Quantum Machine Learning: Foundation, New Techniques, and Opportunities for Database Research

SIGMOD'23 **Tutorial**

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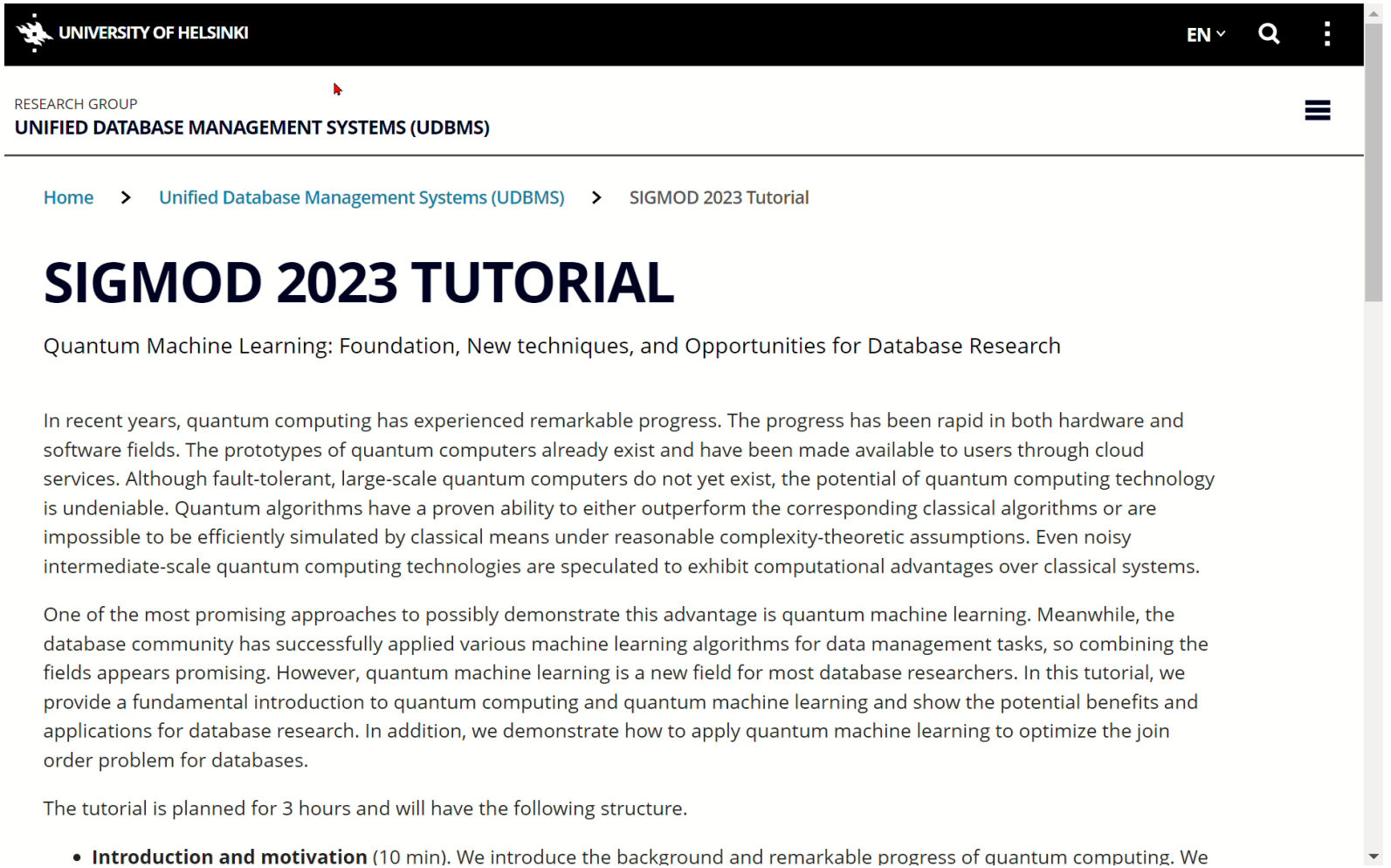
Tutorial Page

- Additional material (slides/links etc.): https://www.helsinki.fi/en/researchgroups/unified-database-management-systems-udbms/sigmod-2023-tutorial



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SIGMOD 2023 TUTORIAL

Quantum Machine Learning: Foundation, New techniques, and Opportunities for Database Research

In recent years, quantum computing has experienced remarkable progress. The progress has been rapid in both hardware and software fields. The prototypes of quantum computers already exist and have been made available to users through cloud services. Although fault-tolerant, large-scale quantum computers do not yet exist, the potential of quantum computing technology is undeniable. Quantum algorithms have a proven ability to either outperform the corresponding classical algorithms or are impossible to be efficiently simulated by classical means under reasonable complexity-theoretic assumptions. Even noisy intermediate-scale quantum computing technologies are speculated to exhibit computational advantages over classical systems.

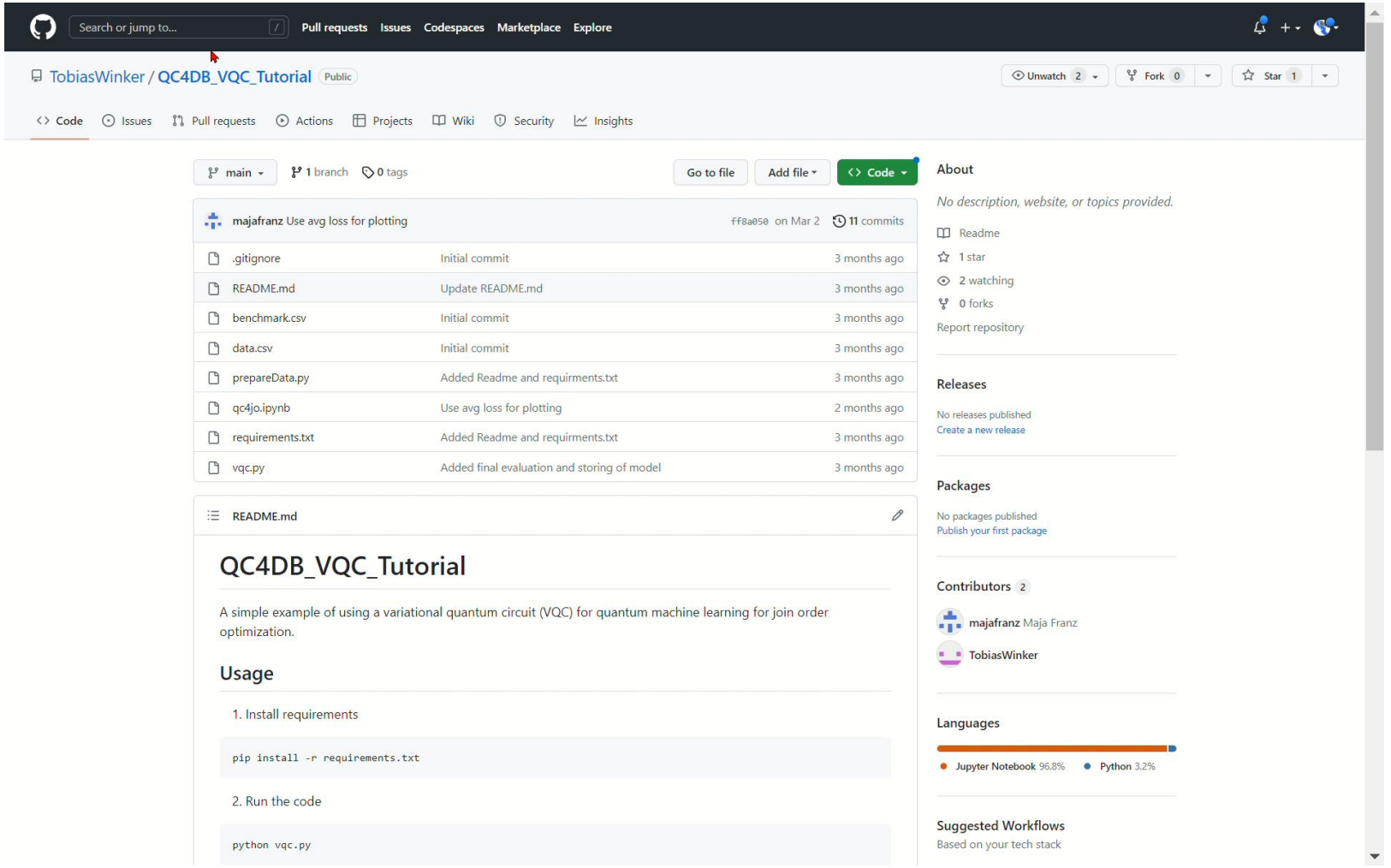
One of the most promising approaches to possibly demonstrate this advantage is quantum machine learning. Meanwhile, the database community has successfully applied various machine learning algorithms for data management tasks, so combining the fields appears promising. However, quantum machine learning is a new field for most database researchers. In this tutorial, we provide a fundamental introduction to quantum computing and quantum machine learning and show the potential benefits and applications for database research. In addition, we demonstrate how to apply quantum machine learning to optimize the join order problem for databases.

The tutorial is planned for 3 hours and will have the following structure.

- **Introduction and motivation** (10 min). We introduce the background and remarkable progress of quantum computing. We

Code

- Python code for first steps:
  quantum machine learning optimizes join orders
  https://github.com/TobiasWinker/QC4DB_VQC_Tutorial



Publication

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ABSTRACT

In the last few years, the field of quantum computing has experienced remarkable progress. The prototypes of quantum computers already exist and have been made available to users through cloud services (e.g., IBM Q experience, Google quantum AI, or Xanadu quantum cloud). While fault-tolerant and large-scale quantum computers are not available yet (and may not be for a long time, if ever), the potential of this new technology is undeniable. Quantum algorithms have the proven ability to either outperform classical approaches for several tasks, or are impossible to be efficiently simulated by classical means under reasonable complexity-theoretic assumptions. Even imperfect current-day technology is speculated to exhibit computational advantages over classical systems. Recent research is using quantum computers to solve machine learning tasks. Meanwhile, the database community has already successfully applied various machine learning algorithms for data management tasks, so combining the fields seems to be a promising endeavour. However, quantum machine learning is a new research field for most database researchers. In this tutorial, we provide a fundamental introduction to quantum computing and quantum machine learning and show the potential benefits and applications for database research. In addition, we demonstrate how to apply quantum machine learning to the join order optimization problem in databases.

CCS CONCEPTS

• **Computer systems organization** → **Quantum computing**; • **Computing methodologies** → **Machine learning**; • **Information systems** → **Data management systems**.

KEYWORDS

Quantum machine learning, quantum computing, databases

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Figure 1: Timeline of quantum computing and quantum machine learning papers, and quantum computers (including roadmaps). Figure is extended from [24].

1 INTRODUCTION

Considering the timeline of available and future quantum computers in relation to the number of supported qubits in Figure 1, there seems to be an exponential growth trend in the number of supported qubits. The roadmap of major players contains quantum computers (QC) allowing to scale in 2023 (IBM), supporting 4000 qubits in 2025 (IBM) and 10000 qubits in 2029 (Google). Although the number of qubits is known to be a problematic measure for general QC capabilities (and other metrics such as quantum volume [13] have been proposed), the prestigious race for the most qubits is a driver of the current hype in quantum technologies promising numerous quantum applications in practice within this decade.

A quite obvious correlation exists between the availability of quantum computers supporting more qubits and the publication performance of researchers in the areas of quantum computing and quantum machine learning (see Figure 1). There seem to be differences in the absolute numbers of published papers in the addressed areas for different scientific communities: In 2022, there have been 6.8 times more papers published on nature.com (aiming to publish journal articles in the areas of natural sciences) containing 'quantum computing' and 4.7 times more papers containing 'quantum machine learning' in the title than are included in the dblp computer science bibliography (providing open bibliographic

Agenda

- Introduction and motivation
- **Basics** of Quantum Computing
- **Quantum machine learning** (+ coffee break)
- Demo: **quantum machine learning optimizes join orders**
- Open problems and **challenges** for database research
- QA session

Golden Age of Quantum Computing ? 1/3

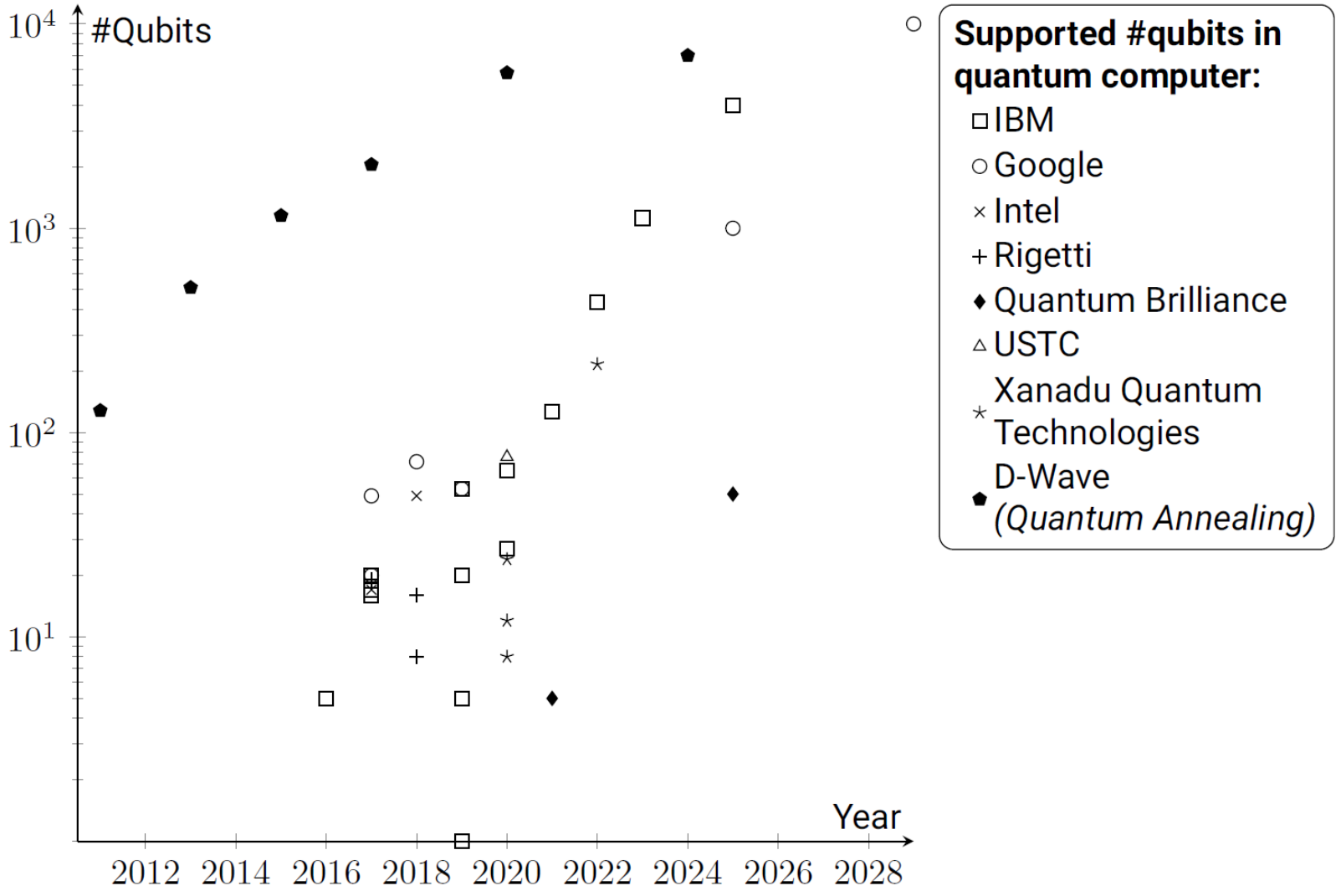
- **„Billion USD-race“** of funding quantum computing technologies between nations, e.g.:
  - more than 55 billion USD in state-sponsored research and development initiatives worldwide[1] (Jan.’23)
    - China: 20,0 billion USD
    - EU: 7,2 billion USD
    - Germany: 6,4 billion USD
    - USA: 3,7 billion USD
    - UK: 2,5 billion USD
    - France: 2,3 billion USD
    - Japan: 1,8 billion USD
    - Canada: 1,6 billion USD
    - India 1,1 billion USD
  - Germany: recently announced additional 3 billion Euros[2]

