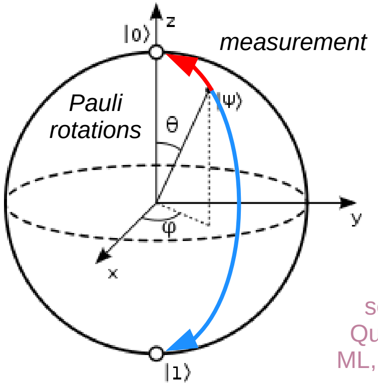
Secrets revealed in this session:

*To explore the practical aspects of 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*
*QML readings*
*Qiskit demo and tasks (TS curve fitting)*
*Summary and Q&A*

# Quantum Algorithms and Data Encoding for QML with Qiskit


**Jacob L. Cybulski**
*Enquanted, Australia*

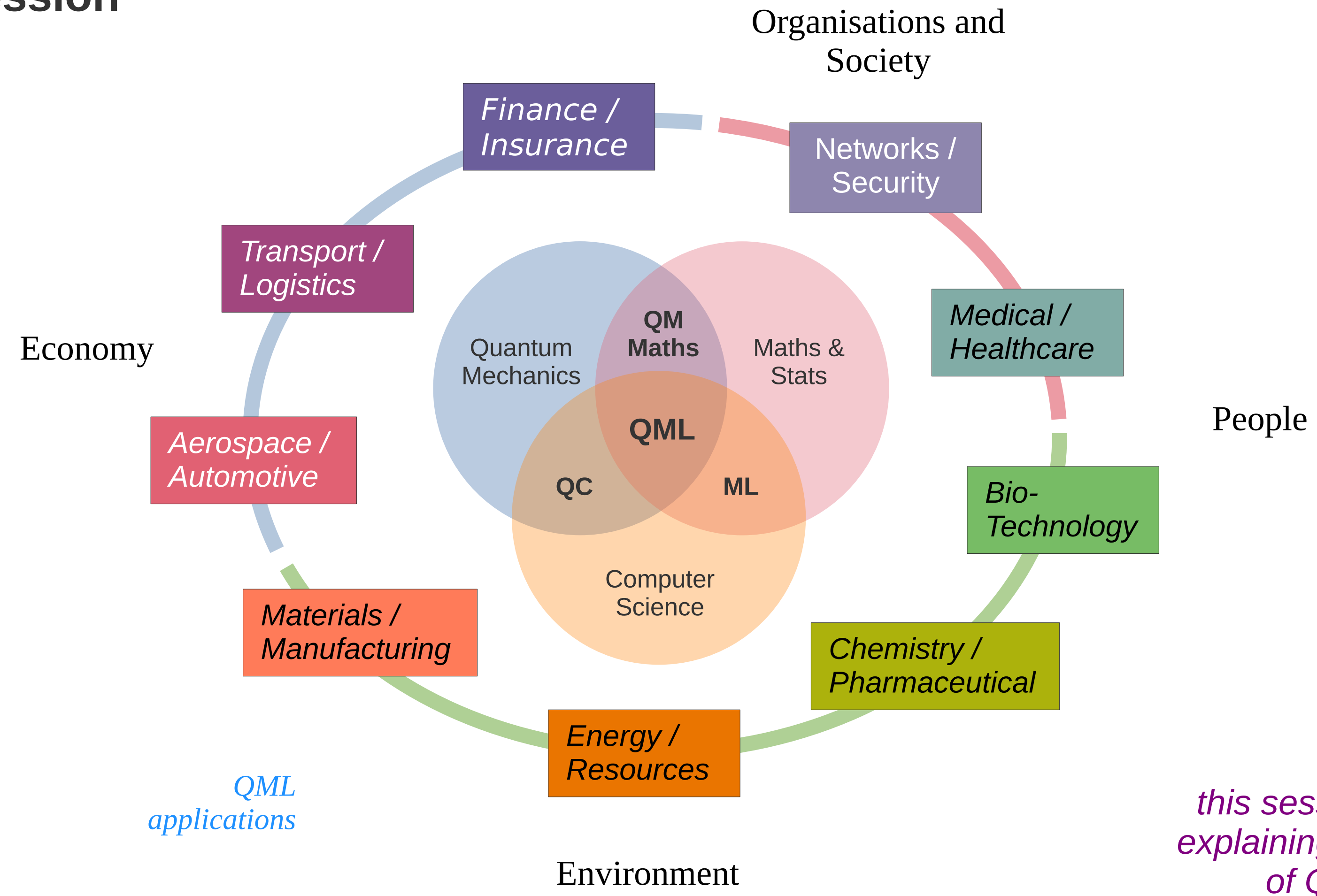

We will assume some knowledge of Quantum Computing ML, Qiskit and Python


*August 9-10 and 23-24, 2025, Qbronze-167 Workshop, Qindia / QWorld*

# Quantum ML

## aims of this session

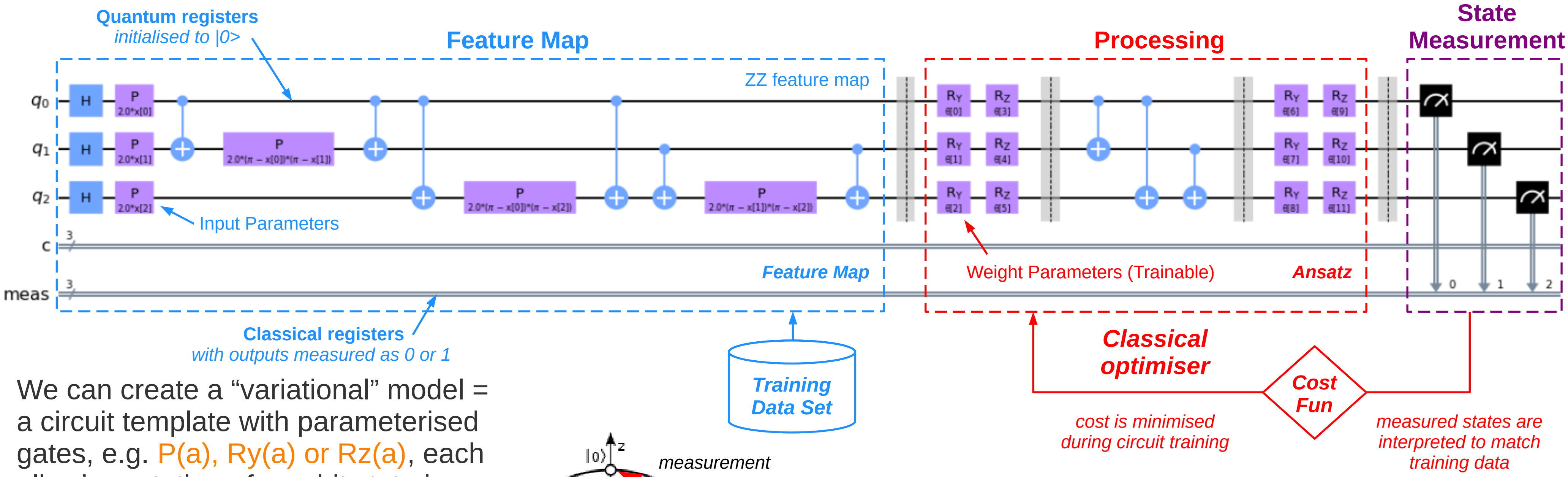
**Jacob Cybulski**, Founder
Enquanted, Australia




*this session aims at explaining the nature of QML models*

# Variational Quantum Circuits
## *and Variational Quantum Algorithms*

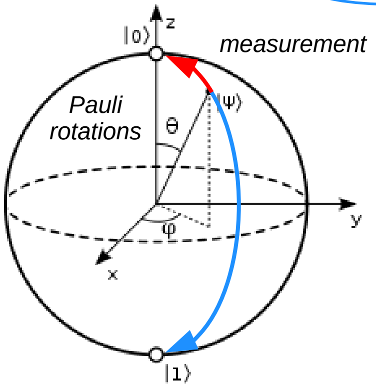
*Variational quantum circuits are not executable!*
*They must first be instantiated, i.e. all of their*
*input and weight parameters must be assigned values!*




