Secrets revealed in this session:

To explore the principles of quantum machine learning models, their parameterisation and optimisation

Quantum Machine Learning

Introduction

Jacob L. Cybulski
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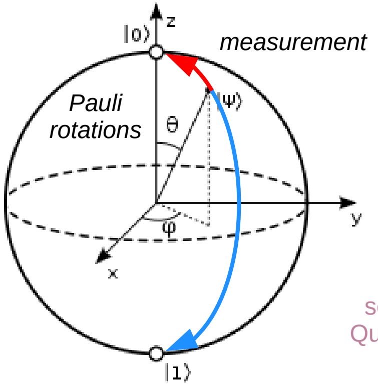

We will assume some knowledge of Quantum Computing ML and Python

12-13 April 2025, QPoland, Fundacja Quantum AI

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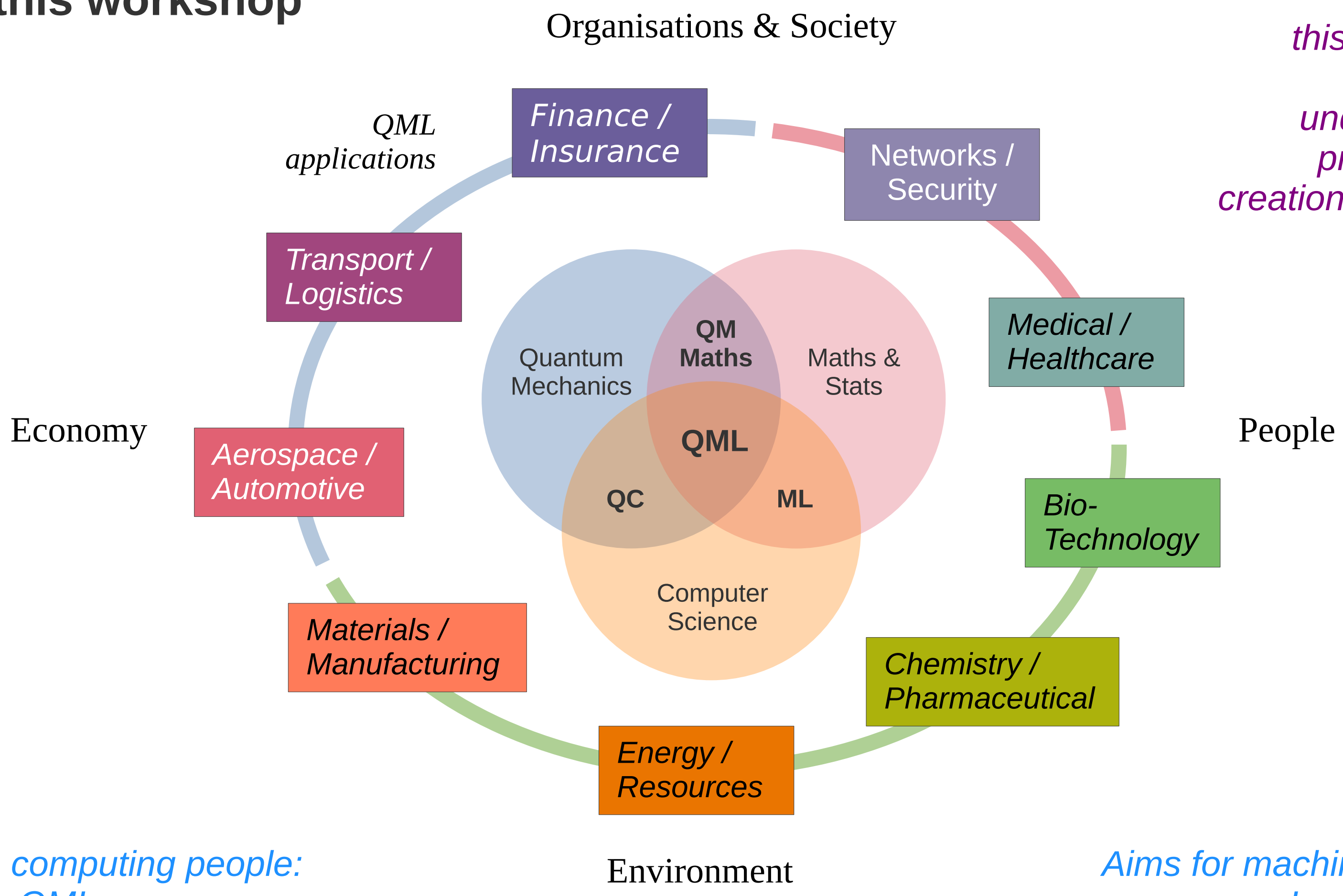
Jacob L. Cybulski, Quantum Computing Intro Series (SheQuantum, Assoc of Polish Profs in Australia)
2021-2025

Quantum ML
aims of this workshop



this workshop aims at developing the understanding of and practical skills in the creation and application of QML models

