^N a_i |\psi_i\rangle$, where the $a_i \in \mathbb{C}$ are the **amplitudes**.
- ► The effect of applying O to an element $|\psi\rangle \in \mathbb{C}^N$ is fully defined by the eigenvalue equations $O|\psi_i\rangle = \lambda_i|\psi_i\rangle$ with eigenvalues λ_i . Expectation values of the observable property are calculated by $\mathbb{E}(O) = \langle \psi|O|\psi\rangle$.
- The dynamic evolution of a quantum state is represented by a **unitary operator** $U = U(t_2, t_1)$ mapping $|\psi(t_1)\rangle$ to $U(t_2, t_1)|\psi(t_1)\rangle = |\psi(t_2)\rangle$ with $U^{\dagger}U = 1$. U is the solution of the corresponding **Schrödinger equation** $i\hbar \partial_t |\psi\rangle = H |\psi\rangle$ with **Hamiltonian** H.

- 1. Consider a random variable M (measurement) that can take the values (observations) $\{m_1, ..., m_N\}$.
- 2. Assign probabilities $\{p_1, ..., p_N\}$ to these values quantifying our knowledge on how likely an observation is to occur.
- 3. The expectation value of the random variable is defined as

$$\langle M \rangle = \sum_{i=1}^{N} p_i m_i,$$

Use the notation

$$q = \begin{pmatrix} \sqrt{p_1} \\ \vdots \\ \sqrt{p_N} \end{pmatrix} = \sqrt{p_1} \begin{pmatrix} 1 \\ \vdots \\ 0 \end{pmatrix} + \ldots + \sqrt{p_N} \begin{pmatrix} 0 \\ \vdots \\ 1 \end{pmatrix}, \qquad M = \begin{pmatrix} m_1 & \ldots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \ldots & m_N \end{pmatrix}.$$

The expectation value can now be written as

$$\langle M \rangle = q^T M q = \sum_{i=1}^N p_i m_i$$

$$q o \psi = egin{pmatrix} lpha_1 \ dots \ lpha_N \end{pmatrix} \in \mathbb{C}^N, \quad |lpha_i|^2 = p_i$$

$$M \to O_{\text{hermitian}} \in \mathbb{C}^{N \times N}, \quad \text{eig[O]} = \{m_1, \dots, m_N\}$$

$$\langle M \rangle = \psi^T M \psi = \langle \psi | M | \psi \rangle = \sum_{i=1}^N p_i m_i$$

$$\begin{pmatrix} s_{11} & \dots & s_{1N} \\ \vdots & \ddots & \vdots \\ s_{N1} & \dots & s_{NN} \end{pmatrix} \begin{pmatrix} p_1 \\ \vdots \\ p_N \end{pmatrix} = \begin{pmatrix} p_1' \\ \vdots \\ p_N' \end{pmatrix}, \qquad \sum_{i=1}^N p_i = \sum_{i=1}^N p_i' = 1$$

$$\begin{pmatrix} u_{11} & \dots & u_{1N} \\ \vdots & \ddots & \vdots \\ u_{N1} & \dots & u_{NN} \end{pmatrix} \begin{pmatrix} \alpha_1 \\ \vdots \\ \alpha_N \end{pmatrix} = \begin{pmatrix} \alpha_1' \\ \vdots \\ \alpha_N' \end{pmatrix}, \qquad \sum_{i=1}^N |\alpha_i|^2 = \sum_{i=1}^N |\alpha_i'|^2 = 1$$



PHYSICAL CIRCUIT

$$n \begin{bmatrix} |0\rangle \\ \vdots \\ |0\rangle \end{bmatrix}$$

$$2^{n} \begin{bmatrix} |1|^2 = p(0...00) \\ 1+0i \\ 0+0i \\ \vdots \end{bmatrix}$$

$$|0|^2 = p(0...01)$$

```
from pennylane import *

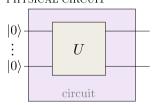
dev = device('default.gubit', wires=2)

def circuit():
    return probs(wires=[8, 1])

print(circuit()) # [1. 8. 8. 8.]
print(dev.state) # [1.+8.j 8.+8.j 8.+8.j 8.+8.j]
```