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), the circuit consists of three blocks:

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

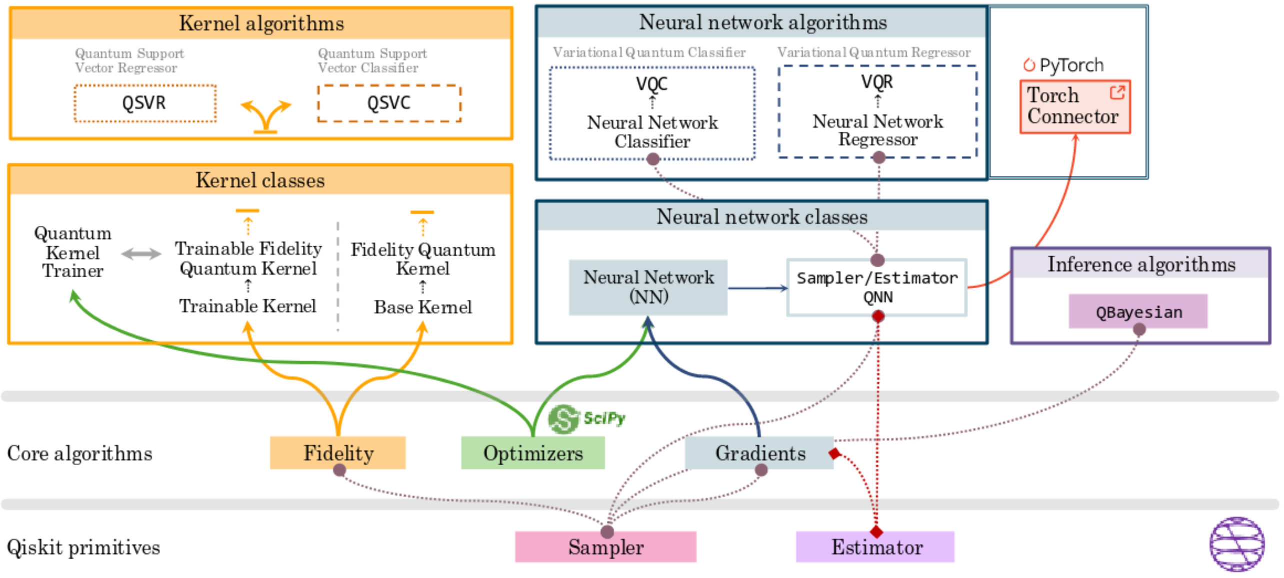



Classical input data is encoded into the feature map's parameters, setting the model's initial quantum state.

The quantum state is 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.

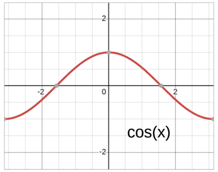
The rotation operators are always available in a quantum platform API, e.g. *Rx*, *Ry*, *Rz*, *P* or *U* (*xyz*).

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

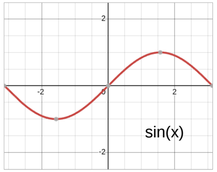
Rotations are *relative to a specific qubit state*, commonly starting at |0⟩ state, or (|0⟩+|1⟩)/sqrt(2), which require qubits to be initialised in these states.

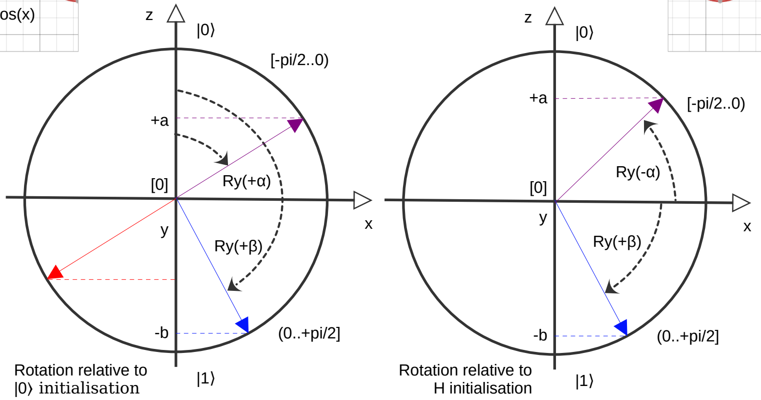
The encoded value could be represented either by the *angular rotation*, or the *amplitude* of the qubit projective measurement (Z).

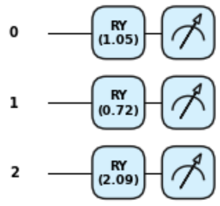
Input data can also be repeatedly encoded and spread around the circuit, which is called *data reuploading*, and which is known to improve the model performance.

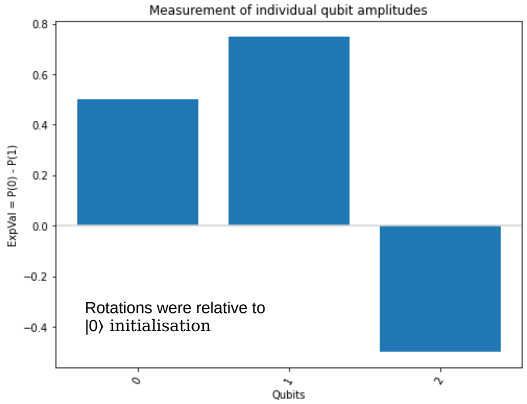



*Note that training will place qubit states in areas x < 0 and arbitrarily around the z axis. Measurements of such states cannot distinguish them from "pure" x > 0 and z = 0.*




**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.

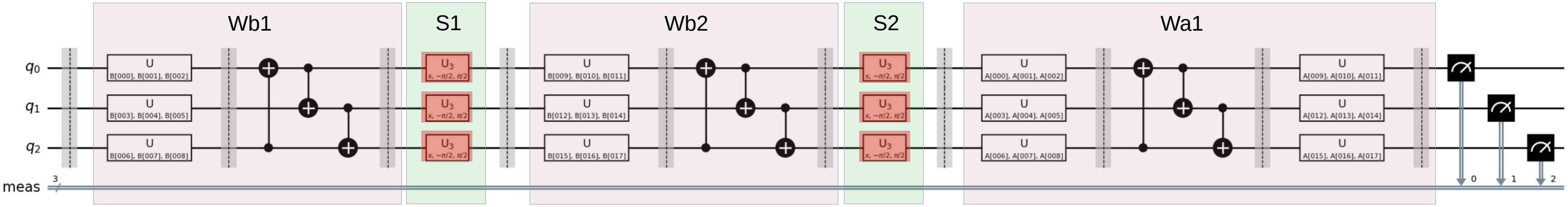
# Ansatz design and training

## 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*

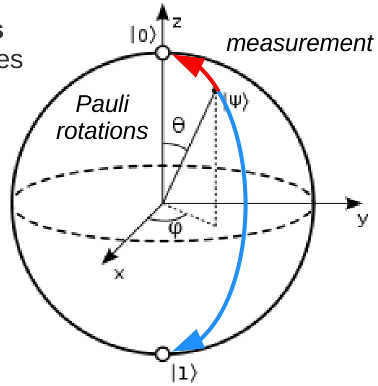
**feature maps vary in:**
structure and function (!!!)

