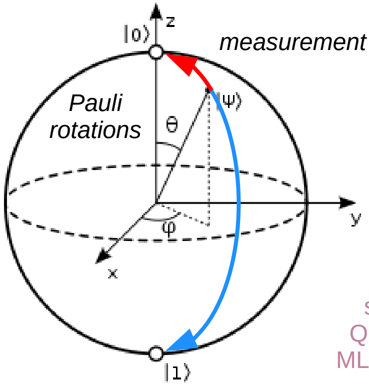
Secrets revealed in this session:

To improve understanding of VQAs and skills in building quantum machine learning models and their optimisation

- QML and its aims
- Parameterised circuits
- Variational quantum algorithms
- Data encoding / angle encoding
- State measurement
- Ansatz design and training
- Model geometry and gradients
- Parameters optimisation
- Curse of dimensionality
- QML readings
- Qiskit demo and tasks (TS forecasting)
- Summary and Q&A

An introduction to Quantum Machine Learning in Qiskit

Jacob L. Cybulski
Enquanted, Australia



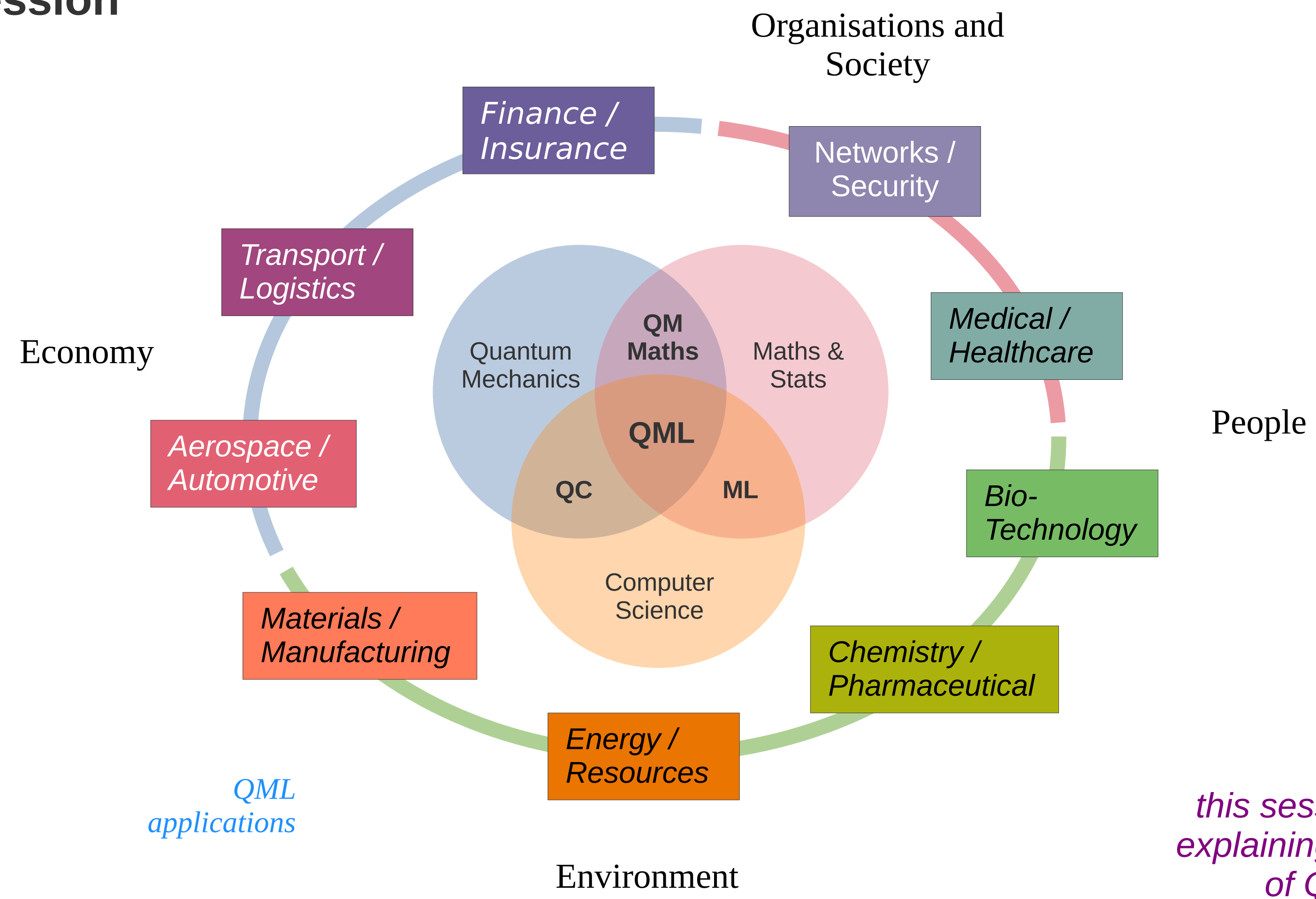
We will assume some knowledge of Quantum Computing ML, Qiskit and Python

October 10, 2025, Adam Mickiewicz University in Poznań, Poland.

Quantum ML

aims of this session

Jacob Cybulski, Founder
Enquanted, Australia

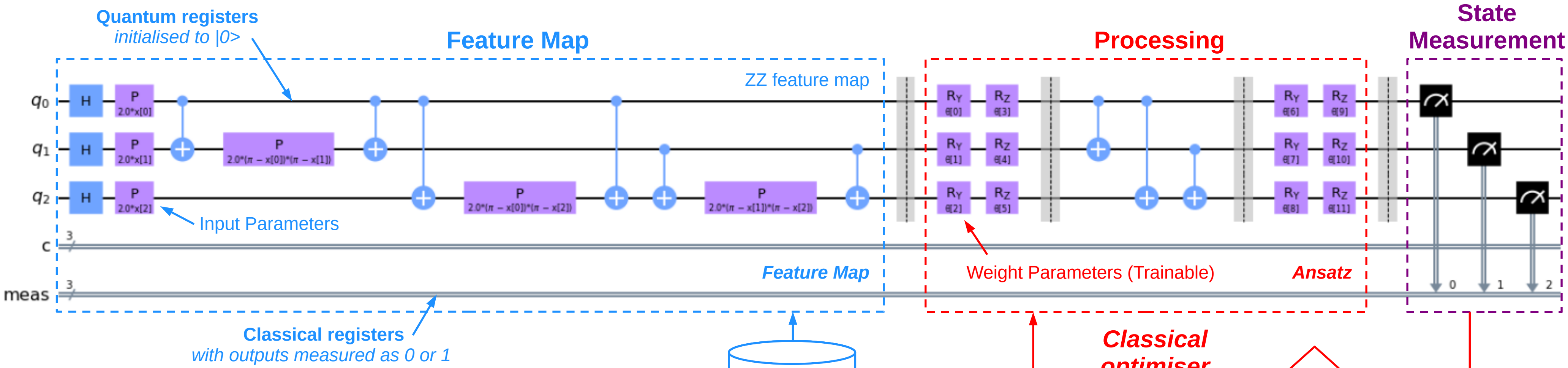


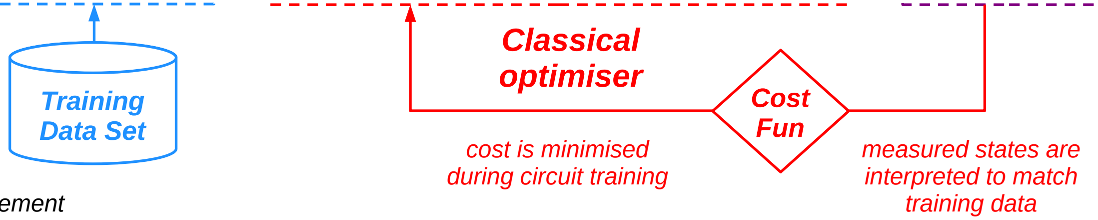
this session aims at explaining the nature of QML models

Parameterised Quantum Circuits

and Variational Quantum Algorithms

Variational quantum circuits are not executable!
They must first be instantiated, i.e. all of their
input and weight parameters must be assigned values!

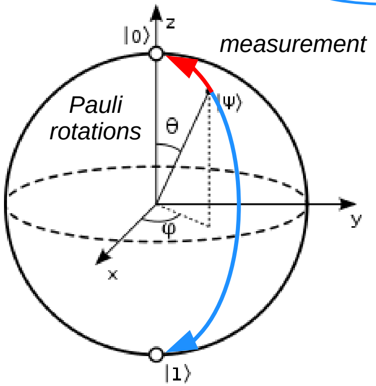




We can create a "variational" model = a circuit template with parameterised gates, e.g. P(a), Ry(a) or Rz(a), each allowing rotation of a qubit state in x, y or z axis (as per Bloch sphere).

