

IBM quantum computer

There is no quantum world. There is only an abstract physical description. It is wrong to think that the task of physics is to find out how nature is. Physics concerns what we can say about nature... (Niels Bohr)

*Quantum computing is modern magic
Quantum machine learning turns data into magic*

Quantum Computing and Quantum Machine Learning

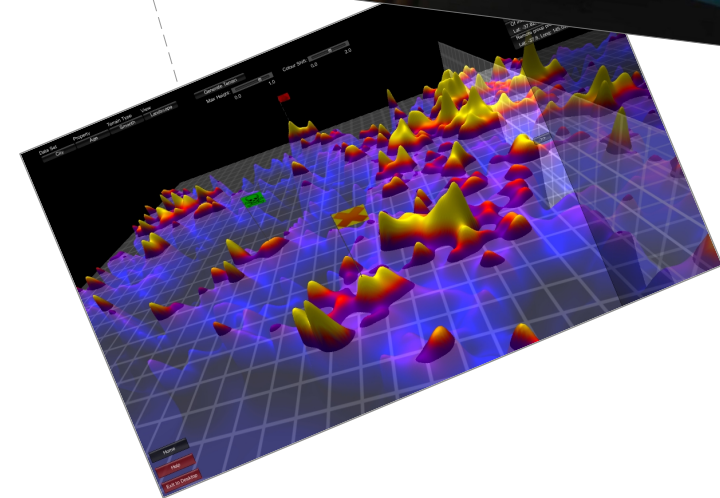
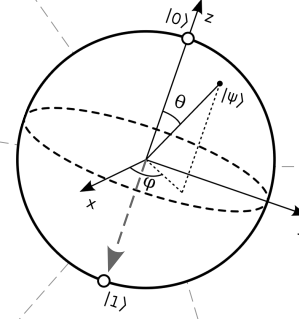
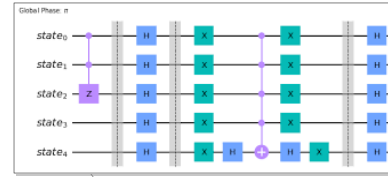
Concepts, Applications and Major Players

Jacob L. Cybulski
School of IT, SEBE, Deakin University

Presenter

Jacob Cybulski

jacob.cybulski@deakin.edu.au

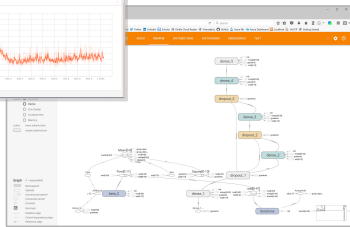
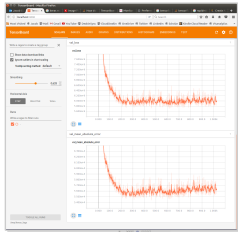


Research

- Quantum Computing
- Quantum Machine Learning
- Classical Machine Learning
- Immersive Data Visualisation
- Business AI

Also

- Recreational Cycling
- Reading Science
- Listening to Weird Music



Quantum Computing and Quantum Machine Learning

General Overview



Quantum Computing & Quantum Machine Learning

- [Quantum mechanics](#), science dealing with the behaviour of matter and light on the atomic and subatomic scale (Britannica.com, 2020)
- It is the foundation of all quantum physics including quantum chemistry, quantum field theory, quantum technology, and quantum information science (Wikipedia.org, 2021)
- [Quantum computation](#) and [quantum information](#) are the study of the information processing tasks that can be accomplished using quantum mechanical systems (Nielsen and Chuang, 2010)
- [Quantum machine learning](#) [...] looks at the opportunities that the current development of quantum computers open up in the context of intelligent data mining (Schuld and Petruccione, 2018)

The popular beliefs of what quantum computers are and what they can do:

- *They are much faster than classical machines (quantum supremacy)*
- *They can break passwords*
- *They work on entirely different principles using qubits which are "0 and 1 at the same time"*
- *They can run programs forward and backwards*
- *Quantum machines use virtually no electricity (at absolute zero 0K)*
- *Quantum computers will soon replace our laptops*
- *They are just a theory*
- *It will take at least 50 years for quantum computing to be useful*
- *You need to have a PhD in Physics to understand quantum computing*
- *You can make big \$\$\$ by investing in quantum computing, ...*

Quantum Devices / Machines

Quantum technologies that are currently being explored include:

- Quantum sensing systems (incl. measuring instruments)
- Quantum information systems (incl. cryptography)
- Quantum communication (incl. networks)
- [Quantum computers](#)
- Quantum inspired systems

Quantum computers may operate using vastly different approaches:

- [Quantum simulators](#) (incl. HPC accelerators)
- Quantum adiabatic / Quantum annealing computers
- Topological quantum computers
- [Quantum circuit/gate models](#)
- Universal quantum computers (Quantum Turing Machines)