**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.

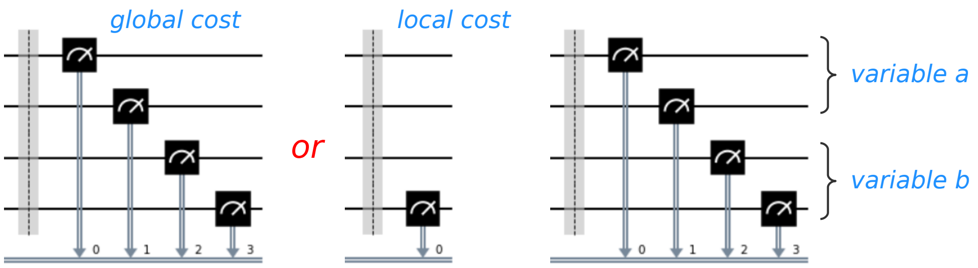
- all qubits (global cost / measurement)
- a few selected qubits (local cost / measurement)
- groups of qubits (each as a variable value)

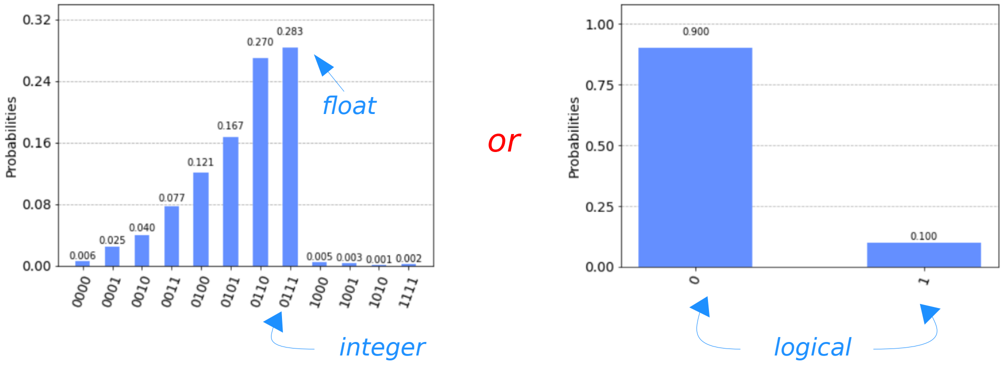
And received in many different formats, e.g.

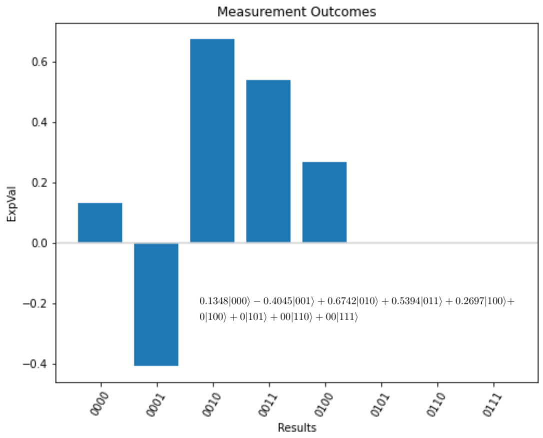
- as counts of outcomes (repeated measurements)
- as probabilities of outcomes (e.g. P(|0111⟩))
- as Pauli expectation values (i.e. of eigenvalues)
- as expectation of interpreted values (e.g. 0 to 15)
- as variance, etc.

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!**

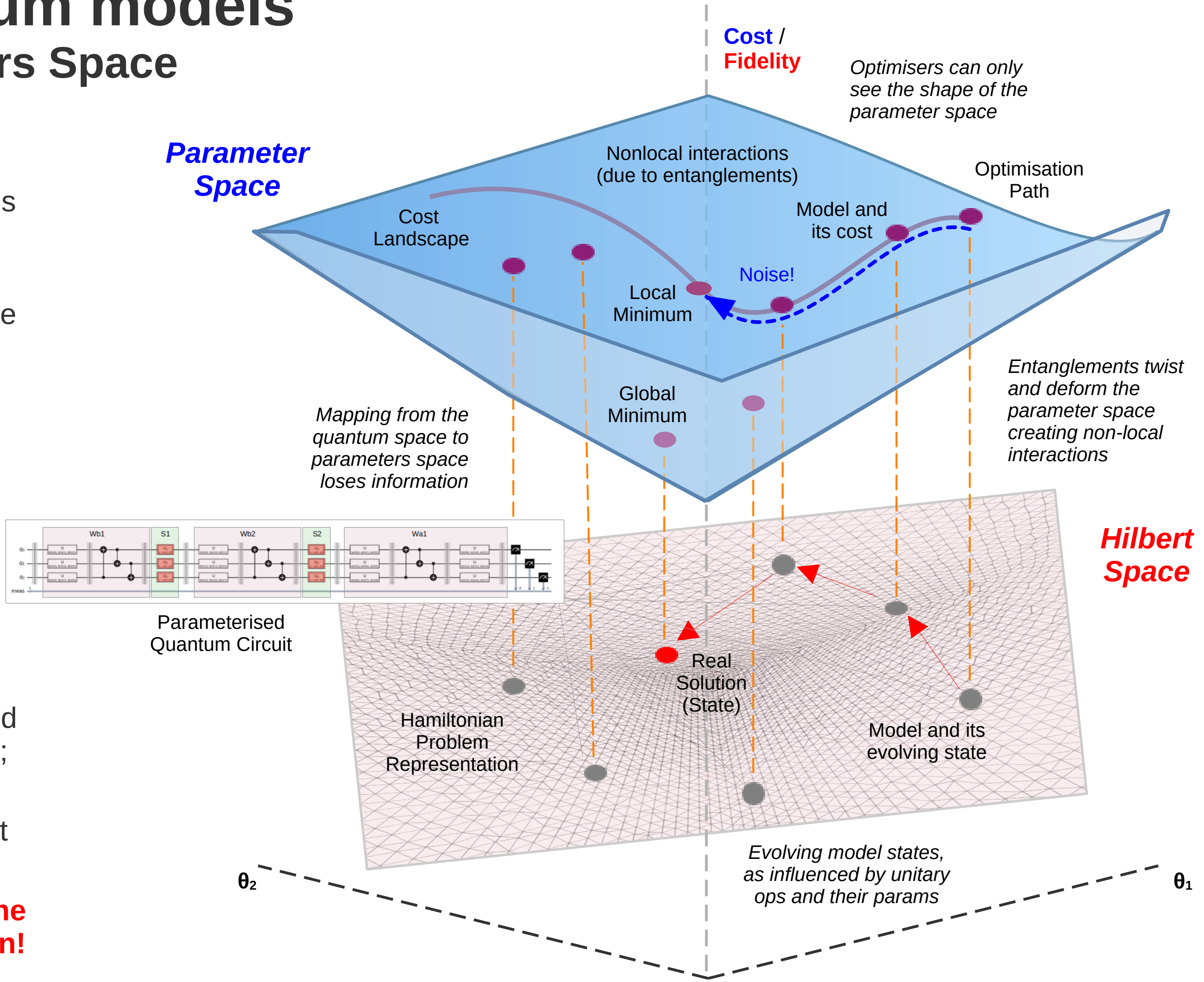
So... having ***n*** measurements leads to ***2**^n^* outcomes

