

**Secrets revealed in this session:**

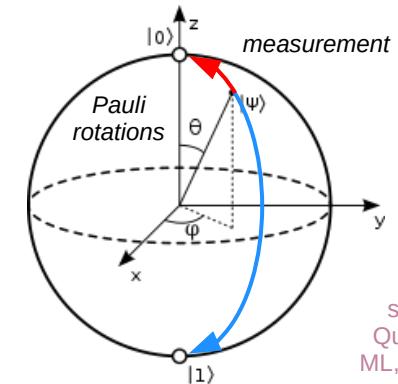
**To explore the practical aspects  
of building quantum machine  
learning models and their  
optimisation**



**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

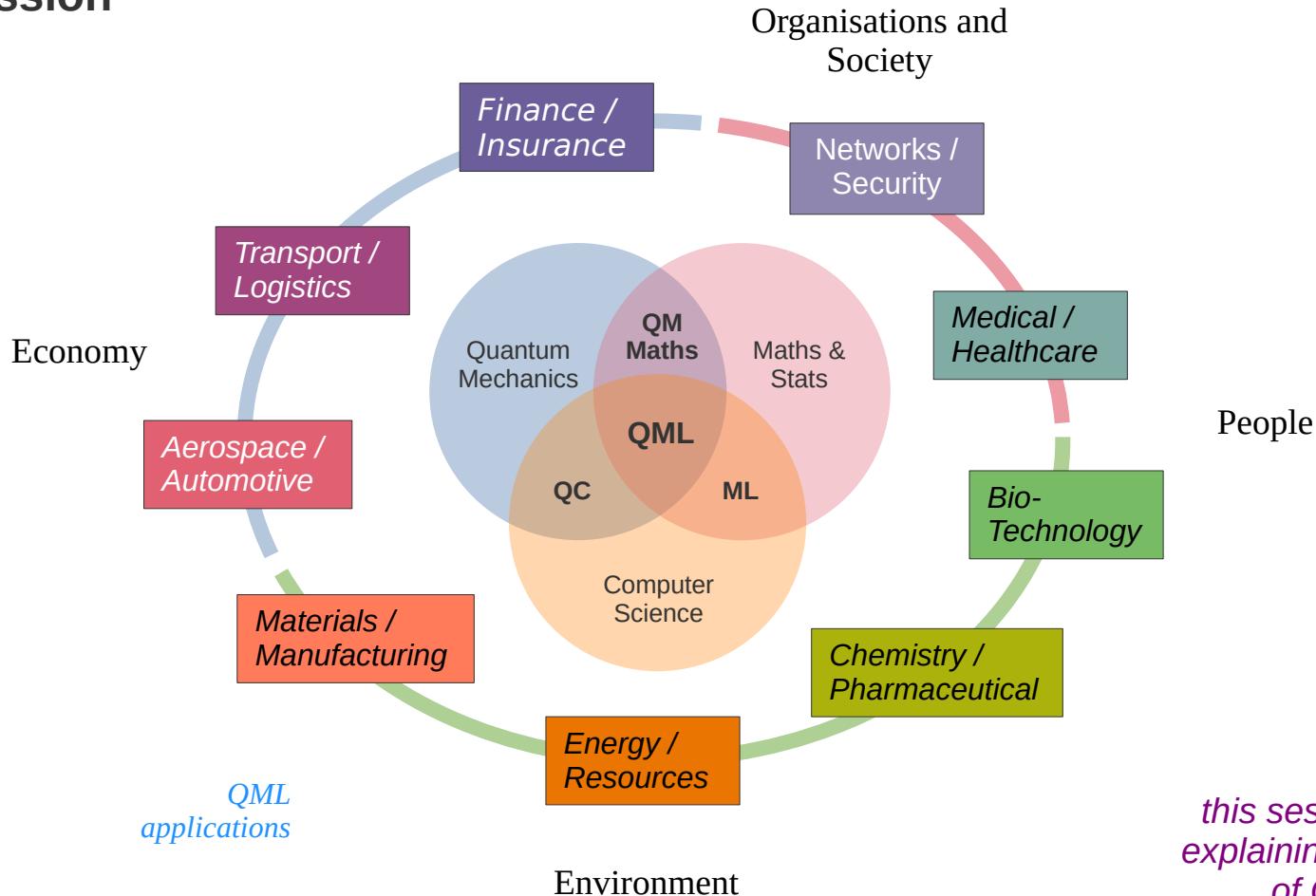
# Quantum ML

## aims of this session

Jacob L. Cybulski, Quantum Business Series (Deakin, RMIT, ACS, Warsaw School of Economics)  
Jacob L. Cybulski, Quantum Computing Intro Series (SheQuantum, Assoc of Polish Profs in Australia)  
2021-2025