[1] https://www.forbes.com/sites/gilpress/2023/01/31/new-funding-for-quantum-computing-accelerates-worldwide/

[2] https://thequantuminsider.com/2023/05/03/germany-announces-3-billion-euro-action-plan-for-a-universal-quantum-computer/

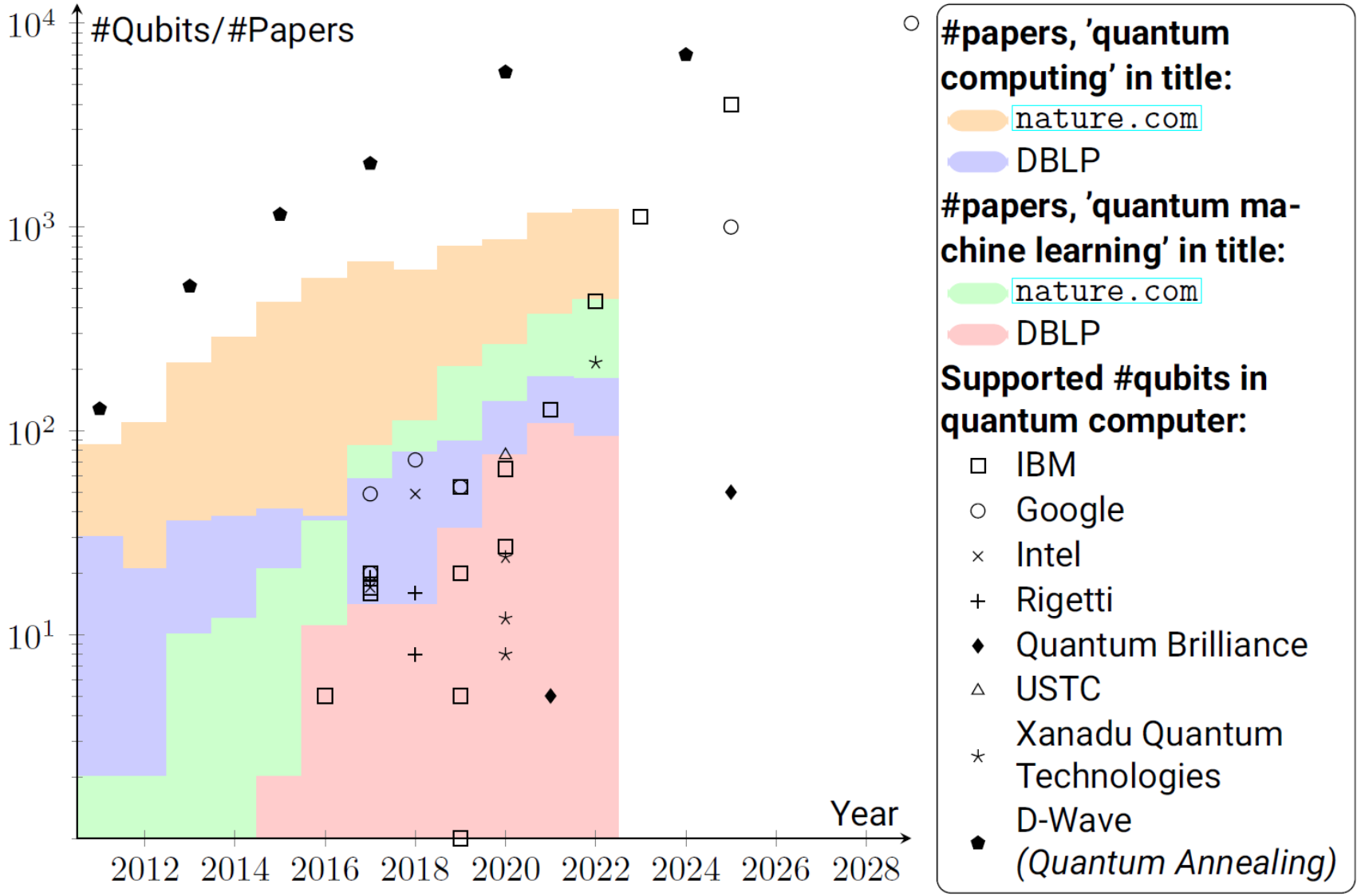
Golden Age of Quantum Computing ? 2/3

- **Exponential growth** in number of **qubits**



Golden Age of Quantum Computing ? 3/3

- **Exponential growth** in number of **papers**
- Research contributions dominated by natural sciences community
- ***We encourage computer scientists*** *(especially from the database community)* ***to consider quantum computing*** *for their research!*



Quantum mechanics from computational perspective

Simulating Physics with Computers

Richard P. Feynman

Department of Physics, California Institute of Technology, Pasadena, California 91107

Received May 7, 1981

Nature isn't classical, dammit, and if you want to make a simulation of nature, you'd better make it quantum mechanical, and by golly it's a wonderful problem, because it doesn't look so easy.

– Richard Feynman

Quantum advantage and hype

BLOG ›

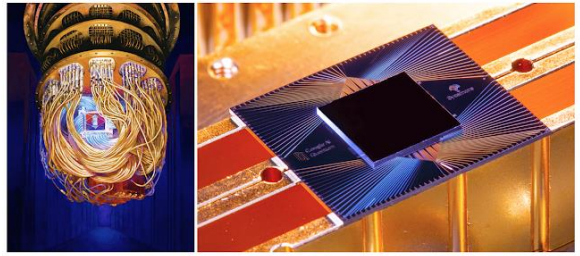
Quantum Supremacy Using a Programmable Superconducting Processor

WEDNESDAY, OCTOBER 23, 2019

Posted by John Martinis, Chief Scientist Quantum Hardware and Sergio Boixo, Chief Scientist Quantum Computing Theory, Google AI Quantum

Physicists have been talking about the power of **quantum computing** for over 30 years, but the questions have always been: will it ever do something useful and is it worth investing in? For such large-scale endeavors it is good engineering practice to formulate decisive short-term goals that demonstrate whether the designs are going in the right direction. So, we devised an experiment as an important milestone to help answer these questions. This experiment, referred to as a **quantum supremacy** experiment, provided direction for our team to overcome the many technical challenges inherent in quantum systems engineering to make a computer that is both programmable and powerful. To test the total system performance we selected a sensitive computational benchmark that fails if just a single component of the computer is not good enough.

Today we published the results of this quantum supremacy experiment in the *Nature* article, "**Quantum Supremacy Using a Programmable Superconducting Processor**". We developed a new 54-qubit processor, named "Sycamore", that is comprised of fast, high-fidelity **quantum logic gates**, in order to perform the benchmark testing. Our machine performed the target computation in 200 seconds, and from measurements in our experiment we determined that it would take the world's fastest supercomputer 10,000 years to produce a similar output.



***Left:** Artist's rendition of the Sycamore processor mounted in the cryostat. (**Full Res Version**; Forest Stearns, Google AI Quantum Artist in Residence) **Right:** Photograph of the Sycamore processor. (**Full Res Version**; Erik Lucero, Research Scientist and Lead Production Quantum Hardware)*

Article | Open Access | Published: 01 June 2022

Quantum computational advantage with a programmable photonic processor

Lars S. Madsen, Fabian Laudenbach, Mohsen Falamarzi. Askarani, Fabien Rortais, Trevor Vincent, Jacob F. F. Bulmer, Filippo M. Miatto, Leonhard Neuhaus, Lukas G. Helt, Matthew J. Collins, Adriana E. Lita, Thomas Gerrits, Sae Woo Nam, Varun D. Vaidya, Matteo Menotti, Ish Dhand, Zachary Vernon, Nicolás Quesada & Jonathan Lavoie

Nature **606**, 75–81 (2022) | Cite this article

107k Accesses | **104** Citations | **1282** Altmetric | Metrics

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Science Bulletin

Volume 67, Issue 3, 15 February 2022, Pages 240-245

Article

Quantum computational advantage via 60-qubit 24-cycle random circuit sampling

Qingling Zhu [a b c], Sirui Cao [a b c], Fusheng Chen [a b c], Ming-Cheng Chen [a b c], Xiawei Chen [b], Tung-Hsun Chung [a b c], Hui Deng [a b c], Yajie Du [b], Daojin Fan [a b c], Ming Gong [a b c], Cheng Guo [a b c], Chu Guo [a b c], Shaojun Guo [a b c], Lianchen Han [a b c], Linyin Hong [d], He-Liang Huang [a b c e], Yong-Heng Huo [a b c], Liping Li [b], Na Li [a b c], Shaowei Li [a b c]... Jian-Wei Pan [a b c]

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REPORT

Quantum computational advantage using photons

HAN-SEN ZHONG, HUI WANG, YU-HAO DENG, MING-CHENG CHEN, LI-CHAO PENG, YI-HAN LUO, JIAN QIN, DIAN WU, XING DING, [...] AND JIAN-WEI PAN +14 authors Authors Info & Affiliations

SCIENCE · 3 Dec 2020 · Vol 370, Issue 6523 · pp. 1460-1463 · DOI: 10.1126/science.abe8770

18,637 760

A light approach to quantum advantage

Article | Open Access | Published: 14 June 2023

Evidence for the utility of quantum computing before fault tolerance

Youngseok Kim, Andrew Eddins, Sajant Anand, Ken Xuan Wei, Ewout van den Berg, Sami Rosenblatt, Hasan Nayfeh, Yantao Wu, Michael Zaletel, Kristan Temme & Abhinav Kandala

Nature **618**, 500–505 (2023) | Cite this article

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Basics of Quantum Computing

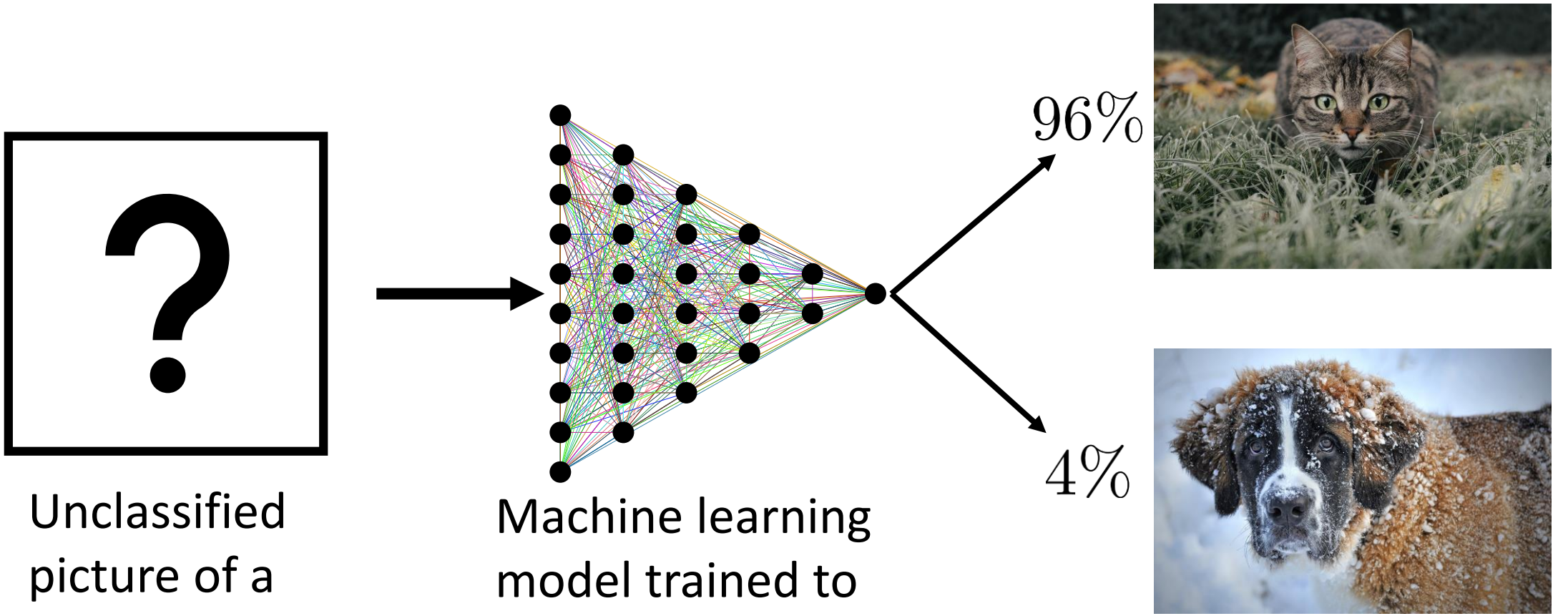
What is quantum computing?

Quantum computing is a computing paradigm which utilizes quantum mechanical properties, such as entanglement, superposition and interference, to perform computations.