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

# Working with quantum models

## Hilbert Space vs Parameters Space

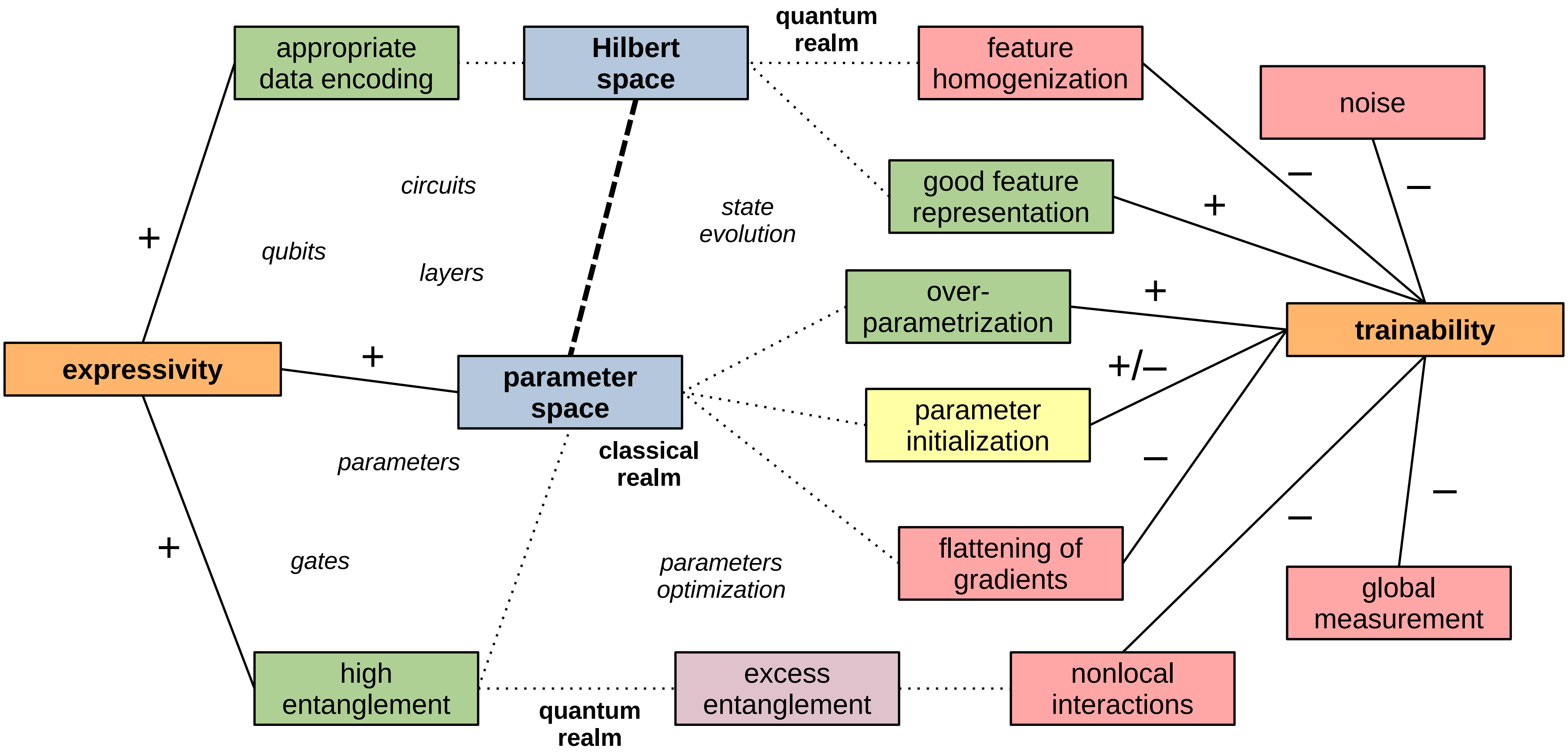
- **Hilbert state space** (dim = the number of qubits) is the quantum realm where the models and their states evolve in response to unitary operations as defined by the circuit gates;
- **Data encoding** brings in classical data into the Hilbert space as unique and correlated quantum states during the model execution;
- **Layers of circuit gates** determine the evolution of the quantum model's initial state into its final state;
- **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!**



# Expressivity vs. Trainability

**Model expressivity:** ability to effectively represent time series data in quantum space.

**Model trainability:** capacity to learn and generalise for predictive accuracy and efficiency in the process of model optimisation.




Jacob L. Cybulski and Sebastian Zajac. “Quantum Modelling of Time Series: Expressivity vs. Trainability”, 20 August 2025, Preprint (Version 1) available at Research Square [https://doi.org/10.21203/rs.3.rs-7253212/v1].

# 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 curve fitting):

- Add ML 0.8.3 package to Qiskit 1.4.4 (Python 3.11)
- Create a few simple models to fit samples of data
- Learn to initialise model weights
- Learn the interaction b|n data encoding and ansatz
- Understand how observables / measurements work
- Explore the impact of ansatz structure on performance
- **Challenge:** Apply your skills to complex data
- **Reflection:** Refine your QML development process

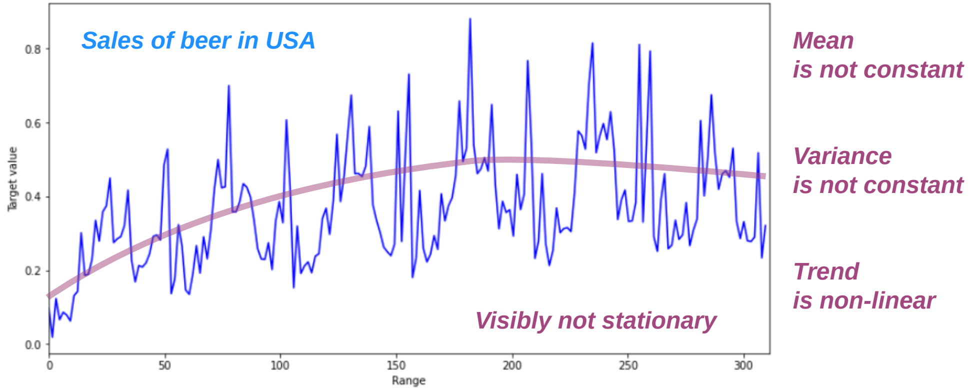
## Key takeaways:

- Plan model development, tests and experiments
- More params and entanglements improve *expressivity*
- Data reuploading makes a huge difference!
- More width / depth / params reduce *trainability* = *the curse of dimensionality*
- More entanglements reduce *trainability*
- High dimensional param space upsets even non-gradient optimisers due to *model sparsity*
- Bad data encoding spoils the bunch!
- Carefully consider your quantum model initialisation
- Surprise - a single qubit model still works! (and well)
- More training often does not eliminate problems!

# QML for time series analysis

## Quantum time series analysis is hard!

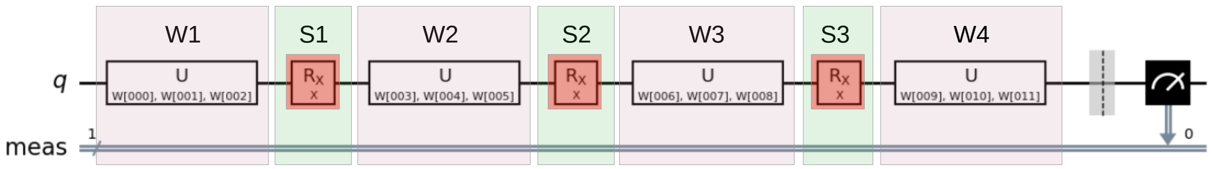
- Time series (TS) analysis aims to *identify patterns* in historical time data and to *create forecasts* of what data is likely to be collected in the future
- *Many TS applications*, including heart monitoring, weather forecasts, machine condition monitoring, etc.
- Time series can be *univariate*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



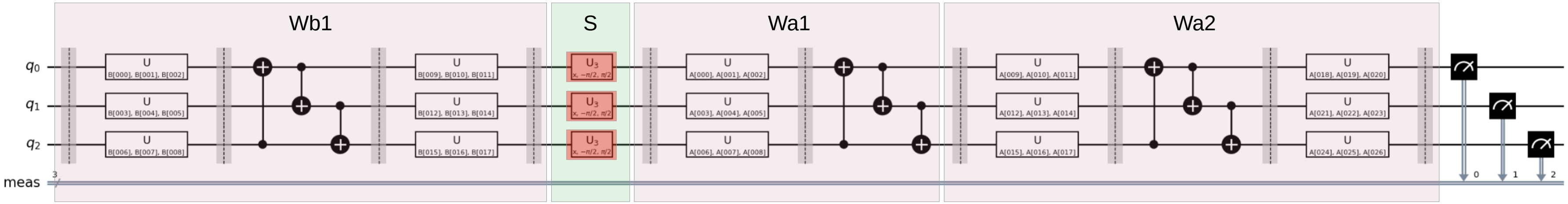

- TS values are dependent on the preceding values!
- Distinction between consecutive TS values is small!
- There are several different types of TS models, e.g.
  - The first group are *curve-fitting models*, which are trained to fit a function to a sample of data points, to predict data values at specific 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!