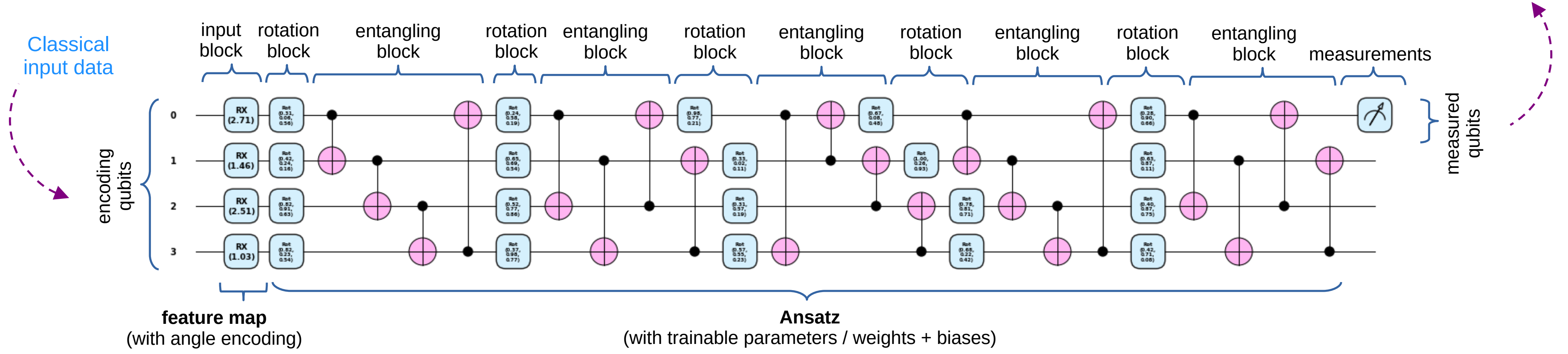
Aims for quantum computing people: Learn about ML in QML

Aims for machine learning people: Learn about Q in QML

Variational Quantum Models

= *Parameterised Quantum Circuits*

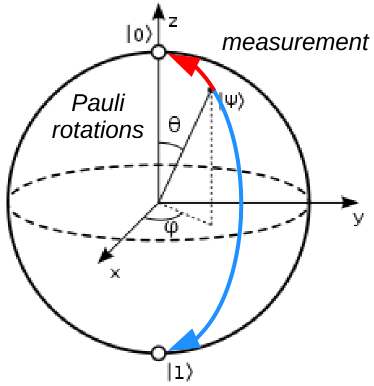
Ansatz parameters are trainable.
Each parameter defines a dimension in the model's parameter space.



We can create a "variational" model = a circuit template with parameterised gates, e.g. P(a), Ry(a) or Rz(a), each allowing rotation of a qubit state in x, y or z axis (as per Bloch sphere).

Typically, but now always, the circuit consists of three blocks:

- a feature map (input)
- an ansatz (processing)
- measurements (output)



Classical input data is encoded into the feature map's parameters, setting the model's initial quantum state.

The quantum state is then altered by an ansatz, which consists of parameterised gates (operations), which alter the initial quantum state.

The quantum state of the circuit is then measured and interpreted as the model's output in classical data form, e.g. as binary values, integer or real value, a single event's probability or the probability distribution.

Data encoding strategies

Data encoding

There are many methods of data embedding, such as: the *basis*, *angle*, *amplitude*, *QRAM*, ... encoding,

In this workshop we will rely on *angle encoding* realised as qubit state rotation by the angle defined by the data.

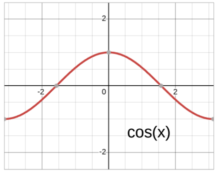
The rotation operators are always available in a quantum platform API (e.g. *Rx*, *Ry*, *Rz* or *Rxyz*).

Typically, the encoding rotation is performed around x or y axis, or both (allowing two values per qubit).

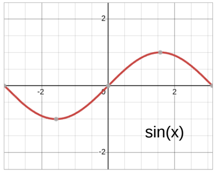
Rotations are *relative to a specific qubit state*, commonly starting at |0⟩ state, or (|0⟩+|1⟩)/sqrt(2), which require qubits to be initialised in these states.

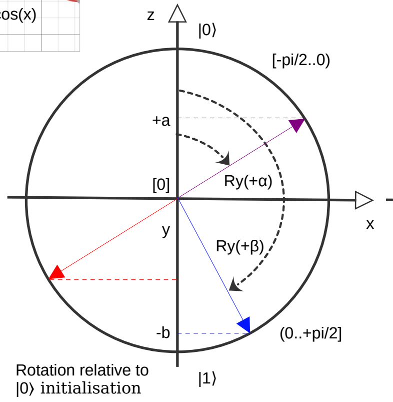
The encoded value could be represented either by the *angular rotation*, or the *amplitude* of the qubit projective measurement (Z).

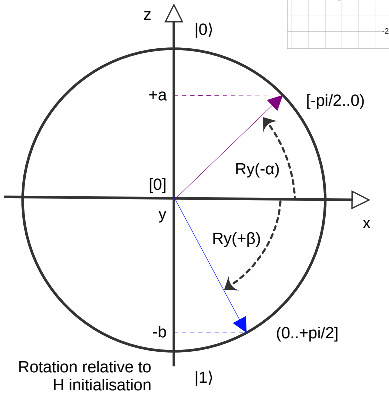
In some cases, input data is repeatedly encoded and interspersed with ansatz layers, called *data reuploading*, which improves the model performance.