Outline of the basics

- Gaining intuition about quantum computing through ML and probabilistic computing
- Introduction to quantum circuit model
- Practical approach to quantum computing

We are used to think probabilistically, especially when developing ML models



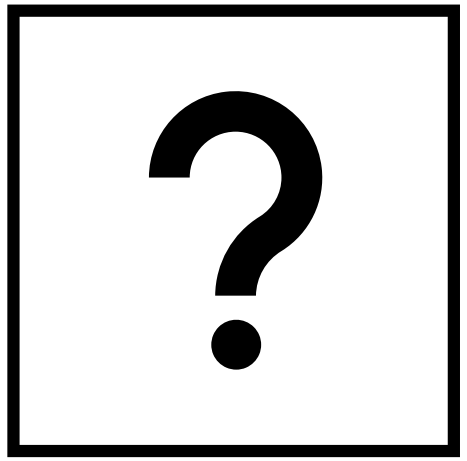
Unclassified picture of a cat or a dog

Machine learning model trained to identify cats and dogs

Classification output

Developing the previous probabilistic approach

Initial system



0.5 0.5

cat dog

p_0 p_1

Probabilistic bit

$$p = ap_0 + bp_1$$

where $0 \leq a, b \leq 1$ and $a + b = 1$.

Probabilistic functions respect conditions

$0 \leq a, b \leq 1$ and $a + b = 1$.

State of the system after classification

$0.96p_0$

$0.04p_1$

Quantum circuit model

From probabilistic bits to quantum bits

Required changes:

- Computations (excluding measurements) must be reversible
- Quantum bits comprise generalized probabilities over complex numbers
- Mappings between quantum bits follow the dynamics of quantum mechanics

Let’s define a computation model which satisfies the previous properties!

Quantum computing follows the dynamics of quantum mechanics

The postulates of quantum mechanics [Nielsen & Chuang]:

1. State space of a single quantum bit system
2. Evolution
3. State space of a composite system
4. Quantum measurement

Qubits form the basis for quantum computation

Classical computing is based on **bits**

$$0 \qquad 1$$

Quantum computing is based on **qubits**

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

A state of a single qubit can be expressed as a linear combination of the basis states

$$|\varphi\rangle = \alpha|0\rangle + \beta|1\rangle,$$

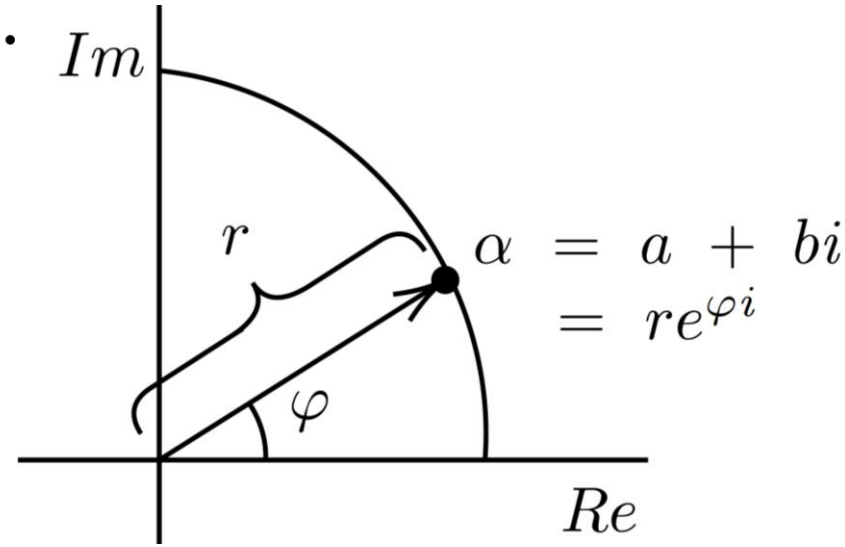
where $\alpha, \beta \in \mathbb{C}$ and $|\alpha|^2 + |\beta|^2 = 1.$

Superposition allows qubits to simultaneously exist in multiple states.

Bloch sphere visualizes a single qubit

We can find an angle θ so that (Pythagorean identity)

$$|\alpha|^2 + |\beta|^2 = \cos^2\left(\frac{\theta}{2}\right) + \sin^2\left(\frac{\theta}{2}\right) = 1.$$



Thus, we can rewrite the state the following way

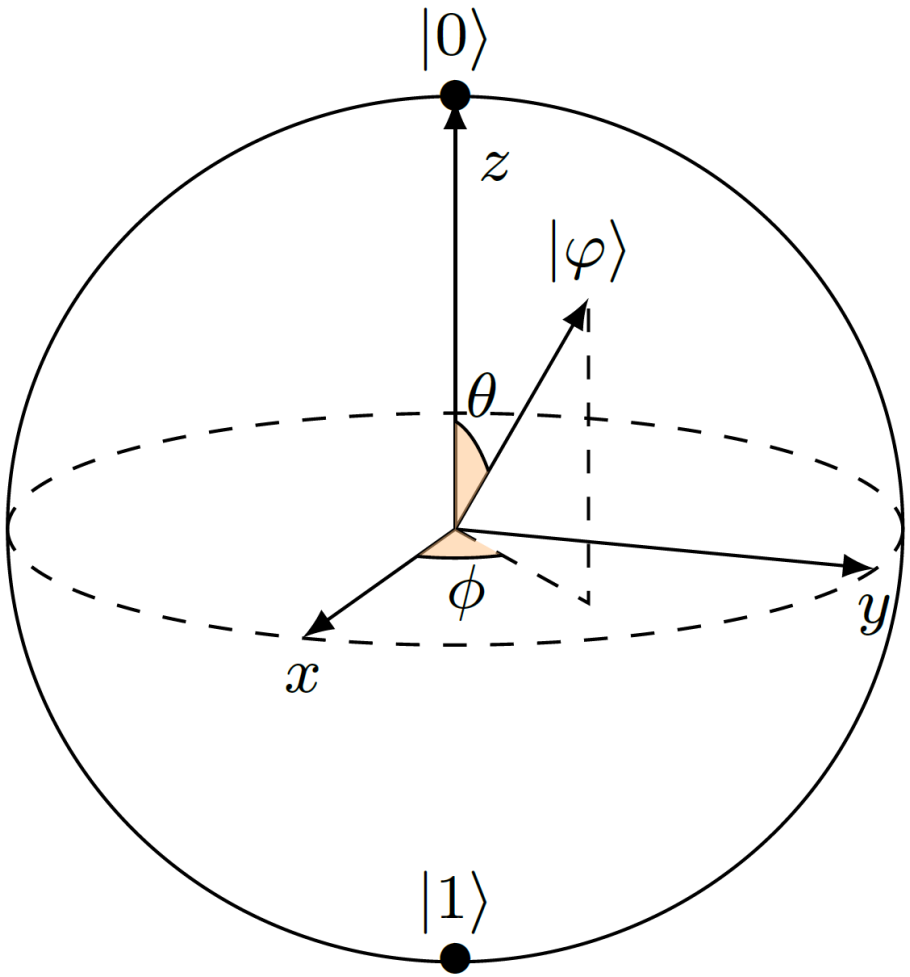
$$|\varphi\rangle = \alpha|0\rangle + \beta|1\rangle$$

$$= e^{i\gamma}(\cos\left(\frac{\theta}{2}\right)|0\rangle + e^{i\phi}\sin\left(\frac{\theta}{2}\right)|1\rangle).$$

The factor $e^{i\gamma}$ has no observable effects. Effectively,

$$|\varphi\rangle = \alpha|0\rangle + \beta|1\rangle = \cos\left(\frac{\theta}{2}\right)|0\rangle + e^{i\phi}\sin\left(\frac{\theta}{2}\right)|1\rangle.$$

Bloch sphere visualizes a single qubit



Quantum computation evolves by applying quantum logic gates to the states

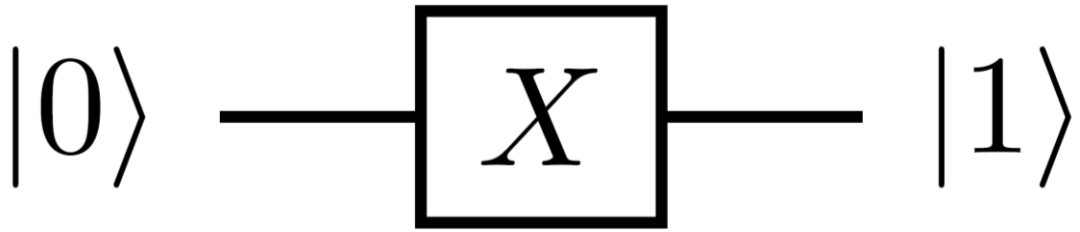
Quantum logic gates are defined by complex-valued unitary matrices U.

Matrix U is unitary if its conjugate transpose is its inverse:

$$UU^\dagger = U^\dagger U = I.$$

Conjugate transpose $U^\dagger$ is the matrix which is obtained by transposing U and applying complex conjugate on its each entry.

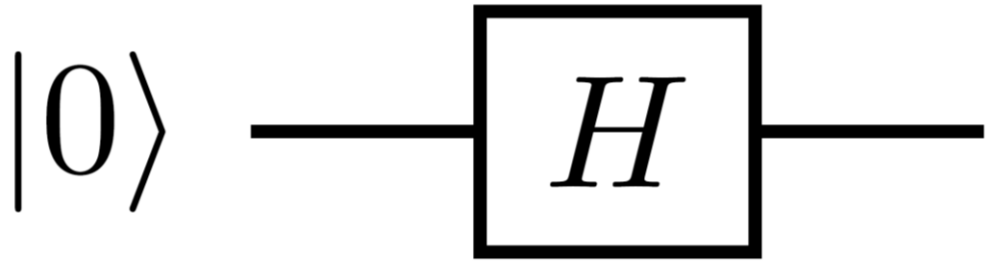
Quantum computation evolves by applying quantum logic gates to the states



For example, the NOT gate's unitary matrix is

$$X = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}.$$

Quantum computation evolves by applying quantum logic gates to the states



For example, the Hadamard gate's unitary matrix is

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

Example: Apply Hadamard-gate to the basis state

$$
\begin{aligned}
H|0\rangle &= \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} \\
&= \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix} \\
&= \frac{1}{\sqrt{2}} (|0\rangle + |1\rangle)
\end{aligned}
$$

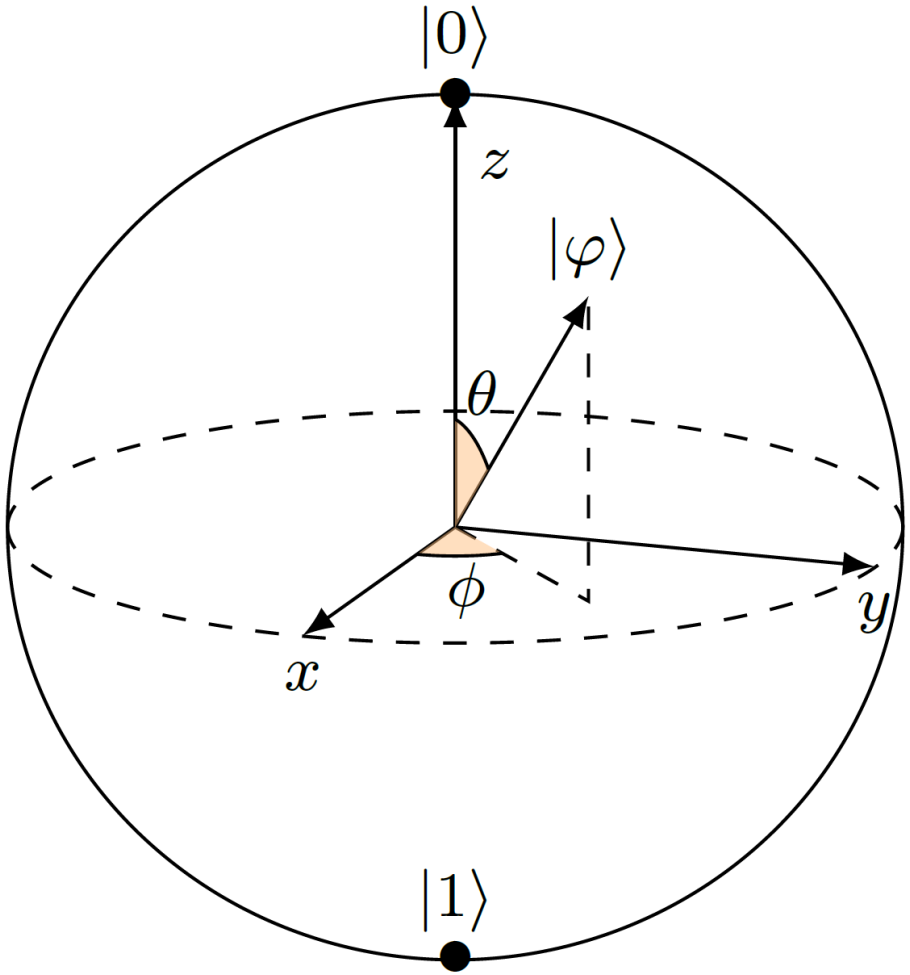
Parameterized gates are important in quantum machine learning

$$R_x(\theta) = \begin{pmatrix} \cos(\theta/2) & -i\sin(\theta/2) \\ -i\sin(\theta/2) & \cos(\theta/2) \end{pmatrix}$$

$$R_y(\theta) = \begin{pmatrix} \cos(\theta/2) & -\sin(\theta/2) \\ \sin(\theta/2) & \cos(\theta/2) \end{pmatrix}$$

$$R_z(\theta) = \begin{pmatrix} e^{(-i\theta/2)} & 0 \\ 0 & e^{i\theta/2} \end{pmatrix}$$

Bloch sphere can visualize how the rotation gates rotate the qubit on the sphere



State space of a composite system

The state space of a composite system is the tensor product of the state spaces of the component systems.

$$|0\rangle \otimes |0\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \otimes \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} 1 \cdot \begin{pmatrix} 1 \\ 0 \end{pmatrix} \\ 0 \cdot \begin{pmatrix} 1 \\ 0 \end{pmatrix} \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix} = |00\rangle.$$

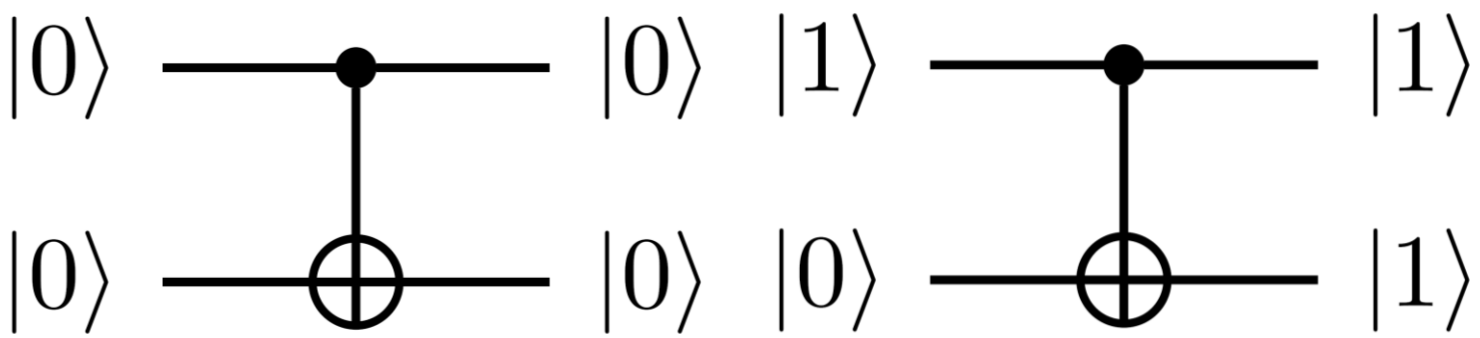
2^n

For example, the two-qubit quantum system has the basis states $|00\rangle, |10\rangle, |01\rangle, \text{and } |11\rangle.$

Entanglement

Quantum entanglement means that the quantum state of each component system of the whole system cannot be described independently of the state of the others.