# Curve-fitting models

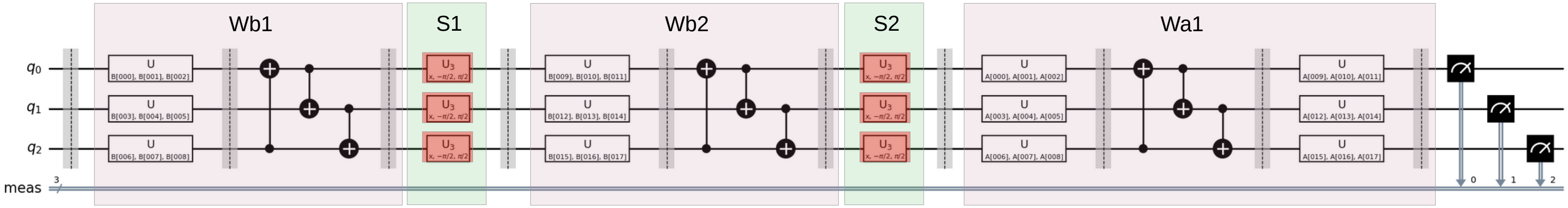
Serial



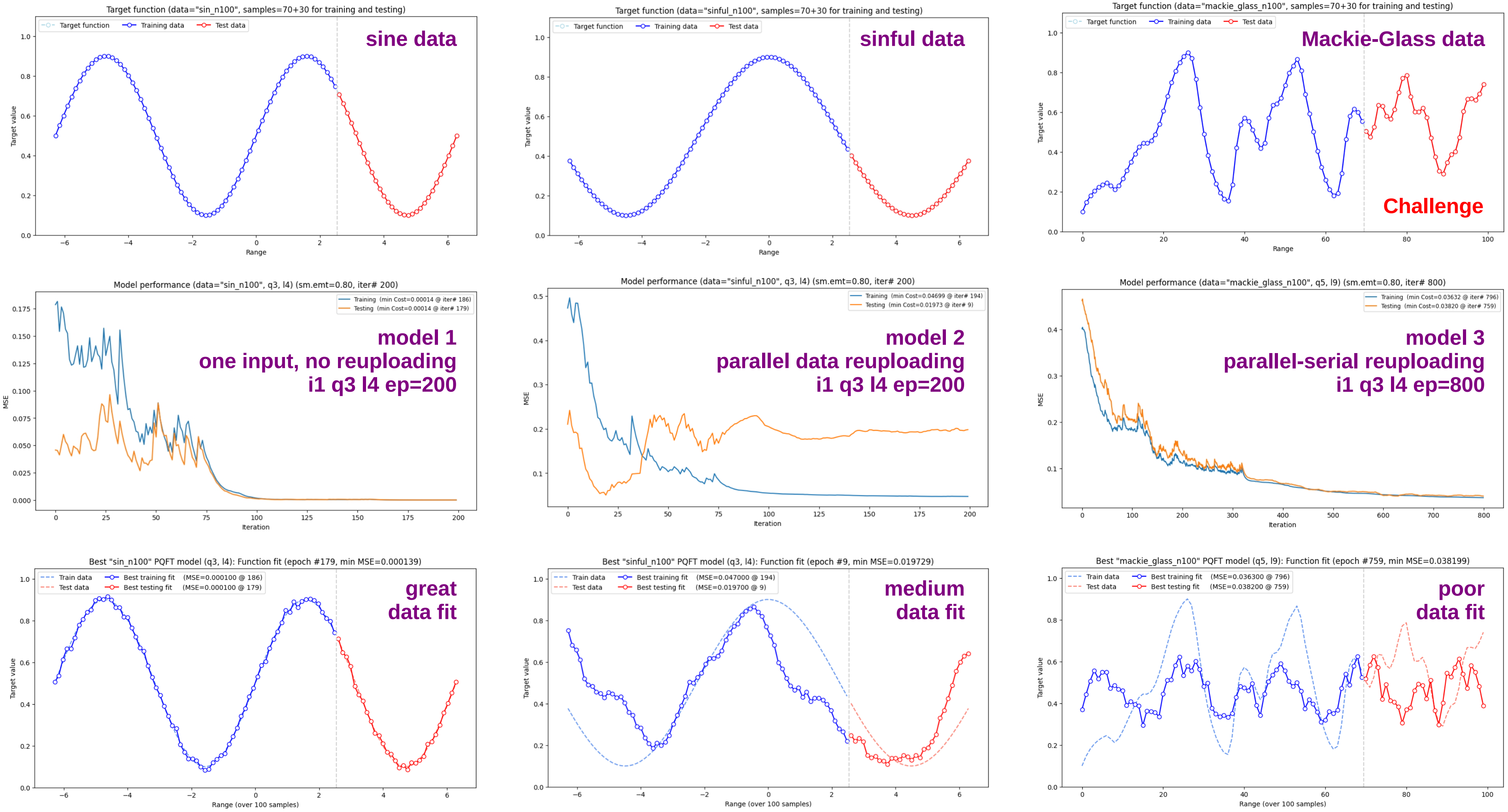

Parallel




Parallel-Serial

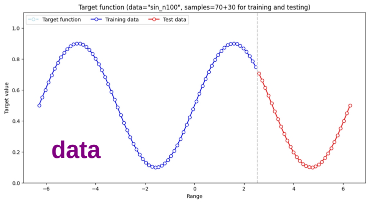


# Data and some results




**Approach to quantum TS modelling is data dependent!**

# Qiskit
## circuit creation




*Sample data needs to be prepared, cleaned and split into training and test partitions.*

```
##### Model 1 - Single input
def qnn_model_1(qubits_no, layers_no, add_meas=False):
    qr = QuantumRegister(qubits_no, 'q')
    ansatz = QuantumCircuit(qr, name="ansatz")
    param_x = Parameter('X')
    ansatz.rx(param_x, 0)

    for l in range(layers_no):
        ansatz.barrier()
        for q in range(qubits_no):
            ansatz.rx(Parameter(f'P{l:02d}_A{q:02d}'), q)
            ansatz.ry(Parameter(f'P{l:02d}_B{q:02d}'), q)
            ansatz.rz(Parameter(f'P{l:02d}_C{q:02d}'), q)
        for q in range(qubits_no-1):
            ansatz.cx(q, q+1)
        if qubits_no > 1:
            ansatz.cx(qubits_no-1, 0)
    if add_meas:
        ansatz.measure_all()
    return ansatz
```

**define a quantum model** 1

```
##### Model settings for models with 1 input

inputs_no = 1          # Number of inputs
qubits_no = 3          # Number of qubits
layers_no = 4          # Number of layers
epochs = 200           # Tra
shots = 1000           # Ig
print_fract = 0.1      # Fr
weights_scaler = 1.00 # Sc
```

**and its meta-params** 2

**Here we present a simple curve-fitting quantum model developed in Qiskit.**

The model's architecture consists of a feature map of a single Rx gate and several layers (4), each layer providing trainable parameters (Rx, Ry, Rz) spanning all qubits (3 x 3), as well as, an entangling block of CNOT gates arranged in a circular fashion (3).

The following code illustrates model creation and its preparation for training:

- [1] Function creating parameterised model circuit (inputs_no, qubits_no, layers_no).
- [2] Meta-parameters defining the model and its training (epochs, shots, weight_scaler).
- [3] Selection of the model function, loss function and optimiser.
- [4] Creation of the circuit and a vector of initial weight values.