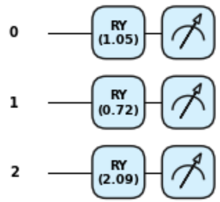


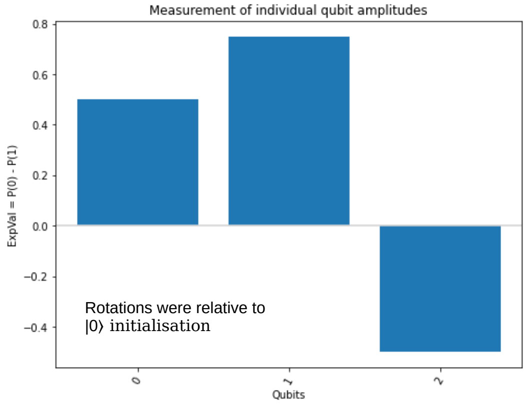
Note that training will place qubit states in areas x < 0 and arbitrarily around the z axis. Measurements of such states cannot distinguish them from "pure" x > 0 and z = 0.











Input

Values entered: [np.arccos(0.5), np.arccos(0.75), np.pi-np.arccos(0.5)]
Ry angles used: [1.047, 0.723, 2.094]

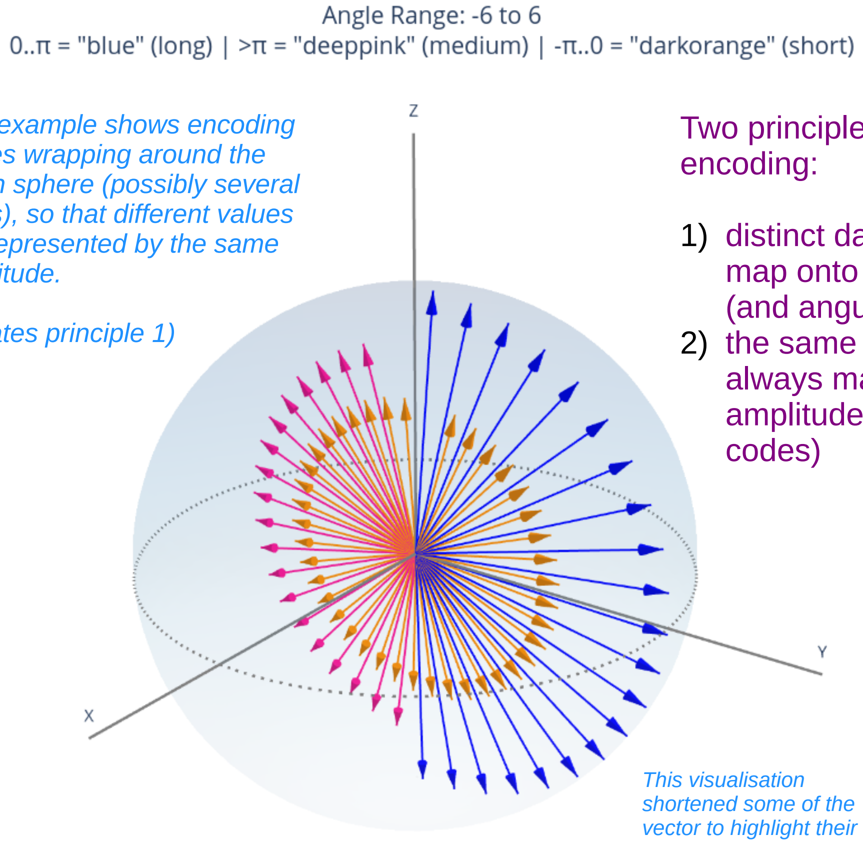
Measurements

Probabilities: [[0.25, 0.75], [0.562, 0.438], [0.25, 0.75]]
Amplitudes: [0.5, 0.75, -0.5]

Maria Schuld and Francesco Petruccione.
Machine Learning with Quantum Computers. 2nd ed. Springer, 2021.

Angle encoding

The Good, the Bad and the Ugly



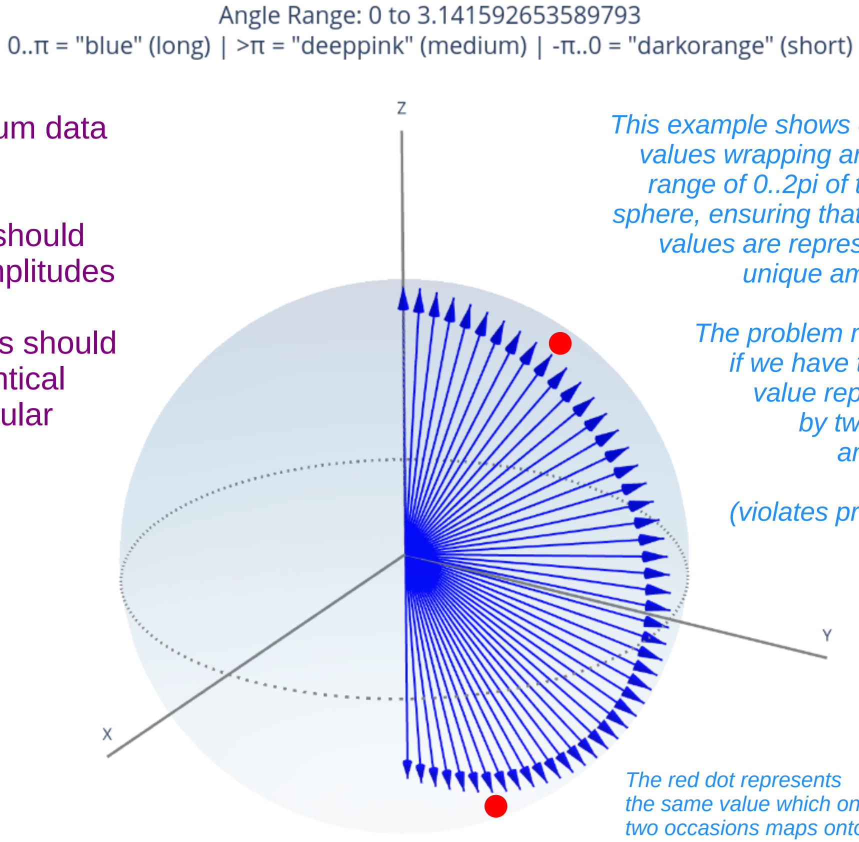
This example shows encoding values wrapping around the Bloch sphere (possibly several times), so that different values are represented by the same amplitude.