Typically (but now always), such circuits consist of three blocks:

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

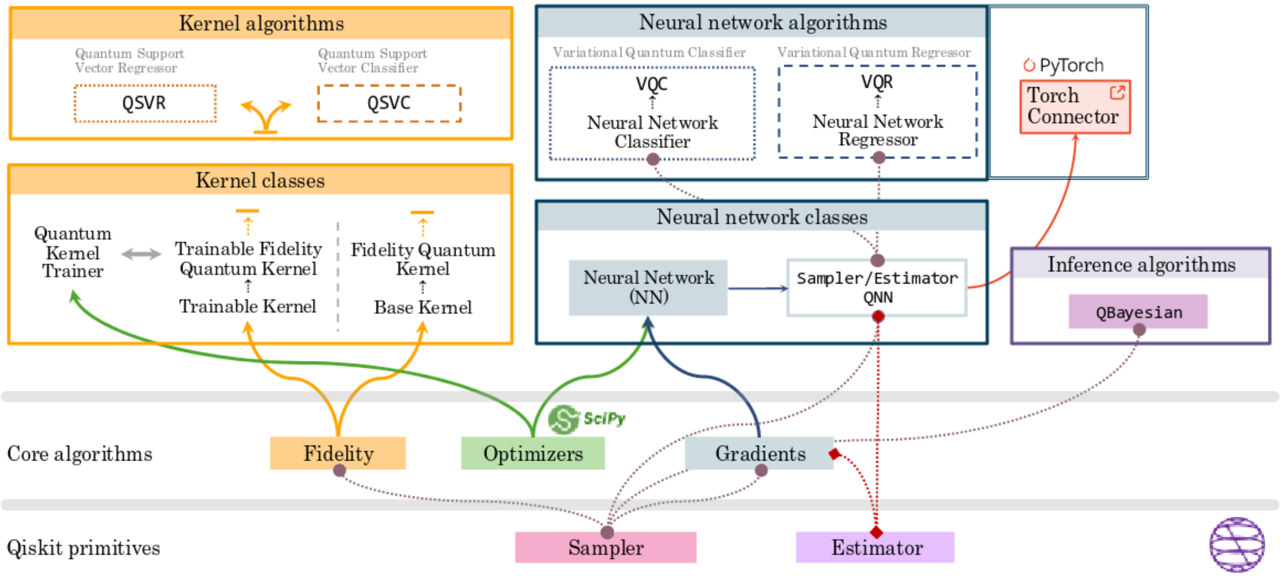


Classical input data is encoded into the feature map's parameters, setting the model's initial quantum state.

The quantum state is altered by an ansatz, of parameterised gates (operations), which are trained by an optimiser

The final quantum state of the circuit is then measured and interpreted as the model's output in the form of classical data.

Qiskit ML Resources



Qiskit ML models and related algorithms:

- Quantum Neural Networks (QNN, VQC/R, QCNN, qGAN)
- Quantum Kernel Methods (Feature Maps, Estimators)
- Quantum Support Vector Machines (QSVM, QSVC/R)
- Quantum Bayesian Modelling (Qbayesian)
- Quantum Kernel Principal Components Analysis (QKPCA)
- Quantum Clustering Algorithms (QCA k-NN, DQC)
- Quantum Optimisation Algorithms (QAOA, QUBO)

Sahin, M.E., Altamura, et al., 2025. Qiskit Machine Learning: an open-source library for quantum machine learning tasks at scale on quantum hardware and classical simulators. ArXiv.2505.17756.

Olivier Ezratty, Understanding Quantum Technologies (2024)

Other open source or published algorithms

- Quantum Fourier Analysis (QFT, QFFT)
- Quantum Sequence Models (QRNN, QLSTM, QGRU)
- Quantum Annealing / Quantum Adiabatic Algorithm (QAA)
- Quantum Boltzmann Machines (QBM, QRBM))
- Quantum Self-Attention and Transformers
- Quantum Random Forest (QRF)
- Quantum k-Nearest Neighbour (QkNN)
- Quantum Hopfield Associative Memory (QHAM)
- Quantum Reinforcement Learning (QRL)
- Quantum Genetic Algorithms (QGA)

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*, *P* or *U* (*xyz*).

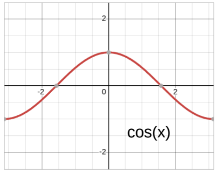
Typically, the encoding rotation is performed around x or y axis, or both (allowing two values per qubit).

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.

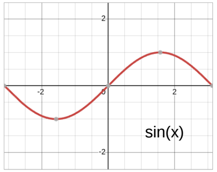
The encoded value could be represented either by the *angular rotation*, or the *amplitude* of the qubit projective measurement (Z).

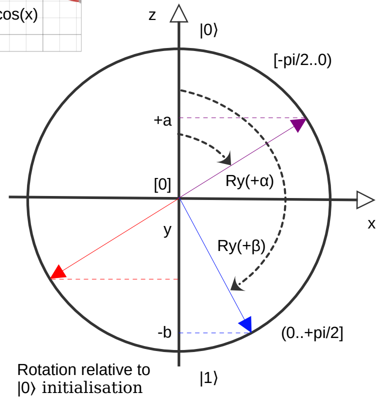
Input data can also be repeatedly encoded and spread around the circuit, which is called *data reuploading*, and which is known to improve the model performance.

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

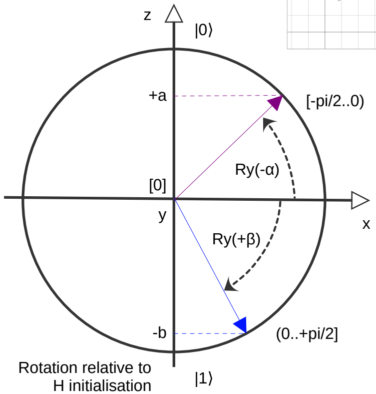


Note that training will place qubit states in areas x < 0 and arbitrarily around the z axis. Measurements of such states cannot distinguish them from "pure" x > 0 and z = 0.

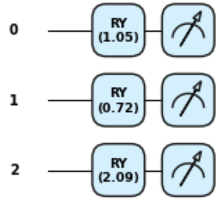


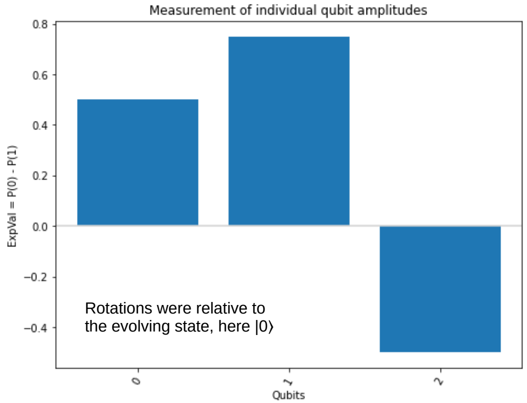


Rotation relative to
|0⟩ initialisation



Rotation relative to
H initialisation





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]

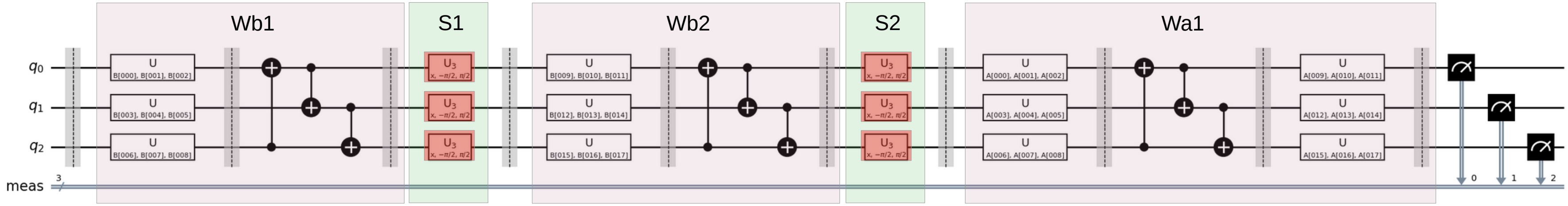
Ansatz design and training

A sample curve fitting model ...

Beware that
adding qubits adds
parameters and entanglements!