Prerequisite Knowledge to entering QC / QML research

Quantum Computing

A subset of Quantum Mechanics

- Complex numbers
- Linear algebra
- Probability theory
- Statistics

Quantum Hardware

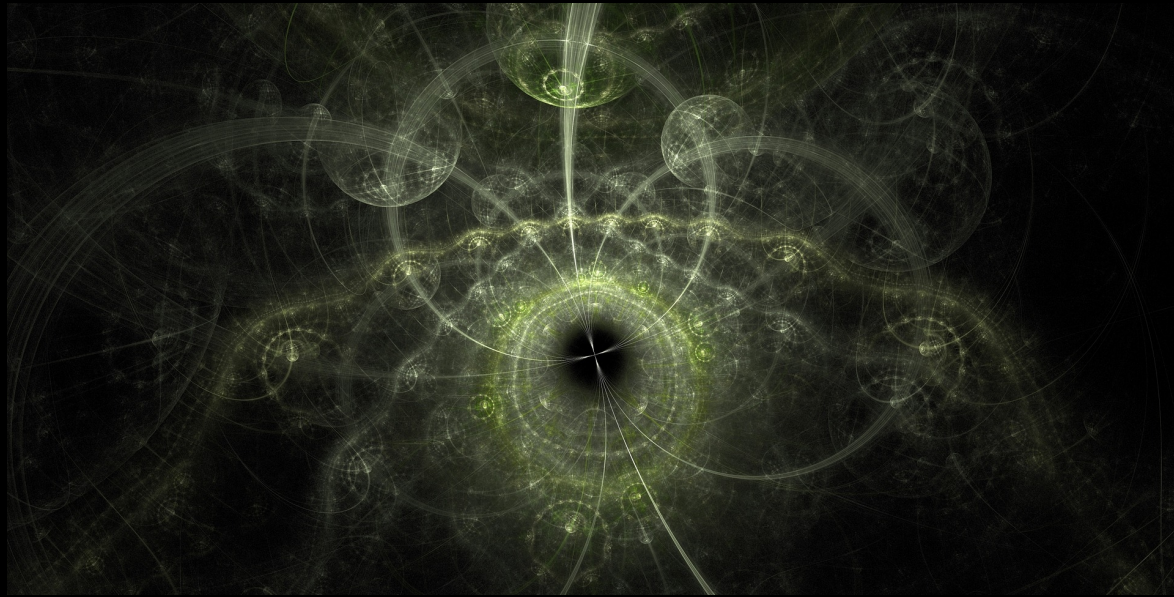
- Configuration
- Calibration
- Error mitigation

Quantum Machine Learning

- Data science
Maths and algorithms
 - ✓ **Calculus**
incl. differential equations, PDE
 - ✓ **Optimisation techniques**
incl. gradient descent, quadratic programming
 - ✓ **Machine learning**
incl. algorithms, models, training, validation, differential programming, and more...

Quantum Computing and Quantum Machine Learning

Fundamental Concepts in Depth

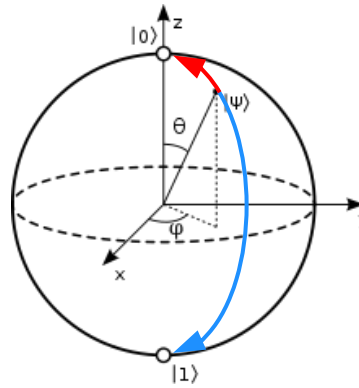


Single qubit

Unit of quantum information

↓ Elementary particle, e.g. electron or photon

- **Qubit** is a device representing a unit of quantum information
- **Qubit state** ψ is a vector in **superposition** (linear combination) of two basis vectors:
↓ Dirac or bra-ket notation Computational basis $\rightarrow \{|0\rangle, |1\rangle\}$
 $|\psi\rangle = \alpha |0\rangle + \beta |1\rangle$ and $|\alpha|^2 + |\beta|^2 = 1$
where α and β are complex numbers, referred to as **probability amplitudes**.
- The qubit state can be described by four numbers (α and β real and imaginary parts), however, because a qubit is a unit vector it only has 3 degrees of freedom, and so can be depicted in 3D space, e.g. as a **Bloch sphere** (see diagram)
- Bloch sphere represents a single qubit state in x, y, z coordinates, as well as by θ and ϕ in polar coordinates (**amplitude** and **phase**)



When measured, the qubit state “collapses” into one of the basis states $|0\rangle$ and $|1\rangle$ resulting in a value of “0” or “1” to be observed

Probability amplitudes α and β can be used to determine the **probability of measurement outcome**:

$$p(0) = |\alpha|^2 \text{ and } p(1) = |\beta|^2$$

Note: Phase ϕ has no impact on the outcome of a qubit measurement! (self-evident, see the figure)

Note: In this visualisation the angle θ between $|0\rangle$ and $|1\rangle$ is π rather than the actual value $\pi/2$

Conversion of polar coordinates into probability amplitudes takes into consideration the Bloch sphere peculiarities (note $\theta/2$ adjustments):

$$\alpha = \cos\left(\frac{\theta}{2}\right) \text{ and } \beta = e^{i\phi} \sin\left(\frac{\theta}{2}\right)$$

Note: The qubit state can be placed half-way between the basis states (using the Hadamard gate “H”), then its measurements “0” and “1” will be produced with equal probabilities.