(violates principle 1)

This visualisation shortened some of the vector to highlight their difference, however, they are all of length 1.

Two principles of quantum data encoding:

1) distinct data values should map onto distinct amplitudes (and angular codes)
2) the same data values should always map into identical amplitudes (and angular codes)



This example shows encoding values wrapping around the range of 0..2pi of the Bloch sphere, ensuring that different values are represented by unique amplitudes.

The problem may arise if we have the same value represented by two distinct amplitudes

(violates principle 2)

The red dot represents the same value which on two occasions maps onto two different angles and thus two amplitudes.

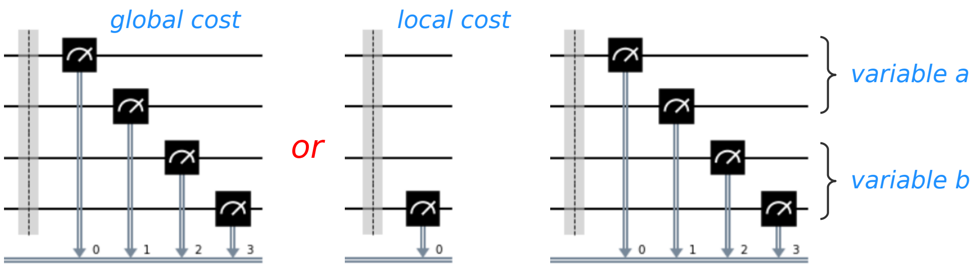
Commonly used
measurements and interpretation

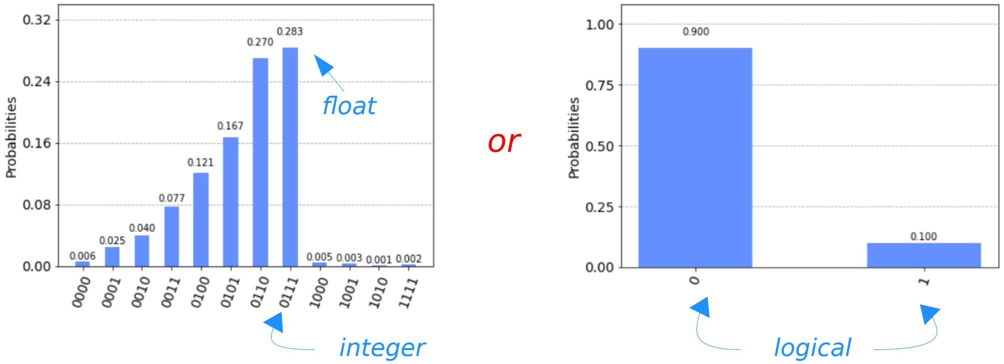
There are many ways of obtaining the outcome of a circuit execution, e.g. we can measure:

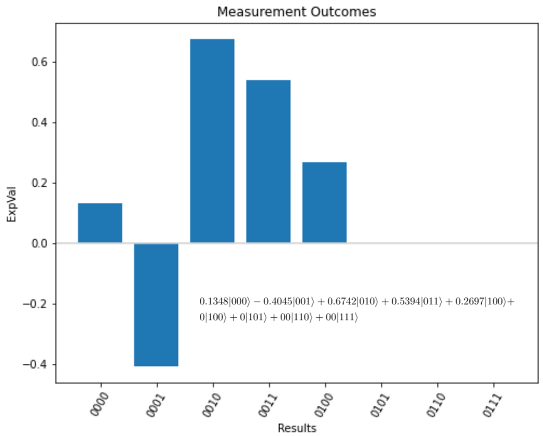
- all qubits (global cost / measurement)
- a few selected qubits (local cost / measurement)
- groups of qubits (each as a variable value)
- as counts of outcomes (repeated measurements)
- as probabilities of outcomes (e.g. P(|0111⟩))
- as Pauli expectation values (i.e. of eigenvalues)
- as expectation of interpreted values (e.g. 0 to 15)
- as variance, etc.