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

Encoding of classical data in a quantum circuit is ***not*** *what our ML experience tells us about* ***inputs*** *!*



Data ***reuploading*** *across circuit's width and depth*

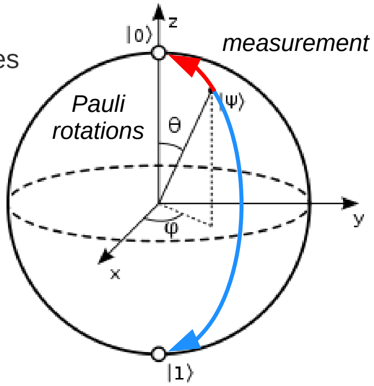
feature maps vary in:
structure and function (!!!)

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)

Commonly used
measurements and interpretation

Quantum circuits can be measured in many ways, e.g.

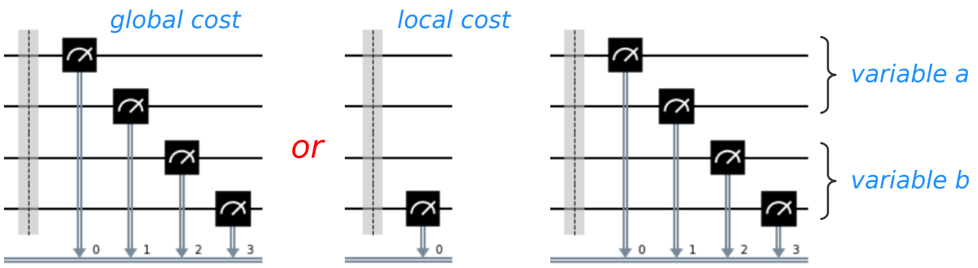
- all qubits (global cost / measurement)
- a few selected qubits (local cost / measurement)
- groups of qubits (each as a variable value)

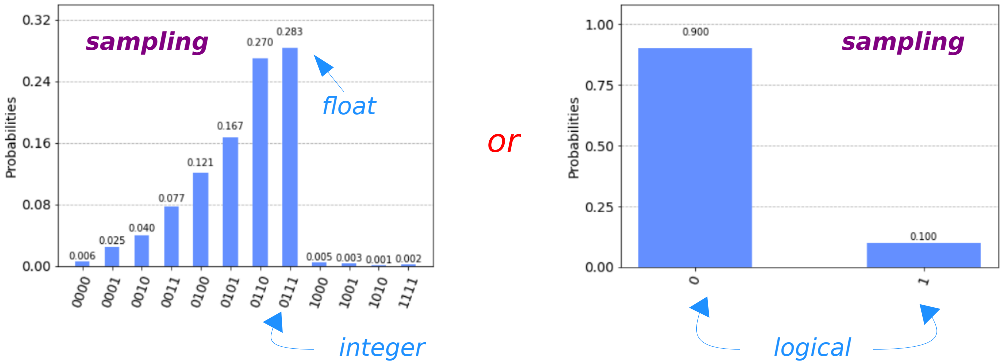
And received in many different formats, e.g.

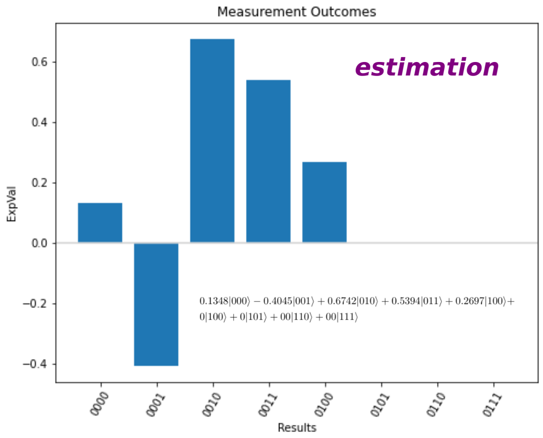
- as counts of outcomes (repeated measurements)
- as probabilities of outcomes (e.g. P(|0111⟩))
- as Pauli expectation values (i.e. of eigenvalues)
- as expectation of interpreted values (e.g. 0 to 15)
- as variance, etc.

Repeated 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 in the range [-1..+1]

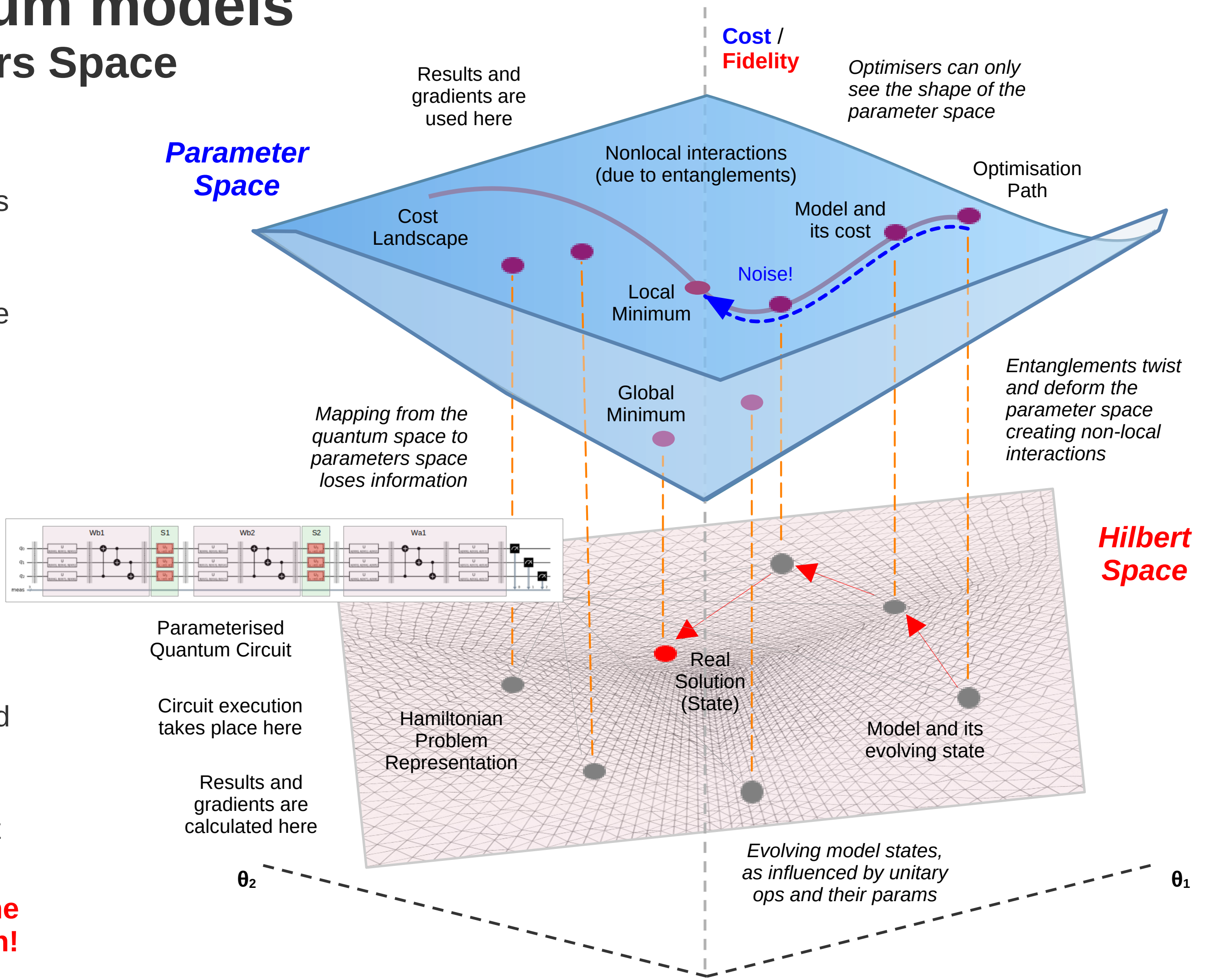
Beware that
adding 1 measurement → doubles the number of outcomes!

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

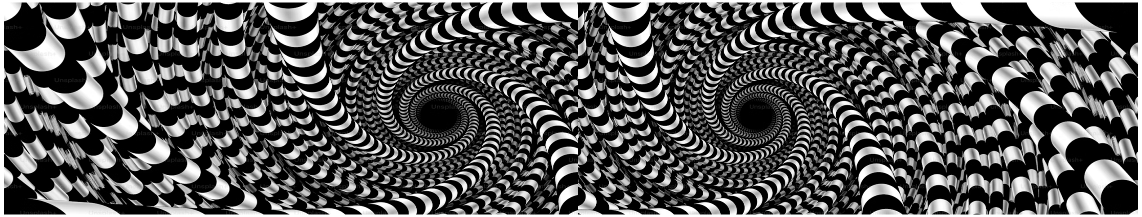
Maria Schuld and Francesco Petruccione.
Machine Learning with Quantum Computers. 2nd ed. Springer, 2021.