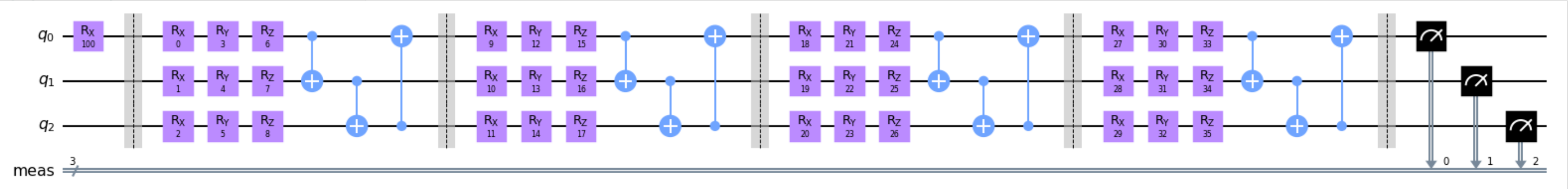
**Qiskit**

```
mfun = qnn_model_1
loss_fun = L2Loss()
optimizer = COBYLA(maxiter=epochs)
```

**Select model, loss function and optimiser** 3

```
### Create and initialise a quantum model
model = mfun(qubits_no, layers_no)
init_weights = weights_scaler * 2 * np.pi * \
    algorithm_globals.random.random(model.num_parameters-inputs_no)
```

**create model circuit calculate initial weights** 4




**model circuit**

# Training a simple

## Qiskit estimator

```
### Define a QNN estimator

obs = SparsePauliOp.from_list([("Z" * model.num_qubits, 1)])
estimator = StatevectorEstimator(seed=seed)
regr_qnn = EstimatorQNN(
    circuit=model,
    input_params=[model.parameters[-inputs_no]],
    weight_params=model.parameters[:-inputs_no],
    observables=obs,
    estimator=estimator,
    gradient=ParamShiftEstimatorGradient(estimator),
)
```

5

estimator

```
### Define and fit regressor

regr_callback = create_callback(epochs, print_fract=print_fract)

regressor = NeuralNetworkRegressor(
    neural_network=regr_qnn,
    loss=loss_fun,
    optimizer=optimizer,
    initial_point=init_weights,
    callback=regr_callback
)
```

regressor

6

```
### Select the loss function (here, MSE cost)
loss_fun = L2Loss()

### Select the optimiser (here, non-gradient based)
optimizer = COBYLA(maxiter=epochs)
```

```
regressor.fit(X_train, y_train)
```

training loop

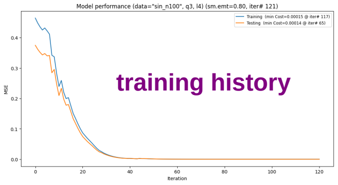
7

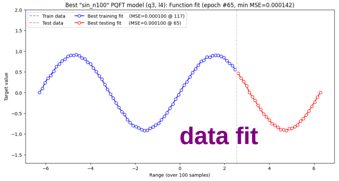
training log

```
Model training started

(00:00:00) - Iter#:   0 / 200, Cost: 0.178608
(00:00:01) - Iter#:  20 / 200, Cost: 0.176996
(00:00:02) - Iter#:  40 / 200, Cost: 0.028761
(00:00:03) - Iter#:  60 / 200, Cost: 0.008521
(00:00:05) - Iter#:  80 / 200, Cost: 0.004425
(00:00:06) - Iter#: 100 / 200, Cost: 0.001005
(00:00:07) - Iter#: 120 / 200, Cost: 0.000322
(00:00:09) - Iter#: 140 / 200, Cost: 0.000784
(00:00:10) - Iter#: 160 / 200, Cost: 0.000176
(00:00:11) - Iter#: 180 / 200, Cost: 0.000145

Total time 00:00:12, min Cost=0.000144
```




In Qiskit it is possible to create variety of different quantum models.

Here we build a circuit using a Qiskit state vector estimator and a QNN regressor.

callback function

8

```
##### Callback function use to collect training data

objfun_vals = []   # To store objective function values
params_vals = []   # To store parameter values

def create_callback(epochs, print_fract=0.1):

    global objfun_vals, params_vals
    objfun_vals = []
    params_vals = []
    elapsed = 0
    start_time = time.time()

    def callback_func(weights, obj_func_eval):
        nonlocal epochs, print_fract, start_time, elapsed
        global objfun_vals, params_vals

        iters = len(objfun_vals)
        objfun_vals.append(obj_func_eval)
        params_vals.append(weights)
        elapsed = time.time() - start_time
        time_str = time.strftime("%H:%M:%S", time.gmtime(elapsed))
        if (print_fract == 0) or (iters % int(print_fract*epochs) == 0):
            print(f"({time_str}) - Iter#: {iters:3d} / {epochs:3d}, "+\
                  f"Cost: {obj_func_eval:.6f}")

    return callback_func
```

***Estimator*** [5] which computes the the *circuit* expectation values, with respect to given *observables*, and considering the circuit's *input parameters* and *weight parameters*, a *gradient method*, and an *estimator primitive* (hardware specific)

***Regressor*** [6] which predicts continuous values using an *optimiser*, a *loss function*, and the model *initial parameters*. We can access, save and print or plot, all intermediate optimisation steps via a *callback function* [8].

Qiskit ML provides a utility *function "fit"* which executes a ***training loop*** [7], folding into one: a *forward* pass which applies the model with its current parameters to training data, *cost calculation*, and a *backward* pass to improve the model parameters.

# Quantum model performance:

## Scoring your quantum model

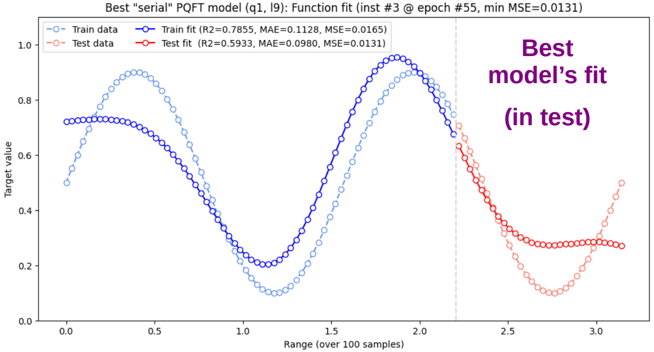
Quantum model training relies on the training data and a loss function to guide the optimiser, e.g. L2Loss (MSE cost), however, other performance metrics may also be needed, e.g. MSE, MAE or $R^2$, calculated for training, validation and test data.

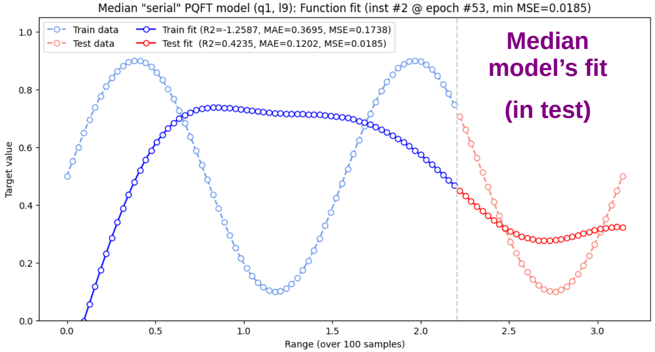
Therefore, at each optimisation step, the model parameters are saved for later use. These parameters values can be assigned to the weights of the model circuit, which can then be scored using all data partitions, against the expected values (figure bottom-left).