PHYSICAL CIRCUIT



$$|1|^{2} = p(0...00)$$

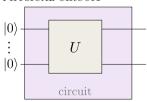
$$u_{ij}$$

$$\begin{vmatrix} 1 + 0i \\ 0 + 0i \\ \vdots \end{vmatrix}$$

$$|0|^{2} = p(0...01)$$



PHYSICAL CIRCUIT



$$|\psi_1|^2 = p(0...00)$$



$$|\psi_2|^2 = p(0...01)$$

```
from pennylane import *
import numpy as np

dev = device('default.gubit', wires=2)

U = np.array([[8., -0.70710678, 8., 0.70718678],

[8.70710678, 8., -0.70710678, 0.],

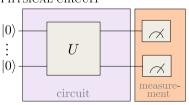
[8., -0.70710678, 8., -0.70718678]])

genode(dev)
def circuit():
    QubitUnitary(U, wires=[0, 1])
    return probs(wires=[6, 1])

print(circuit()) # [8. 8.5 8.5 8.]
print(dev.state) # [8.+8.] 0.787+8.] 0.787+8.] 0.787+8.]
```



PHYSICAL CIRCUIT



```
from pennylane import *
import numby as inp

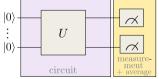
dev = device('default.qubit', wires=2, shots=1)

U = np.array([[0., -0.78710678, 0., 0.70918678], 0., 0.70918678], 0., 0.70918678, 0., 0.70918678, 0., 0., 0.70918678]]

Quitental control c
```



PHYSICAL CIRCUIT $|0\rangle$





```
from pennylane import *
import numpy as np

dev = device('default.qubit', *ires=2, *hots=1)

U = np.array([[0., -0.78718678, 0., 0.78719678],
[0.78718678, 0., -0.78718678, 8. ],
[0., -0.78718678, 0., -0.78718678, 8. ],

@qnode(dev)

def circuit():
    QubitUnitary([], *ires=[0, 1])
    return expval(PauliZ(wires=0)), expval(PauliZ(wires=1))

print(circuit()) # [8., 8.]

print(dev.state) # [8.-0.] 8.787+0.] 8.787+0.] 8.+8.]]
```







PHYSICAL CIRCUIT $|0\rangle$ \vdots $|0\rangle$ measurementment



```
from pennylane import *

dev = device('default.qubit', wires=2)

equods(dev)

def circust(phi):

RX(phi, wires=0)

CNOT(wires=[0, 1])

Hadamard(wires=0)

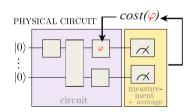
PauliZ(wires=1)

return expval(PauliZ(wires=0)), expval(PauliZ(wires=1))

print(circust(0,2)) # [0.8.98086658]

print(dev.state) # [6.78+0.] 8.+0.67] 8.76+0.] 8.-0.678]
```



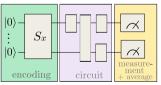


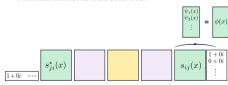


```
from pennylane import *
dev = device('default.qubit', wires=1)
Manade (dev)
def circuit(phi):
   Hadamard(wires=0)
   RY(phi, wires=0)
    return expval(PauliZ(wires=0))
phi = 0.2
opt = GradientDescentOptimizer(stepsize=0.2)
   phi = opt.step(circuit, phi)
   print(phi)
    # 0.39601331556824826
   # 0.5805345472544579
    # 0.7477684644009802
    # 0.8944100937922911
    # 1.0196058853338432
```



PHYSICAL CIRCUIT



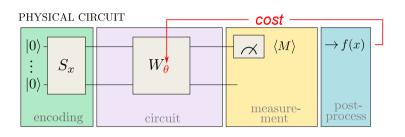


```
from pennylane import *
dev = device('default.qubit', wires=2)
Ranode(dev)
def circuit(phi, x=None):
   RX(x, wires=[0])
   CNOT(wires=[0, 1])
   RY(phi, wires=[1])
    return expval(PauliZ(wires=[1]))
print(circuit(0.2, x=0.1)) # 0.975
print(circuit(0.2, x=0.5)) # 0.860
```

```
from torch autograd import Variable
                                                            from torch autoored import Verieble
data = torch.tensor([(0., 0.), (0.1, 0.1), (0.2, 0.2)]) =
                                                            data = [(0., 0.), (0.1, 0.1), (0.2, 0.2)]
                                                            dev - device( default qubit, mines-2)
 ief medel(phi: x=None);
                                                            def circult(shi, x-bone);
    return wents
                                                                templates.AngleEmbedding(features=[x], =====[0])
                                                                templates SasicEntanglerLayers(unimfumph) wires[8, 1])
                                                                return exeval(PauliZ(nirus-[1]))
                                                             HOT LASSIA - BIT
dof loss(o b):
    return torch abs(a - b) we 2
                                                                roboto torch abs(a - b) ex 2
dof av loss(phi):
    c += loss(model(phi, =x), y)
                                                                c += toss(circuit(ohi, ==x), y)
phi = Variable(terch.tensor(0:1), remainer erass(res) 24
                                                            cht = Variable(torch tencor([]0.1 0.21 [-0.5 0.11]) requires gradulents)
opt = torch.outim.Admo([phi.], | =8.82)
                                                            opt = torch.optim.Adam([phi 1, 1/=0.02)
                                                                l = av loss(phi )
                                                                1.backward()
    1. backward()
    ont.sten()
                                                                cot step()
```

MODELS

Parametrised quantum computations can be used as ML models.