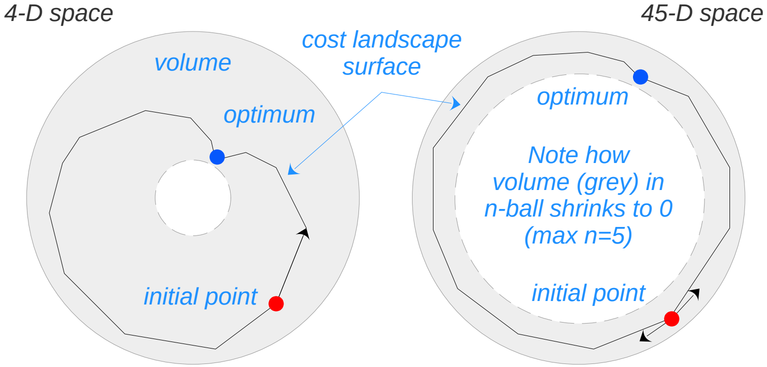
Working with quantum models
Hilbert Space vs Parameters Space

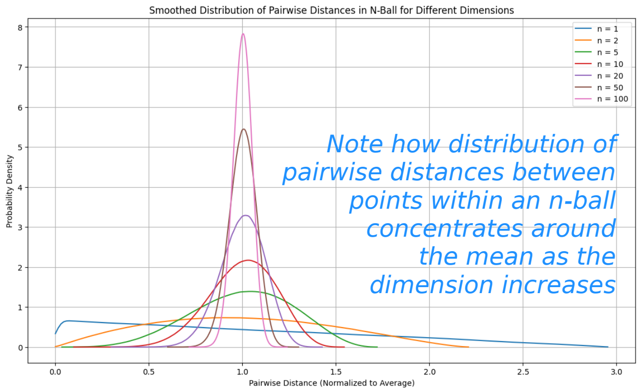
- **Hilbert state space** (dim = the number of qubits) is the quantum realm where the models and their states evolve in response to unitary operations as defined by the circuit gates
- **Data encoding** brings in classical data into the Hilbert space as unique and correlated quantum states during the model execution
- **Layers of circuit gates** determine the evolution of the quantum model's initial state into its final state during the circuit execution
- **Trainable parameter space** is a classical multi-dimensional space of circuit gate parameters, which the optimiser navigates
- **Entanglements** (defined by CNOTs) create and correlate non-separable qubit states, which alter the parameter space geometry, and also the cost landscape used by the optimiser
- **Measurement** of individual qubits collapses their states, consequently projecting the circuit state onto classical outcomes
- **The mapping from the quantum space to the classical parameter loses some information!**



The curse of dimensionality







Cybulski, J.L., Nguyen, T., 2023. “Impact of barren plateaus countermeasures on the quantum neural network capacity to learn”, Quantum Inf Processing 22, 442.

Barren Plateaus (too many dimensions)

- Pairwise distances between uniformly distributed points in high-dimensional space become (almost) identical, and the surface of such a space is almost flat (n-ball value is near its surface).
- In a quantum model with a high-D parameter space, the cost landscape is nearly flat, the situation called *barren plateau (BP)*.
- In high-D parameter space, models sampled by the optimiser are very sparse in both Hilbert space and parameter space.
- When BPs emerge, the optimiser struggles finding the optimum.
- Selecting the optimisation initial point far from the optimum (e.g. random) makes it even more difficult !

There are some well-known BP countermeasures

- use fewer qubits / layers / parameters
- use local cost functions (do not measure all qubits)
- use non-Euclidean metrics (e.g. Fisher Information Metric)
- beware of random params initialisation (and keep them small)
- use BP-resistant model design (e.g. layer-by-layer dev)
- use BP-resistant models (e.g. QCNNs)

Qiskit QML
Workshop

Why Qiskit?

- Accessible from *Python*, *Rust*, *C++ and more...*
- Has a standard set of *quantum state operations*
- Supports creation of flexible QML *algorithms*
- Executes on *simulators* and *quantum hardware*
- Supports hardware *accelerators (e.g. GPUs)*
- Provides tools for *error mitigation*
- Utilises variety of *quantum gradients models*
- Supports *hybrid quantum-classical models*
- Provides many QML models, e.g. *QNNs*, *QCNN*, *QAE*, *QSVM* and *Bayesian models*
- Can be extended with *PyTorch* and *TensorFlow*
- Among quantum SDKs, it is *the best performer*
- It is largely *hardware agnostic via vendor backends*
- Supports *IBM quantum backend and runtime*
- It is *complex* and its *core design changes too often!*

Qiskit QML tasks (time series forecasting):

- Add ML 0.8.3 package to Qiskit 1.4.4 (Python 3.11)
- Create standard and custom models to fit simple data
- Learn the interaction b|n estimator and regressor
- Explore the impact of ansatz structure on performance
- Explore the impact of observables on performance
- Explore the impact of optimiser on performance
- **Challenge:** Apply your skills to chaotic data
- **Reflection:** Refine your QML development process

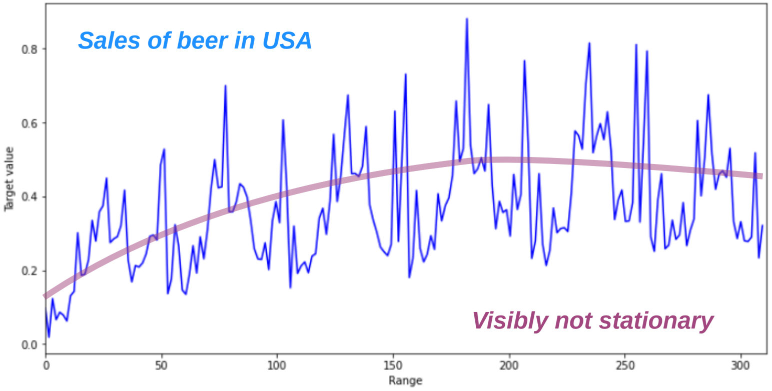
Key takeaways:

- Plan model development, tests and experiments
- Data encoding is crucial to model performance
- Carefully consider your quantum model initialisation
- More params and entanglements improve *expressivity*
- More params and entanglements reduce *trainability*
- Dealing with *the curse of dimensionality*
- High dimensional parameter space upsets even non-gradient optimisers due to *model sparsity*
- More training often does not eliminate problems!
- Selection of appropriate optimisers, observables and custom models, may be necessary to break the performance swamp

QML for time series analysis

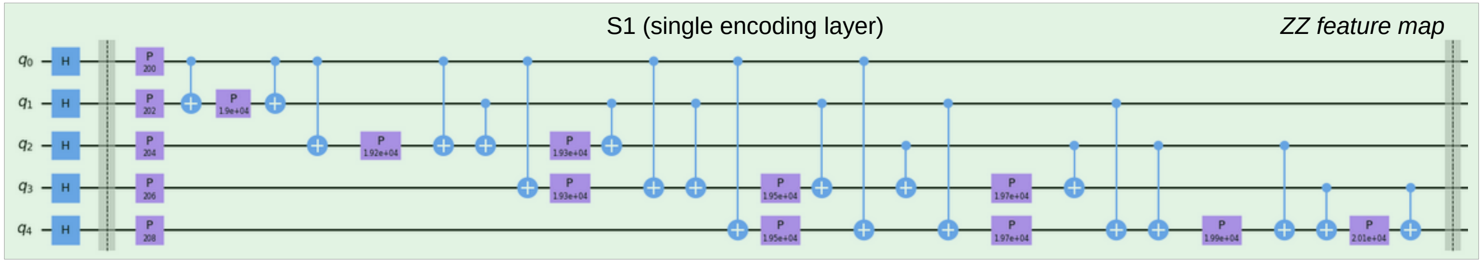
Quantum time series analysis is hard!