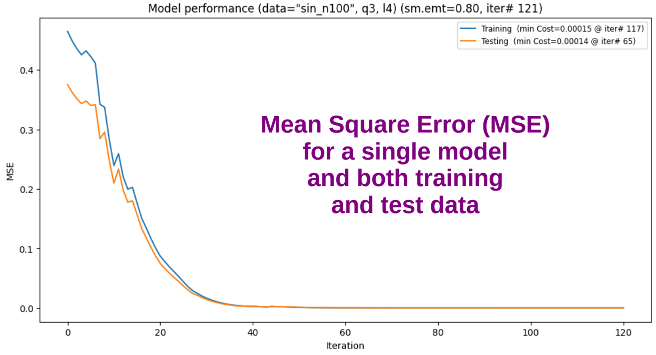
However, as a quantum model performance is highly sensitive to its initialisation, it is also advisable to run multiple, differently initialised, instances of the same model. Subsequently we can analyse a distribution of their performance results, e.g. here we present 5 instances of the same model with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

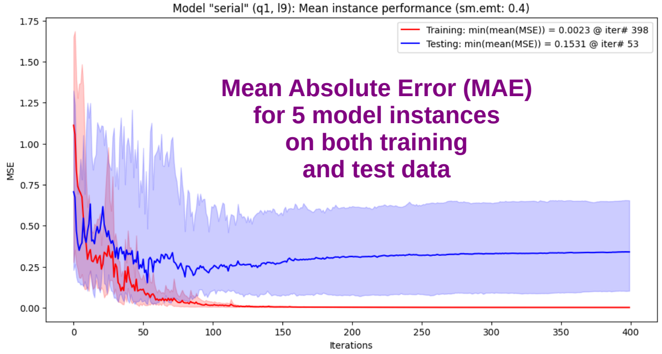
When doing so, it is also possible to present the level of model's fit to data, depending on it best, median or worst instance performance (figures right).

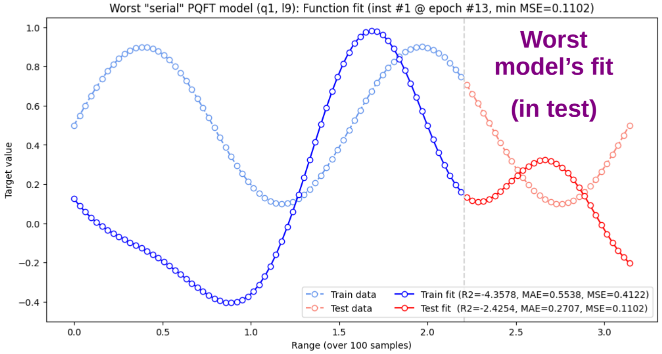
In doing so, our performance assessment can be reported in honest and unbiased way.



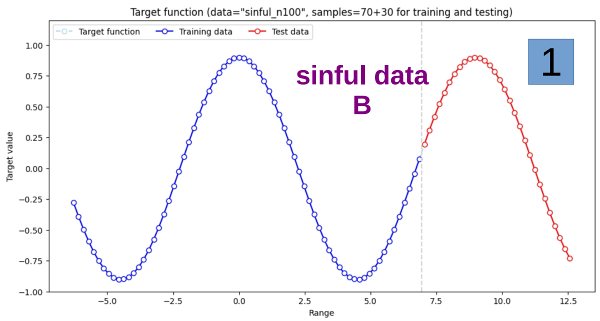



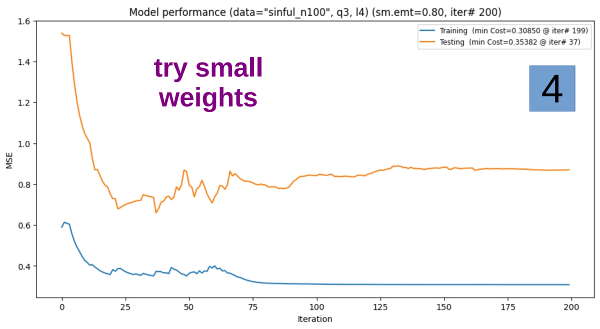



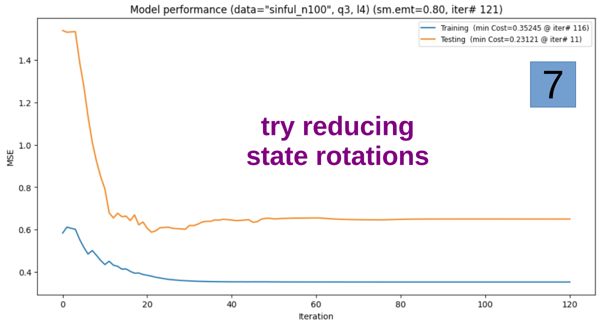



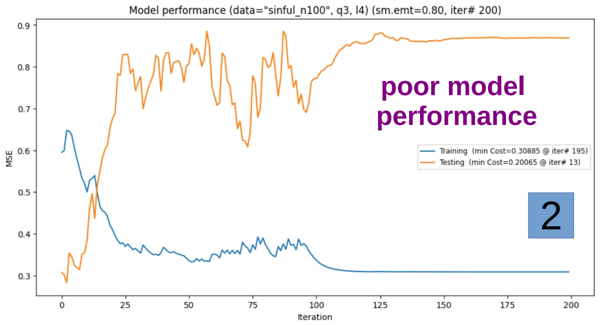



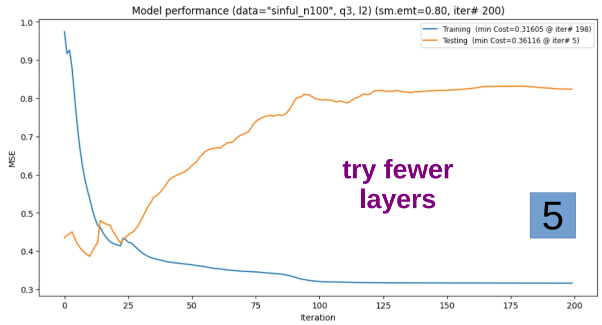
# In search of solution!