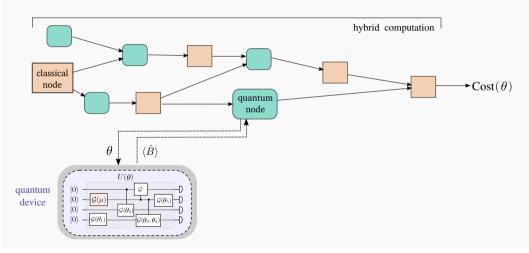


MATHEMATICAL DESCRIPTION

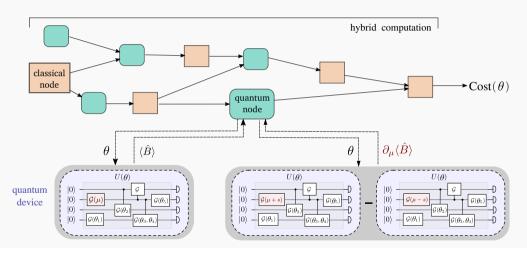


Farhi & Neven 1802.06002, Schuld et al. 1804.00633, Benedetti et al. 1906.07682

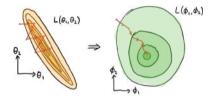
1. How to optimise quantum circuits?

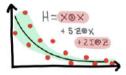


Guerreschi et al. 1701.01450, Mitarai et al. 1803.00745, Schuld et al. 1811.11184, Mari et al. 2008.06517



Guerreschi & Smelyanskiy 1701.01450, Mitarai et al. 1803.00745, Schuld et al. 1811.11184





Barren plateaus in quantum neural network training landscapes

Jarrod R. McClean, ^{1, *} Sergio Boko, ^{1, †} Vadim N. Smelyanskiy, ^{1, †} Ryan Babbush, ¹ and Hartmut Neven [†] Coogle Inc., ³⁴⁰ Main Street, Venice, CA 96291, USA (1998).

Many experimental proposals for noisy intermediate scale quantum devices invelve training a parameterized quantum circuit with a classical optimization length. Such hybrid quantum circuit with a classical optimization length such which parameterized algorithms are popular for applications in quantum simulation, optimization, and machine learning. Due to its simplicity and hardware efficiency, candom circuits are often proposed as initial guesses for exploring the space of quantum states. We show that the exponential dimension of Hilbert space and the gradient estimated complexity make this choice unsuitable for leybrid quantum-classical algorithms run on more than a few quibts. Specifically, we show that for a wide close of reasonable parameterized quantum circuits, the probability that the gradient along any reasonable direction is mon-zero to some fixed precision is exponentable small as a function of the number of quibts. We argue that this is related to the 2-design characteristic of random circuits, and that solutions to this problem must be studied.

Rapid developments in quantum hardware have motivated advances in algorithms to run in the so-called noisy intermediate scale quantum (NISQ) regime [1]. Many of the most promising application-oriented approaches are hybrid quantum-classical algorithms that refy on optimization of a parameterized quantum circuit [2–8]. The resilience of these approaches to certain types of errors and high flexibility with respect to coherence time and gate requirements make them especially attractive for NISQ intelementations [3, 9–1].

The first implementation of such algorithms was de-

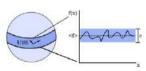
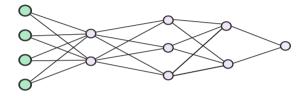


FIG. 1. A cartoon of the general geometric results from this work. The sphere depicts the phenomenon of concentration of

2. What *are* these models?

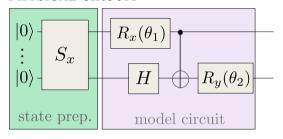
MODEL



MATHEMATICAL DESCRIPTION

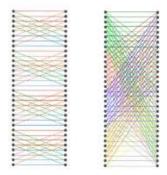


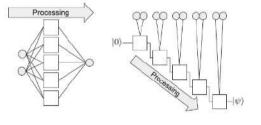
PHYSICAL CIRCUIT

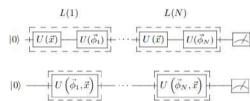


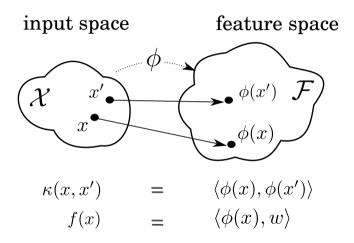
MATHEMATICAL DESCRIPTION











Quantum feature map:

$$x \to \Phi(x) \in \mathbb{C}^{2^{n_{\text{qubits}}}}$$

Quantum feature map:

$$x \to \Phi(x) \in \mathbb{C}^{2^{n_{\text{qubits}}}}$$

Measurement:

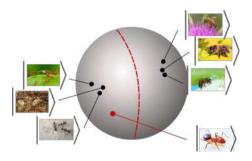
$$\Phi(x)^{\dagger}M\Phi(x)$$

Measurement:

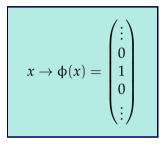
$$\phi(x)^{T} M \phi(x)$$

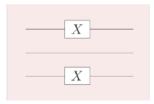
$$= \phi(x)^{\dagger} w w^{\dagger} \phi(x)$$

$$= |\phi(x)^{\dagger} w|^{2}$$



Data encoding defines a "quantum kernel".



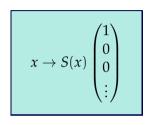


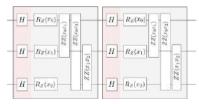
Data encoding defines a "quantum kernel".

$$x \to \phi(x) = \begin{pmatrix} x_1 \\ x_2 \\ x_3 \\ \vdots \end{pmatrix}$$

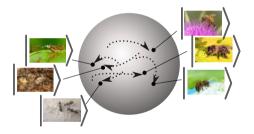
$$\begin{pmatrix} x_1 \\ x_2 \\ \vdots \\ x_N \end{pmatrix}$$

Data encoding defines a "quantum kernel".

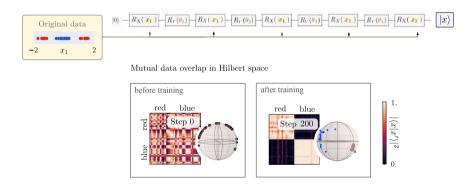




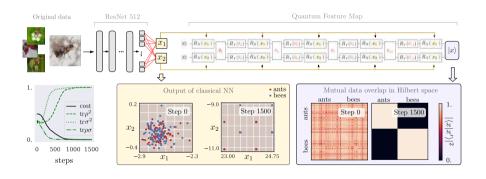
We can engineer/train our features.



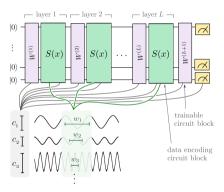
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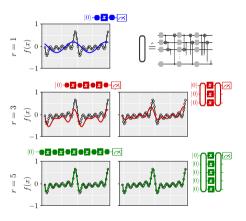
We can engineer/train our features.



Quantum circuits are partial Fourier series.



Quantum circuits are partial Fourier series.



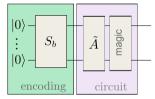
ALGORITHMS

1. Exploit the linear algebra structure

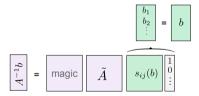
Quantum computers can invert exponentially large matrices.*

Assumption: the bottleneck of my ML algorithm is matrix inversion: $Ax = b \rightarrow x = A^{-1}b$.





MATHEMATICAL DESCRIPTION



Quantum computers can invert exponentially large matrices.*

- 1. Prepare ψ_b .
- 2. Apply \tilde{A} ψ_b (where $\tilde{A} = e^{-iA}$, but that is not so important).

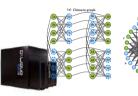
$$\begin{split} \tilde{A}\psi_b &= \tilde{A} \left(\langle a_1, \psi_b \rangle a_1 + \dots + \langle a_N, \psi_b \rangle a_N \right) \\ &= \langle a_1, \psi_b \rangle \lambda_1 a_1 + \dots + \langle a_N, \psi_b \rangle \lambda_N a_N \\ &\Rightarrow \langle a_1, \psi_b \rangle \frac{1}{\lambda_1} a_1 + \dots + \langle a_N, \psi_b \rangle \frac{1}{\lambda_N} a_N \\ &= \psi_x \end{split}$$

3. Use ψ_b to do something interesting.

2. Use QC as samplers

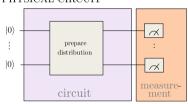
Quantum computers can train Boltzmann machines.*