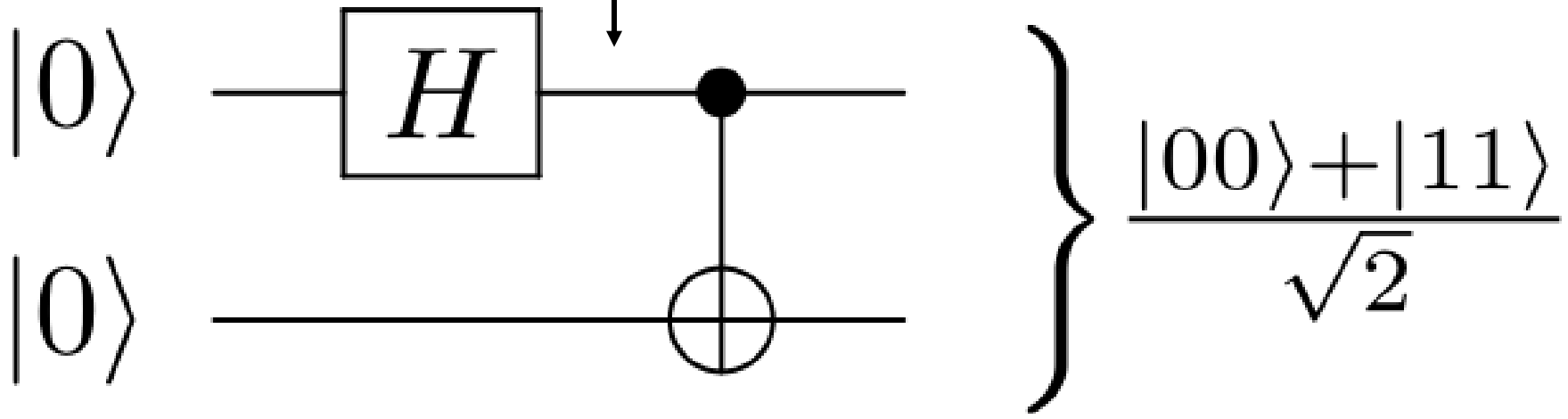
Controlled NOT i.e. CNOT-gate



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

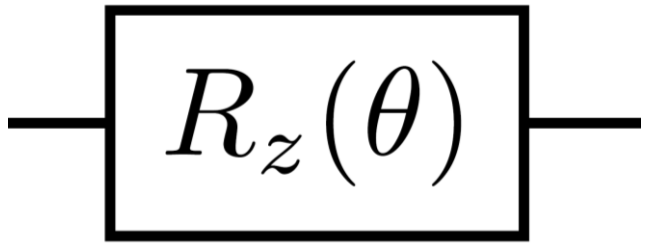
Entanglement + superposition: Bell state

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

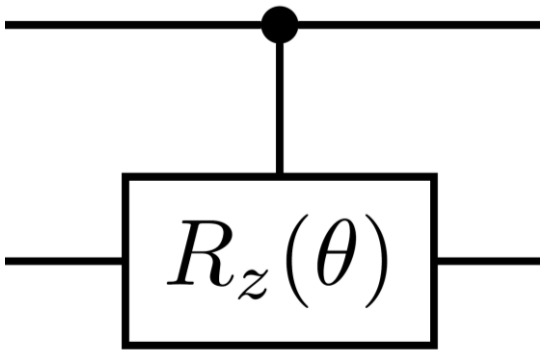


Parameterized gates have controlled versions which are important in quantum machine learning

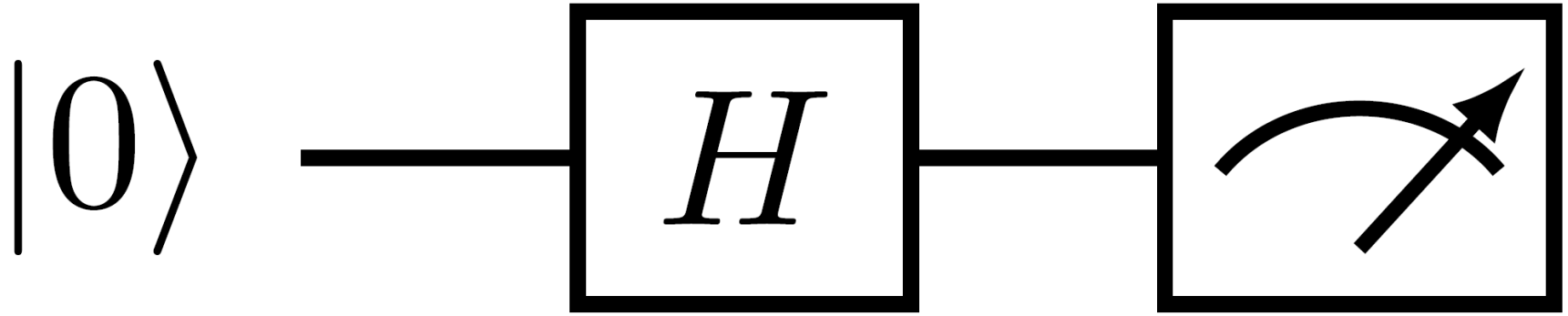
$$R_z(\theta) = \begin{pmatrix} e^{(-i\theta/2)} & 0 \\ 0 & e^{i\theta/2} \end{pmatrix}$$



$$CR_z(\theta) = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & e^{(-i\theta/2)} & 0 \\ 0 & 0 & 0 & e^{i\theta/2} \end{pmatrix}$$



Measurement collapses the state and produces a classical bit



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

50% probability to measure 1

50% probability to measure 0

Measurement formally

Let $O = \{m_1, \ldots, m_n\}$ be the set of measurement outcomes that may occur in the experiment.

Quantum measurements are defined by a collection $\{M_m \mid m \in O\}$ of measurement operators.

The probability of measuring the outcome $m \in O$ is given by

$$p(m) = \langle \varphi | M_m^\dagger M_m | \varphi \rangle.$$

Measurement formally

The most important measurement is the measurement in the computational basis.

In the case of a single qubit, the collection of the measurement operators is given by

$$M_0 = |0\rangle\langle 0| = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix},$$

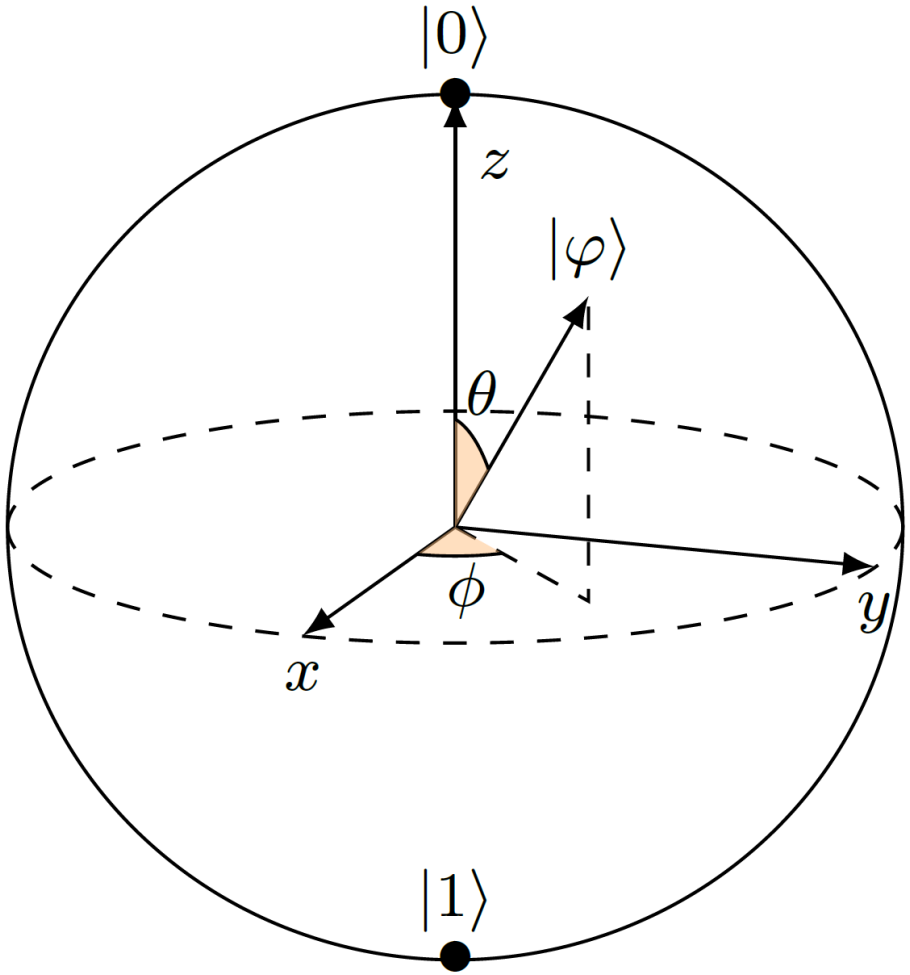
$$M_1 = |1\rangle\langle 1| = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}.$$

Measurement example

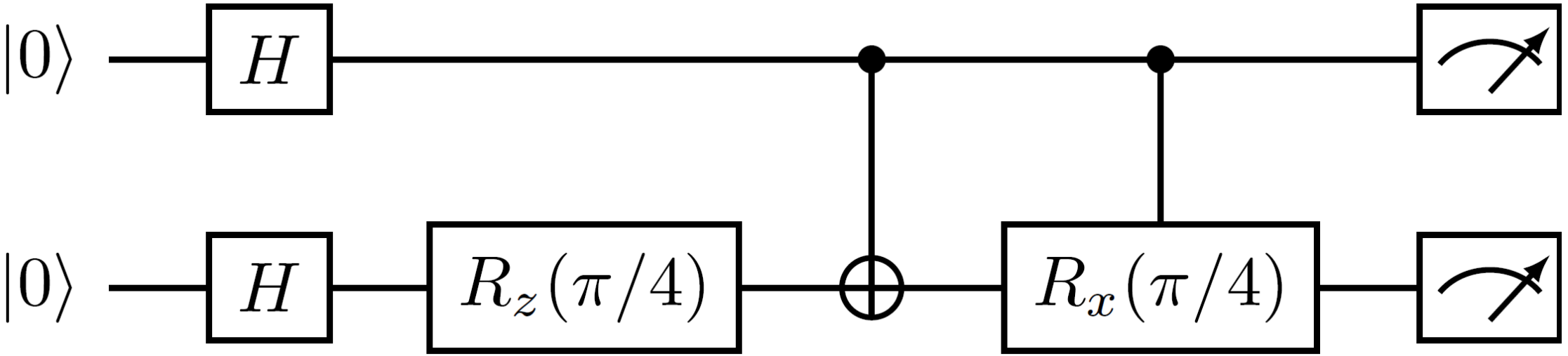
If $|\varphi\rangle = \alpha|0\rangle + \beta|1\rangle$, then the probability to measure 0 is

$$p(0) = \langle\varphi|M_0^\dagger M_0|\varphi\rangle = \langle\varphi|M_0|\varphi\rangle = |\alpha|^2.$$

Measurement from the Bloch sphere perspective



Summary on the quantum circuit model



Modern quantum computing in practice: Noisy Intermediate Scale Quantum (NISQ) hardware

METHOD	Superconducting	Ion traps	Photonic	Topological
Company support	Google, IBM, IQM, Rigetti	IonQ, Quantinuum	Xanadu	Microsoft

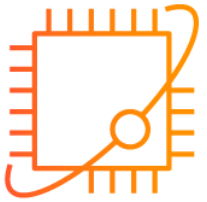
METHOD	Silicon	Diamond	Annealing	Classical simulators
Company support	Intel	Quantum Brilliance	D-Wave	IBM, Amazon, NVIDIA, Fujitsu

Modern quantum computing in practice: Software libraries and platforms for quantum computing

Q#

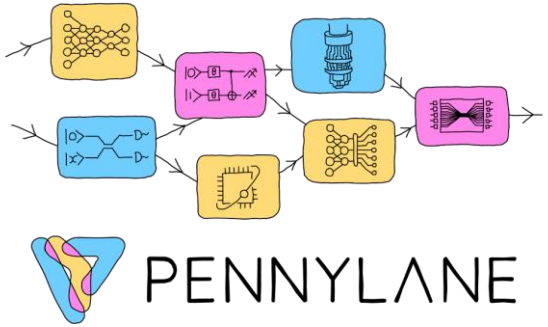
Cirq

TensorFlow Quantum



Amazon Braket

Microsoft Azure Quantum



PENNYLANE

Qiskit

IBM Quantum

Xanadu Cloud

(tket) CQ

Introduction materials

- A practical introduction to quantum computing: from qubits to quantum machine learning and beyond by Elias Fernandez-Combarro Alvarez (Universidad de Oviedo (ES))
- Quantum Computing by Prof. Dr. Sven Groppe
- Nielsen, M. A., Chuang, I. L. (2000). Quantum Computation and Quantum Information. India: Cambridge University Press.
- Quantum Algorithm Zoo: https://quantumalgorithmzoo.org/

Learn to code quantum algorithms:

- Xanadu's Quantum Codebook. https://codebook.xanadu.ai/
- Qiskit Tutorials. https://qiskit.org/documentation/tutorials.html
- IQM Academy. https://www.iqmacademy.com/

Quantum Machine Learning

Overview

1. Motivation
2. (Classical) Machine learning
3. Optimization
4. Hybrid algorithms
5. Variational quantum circuits
   - Structure
   - Encoding
   - Decoding

Machine learning

Function approximation

Problem

- x : Input data
- y : Desired output
- g : An unknown function mapping $y = g(x)$

Goal

A model f which approximates g

Solution

Use parameterized function $f(x, \theta)$ to approximate $g(x)$
Find θ_o for which $f(x, \theta_o)$ is best approximation of $g(x)$

Machine learning

Methods

Supervised learning

Learning from data:

- Input: x
- Desired Output: y
- Error function: $E(f(x, \theta), y)$

Goal: $\arg\min_{\theta} E(f(x, \theta), y)$

Training data

x_0	y_0
x_1	y_1
x_2	y_2
x_3	y_3

Model $f(x, \theta)$

x_{new}	$f(x_{new}, \theta)$

Machine learning

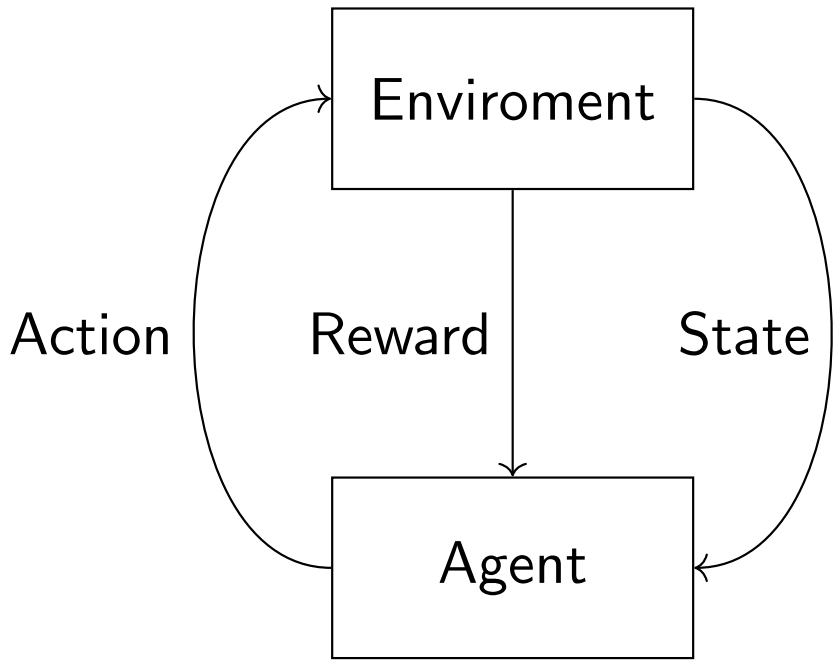
Methods

Reinforcement Learning

Agent with environment:

- Initial state x_0
- Policy $f(x_n)$
- Reward $R(x_n, f(x_n, \theta))$
- Next state
  $x_{n+1} = P(x_n, f(x_n))$

Goal: $\arg\max_{\theta} \sum_{n=0}^{\inf} P(f(x_n, \theta))$



Optimizer

Gradient descent

Use gradient of loss function to determine parameter change

- Loss function has to be differentiable
- Problem of barren plateau

Optimizer

Evolutionary algorithm

Inspired by natural evolution

- Parameter vectors are members of a population
- New members are created by mutation and crossover
- Best members are selected by a fitness function
- Any fitness function is possible
- Many variants

Hybrid Algorithm

Quantum machine learning

Problem

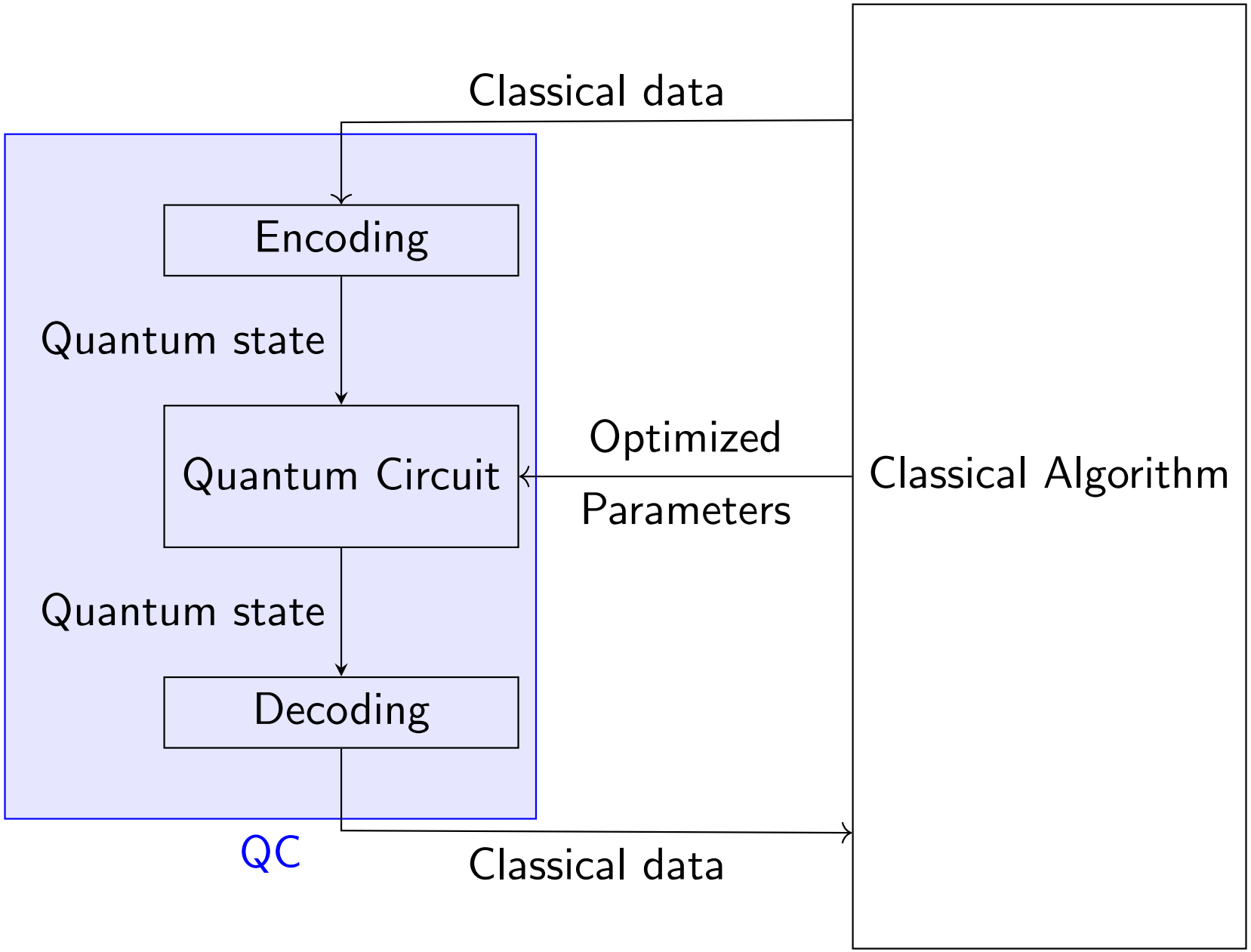
Limited number of qubits and circuit depth for NISQ and simulators

Solution

Use QC as subroutine in a classical algorithm

- Utilization of quantum computers, without a full quantum algorithms
- Circuits are smaller and shorter better suited for NISQ era
- Measurement required $\Rightarrow$ Alters quantum state $\Rightarrow$ No continues interaction $\Rightarrow$ QC as function
- Quantum model in machine learning

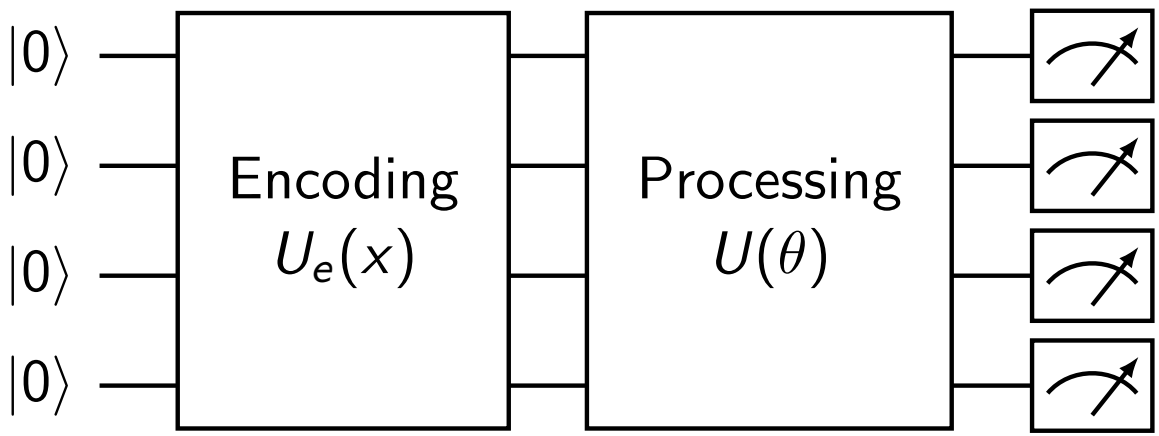
Hybrid Algorithm



VQC

Variational quantum circuits

- Quantum circuit with parameters
- 3 Components:
  - Encoding
  - Processing
  - Measurement
- Proven universal approximator
- Possible machine learning model



VQC

Processing Layer

Turns quantum state representing the input into quantum state representing the output

Required:

- Parameterized operation e.g. Rotation gates
- Entanglement operation e.g. controlled Pauli gates

Common:

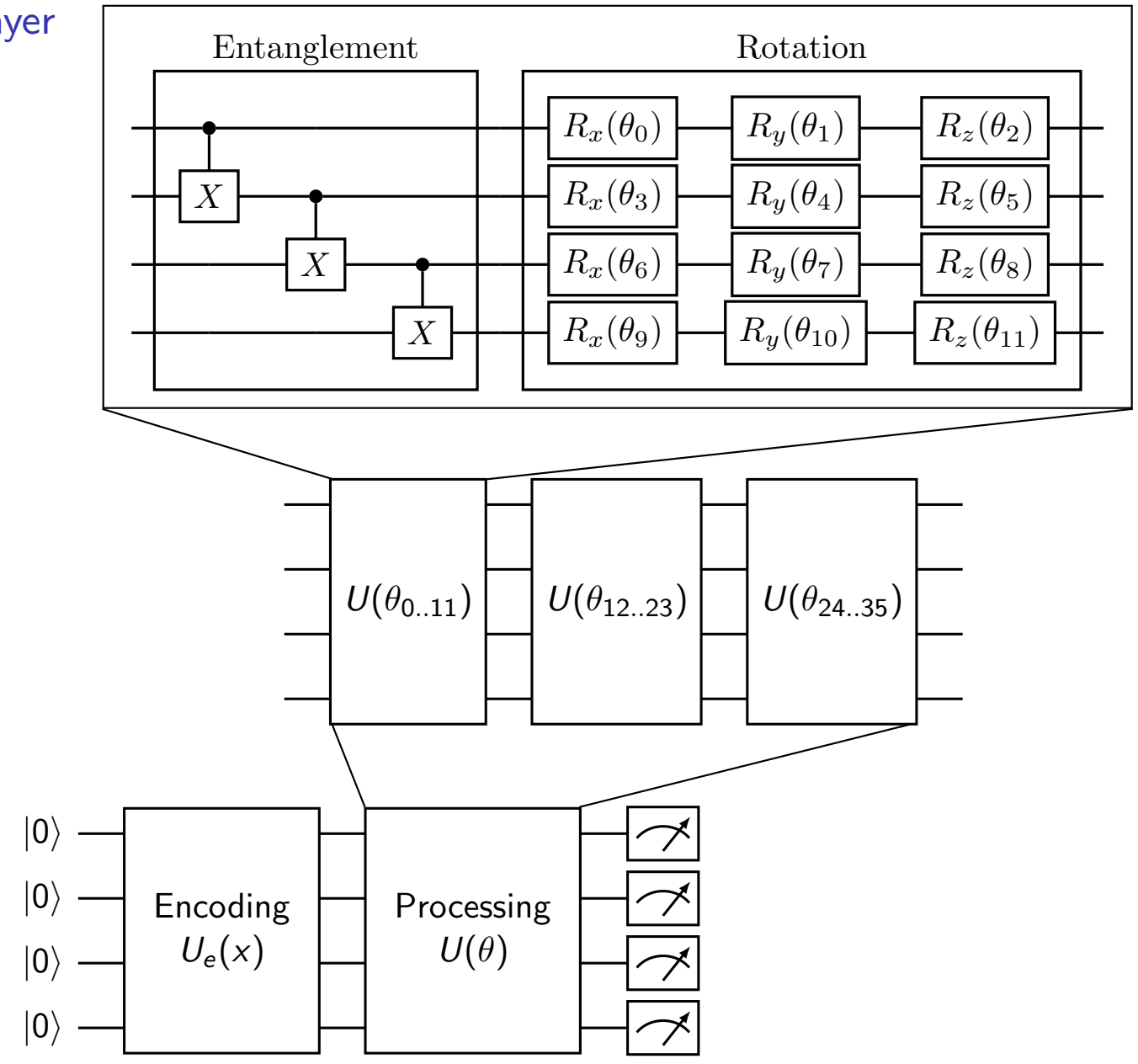
- Alternating entanglement and rotation layers
- Repetition of the same layer

Optional:

- Re-uploading

VQC

Processing Layer



Processing Layer

Entanglement

Entanglement effects depth of layer as rotation part is constant length. Entanglement layout:

- Linear
- Circle
- Full
- Tree
- Pairwise
- Shifted-circular-alternating (SCA)