Repeated circuit measurement can be interpreted as outcomes of different types, e.g.

- as a probability distribution (as is)
- as a series of values (via expvals)
- as a binary outcome:
  single qubit measurement or parity of kets
- as an integer:
  most probable ket in multi-qubit measurement
- as a continuous variable:
  probability of the selected ket (e.g. $|0^n\rangle$)







Or we can measure expectation values of the circuit state and interpret them as a series of values

Beware that adding 1 measurement → doubles the number of outcomes!

So... having ***n*** measurements leads to 2^n outcomes

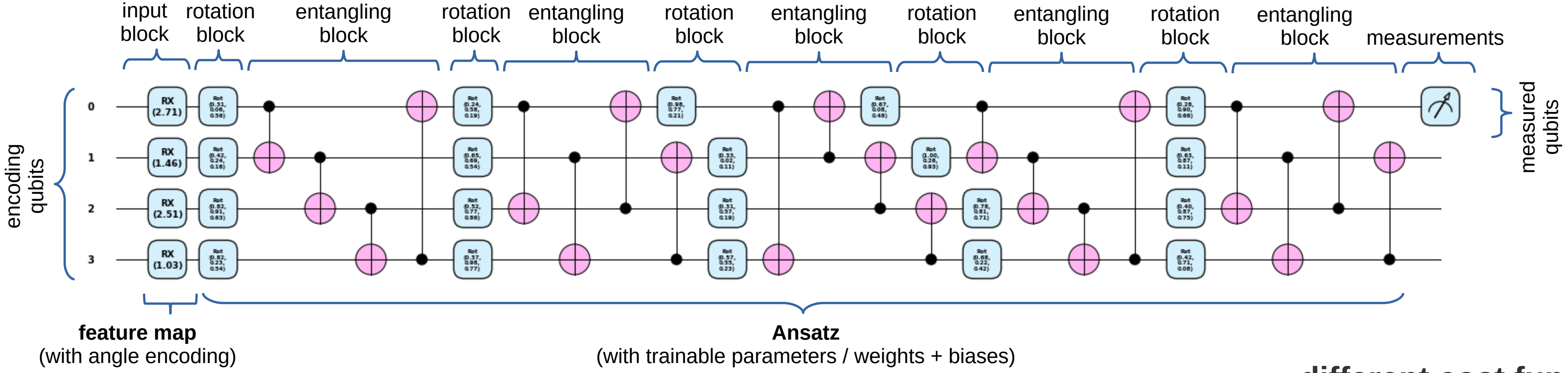
Maria Schuld and Francesco Petruccione.
Machine Learning with Quantum Computers. 2nd ed. Springer, 2021.

Ansatz design and training

A simple quantum classifier ...

Beware that
adding qubits adds
parameters and entanglements!

The number of states represented by the circuit grows exponentially with the number of qubits!



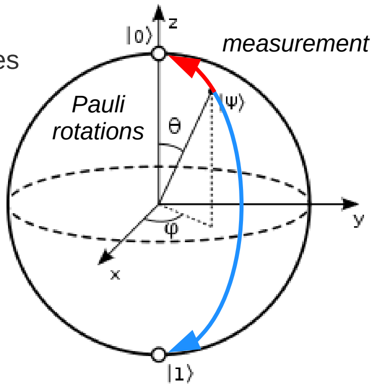
feature maps vary in:
structure and function

ansatze vary in:

- width (qubits #)
- depth (layers #)
- dimensions (param #)
- structure (e.g. funnelling)
- entangling (circular, linear, sca)

ansatz layers consist of:
rotation blocks and entangling blocks of R(x, y, z) and CNOT gates
(rotation) (entanglement)