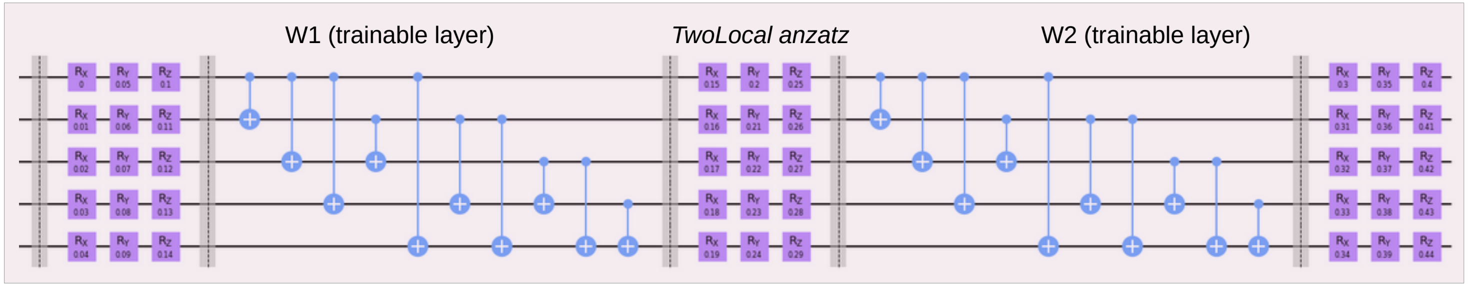
- Time series (TS) analysis aims to *identify patterns* in historical time data and to *create forecasts* of what data is likely to be collected in the future
- *Many TS applications*, including heart monitoring, weather forecasts, machine condition monitoring, etc.
- Time series can be *univariate* or *multivariate*
- Time series often show *seasonality* in data, i.e. some patterns repeating over time



- TS values are dependent on the preceding values!
- Distinction between consecutive TS values is small!
- There are several different types of TS models, e.g.
  - The first group are *curve-fitting models*, which are trained to fit a function to a sample of data points, to predict data values at specific points in time
  - The second group are *forecasting models*, which are trained to predict future data points from their preceding temporal context (a fixed-size window sliding over TS)
- Majority of statistical forecasting methods require *strict data preparation*, such as dimensionality reduction, TS aggregation, imputation of missing values, removal of noise and outliers, adherence to normality and homoskedasticity, they need to be stationary
- QML methods do not have such strict requirements, and are promising for effective time series analysis and forecasting!

Forecasting models

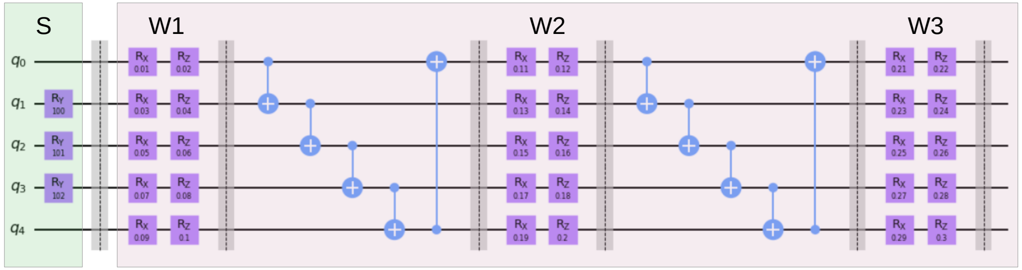




xqnn_standard_model

This QNN model consists of two components, i.e. (1) the ZZ feature map, and (2) a TwoLocal ansatz.

This QNN architecture is commonly used and considered to enhance expressivity of the quantum circuit.



xqnn_custom_model

This is a custom-built QNN model. It is composed of (1) an angle encoding feature map of Ry rotation gates; and (2) an ansatz that is wider than the encoding layers and consisting of several trainable layers of Rx, Ry and Rz parameterised blocks interspersed with entangling blocks of CNOT gates arranged in a circular fashion.

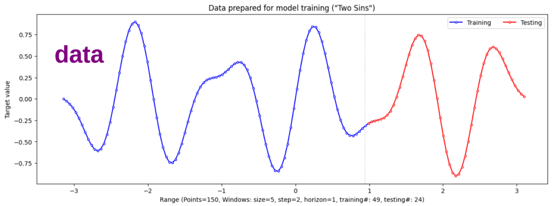
Custom models are often used when facing training difficulties, e.g. to improve the circuit trainability by reducing the its entanglement (fewer CNOT gates) or to add trainable parameters to enhance its expressivity.

In this workshop we provide two alternative QNN models. The first features the commonly used circuit structure relying on Qiskit supplied parameterised circuits. The second is custom made and is created from the Qiskit basic building blocks (gates and parameters).

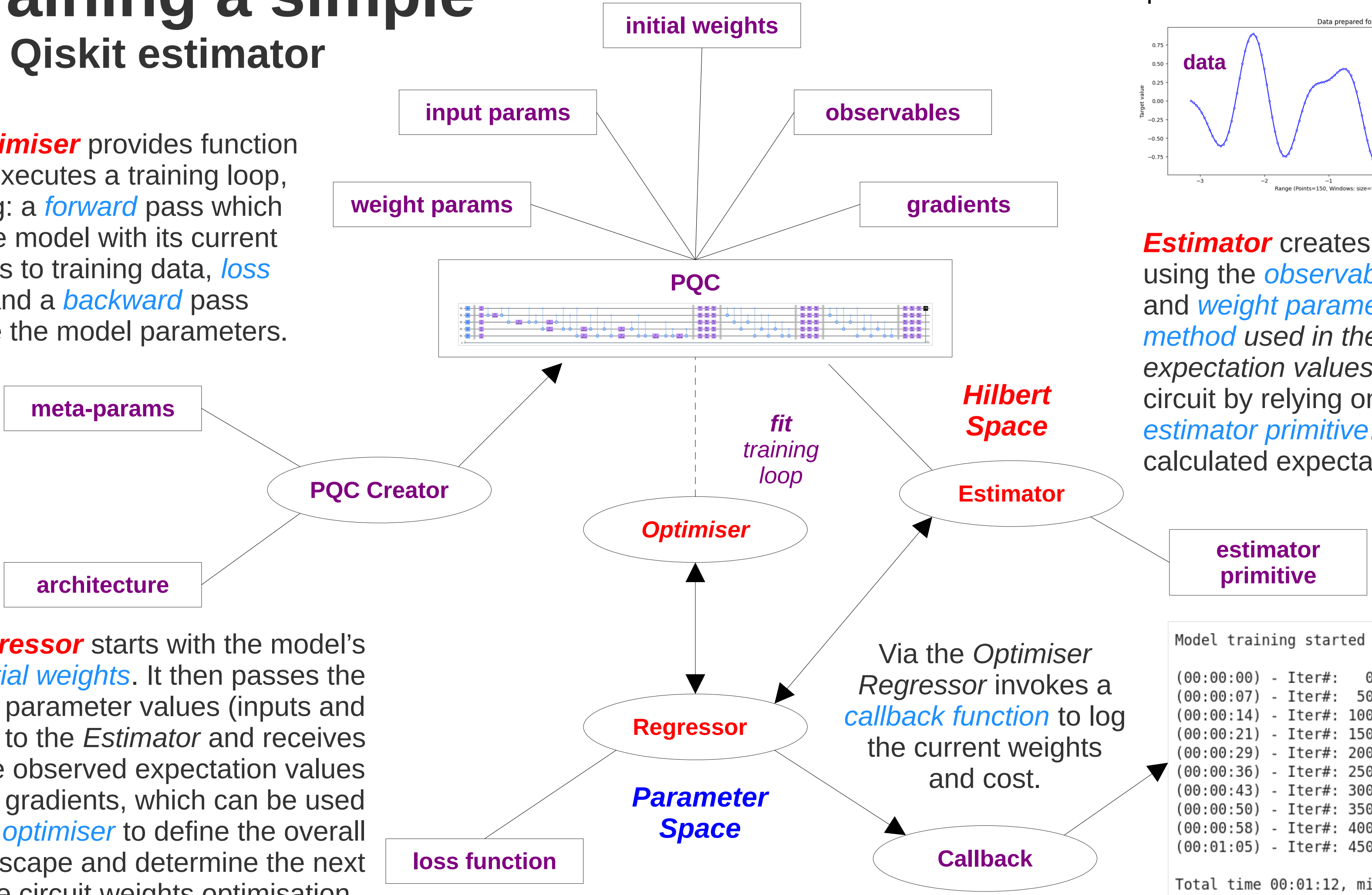
Training a simple

TS Qiskit estimator

Dataset is to be prepared, cleaned and partitioned for training and testing.



Qiskit ***Optimiser*** provides function ***fit*** which executes a training loop, performing: a *forward* pass which applies the model with its current parameters to training data, *loss function*, and a *backward* pass to improve the model parameters.