Processing Layer

Structures

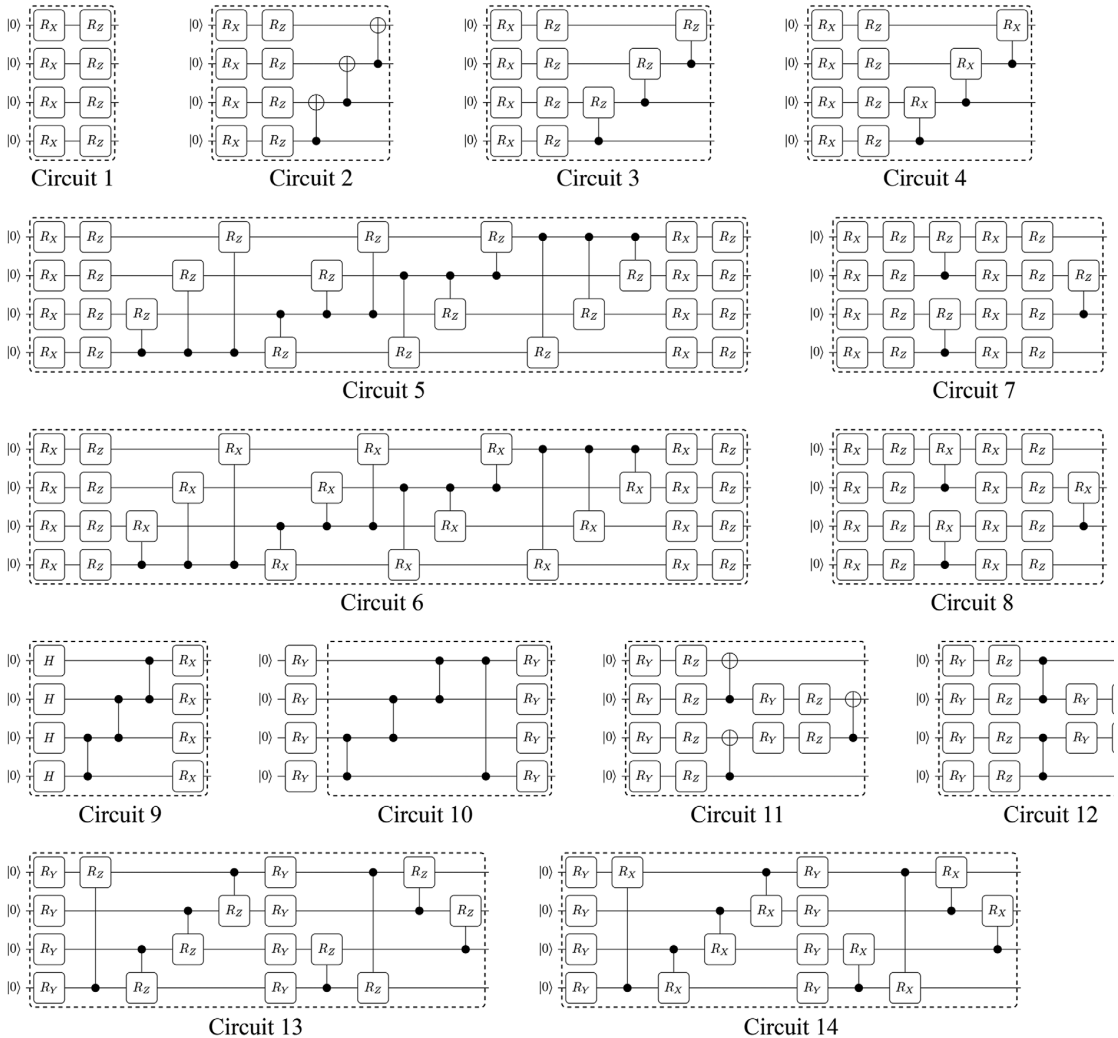


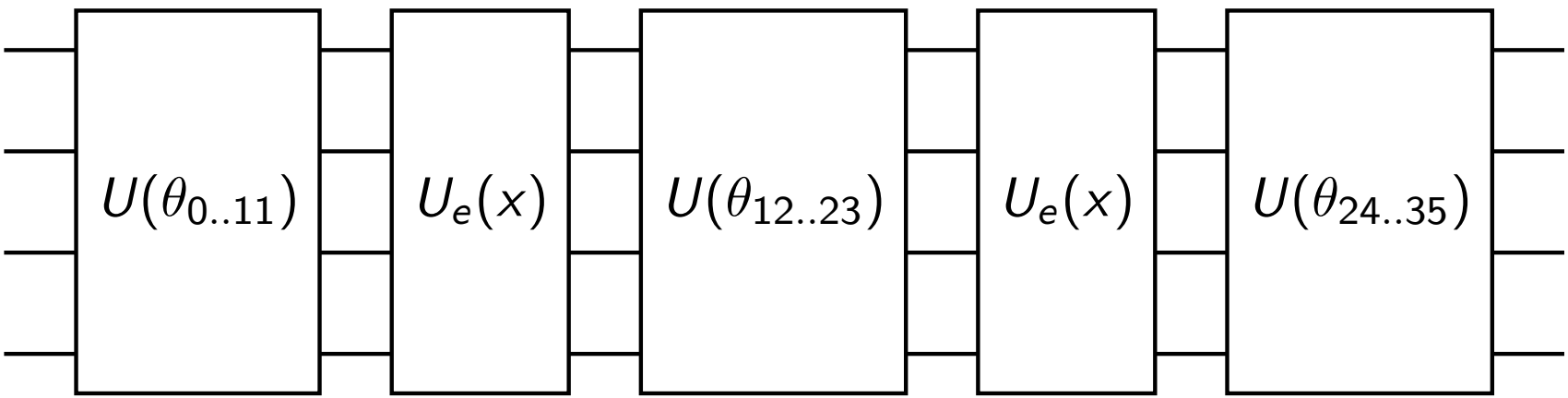
Figure: Expressibility and Entangling Capability of Parameterized Quantum Circuits for Hybrid Quantum-Classical Algorithms by Sukin Sim, Peter D. Johnson, and Alán Aspuru-Guzik

Processing layer

Reuploading

Reapply encoding layer

- Possible because encoding is unitary operation and not setting values
- Increases effect of input
- Allows universality



Encoding

Making our data quantum

Goal:

We require a quantum state $|\varphi\rangle$ representing our classical data x

Solution:

Use a unitary U_e operator depending on x

$$|\varphi\rangle = U_e(x)\,|0\rangle$$

Choice of U_e affects

- Possible data values
- Number of qubits
- Depth of encoding circuit

Encoding Methods

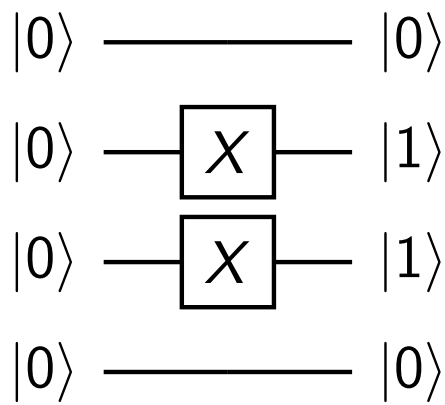
Basis encoding

Turn a classical bit into a qubit

$$U_e(0)\,|0\rangle = |0\rangle\,, U_e(1)\,|0\rangle = |1\rangle$$

- Only allows binary data
- One qubit per classical bit
- Depth: 1 gate

Encoding 0110 using X gate:



Encoding Methods

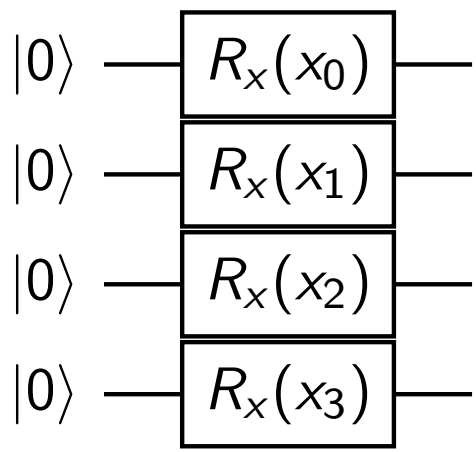
Angle encoding

Use rotation gates to encode one value into one bit

$$U_e(x_i)\,|0\rangle = \cos(x_i/2)\,|0\rangle + \sin(x_i/2)\,|1\rangle$$

- Allows encoding of real value
- One qubit per classical value
- Depth: 1 gate
- Values in interval $[0, 4\pi)$ for injective encoding

Encoding of 4 values using R_x gates:



Encoding Methods

Amplitude encoding

Encode values into amplitudes of quantum state

$$U_e(x)\,|0\rangle = \frac{1}{n}\sum_{i=0}^{n-1} x_i$$

- Allows encoding of real value with sum of 1
- $\log_2(n)$ qubits for n values
- Depth: $O(n)$
- Requires a complex circuit to create
- Values encoded in total state not a single qubit

Encoding Methods

Comparison

- Amplitude encoding densest, but highest depth
- Angle and amplitude encoding require scaling of data
- Angle encoding often a good compromise
- Hybrid methods

Method	Data	Qubits	Depth
Basis encoding	String of n bits	$O(n)$	$O(1)$
Angle encoding	n real values	$O(n)$	$O(1)$
Amplitude encoding	n real values	$O(\log(n))$	$O(n)$

Output decoding

Receiving a classical result

Option 1 Use measurement as binary string

- Returns one basis state of the superposition
- Result is string of n bit
- Probabilistic

Option 2 Use probabilities

- 2^n continues values in interval $[0, 1]$ with sum of 1
- Probability easily acquired on simulator
- Require repeat execution to approximate on real quantum computers

Optimizer

Parameters of a VQC are adjusted by a classical optimizer

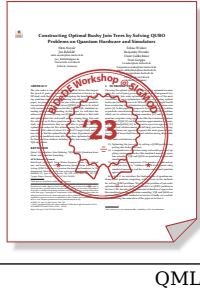
- Gradient based (SGD, Adam)
- Evolutionary algorithms

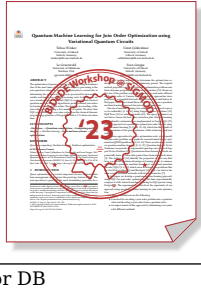
Parameter shift rule

Calculation of gradients

- Run two copies with one parameter slightly shifted
- Requires $2n$ runs for n parameters

Quantum-DB work so far

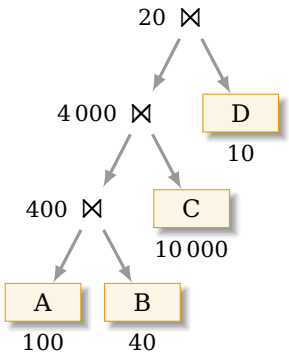




Demonstration

Quantum Machine Learning for Join Ordering

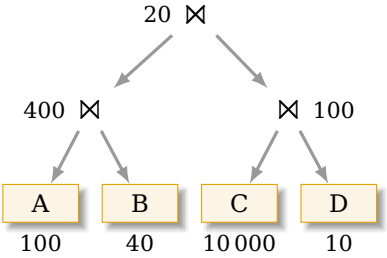
```
SELECT ...  FROM A,B,C,D WHERE ...
```



Costs

$$C = 400 + 4000 + 20 = 4420$$

```
SELECT ...  FROM A,B,C,D WHERE ...
```

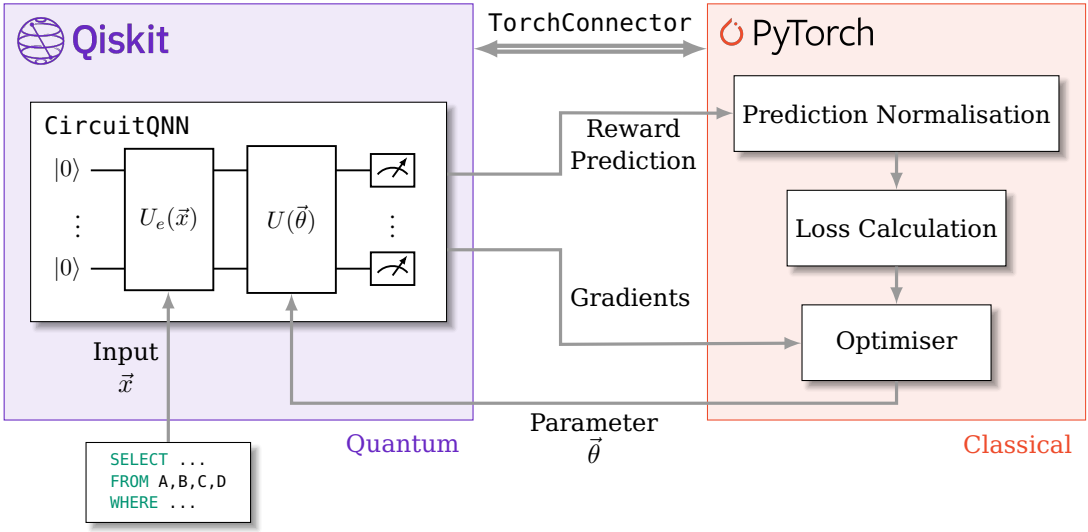


Costs

$$C = 400 + 100 + 20 = 520$$

Demo Overview

1. Create the Variational Quantum Circuit (VQC)
2. Load the Data
3. Create the *Quantum Neural Network*
4. Train the Model
5. Evaluate the Model


Qiskit
TorchConnector
PyTorch
CircuitQNN
$|0\rangle$
$|0\rangle$
$U_e(\vec{x})$
$U(\vec{\theta})$
Reward
Prediction
Prediction Normalisation
Loss Calculation
Gradients
Optimiser
Input
$\vec{x}$
Parameter
$\vec{\theta}$
Quantum
Classical
SELECT ...
FROM A,B,C,D
WHERE ...