rotation gates
alter qubit states around x, y, z axes



To execute a circuit we just apply it to input data and the optimum parameters

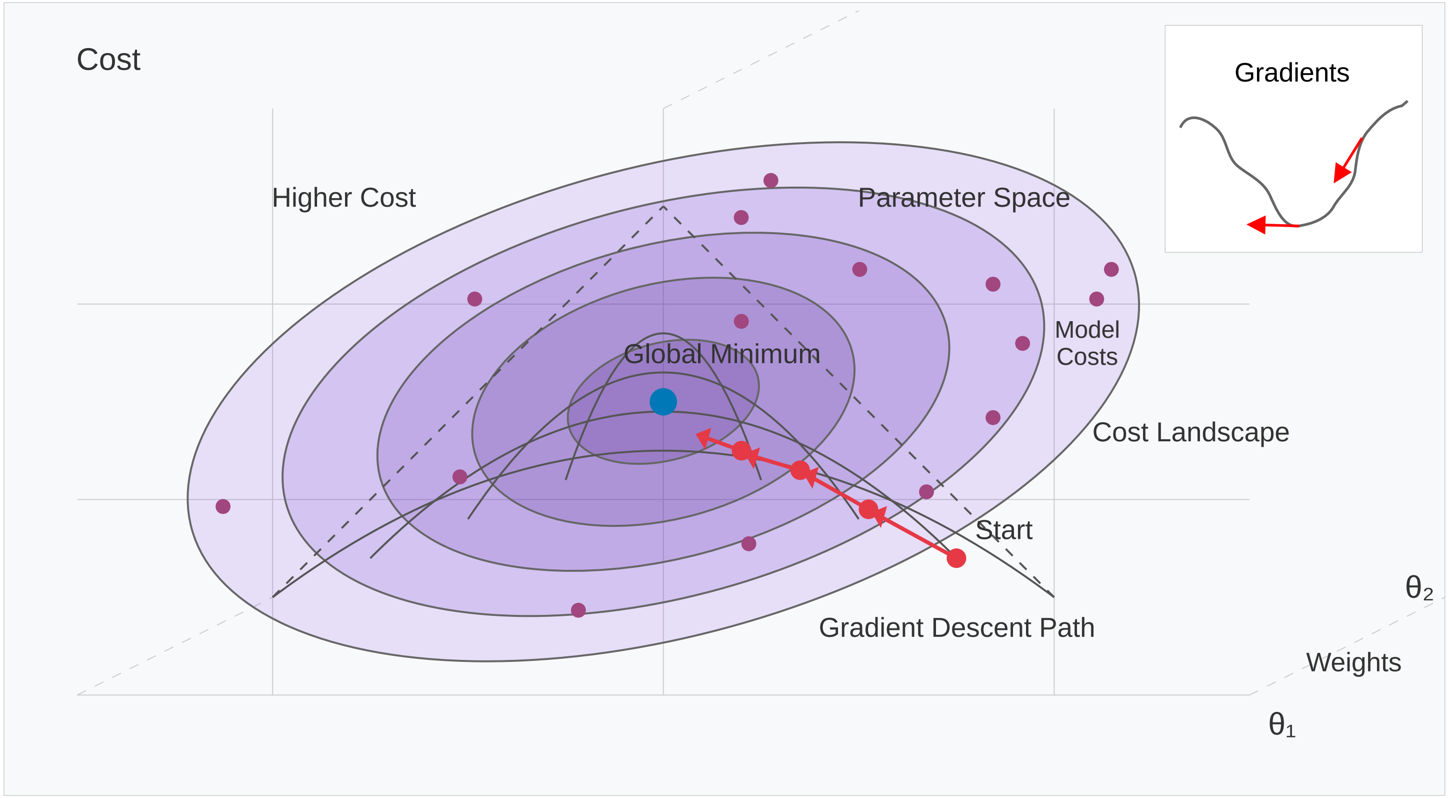
different cost functions:
R2, MAE, MSE, Huber, Poisson, cross-entropy, hinge-embedding, Kullback-Leibner divergence

different optimisers:
gradient based (Adam, NAdam and SPSA)
linear approximation methods (COBYLA)
non-linear approximation methods (BFGS)
quantum natural gradient optimiser (QNG)

circuit execution on:
simulators (CPUs), accelerators (GPUs) and real quantum machines (QPUs)

Problem-solving with DL models

Classical model optimisation



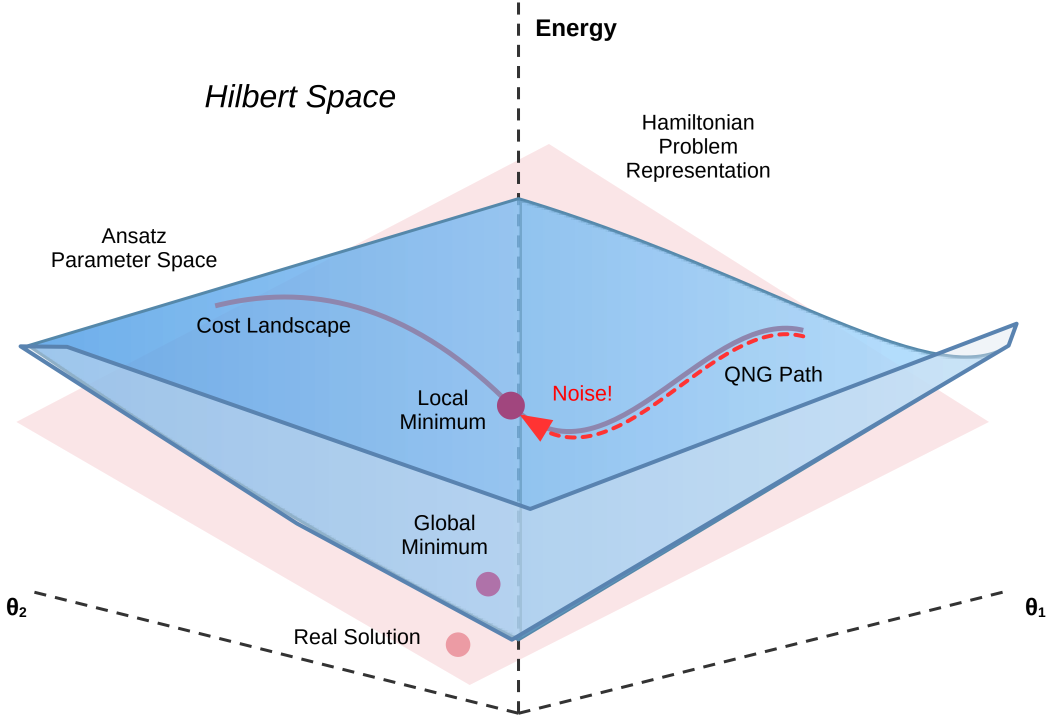
Gradients are local, i.e. their changes influence only their immediate neighbourhood

- A Deep Learning model aims to *represent the problem*.
- It is parameterised with *weights* and *biases*.
- The model quality is linked to the *cost function*, where the lower the cost, the better is the model.
- The costs of all possible model parameterisations, form a multi-dim surface, or the *cost landscape*.
- The *optimisation process* relies on the shape of the landscape, which in turn is reflected in the *gradient* of points on the cost surface.
- *Gradient descent* algorithms can assist in the identification of the model with the *minimum cost*.
- *Backpropagation* can also be used to very efficiently re-calculate NN weights.