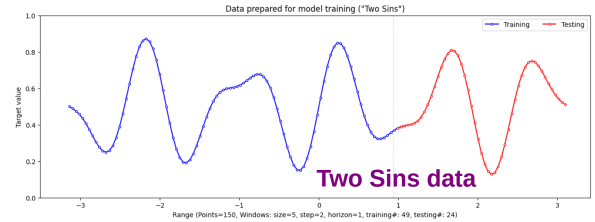
Estimator creates the physical circuit using the *observables*, *input parameters* and *weight parameters*, and the *gradient method used in the calculation of expectation values.* It then executes the circuit by relying on a hardware specific *estimator primitive*. It returns the calculated expectation values.

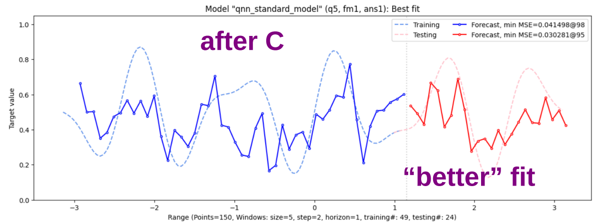
Regressor starts with the model's *initial weights*. It then passes the current parameter values (inputs and weights) to the *Estimator* and receives back the observed expectation values and their gradients, which can be used by an *optimiser* to define the overall cost landscape and determine the next step in the circuit weights optimisation.

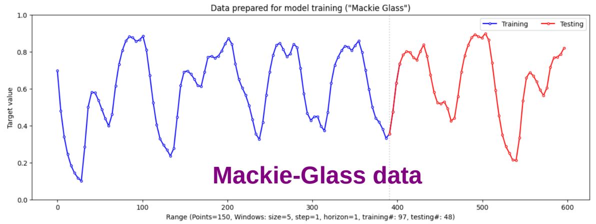
training log

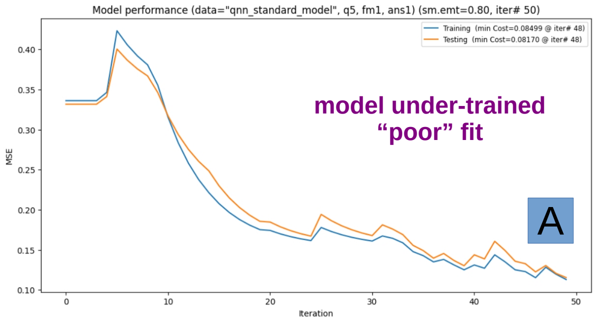
```
Model training started

(00:00:00) - Iter#:   0 / 500, Cost: 0.238564
(00:00:07) - Iter#:  50 / 500, Cost: 0.162685
(00:00:14) - Iter#: 100 / 500, Cost: 0.126066
(00:00:21) - Iter#: 150 / 500, Cost: 0.073866
(00:00:29) - Iter#: 200 / 500, Cost: 0.053152
(00:00:36) - Iter#: 250 / 500, Cost: 0.038513
(00:00:43) - Iter#: 300 / 500, Cost: 0.033054
(00:00:50) - Iter#: 350 / 500, Cost: 0.029146
(00:00:58) - Iter#: 400 / 500, Cost: 0.027865
(00:01:05) - Iter#: 450 / 500, Cost: 0.026759

Total time 00:01:12, min Cost=0.026013
```

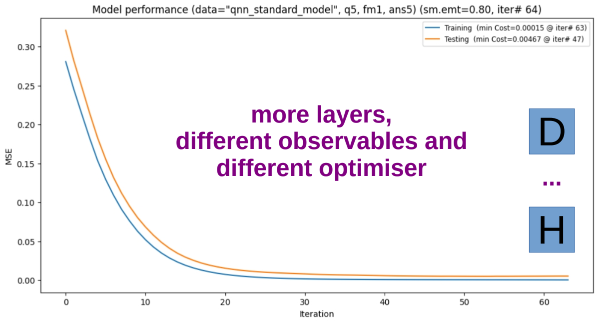
In search of a solution!