Multiple qubits

What happens when we have two qubits q_1 and q_2 each placed in some state ψ_1 and ψ_2 ?

$$|\psi\rangle_1 = \alpha_1 |0\rangle_1 + \beta_1 |1\rangle_1 \text{ and } |\alpha_1|^2 + |\beta_1|^2 = 1$$

$$|\psi\rangle_2 = \alpha_2 |0\rangle_2 + \beta_2 |1\rangle_2 \text{ and } |\alpha_2|^2 + |\beta_2|^2 = 1$$

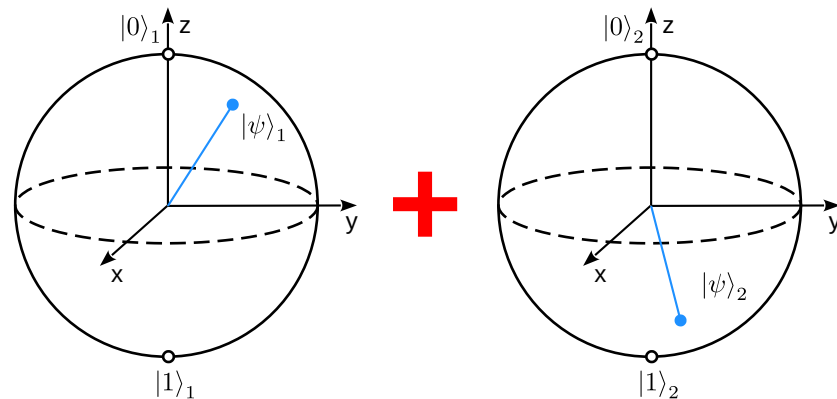
In this case, the state of a quantum system consisting of these two qubits can be described in terms of their combined state space as:

Tensor product

$$|\psi\rangle_1 \otimes |\psi\rangle_2 = \alpha_1\alpha_2 |0\rangle_1 \otimes |0\rangle_2 + \alpha_1\beta_2 |0\rangle_1 \otimes |1\rangle_2 + \beta_1\alpha_2 |1\rangle_1 \otimes |0\rangle_2 + \beta_1\beta_2 |1\rangle_1 \otimes |1\rangle_2$$

Which can be simplified as follows:

$$|\psi\rangle_1 \otimes |\psi\rangle_2 = \alpha_1\alpha_2 |00\rangle + \alpha_1\beta_2 |01\rangle + \beta_1\alpha_2 |10\rangle + \beta_1\beta_2 |11\rangle$$



And this in general coordinates this is:

$$|\psi\rangle_1 \otimes |\psi\rangle_2 = \alpha_{00} |00\rangle + \alpha_{01} |01\rangle + \alpha_{10} |10\rangle + \alpha_{11} |11\rangle$$

Which is a superposition of the following computational basis:

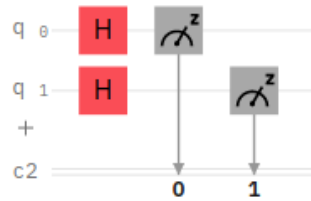
$$\{|00\rangle, |01\rangle, |10\rangle, |11\rangle\}$$

Note that the dimension of the combined state space is exponential of the number of qubits!

Multiple qubits

Entanglement

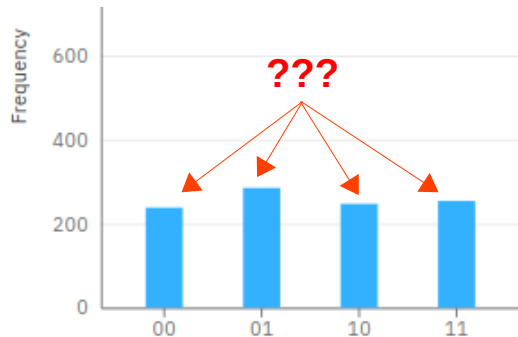
- When two qubits are independent, their measurements are also independent
- Take the following two independent qubits, their measures of “0” or “1” are with equal probability:



The state of two qubits can be described as a superposition of their computational bases $|00\rangle$, $|01\rangle$, $|10\rangle$ and $|11\rangle$

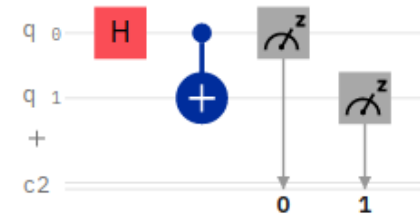
- When the circuit is executed repeatedly, all possible outcomes are produced with **equal probability**.

Distribution of results obtained from 1024 runs reflects a truly random nature of qubit measurement

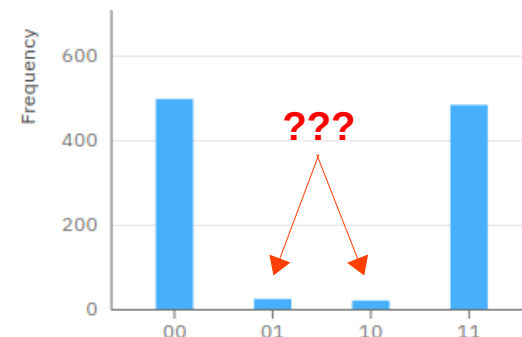


The circuits are now executed on a NISQ machine 1024 times

- Changes to qubits states and their interaction can be designed using *quantum gates*, arranged into *circuits*, which can be executed and their measurements investigated.
- However, when the qubits are *entangled*, i.e. their measurements are correlated.
- Take as an example the following qubits entangled in a *Bell state*:

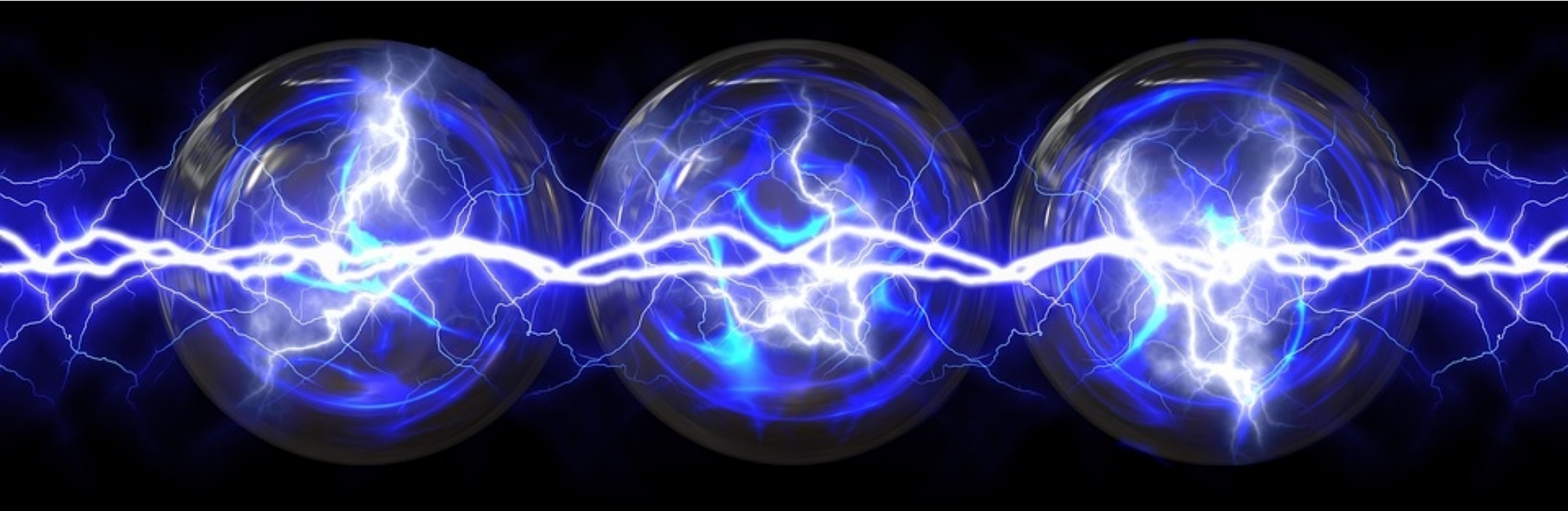


- Their measurements are **always** the same, though their measured values are random.



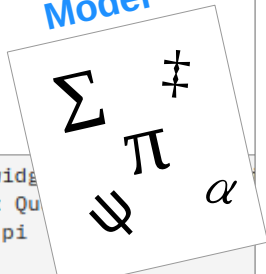
Noise can cause decoherence and thus break entanglement

Quantum Computing and Quantum Machine Learning Solutions and Applications



Quantum solutions take many forms
 ... and they are all equivalent
 ... their execution will yield the same results

Mathematical Model



OpenQASM

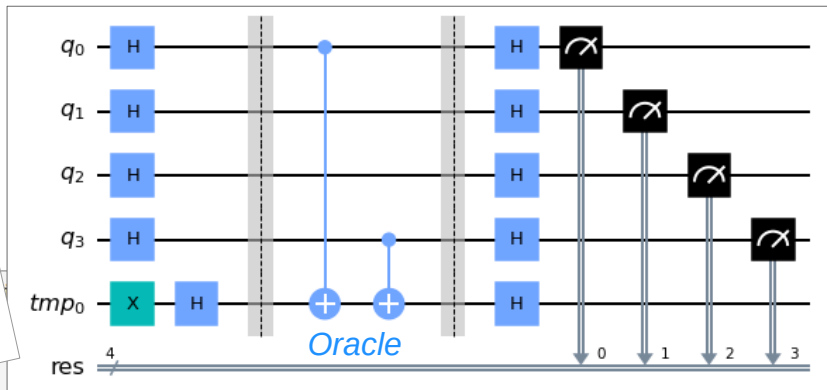
```

1 OPENQASM 2.0;
2 include "qelib1.inc";
3
4 qreg q[5];
5 creg c[5];
6
7 h q[0];
8 h q[1];
9 h q[2];
10 h q[3];
11 x q[4];
12 h q[4];
13 barrier q[0],q[1],q[2],q[3],q[4];
14 cx q[0],q[4];
15 cx q[3],q[4];
16 barrier q[1],q[0],q[2],q[3],q[4];
17 h q[0];
18 h q[1];
19 h q[2];
20 h q[3];
21 h q[4];
22 measure q[0] -> c[0];
23 measure q[1] -> c[1];
24 measure q[2] -> c[2];
25 measure q[3] -> c[3];
    
```

```

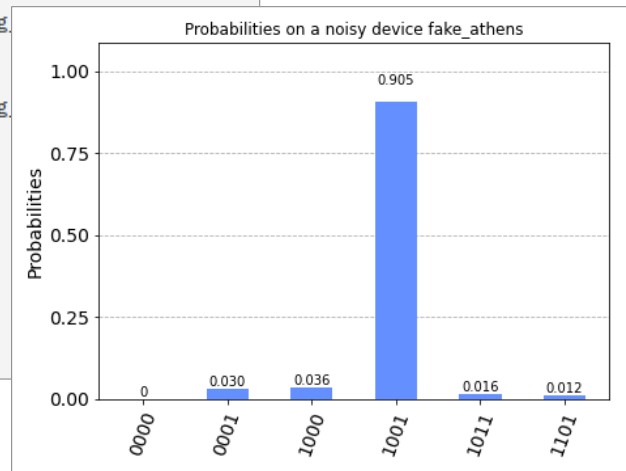
1 from ibm_quantum_wide
2 from qiskit import Qu
3 from numpy import pi
4
5 qreg_q = QuantumRegister(5, 'q')
6 creg_c = ClassicalRegister(5, 'c')
7 circuit = QuantumCircuit(qreg_q, creg_c)
8
9 circuit.h(qreg_q[0])
10 circuit.h(qreg_q[1])
11 circuit.h(qreg_q[2])
12 circuit.h(qreg_q[3])
13 circuit.x(qreg_q[4])
14 circuit.h(qreg_q[4])
15 circuit.barrier(qreg_q[0], qreg_q[1], qreg_q[2], qreg_q[3], qreg_q[4])
16 circuit.cx(qreg_q[0], qreg_q[4])
17 circuit.cx(qreg_q[3], qreg_q[4])
18 circuit.barrier(qreg_q[1], qreg_q[0], qreg_q[2], qreg_q[3], qreg_q[4])
19 circuit.h(qreg_q[0])
20 circuit.h(qreg_q[1])
21 circuit.h(qreg_q[2])
22 circuit.h(qreg_q[3])
23 circuit.h(qreg_q[4])
24 circuit.measure(qreg_q[0], creg_c[0])
25 circuit.measure(qreg_q[1], creg_c[1])
26 circuit.measure(qreg_q[2], creg_c[2])
27 circuit.measure(qreg_q[3], creg_c[3])
    
```