Problem-solving with QML

Quantum model optimisation

- The abstract mathematical model represents the problem to be solved, e.g. in the form of a *Hamiltonian*
- The Hamiltonian defines some geometry in *Hilbert space* with the optimum solution associated with the optimum energy
- The *ansatz* of a quantum circuit approximates the Hamiltonian and therefore the problem
- The parameters of the ansatz define a *parameter space* that overlaps and intersects the Hamiltonian problem space
- Our search for the problem solution is hence restricted to the ansatz parameter space
- Ideally, the selected *optimiser* and the *cost function* should understand the principles and processes of quantum models, e.g. Quantum Natural Gradient (QNG) optimiser
- The QNG method defines gradients, which are then calculated for the *cost landscape* (or the manifold), which spans the ansatz geometry
- The QNG optimiser can then identify a *local optimum* solution for this ansatz
- Noise can prevent finding the local optimum

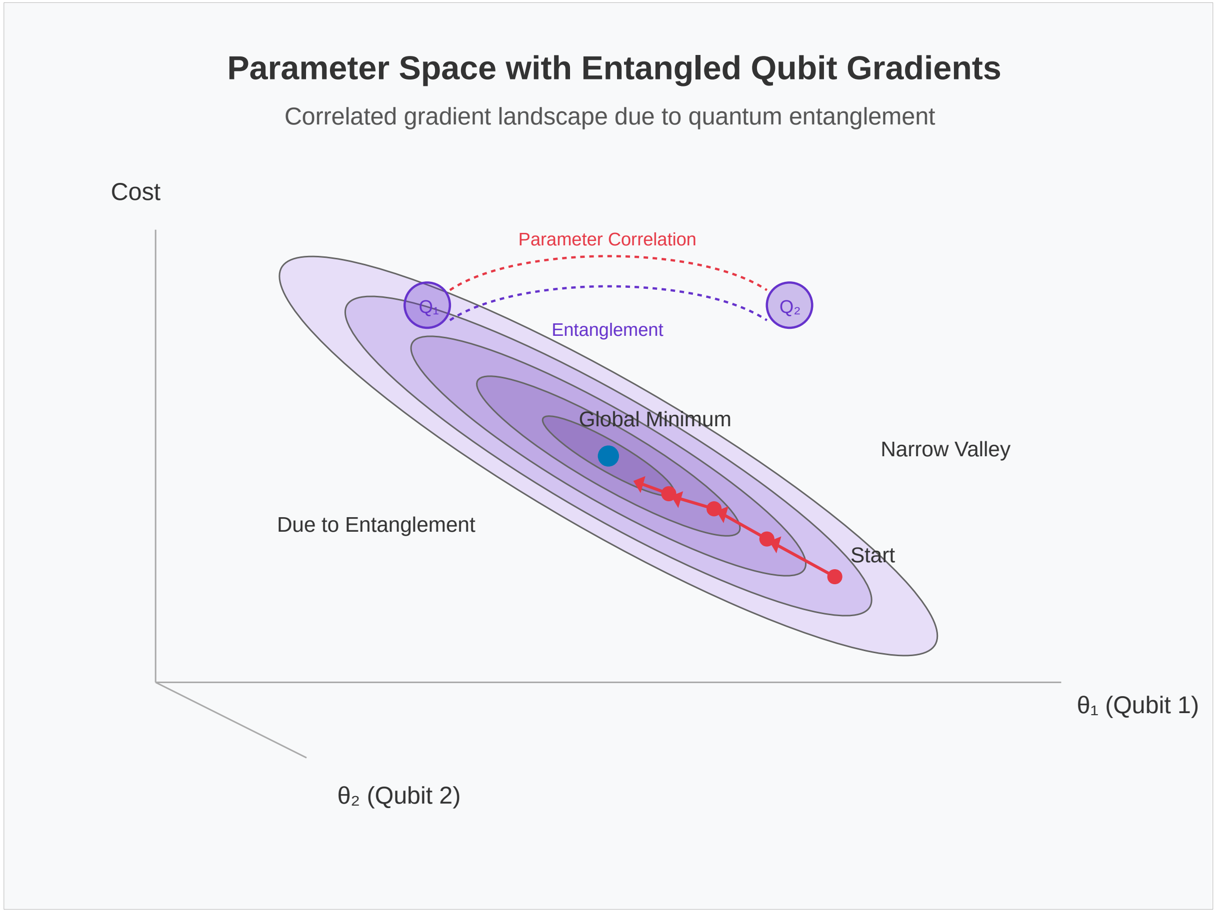


It is more complex than problem-solving with classical models

Quantum model optimisation

- Optimisation of quantum model needs unique approaches due to the emergence of *non-local gradients*
- *Entangled qubits* result in *correlated parameters and gradients*, so the changes to one are reflected in the distant others

- The cost landscape of highly entangled circuits commonly features *narrow valleys*
- Also, *backpropagation* cannot be used directly in training quantum circuits, as their state is not directly accessible and the measurement collapses the state
- *Gradient descend* can still be used with *global gradients*, i.e. those derived from the geometry of the cost landscape
- *Stochastic optimisation techniques* are highly effective when the cost landscape is smooth (no quantum moise)
- Other techniques are also available, such as *particle swarm optimisers*, these however are applicable to smaller models



PennyLane Demo
Everything is a function!