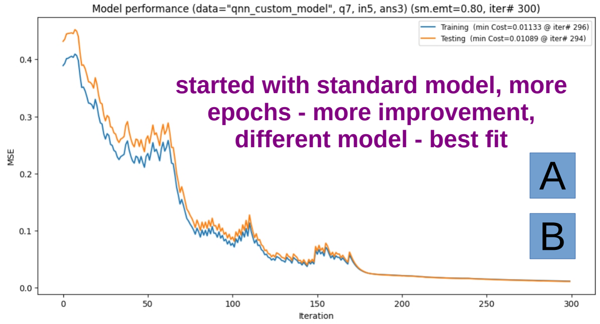


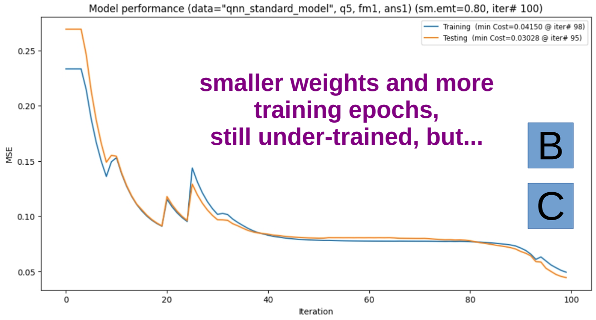


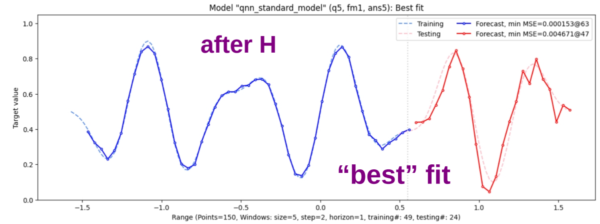


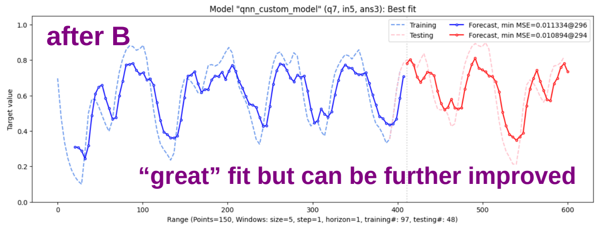










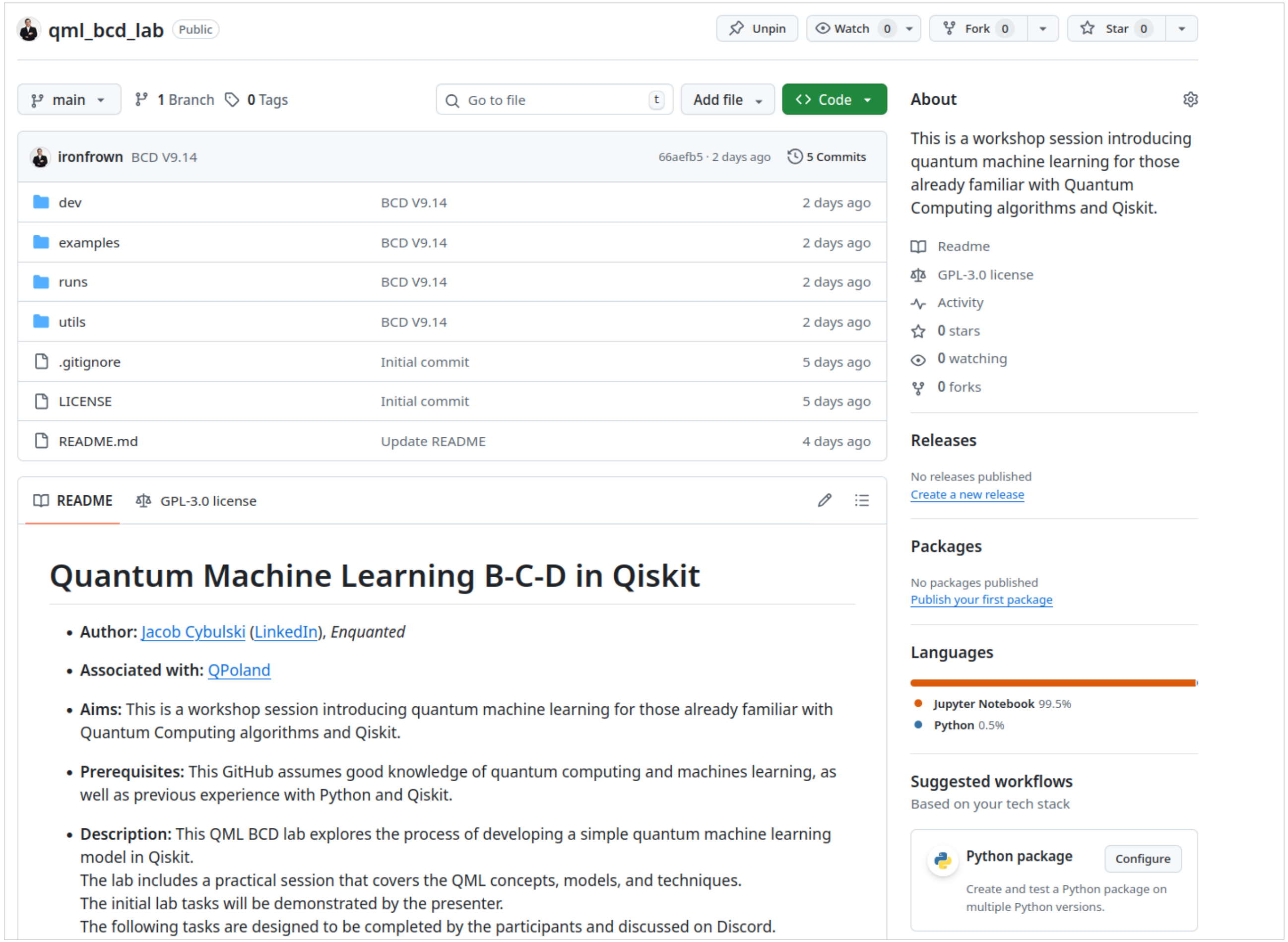


Change: new dataset using the standard and custom QNN model

Often incremental changes result only in small improvements, we may need a drastic change: a model, optimiser or observables

Task: improve a forecasting model for two datasets

Let’s look at the code



qml_bcd_lab Public

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main | 1 Branch | 0 Tags | Go to file | t | Add file | Code

ironfrown BCD V9.14 — 66aefb5 · 2 days ago — 5 Commits

dev	BCD V9.14	2 days ago
examples	BCD V9.14	2 days ago
runs	BCD V9.14	2 days ago
utils	BCD V9.14	2 days ago
.gitignore	Initial commit	5 days ago
LICENSE	Initial commit	5 days ago
README.md	Update README	4 days ago

README | GPL-3.0 license

Quantum Machine Learning B-C-D in Qiskit

- **Author:** Jacob Cybulski (LinkedIn), *Enquanted*
- **Associated with:** QPoland
- **Aims:** This is a workshop session introducing quantum machine learning for those already familiar with Quantum Computing algorithms and Qiskit.
- **Prerequisites:** This GitHub assumes good knowledge of quantum computing and machines learning, as well as previous experience with Python and Qiskit.
- **Description:** This QML BCD lab explores the process of developing a simple quantum machine learning model in Qiskit.
  The lab includes a practical session that covers the QML concepts, models, and techniques.
  The initial lab tasks will be demonstrated by the presenter.
  The following tasks are designed to be completed by the participants and discussed on Discord.

About

This is a workshop session introducing quantum machine learning for those already familiar with Quantum Computing algorithms and Qiskit.

Readme
GPL-3.0 license
Activity
0 stars
0 watching
0 forks

Releases

No releases published
Create a new release

Packages

No packages published
Publish your first package

Languages

Jupyter Notebook 99.5%
Python 0.5%

Suggested workflows

Based on your tech stack

Python package — Configure
Create and test a Python package on multiple Python versions.

Resources for this session, see:
ironfrown (Jacob L. Cybulski, Enquanted)
https://github.com/ironfrown/qml_bcd_lab

Quantum model performance:

Scoring a quantum model (different example)

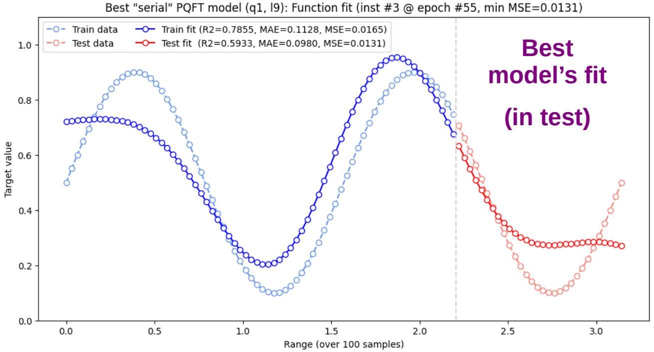
Quantum model training relies on the training data and a loss function to guide the optimiser, e.g. L2Loss (MSE cost), however, other performance metrics may also be needed, e.g. MSE, MAE or R^2, calculated for training, validation and test data.

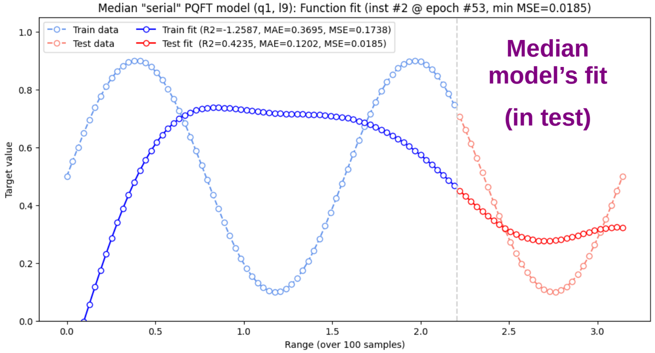
Therefore, at each optimisation step, the model parameters are saved for later use. These parameters values can be assigned to the weights of the model circuit, which can then be scored using all data partitions, against the expected values (figure bottom-left).

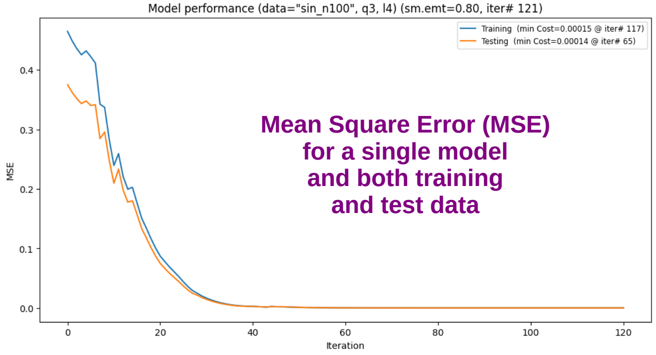
However, as a quantum model performance is highly sensitive to its initialisation, it is also advisable to run multiple, differently initialised, instances of the same model. Subsequently we can analyse a distribution of their performance results, e.g. here we present 5 instances of the same model with identical configurations (figure bottom-middle).

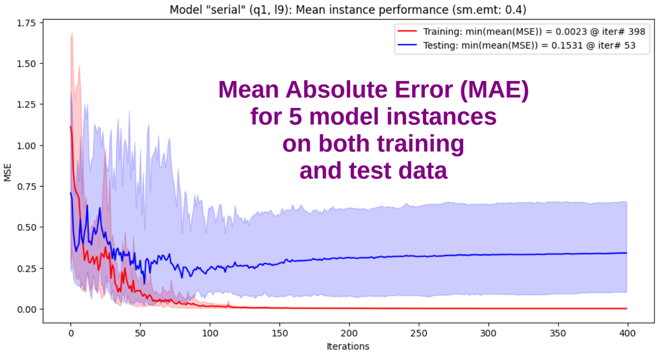
When doing so, it is also possible to present the level of model's fit to data, depending on it best, median or worst instance performance (figures right).

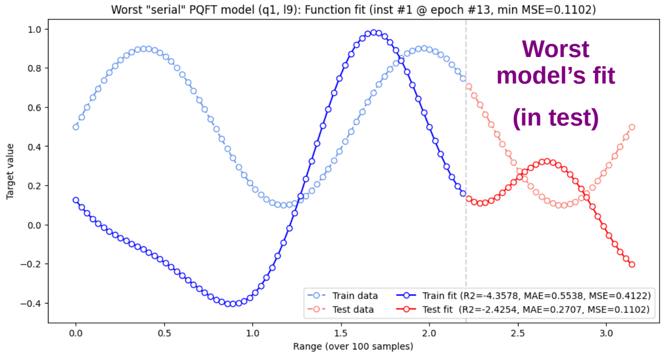
In doing so, our performance assessment can be reported in honest and unbiased way.