Python + Qiskit



Circuit Diagram

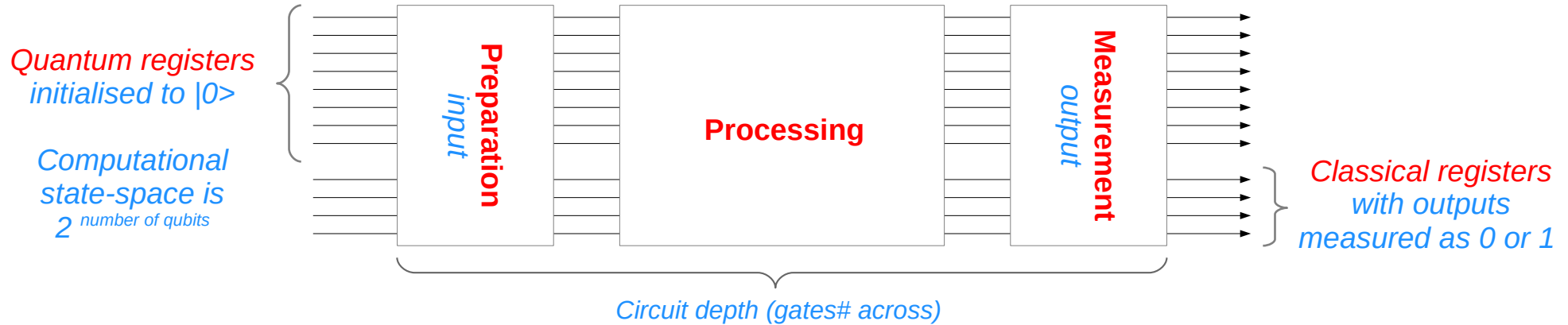
Result



Berstein-Vazirani Oracle

Building a quantum solution

A typical setup of a circuit



In the process of quantum circuit design, we usually perform three tasks, i.e.

- 1) **Preparation** of quantum information, which involves setting each qubit to a specific state (by rotation)
 - 2) **Processing** of quantum information, which applies inter-related gates to these qubits
 - 3) **Measurement** of qubits to obtain classical information about their state.
- A circuit can then be executed on a quantum machine or a simulator and outputs obtained
 - When the circuit is too complex (too deep), the computation may take longer than its coherence time, in which case errors will be produced
 - Effect of noise may require a manual circuit redesign

Examples of Quantum Applications

Selected Areas

- *Cyber security*
- *Financial services*
- *Materials / manufacturing*
- *Transport / logistics*
- *Aerospace / automotive*
- *Energy / resources*
- *Medical / healthcare*
- *Chemistry / pharmaceutical*
- *Bio-tech / genetics / omics*
- *Sensors / measurements*
- *and more...*

Illustrative Examples

Breaking classical encryption, new quantum methods

Portfolio optimisation, fraud indicators, credit scoring

Structural analysis, efficient batteries, costs and risks

Supply chain / inventory / distribution optimisation

Efficient fuels, effective assembly, route planning

Energy distribution, planning and optimisation

Results of therapies, prediction of adverse effects

New chemicals and drugs, personal medicine

Protein folding, study of genetic diseases

Precise instruments, timing, navigation, imaging

Quantum Computing and Quantum Machine Learning Technology and Major Players



Government Funded Quantum Initiatives

- Australia (US\$94M)
- Canada (US\$66M+US\$360M)
- **China (US\$10B)**
- **EU (US\$1.1B)**
- Finland (US\$25M)
- **France (US\$1.8B)**
- **Germany (US\$3.1B)**
- **India (US\$1B)**
- Israel (US\$360M)
- Japan (US\$470M)
- Netherlands (US\$740M)
- New Zealand (US\$25.5M)
- Russia (US\$663M)
- Singapore (US\$109M+US\$74.8M)
- South Korea (US\$37M)
- Sweden (US\$115M)
- **UK (US\$1B)**
- **USA (US\$1.275B)**