PennyLane (PL) …

- Supports *differentiable programming paradigm*
- Integrates seamlessly with the *Python*
- Has a range of operations for *state preparation*, *gates* and *measurements*
- Supports creation of flexible *quantum algorithms*
- Executes on *simulators* and *quantum hardware*
- Supports *error mitigation*
- Extends its *quantum gradients* with those from JAX, PyTorch, Keras, TensorFlow, or NumPy
- Supports *hybrid quantum-classical models*
- Allows training with *hardware-compatible gradients* and *higher-order derivatives*
- Provides numerous quantum models, such as: *QNNs*, *quantum kernels* and *Fourier models*
- Can be extended with models and optimisers from other SDKs, e.g. *PyTorch* and *TensorFlow*

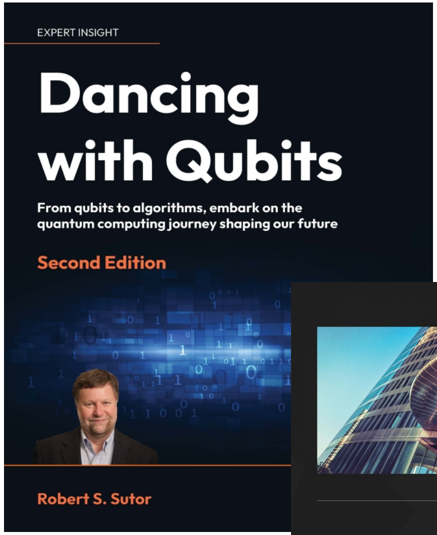
PennyLane Demo:

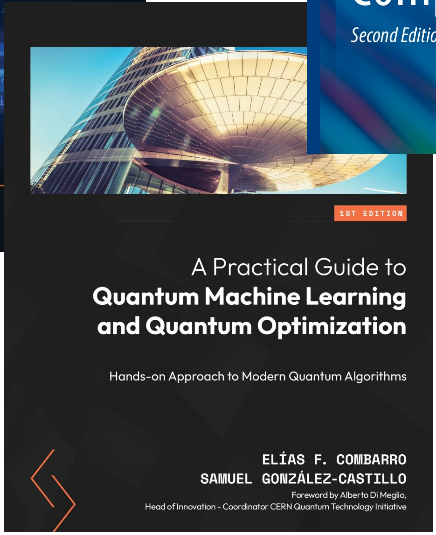
- Create a simple PL model to fit a simple function
- Learn to initialise model weights
- Explore the impact of ansatz structure on performance
- Create minimalistic quantum models
- Learn the interaction of data encoding and ansatz
- Investigate different types of entangling
- Apply the best solution to more complex data
- Learn about stamina and wisdom in QML development

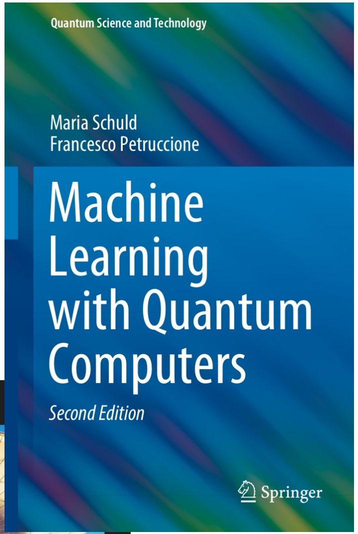
Key takeaways:

- Plan model development, tests and experiments
- Bad data encoding spoils the bunch!
- Strong entanglement improves the data fit
- More width and depth = the curse of dimensionality
- Carefully consider your quantum model initialisation
- Surprise - a single qubit model still works! (and well)
- More training does not solve the problems
- Data reuploading makes a huge difference!

Recommended reading
on QML







PennyLane: Automatic differentiation of hybrid quantum-classical computations

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14 Feb 2020

Modern applications of machine learning in quantum sciences

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June 23, 2022

Abstract

In these Lecture Notes, we provide a comprehensive introduction to the most recent advances in the application of machine learning methods in quantum sciences. We cover the use of deep learning and kernel methods in supervised, unsupervised, and reinforcement learning algorithms for phase classification, representation of many-body quantum states, quantum feedback control, and quantum circuits optimization. Moreover, we introduce and discuss more specialized topics such as differentiable programming, generative models, statistical approach to machine learning, and quantum machine learning.

1

Thank you!

Any questions?

Photos from Unsplash
Enquanted is being somewhere in-between Enchanted and Entangled