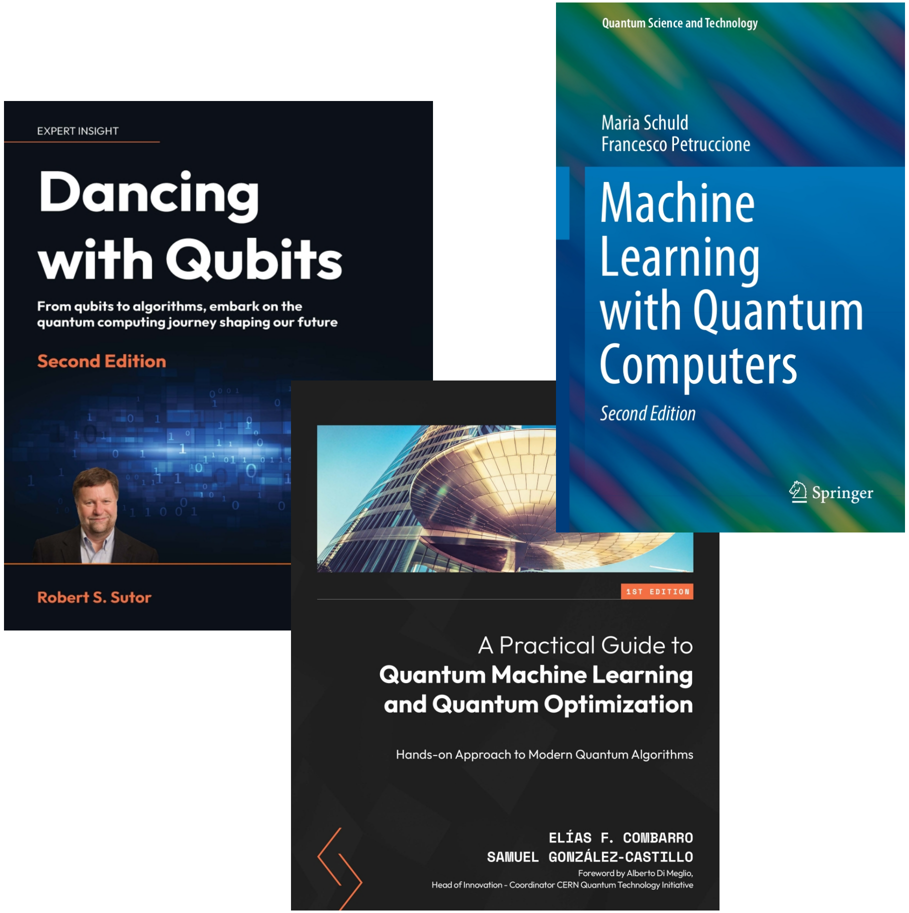






Recommended reading

on QML with Qiskit



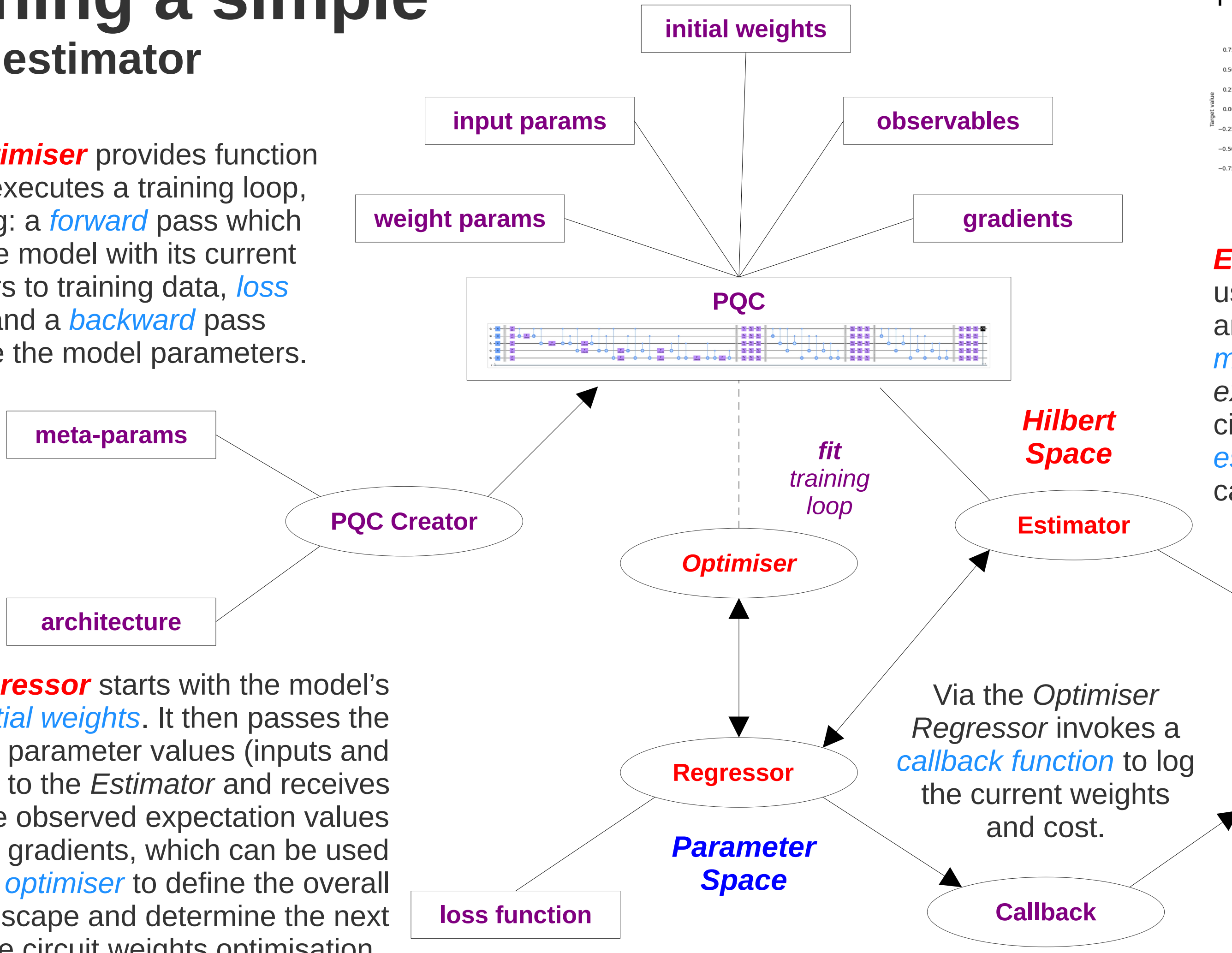
Thank you!

Any questions?

Available resources, see:
ironfrown (Jacob L. Cybulski, Enquanted)
https://github.com/ironfrown/qml_bcd_lab

Training a simple
Qiskit estimator

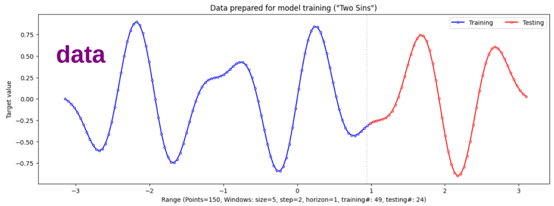
Qiskit ***Optimiser*** provides function ***fit*** which executes a training loop, performing: a *forward* pass which applies the model with its current parameters to training data, *loss function*, and a *backward* pass to improve the model parameters.



Regressor starts with the model's *initial weights*. It then passes the current parameter values (inputs and weights) to the *Estimator* and receives back the observed expectation values and their gradients, which can be used by an *optimiser* to define the overall cost landscape and determine the next step in the circuit weights optimisation.

Via the *Optimiser Regressor* invokes a *callback function* to log the current weights and cost.

Dataset is to be prepared, cleaned and partitioned for training and testing.



Estimator creates the physical circuit using the *observables*, *input parameters* and *weight parameters*, and the *gradient method used in the calculation of expectation values.* It then executes the circuit by relying on a hardware specific *estimator primitive*. It returns the calculated expectation values.

training log

```
Model training started

(00:00:00) - Iter#:   0 / 500, Cost: 0.238564
(00:00:07) - Iter#:  50 / 500, Cost: 0.162685
(00:00:14) - Iter#: 100 / 500, Cost: 0.126066
(00:00:21) - Iter#: 150 / 500, Cost: 0.073866
(00:00:29) - Iter#: 200 / 500, Cost: 0.053152
(00:00:36) - Iter#: 250 / 500, Cost: 0.038513
(00:00:43) - Iter#: 300 / 500, Cost: 0.033054
(00:00:50) - Iter#: 350 / 500, Cost: 0.029146
(00:00:58) - Iter#: 400 / 500, Cost: 0.027865
(00:01:05) - Iter#: 450 / 500, Cost: 0.026759

Total time 00:01:12, min Cost=0.026013
```