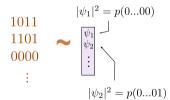




PHYSICAL CIRCUIT



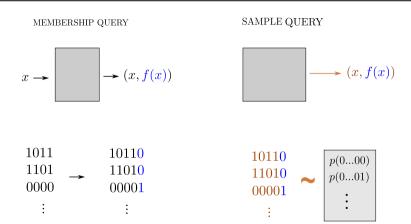
MATHEMATICAL DESCRIPTION



Denil & Freitas 2012(?) https://www.cs.ubc.ca/~nando/papers/quantumrbm.pdf

DATA

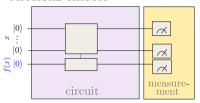
1. Quantum data and learnability



MEMBERSHIP QUERY



PHYSICAL CIRCUIT



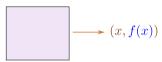
MATHEMATICAL DESCRIPTION

$$|\psi_{1}|^{2} = p(0...00)$$

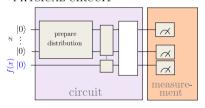
$$10110 \quad \begin{bmatrix} 0 \\ 1 \\ \vdots \end{bmatrix}$$

$$|\psi_{2}|^{2} = p(0...01)$$





PHYSICAL CIRCUIT



MATHEMATICAL DESCRIPTION

10110
11010
00001
:
$$|\psi_1|^2 = p(0...00)$$

$$|\psi_1|^2 = p(0...00)$$

$$|\psi_1|^2 = p(0...00)$$

$$|\psi_2|^2 = p(0...01)$$

A Survey of Quantum Learning Theory

Srinivasan Arunachalam*

Ronald de Wolf†

Abstract

This paper surveys quantum learning theory: the theoretical aspects of machine learning using quantum computers. We describe the main results known for three models of learning: exact learning from membership queries, and Probably Approximately Correct (PAC) and agnostic learning from classical or quantum examples.

Exact learning. In this setting the goal is to learn a target concept from the ability to interact with it. For concreteness, we focus on learning target concepts that are Boolean functions: the target is some unknown $c: \{0,1\}^n \to \{0,1\}$ coming from a known concept class \mathcal{C} of functions, 2 and our goal is to identify c exactly, with high probability, using *membership queries* (which allow the learner to learn c(x) for x of his choice). If the measure of complexity is just the number of queries, the main results are that quantum exact learners can be polynomially more efficient than classical, but not more. If the measure of complexity is *time*, then under reasonable complexity-theoretic assumptions some concept classes can be learned much faster from quantum membership queries (i.e., where the learner can query c on a superposition of x's) than is possible classically.

PAC learning. In this setting one also wants to learn an unknown $c:\{0,1\}^m \to \{0,1\}$ from a known concept class C, but in a more passive way than with membership queries: the learner receives several *labeled examples* (x,c(x)), where x is distributed according to some unknown probability distribution D over $\{0,1\}^n$. The learner gets multiple i.i.d. labeled examples. From this limited "view" on c, the learner wants to generalize, producing a *hypothesis* h that probably agrees with c on "most" x, measured according to the same D. This is the classical Probably Approximately Correct (PAC) model. In the quantum PAC model [BJ99], an example is not a random sample but a superposition $\sum_{x \in [0,1]^n} \sqrt{D(x)} |x,c(x)\rangle$. Such quantum examples can be useful for some

learning tasks with a fixed distribution D (e.g., uniform D) but it turns out that in the usual distribution-independent PAC model, quantum and classical sample complexity are equal up to constant factors, for every concept class \mathcal{C} . When the measure of complexity is *time*, under reasonable complexity-theoretic assumptions, some concept classes can be PAC learned much faster by quantum learners (even from classical examples) than is possible classically.

2. Quantum data as quantum states

What happens if we do QML on "quantum states"?

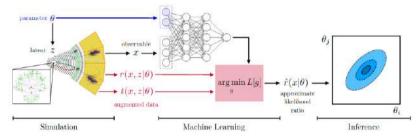


Figure 2. A schematic of machine learning based approaches to likelihood-free inference in which the simulation provides training data for a neural network that is subsequently used as a surrogate for the intractable likelihood during inference. Reproduced from (Brehmer et al.) 2018b).

CONCLUSION

Summary,...

 $machine\ intelligence = data/distributions + algorithm/hardware + models$



...and some open questions.

- ▶ What models are quantum circuits?
- ► Are they actually useful?
- ▶ Will they perform well on larger problem instances?
- Will they perform well under noise?
- What problems are they good for?
- ► Is there a practically relevant problem for which QC are exponentially faster?
- ► Can QC accelerate machine learning?
- ► Can QC push the boundaries of what is learnable?

Thank you!

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