Major Players in Quantum Tech (2021)

Universal / Gate-Based Machines

- IBM (Superconducting / Cooper pair)
- Google (Superconducting)
- Rigetti (Superconducting)
- IonQ (Trapped ion)
- Honeywell (Trapped ion) ←---- merged ----→
- Microsoft (*Majorana Anyons*)
- AQT (Trapped ion)
- CEA Leti (Spin - Silicon / Photonics)
- Quantum Brilliance (Carbon / Room Temp)
- Xanadu (Photonics / Room Temp)

Quantum Adiabatic/Annealing Machines

- D-Wave (Quantum Annealing)

Simulators / Quantum Inspired

- AWS Braket (GPU/TPU, SDK+50 qubits)
- Atos (GPU, 41 qubits)
- Alibaba (Cloud QPD)
- Fujitsu (Digital Annealing)

Software-PaaS / QC

- IBM QE / Qiskit - Qiskit
- Google / Cirq - Cirq
- Microsoft Azure Quantum - Q#
- ETH Zurich - ProjectQ
- CQC (Cambridge) - $t|ket\rangle$ / Pytket
- Classiq - Quantum generator

Software-PaaS / QML

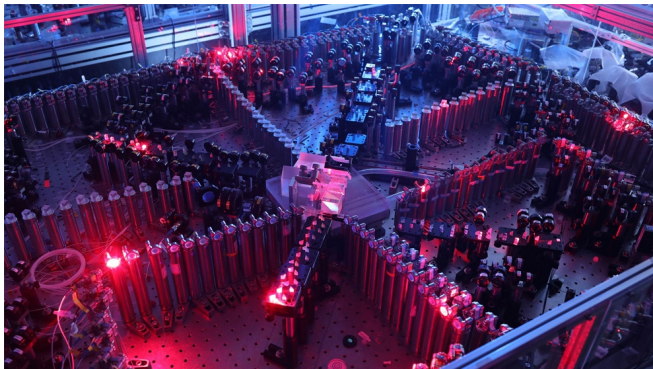
- IBM Quantum / Qiskit - Qiskit ML
- Tensorflow - TFQ (+Cirq)
- Xanadu - PennyLane (+SF)
- Atos - QLM

Applications / Users

- NASA, BASF, Boeing, VW, ...
- Accenture (Business)
- Zapata (Business)
- 1QBit (Medical / Finance)

Quantum Machines

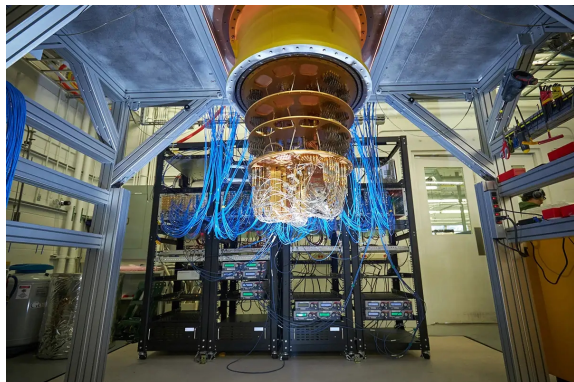
University of Science and Technology of China in Hefei (Jiuzhang - Photonic)



Achieved quantum supremacy performing

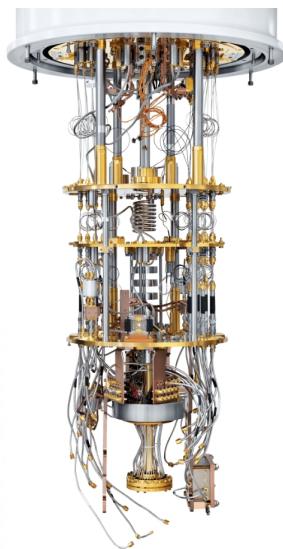
Gaussian Boson Sampling (GBS)

ATOS
(Simulator)



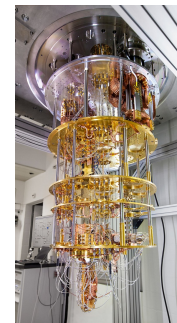
Google (Superconducting)

Rigetti
(Superconducting)



IBM (Superconducting)

Xanadu (Photonic)



Quantum Brilliance
(Diamond)



Which quantum device / machine is best?