Live Demo

https://github.com/TobiasWinker/QC4DB_VQC_Tutorial

Outlook

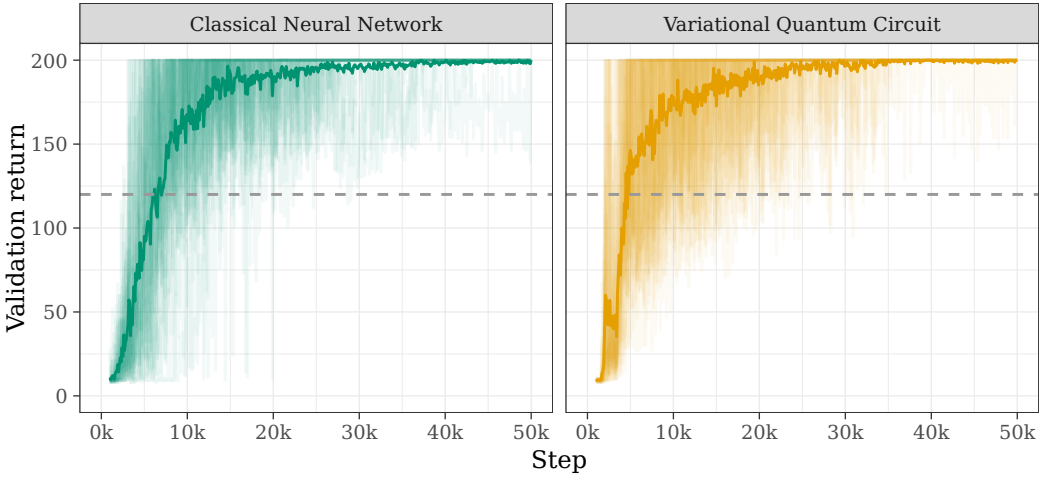
Open Challenges and Future Work

(Quantum) Machine Learning in Databases

Problem		DB Tasks
NP Optimisation	Offline	Knob Tuning
		Index/View Selection
		Partition/-key Selection
	Online	Query Rewrite
		Plan Enumeration
Regression		Cost/Cardinality Estimation
		Index/View Benefit Estimation
		Lateny Estimation
Prediction		Trend Forecast
		Workload Prediction & Scheduling

Table © G. Li, X. Zhou, L. Cao: *Machine Learning for Databases*, Slides, VLDB (2021)

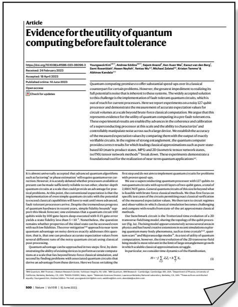
Sampling Complexity



M. Franz, L. Wolf, M. Periyasamy, Ch. Ufrecht, D. D. Scherer, A. Plinge, Ch. Mutschler, W. Mauerer: *Uncovering Instabilities in Variational-Quantum Deep Q-Networks*, J. Franklin Institute (2022)


Article

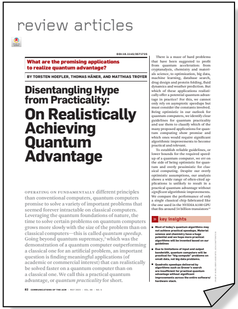
Quantum supremacy using a programmable superconducting processor


Article

Evidence for the utility of quantum computing before fault tolerance


Classically Approximating Variational Quantum Machine Learning with Random Fourier Features

arXiv:2210.13200v1 [quant-ph] 24 Oct 2022


review articles

What are the promising applications to realize quantum advantage?

BY TORSTEN HOEFLER, THOMAS HÄNER, AND MATTHIAS TROYER

Disentangling Hype from Practicality: On Realistically Achieving Quantum Advantage

Open Research Questions

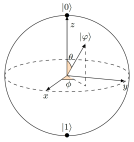
- What are potential advantages of QML?
- Can we achieve quantum advantage in the NISQ era?
- Can quantum hardware-software co-design help?
- How can we build on existing, classical approaches?
- Quantum computing + Large amounts of data = Bad idea?

Publication

- Tobias Winker, Sven Groppe, Valter Uotila, Zhengtong Yan, Jiaheng Lu, Maja Franz, Wolfgang Mauerer. **Quantum Machine Learning: Foundation, New Techniques, and Opportunities for Database Research**. In Companion of the 2023 International Conference on Management of Data (SIGMOD-Companion '23), June 18–23, 2023, Seattle, WA, USA. https://doi.org/10.1145/3555041.3589404


Quantum Machine Learning: Foundation, New Techniques, and Opportunities for Database Research

Bloch sphere visualizes a single qubit

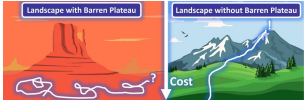


Optimizer

Gradient descent

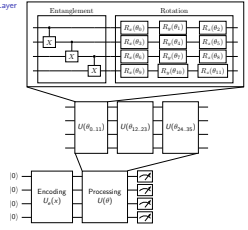
Use gradient of loss function to determine parameter change

- Loss function has to be differentiable
- Problem of barren plateau



VQC

Processing Layer



qc4jo

June 26, 2023

1 Quantum Machine Learning for Join Ordering

This notebook will demonstrate a simple example of using a variational quantum circuit (VQC) in machine learning for join order optimization.

1.1 Imports

[1]:
```
from math import pi
import csv
from collections import deque
import random
import numpy as np

# Qiskit Circuit imports
from qiskit.circuit import QuantumCircuit, QuantumRegister, Parameter,␣
 ↪ParameterVector, ParameterExpression

# Qiskit imports
import qiskit as qk
from qiskit.utils import QuantumInstance
from qiskit import Aer
from qiskit.visualization import plot_histogram

# Qiskit Machine Learning imports
from qiskit_machine_learning.neural_networks import CircuitQNN
from qiskit_machine_learning.connectors import TorchConnector

# PyTorch imports
import torch
from torch import Tensor
from torch.optim import Adam

# Imports for plotting
import matplotlib.pyplot as plt
%matplotlib inline
```

1.2 Create the Variational Quantum Circuit (VQC)

1.2.1 Circuit Hyperparameters

[2]:
```
num_qubits = 4  # Number of qubits
num_layers = 8  # Number of variational layers in the circuit
```

1.2.2 Encoding Layer (Quantum!)

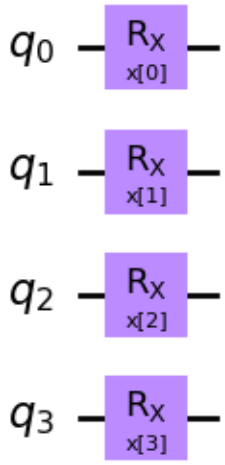
[3]:
```
# Create a quantum circuit
qc = qk.QuantumCircuit(num_qubits)

# Parameters for input
x = qk.circuit.ParameterVector('x', num_qubits)

# Add encoding layer
for i in range(num_qubits):
    qc.rx(x[i], i)
```

[4]:
```
# Draw the circuit
qc.draw("mpl")
```

[4]:



1.2.3 Variational Layers (Quantum!)

[5]:
```
# Parameters for variational layers
thetas = [ qk.circuit.ParameterVector(f'th{l}_', 2*num_qubits) for l in␣
 ↪range(num_layers) ]
```

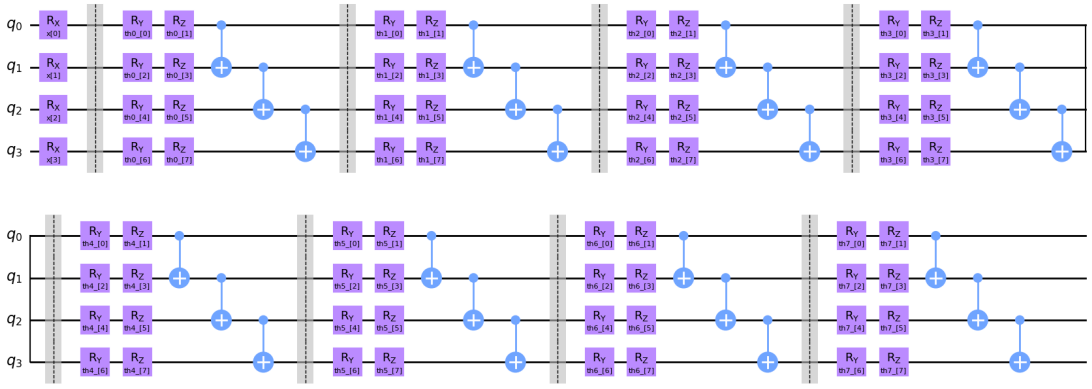
```
# Add variational layers
for l in range(num_layers):
    qc.barrier() # for nicer visualisation

    # Variational part
    for i in range(num_qubits):
        qc.ry(thetas[l][2*i], i)
        qc.rz(thetas[l][2*i+1], i)

    # Entangling part
    for i in range(num_qubits-1):
        qc.cx(i, i+1)
```

[6]:
```
# Draw the circuit
qc.draw("mpl")
```

[6]:



1.2.4 Example: Measure circuit (Quantum!)

[7]:
```
# Generate dummy input
num_inputs = len(x)
dummy_inputs = np.zeros(num_inputs)
print("Inputs:", dummy_inputs)

# Extract the parameters to optimize
params = list(qc.parameters)[:-num_qubits]
num_params = len(params)

# Generate variational parameters randomly in [-pi,pi]
example_param_values = (2*pi*np.random.rand(num_params) - pi)
print("Thetas:", example_param_values)
```

```
Inputs: [0. 0. 0. 0.]
Thetas: [ 0.8047321   0.84461409  0.52073632  2.27864769  0.40968235  2.38381307
```

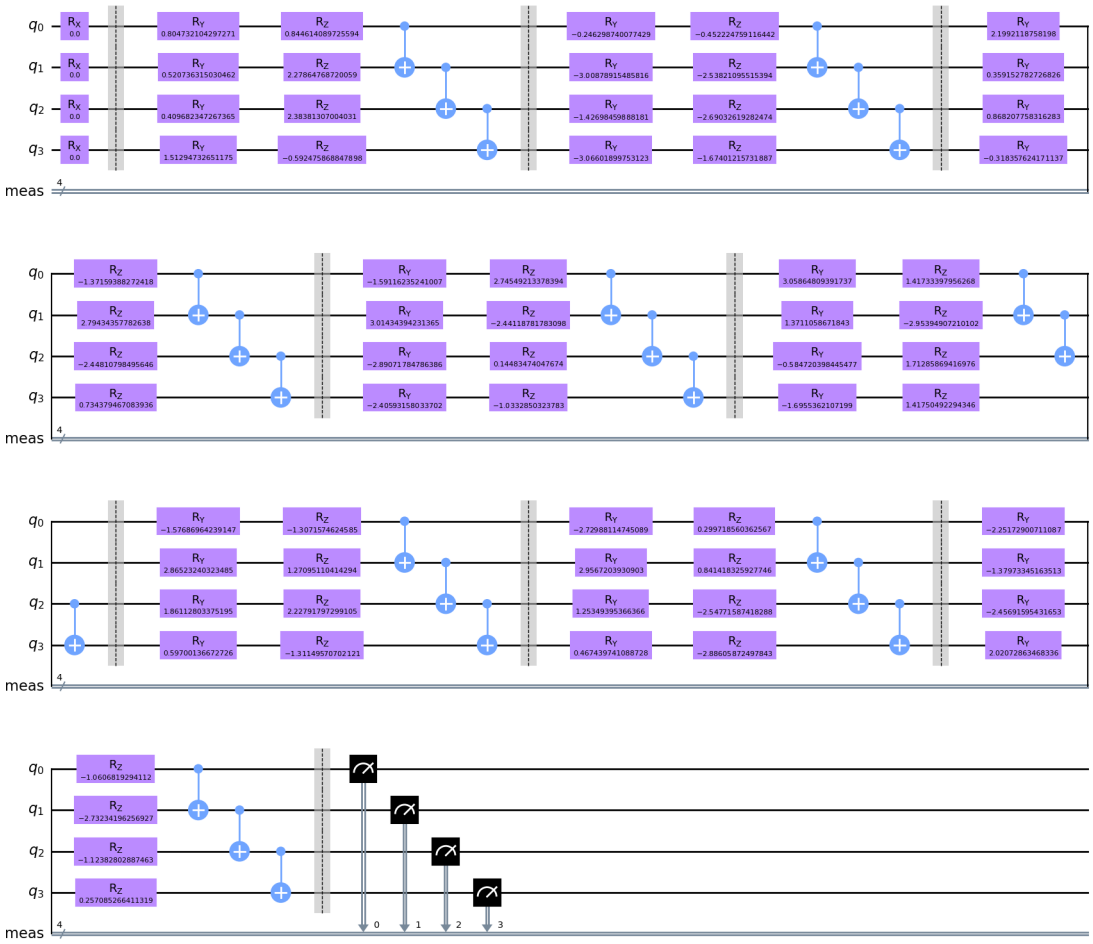
```
 1.51294733 -0.59247587 -0.24629874 -0.45222476 -3.00878915 -2.53821096
-1.4269846  -2.69032619 -3.066019   -1.67401216  2.19921188 -1.37159388
 0.35915278  2.79434358  0.86820776 -2.44810798 -0.31835762  0.73437947
-1.59116235  2.74549213  3.01434394 -2.44118782 -2.89071785  0.14483474
-2.40593158 -1.03328503  3.05864809  1.41733398  1.37110587 -2.95394907
-0.5847204   1.71285869 -1.69553621  1.41750492 -1.57686964 -1.30715746
 2.8652324   1.2709511   1.86112803  2.22791797  0.59700137 -1.31149571
-2.72988115  0.29971856  2.95672039  0.84141833  1.25349395 -2.54771587
 0.46743974 -2.88605872 -2.25172901 -1.06068193 -1.37973345 -2.73234196
-2.45691595 -1.12382803  2.02072863  0.25708527]
```

[8]:
```
# Bind parameters
bound_qc = qc.assign_parameters({p: v for p, v in zip(x, dummy_inputs)})
bound_qc = bound_qc.assign_parameters({p: v for p, v in zip(params,␣
 ↪example_param_values)}) # variational parameters

# Tell Qiskit to measure all qubits
bound_qc.measure_all()

bound_qc.draw("mpl")
```

[8]:



Run the quantum circuit

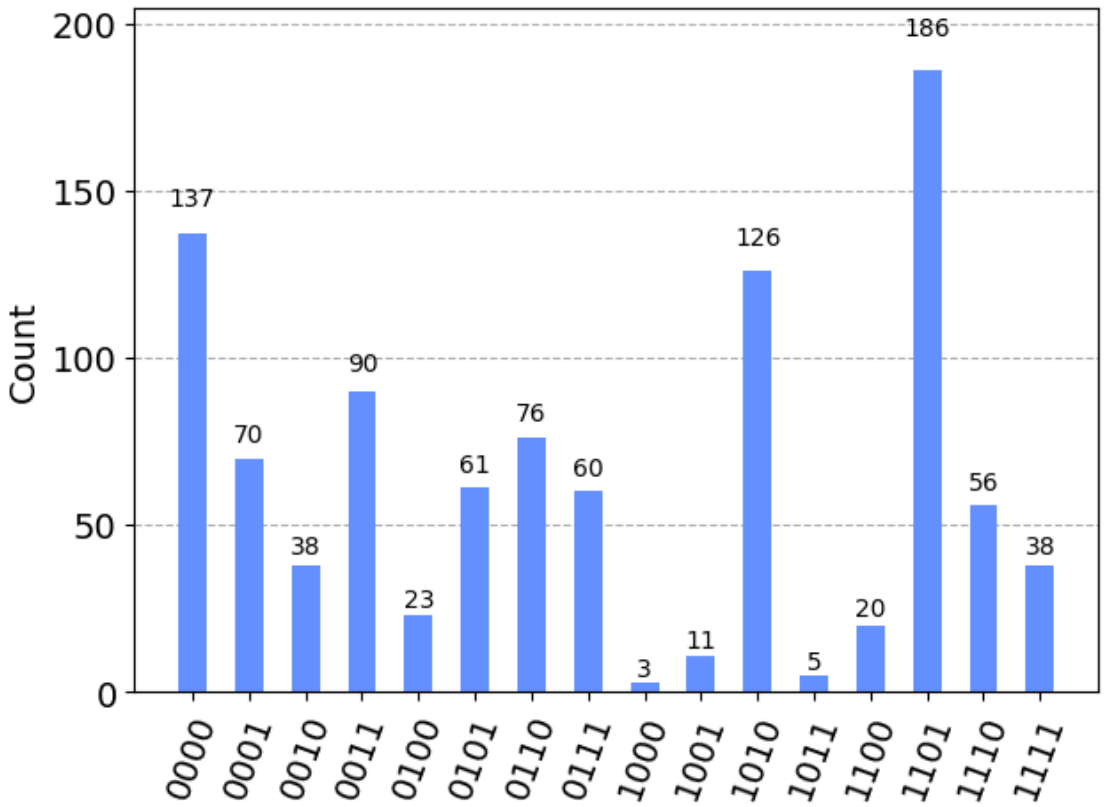
[9]:
```
# Run the quantum circuit on a statevector simulator
backend = Aer.get_backend('aer_simulator_statevector')
shots = 1000
job = backend.run(bound_qc, shots=shots)

# Print result
result = job.result()
counts = result.get_counts()
print(counts)
```

```
{'1011': 5, '1001': 11, '0101': 61, '1110': 56, '1010': 126, '0000': 137,
'0010': 38, '0111': 60, '0011': 90, '1101': 186, '1000': 3, '0110': 76, '1111':
38, '0001': 70, '0100': 23, '1100': 20}
```

[10]:
```
plot_histogram(counts)
```

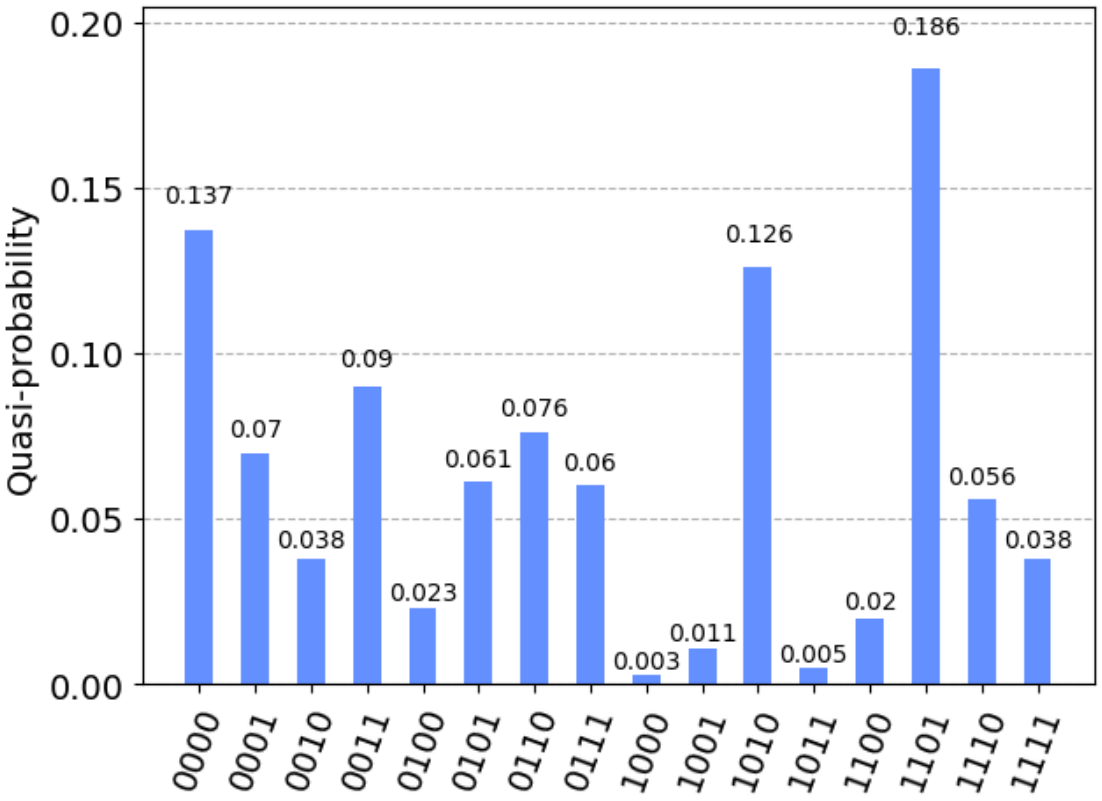
[10]:



[11]:
```
# Calculate probabilities
probs = {v: count/shots for v, count in counts.items()}
print(probs)
plot_histogram(probs)
```

```
{'1011': 0.005, '1001': 0.011, '0101': 0.061, '1110': 0.056, '1010': 0.126,
'0000': 0.137, '0010': 0.038, '0111': 0.06, '0011': 0.09, '1101': 0.186, '1000':
0.003, '0110': 0.076, '1111': 0.038, '0001': 0.07, '0100': 0.023, '1100': 0.02}
```

[11]:



1.3 Load data (Classical!)

[12]:
```
with open('data.csv', newline='') as csvfile:
    data = list(csv.reader(csvfile, delimiter=',', quoting=csv.
 ↪QUOTE_NONNUMERIC))
```

One data_row contains:

[13]:
```
data_row = data[0]
print(data_row)
```

```
[0.2617993877991494, 3.141592653589793, 2.0943951023931953, 1.3089969389957472,
0.0, 0.7964358157055925, 0.8313672111312764, 0.0, 0.0, 0.0, 0.804596018735363,
0.9512026302128396, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 1.0, 0.0]
```

1.3.1 `data_row[0:4]`

Representations of the four tables that should be joined and angle of the encoding rotation gates. These values were created by turning each tablename into an id and mapping them to the interval $[0, \pi]$.

In this case: `[0.2617993877991494, 3.141592653589793, 2.0943951023931953, 1.3089969389957472]`

1.3.2 `data_row[4:20]`

Rewards for the corresponding join orders calculated from the execution times The reward is defined as

$$\frac{t_{\text{best JO}}}{t_{\text{chosen JO}}},$$

where t is the execution time (0 for cross joins).

In this case: `[0.0, 0.7964358157055925, 0.8313672111312764, 0.0, 0.0, 0.0, 0.804596018735363, 0.9512026302128396, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 1.0, 0.0]`

1.4 Create a Quantum Neural Network (Quantum!)

[14]:
```
# Select a quantum backend to run the simulation of the quantum circuit
qi = QuantumInstance(qk.Aer.get_backend('aer_simulator_statevector'))

# Create a Quantum Neural Network
qnn = CircuitQNN(qc, input_params=x, weight_params=params,
                 quantum_instance = qi)
```

1.4.1 Connect to PyTorch (Classical!)

[15]:
```
# Initialize random weights in [-pi,pi]
seed = 42 # Seed for random initialization
np.random.seed(seed)
initial_weights = (2*pi*np.random.rand(num_params) - pi)

# Create PyTorch VQC Wrapper
quantum_nn = TorchConnector(qnn, initial_weights)
```

1.4.2 Define layer which normalises the prediction (Classical!)

[16]:
```
class NormLayer(torch.nn.Module):
    def forward(self, x):
        result = x/x.max()
        return result

# Create a sequential model from the qantum network and the classical norm layer
model = torch.nn.Sequential(quantum_nn, NormLayer())
```

1.5 Train the model

1. The model can be trained by predicting rewards for a corresponding join order defined in a look-up table.
2. A loss is computed over all predicted rewards and the actual rewards stored in the data.
3. The VQCs parameters get updated via backpropagation with respect to the computed loss.

1.5.1 Hyperparameters for Training

[17]:
```
# Use the adam optimizer
optimizer = Adam(model.parameters(), lr=0.005)

# Buffers to store the last 10 rewards and losses
rewards = deque(maxlen=10)
losses = deque(maxlen=10)

num_steps = 40 # number of training steps

random.seed(seed) # set seed for data selection
```

1.5.2 Run the Training

[18]:
```
# save loss and reward for plotting
loss_log, reward_log = [], []

for episode in range(num_steps):

    # Choose a random data entry
    entry = random.choice(data)

    # Predict rewards from the features
    prediction = model(Tensor(entry[0:4])) # Quantum!

    # Choose join order with highest predicted reward
    selected = prediction.argmax()

    # Real reward this selection would give
    current_reward = entry[4+selected]

    # Calculate loss as sum of the squared errors
    loss = 0
    for i in range(0, len(prediction)):
        loss += (prediction[i] - entry[4+i])**2

    # Show quality of current episode
    print("Episode: {}, loss: {:.3f}, Reward : {:.3f}".format(episode, loss.
 ↪item(), current_reward), end="\n")
```

```
    # Store avg loss and reward over the last 10 steps for plotting
    rewards.append(current_reward)
    losses.append(loss.item())
    reward_log.append(sum(rewards)/len(rewards))
    loss_log.append(sum(losses)/len(losses))

    # Optimize using backpropagation
    optimizer.zero_grad()
    loss.backward()       # calculate gradients (partly Quantum!)
    optimizer.step()      # update parameters
```

```
Episode: 0, loss: 3.732, Reward : 0.000
Episode: 1, loss: 5.483, Reward : 0.000
Episode: 2, loss: 3.267, Reward : 0.905
Episode: 3, loss: 3.555, Reward : 0.000
Episode: 4, loss: 5.877, Reward : 0.000
Episode: 5, loss: 3.028, Reward : 0.576
Episode: 6, loss: 3.476, Reward : 0.639
Episode: 7, loss: 3.226, Reward : 0.550
Episode: 8, loss: 3.328, Reward : 0.514
Episode: 9, loss: 3.348, Reward : 0.957
Episode: 10, loss: 3.105, Reward : 0.000
Episode: 11, loss: 5.465, Reward : 0.000
Episode: 12, loss: 2.565, Reward : 1.000
Episode: 13, loss: 4.279, Reward : 0.000
Episode: 14, loss: 3.365, Reward : 0.617
Episode: 15, loss: 3.712, Reward : 0.000
Episode: 16, loss: 3.388, Reward : 0.000
Episode: 17, loss: 3.630, Reward : 0.000
Episode: 18, loss: 2.224, Reward : 0.579
Episode: 19, loss: 3.300, Reward : 0.000
Episode: 20, loss: 2.877, Reward : 0.905
Episode: 21, loss: 3.854, Reward : 0.898
Episode: 22, loss: 4.844, Reward : 0.000
Episode: 23, loss: 4.475, Reward : 0.000
Episode: 24, loss: 2.467, Reward : 0.000
Episode: 25, loss: 2.947, Reward : 0.488
Episode: 26, loss: 3.132, Reward : 0.957
Episode: 27, loss: 3.635, Reward : 0.000
Episode: 28, loss: 2.851, Reward : 0.000
Episode: 29, loss: 4.533, Reward : 0.000
Episode: 30, loss: 4.360, Reward : 0.000
Episode: 31, loss: 3.888, Reward : 0.738
Episode: 32, loss: 3.797, Reward : 0.000
Episode: 33, loss: 6.052, Reward : 0.000
Episode: 34, loss: 3.017, Reward : 0.869
Episode: 35, loss: 2.278, Reward : 1.000
Episode: 36, loss: 2.286, Reward : 1.000
```

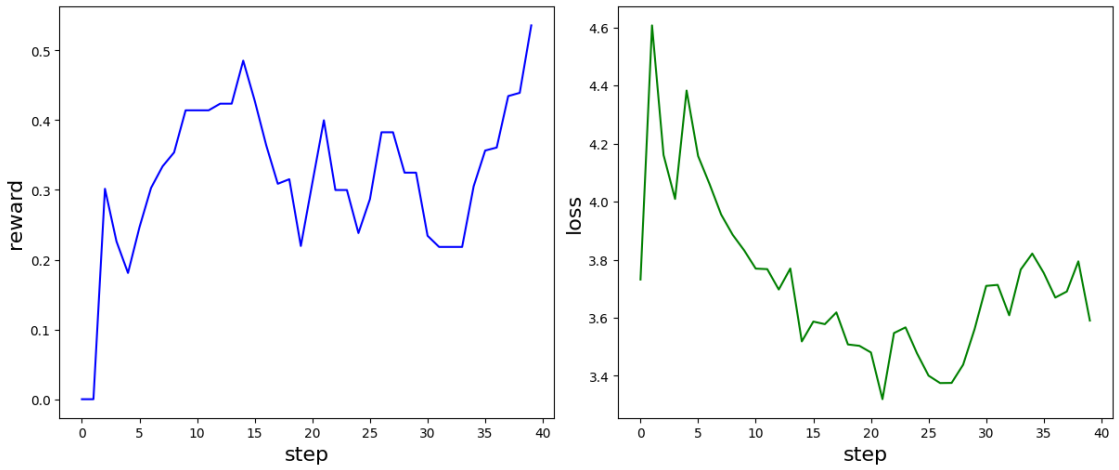
```
Episode: 37, loss: 3.843, Reward : 0.738
Episode: 38, loss: 3.891, Reward : 0.046
Episode: 39, loss: 2.492, Reward : 0.967
```

1.6 Show Training process

[19]:
```
fig, (reward_plot, loss_plot) = plt.subplots(1, 2, figsize=(12, 5),␣
 ↪constrained_layout = True)

loss_plot.set_xlabel('step', fontsize = 16)
loss_plot.set_ylabel('loss', fontsize = 16)
loss_plot.plot(range(num_steps), loss_log, color="green")

reward_plot.set_xlabel('step', fontsize = 16)
reward_plot.set_ylabel('reward', fontsize = 16)
reward_plot.plot(range(num_steps), reward_log, color="blue");
```



1.7 Evaluate the model for all queries

[20]:
```
rewardSum = 0
for entry in data:
    # Predict rewards from the features
    prediction = model(Tensor(entry[0:4]))
    # Choose join order with highest predicted reward
    selected = prediction.argmax()
    # Store the real reward this selection would give
    rewardSum += entry[4+selected]

print("Average reward over all queries: {:.3f}".format(rewardSum/len(data)))
```

```
Average reward over all queries: 0.383
```

1.8 Save model parameters

[21]:
```
torch.save(model.state_dict(), "vqc.model")
```