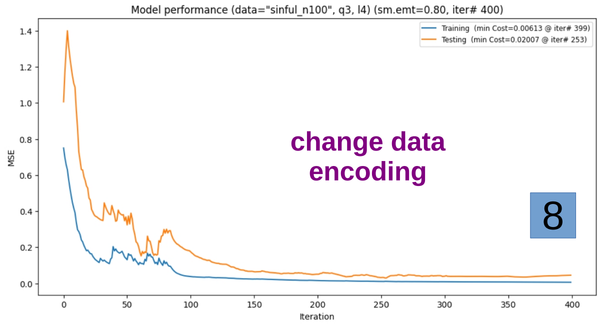


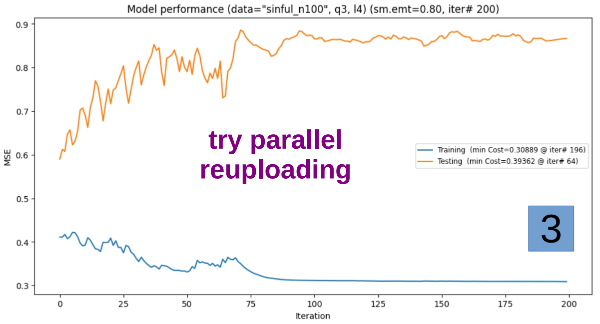



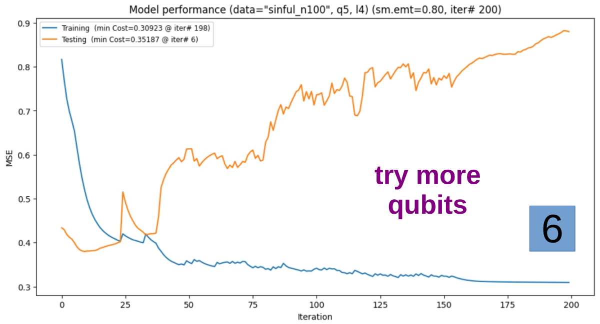



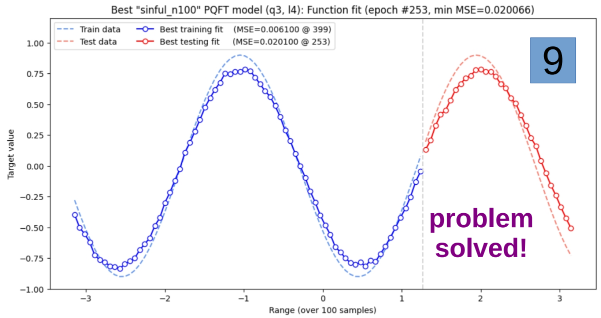



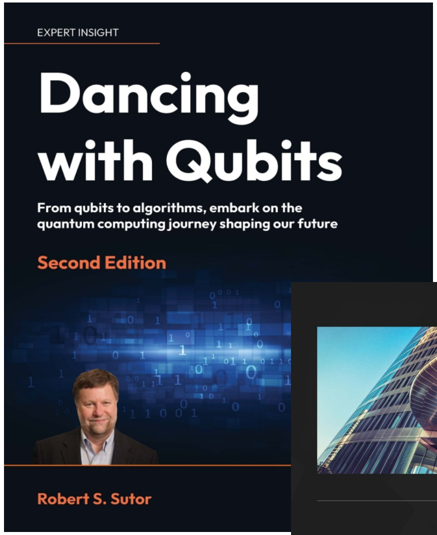



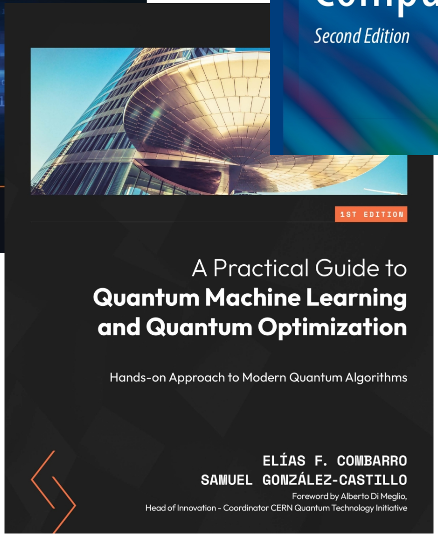



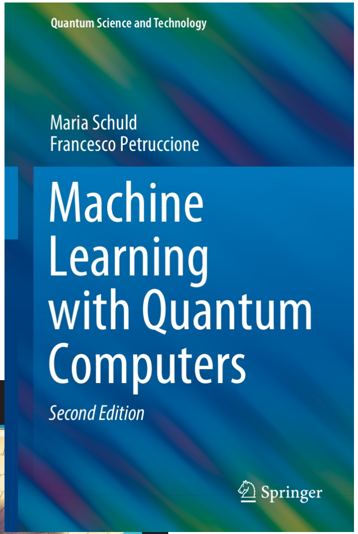

## Task: improve a curve-fitting model for the new dataset

# Recommended reading

## on QML with Qiskit




Quantum computing with Qiskit

Ali Javadi-Abhari,[1] Matthew Treinish,[1] Kevin Krsulich,[1] Christopher J. Wood,[1] Jake Lishman,[2] Julien Gacon,[3] Simon Martiel,[4] Paul D. Nation,[1] Lev S. Bishop,[1] Andrew W. Cross,[1] Blake R. Johnson,[1] and Jay M. Gambetta[1]

[1]IBM Quantum, IBM T. J. Watson Research Center, Yorktown Heights, NY, 10598
[2]IBM Quantum, IBM Research Europe, Hursley, United Kingdom
[3]IBM Quantum, IBM Research Europe, Zürich, Switzerland
[4]IBM Quantum, IBM France Lab, Orsay, France

We describe Qiskit, a software development kit for quantum information science. We discuss the key design decisions that have shaped its development, and examine the software architecture and its core components. We demonstrate an end-to-end workflow for solving a problem in condensed matter physics on a quantum computer that serves to highlight some of Qiskit's capabilities, for example the representation and optimization of circuits at various abstraction levels, its scalability and retargetability to new gates, and the use of quantum-classical computations via dynamic circuits. Lastly, we discuss some of the ecosystem of tools and plugins that extend Qiskit for various tasks, and the future ahead.

[quant-ph] 19 Jun 2024

I. INTRODUCTION

II. DESIGN PHILOSOPHY

We begin by discussing Qiskit's scope within the broader quantum computing software stack, as illustrated in Figure 1. Starting from a computational problem, a quantum algorithm specifies how the problem may be solved with quantum circuits. This step involves translating the classical problem to the quantum domain, for example Fermion to qubit mapping [34, 62]. Circuits at this level can be quite abstract, for example only specifying a set of Pauli rotations, some unitaries, or other high-level mathematical operators. Importantly, these abstract circuits are representable in Qiskit, which contains synthesis methods to generate concrete circuits from them. Such concrete circuits are formed using a standard library of gates, representable using intermediate quantum languages such as OpenQASM [31].

The transpiler rewrites circuits in multiple rounds of passes, in order to optimize and translate it to the target instruction set architecture (ISA). The word "transpiler" is used within Qiskit to emphasize its nature as a circuit-to-circuit rewriting tool, distinct from a full compilation down to controller binaries which is necessary for executing circuits. But the transpiler can also be thought of as an optimizing compiler for quantum programs.

The ISA is the key abstraction layer separating the hardware from the software, and depends heavily on the quantum computer architecture beneath. For example for a physical quantum computer based on superconduct-

Qiskit Machine Learning: an open-source library for quantum machine learning tasks at scale on quantum hardware and classical simulators

M. Emre Sahin,[1] Edoardo Altamura,[1] Oscar Wallis,[1] Stephen P. Wood,[2] Anton Dekusar,[3] Declan A. Millar,[4] Takashi Imamichi,[5] Atsushi Matsuo,[5] Stefano Mensa,[1,*] and Code contributors

[1]The Hartree Centre, STFC, Sci-Tech Daresbury, Warrington, WA4 4AD, United Kingdom
[2]IBM Quantum, IBM T.J. Watson Research Center, Yorktown Heights, NY 10598, USA
[3]IBM Quantum, IBM Research Europe – Dublin, Ireland
[4]IBM Research – UK
[5]IBM Quantum, IBM Research – Tokyo, Tokyo 103-8510, Japan
(Dated: Friday 13th June, 2025)

We present Qiskit Machine Learning (ML), a high-level Python library that combines elements of quantum computing with traditional machine learning. The API abstracts Qiskit's primitives to facilitate interactions with classical simulators and quantum hardware. Qiskit ML started as a proof-of-concept code in 2019 and has since been developed to be a modular, intuitive tool for non-specialist users while allowing extensibility and fine-tuning controls for quantum computational scientists and developers. The library is available as a public, open-source tool and is distributed under the Apache version 2.0 license.

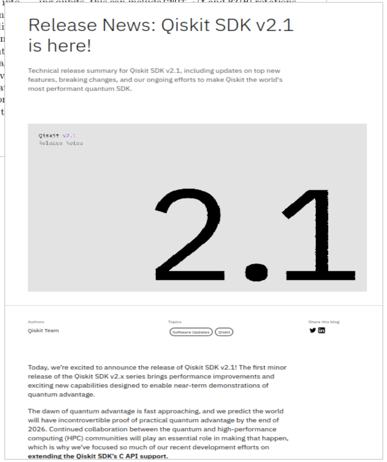
arXiv:2505.17756v1 [quant-ph] 23 May 2025

I. INTRODUCTION

The convergence of quantum computing and machine learning promises a prospective shift in both research and industry. Quantum machine learning (QML) leverages the principles of quantum mechanics to potentially enhance or accelerate classical machine learning algorithms, opening new frontiers in fields ranging from materials science to finance. As the field of QML matures, there is a growing need for accessible and powerful software tools that bridge the gap between theoretical QML algorithms and their practical implementation on emerging quantum hardware and simulators.

II. DESIGN STRUCTURE

[*] stefano.mensa@stfc.ac.uk
[1] github.com/qiskit-community/qiskit-machine-learning



# Thank you!

## Any questions?

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

# 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;
- **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!**