- **Qubit Numbers** is a common and highly inaccurate measure of comparing quantum machines.
- Large number of qubits improves a device functionality.
- Unfortunately, in NISQ (noisy) devices more qubits = more errors.
- We need to use a different measure of quantum device size vs quality.
- **Fidelity** is a measure of closeness (as a %) of results obtained from noisy and theoretical (ideal) gates.
- Some vendors measure median fidelity (%) of single (F1) and two qubit (F2) operations (CZ / XY).
- **Quantum Volume (QV)** was proposed by IBM as an alternative measure of quantum device performance.
- To calculate QV, you repeatedly run a series tests on circuits of different size and consisting of random two-qubit gates acting on a subset of the device's qubits.
- Once probability of "correct" results no longer fits the confidence interval of 97.725%, the largest circuit *depth* (longest path through circuit gates) is used to calculate QV as 2^{depth} .
- Examples (2021):
 - IBM Montreal: qubits=27, QV=128
 - IBM Manhattan: qubits=65, QV=32
 - Honeywell H1: qubits=10, QV=512
 - Rigetti Aspen-9: qubits=31, F2~95.8%
 - Google Sycamore: qubits=53, F2~99%
 - IonQ "claims": qubits=32, F2~99.9% and QV>4,000,000 (calculated for 22 qubits)

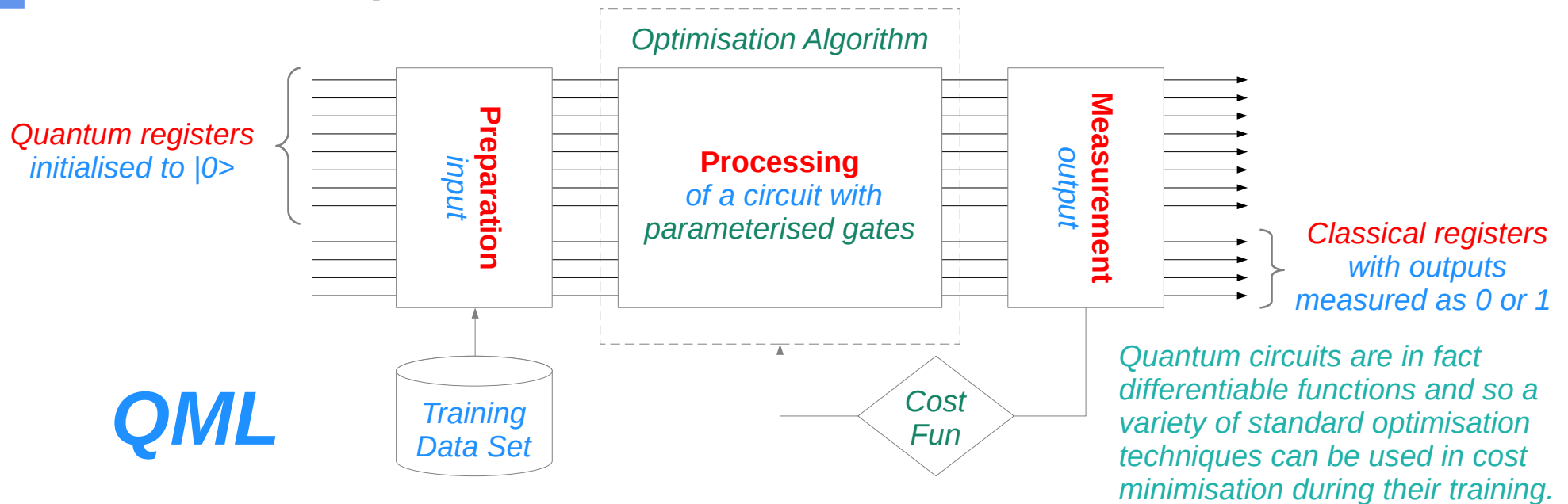
Quantum Computing and Quantum Machine Learning

QML Data to Quantum Models



Quantum Machine Learning

= Variational (parametrised) circuits



Quantum machine learning combines the principles of QC and ML.

QML circuits are created with parametrised gates (e.g. with degree of rotation) which are then optimised using data and ML algorithms

By adopting a specific gate architecture, the circuit may behave as one of the commonly used ML models, e.g. a neural network, in which case a standard optimisation algorithm (e.g. gradient descent) and a cost function (such as MSE) can be used in circuit training

Examples of quantum algorithms and protocols - the ever growing quantum tool-kit!

QC

- Bernstein-Vazirani Algorithm
- Grover's Algorithm
- Shor's Algorithm
- Quantum Fourier Transform
- Quantum Teleportation
- Quantum Key Distribution
- Quantum Image Processing
- HHL Alg. (lin eqs solver) ...

Protocols / Patterns

- Random Number Generation
- Quantum Phase Estimation
- Quantum Counting
- Quantum RAM (qRAM) ...

Variational

- Variational Quantum Eigensolver (VQE)
- Variational Quantum Classifier (VQC)
- Variational Quantum Linear Solver (VQLS)
- Quantum Kernels and Feature Maps ...

QML

- Quantum k-Means and k-NN
- Quantum Approximate Optimization Alg. (QAOA)
- Quantum SVM (QSVM)
- Quantum Neural Nets (QNN) and ConvNets (QCNN)
- Quantum Generative-Adversarial Nets (QGAN)
- Quantum Boltzmann Machines (QBM) and VQBM
- Quantum Reinforcement Learning (QRL)
- Quantum Annealing ...

Quantum Computing and Quantum Machine Learning

Benefits, Risks and Opportunities



QC and QML

Benefits and Risks



Facts

- Quantum computing suits problems that are highly complex but low in data
- Quantum machine learning suits problems that are complex and data rich

Benefits of quantum technologies

- They are efficient sampling devices
- They solve complex problems fast
- They seamlessly integrate algorithms with maths and physical phenomena
- Quantum devices are energy efficient
- Help solving complex scientific problems
- Can be extended with data capabilities

Risks associated with quantum tech

- Threats from new algorithms breaking current practices and standards (costs!)
- Reduced entry cost for the exploration of harmful physical processes, chemicals and biological materials (weapons!)
- High entry cost for business (practice!)
- Rapid pace of developing distinct technologies / standards (obsolescence!)
- Lack of knowledge and skills in applying quantum solutions (education!)
- Shortage of expertise (lab-to-practice!)
- Shortage of development methods for post NISQ devices (future!)

Opportunities right now!



Research

- Study NISQ and Post NISQ methods
- Develop solutions for future quantum devices (millions of qubits)
- Develop new QC / QML user interfaces for non-scientists, business users, specialists
- Create quantum software engineering methodologies and approaches
- Apply QC / QML in established research areas but problems of high complexity, e.g. AI, IoT, frontier materials, epigenetics, fuel / energy systems, cyber security, logistics, ecology, finance and economics, dynamic systems, fluid mechanics, etc.
- Develop new technical areas of QC / QML applications, e.g. 3D data visualisation, robotics, oceanography, space tech, etc.

Education

- Develop programs to educate future QC / QML specialists
- New programs are needed to increase students' awareness of QC / QML issues, esp. NISQ devices
- Programs to industry partners on the opportunities of QC / QML in their domain, e.g. chemistry, finance, etc.
- Organise student and staff teams to participate in QC / QML research, projects, challenges and hackathons
- Take leadership in QC / QML nationally or within the state / region, network, increase visibility
- Develop national and international research centres and grants

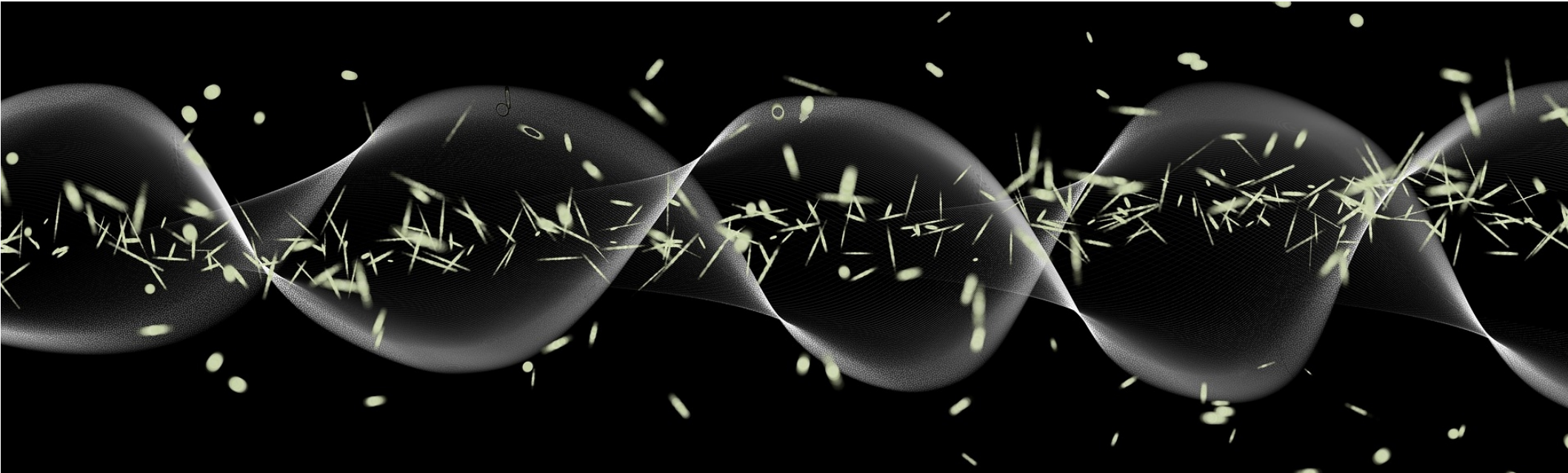
Quantum Computing and Quantum Machine Learning

Questions, References and More...

Opportunities for research

Novel solutions for business

New products and services



New ways of solving hard problems

Variety of new technologies emerging

Exciting discoveries in science

Bibliography for the quantum curious

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Appendix: History of Quantum Computing

An impossibly brief timeline

- 1981: A suggestion to create a quantum computer (by Richard Feynman)
- 1985: An idea of a "universal quantum computer" (by David Deutsch)
- 1994: A quantum algorithm to efficiently factor large numbers (by Peter Shor)
- 1996: A quantum algorithm to efficiently search unstructured databases (by Lov Grover)
- 1998: First 2 qubit quantum computer (by Isaac Chuang and Neil Gershenfeld)
First implementation of a quantum algorithm using a 2-qubit quantum computer running the Deutsch's algorithm (by Jonathan Jones, Michele Mosca and Rasmus Hansen).
- 2001: First implementation of Shor's algorithm (IBM and Stanford University), factoring 15 into its prime factors on a 7-qubit processor.
- 2012: Concept of "quantum supremacy" proposed (by John Preskill)
- 2016: First publicly accessible online quantum computing services (IBM Quantum Experience)
- 2019: First commercial quantum computer (IBM Q System One)
Google claims quantum supremacy on a 53 qubit Sycamore superconducting quantum processor to check the output of random number generator (disputed by IBM)
- 2020: Chinese researchers claim quantum supremacy performing Gaussian Boson Sampling on a 76 qubit Jiuzhang photonic quantum computer
- 2021: The world's largest integrated quantum communication network (China)