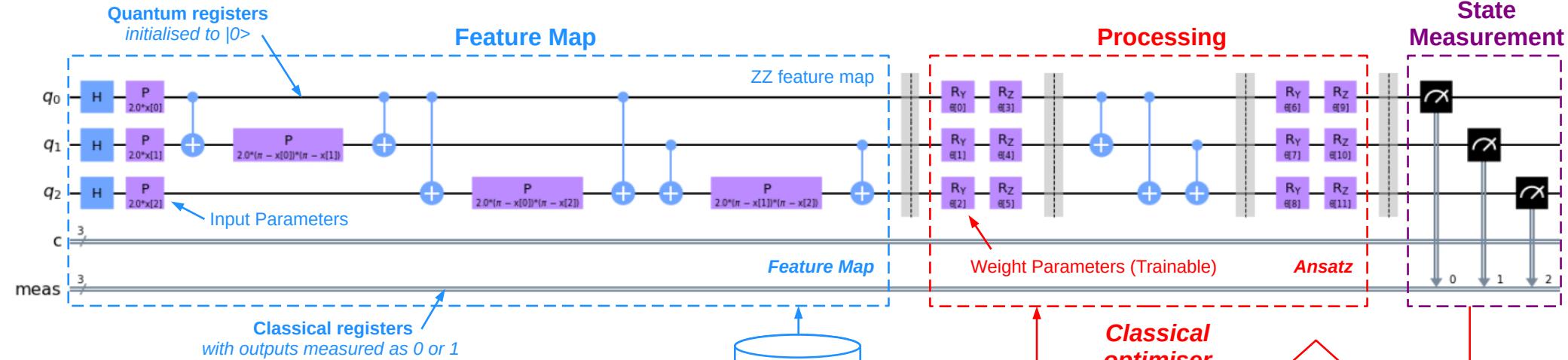
Jacob Cybulski, Founder  
Enquantum, Australia



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

# Variational Quantum Circuits and Variational Quantum Algorithms

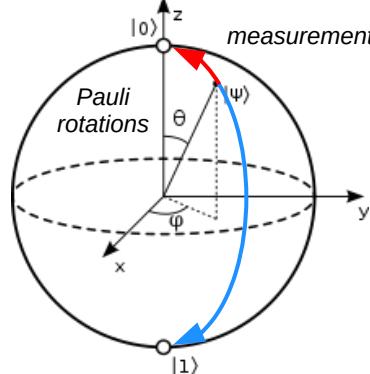
Variational quantum circuits are not executable!  
They must first be instantiated, i.e. all of their input and weight parameters must be assigned values!



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).

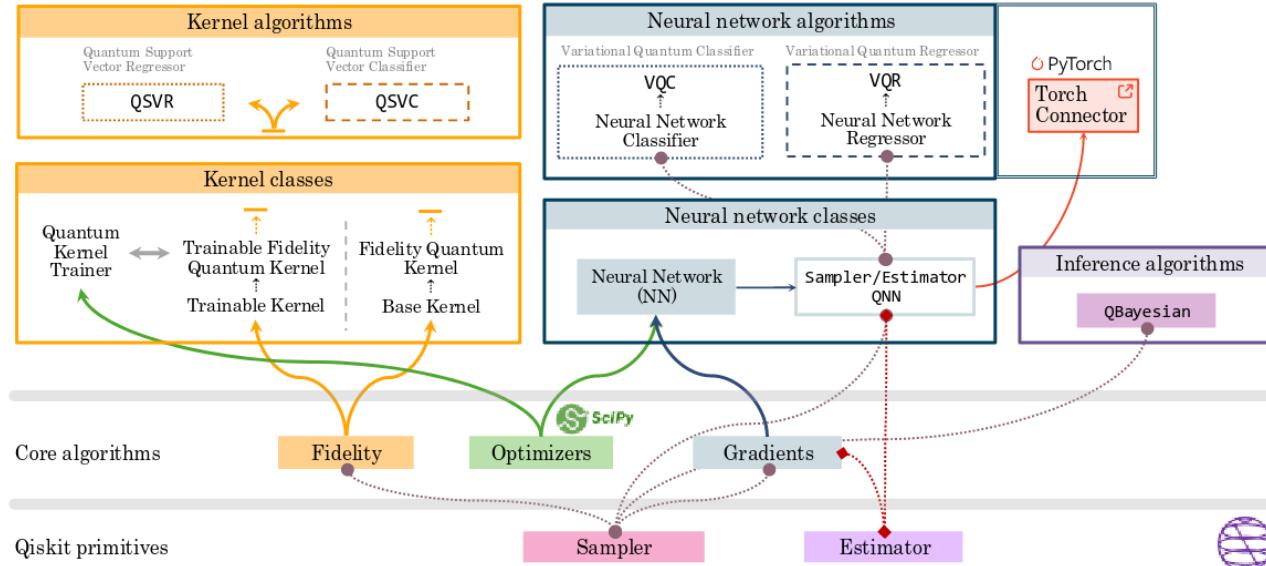
Typically (but now always), the circuit consists of three blocks:

- 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.

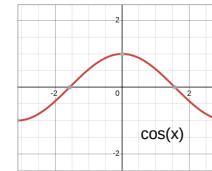
The rotation operators are always available in a quantum platform API, e.g. *Rx*, *Ry*, *Rz*, *P* or *U* (*xyz*).

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

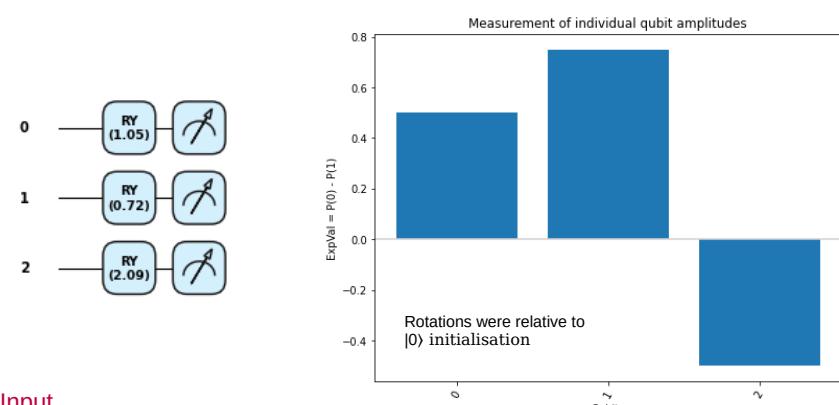
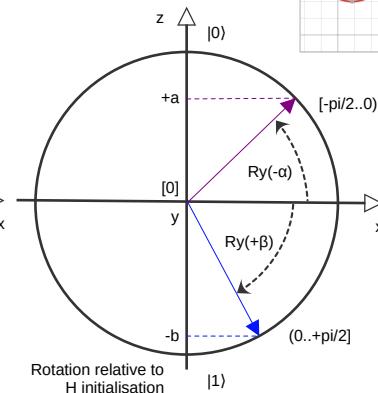
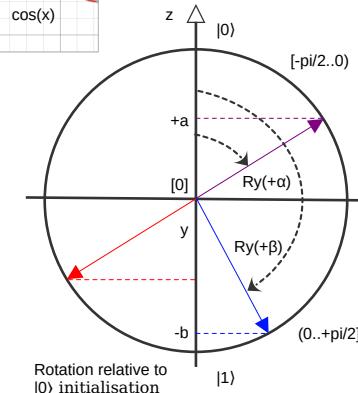
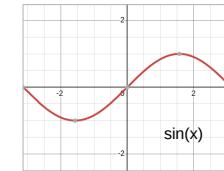
Rotations are *relative to a specific qubit state*, commonly starting at  $|0\rangle$  state, or  $(|0\rangle+|1\rangle)/\sqrt{2}$ , which require qubits to be initialised in these states.

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:  
Ry angles used:  
[ $\text{np.arccos}(0.5)$ ,  $\text{np.arccos}(0.75)$ ,  $\text{np.pi}-\text{np.arccos}(0.5)$ ]  
[1.047, 0.723, 2.094]

### Measurements

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

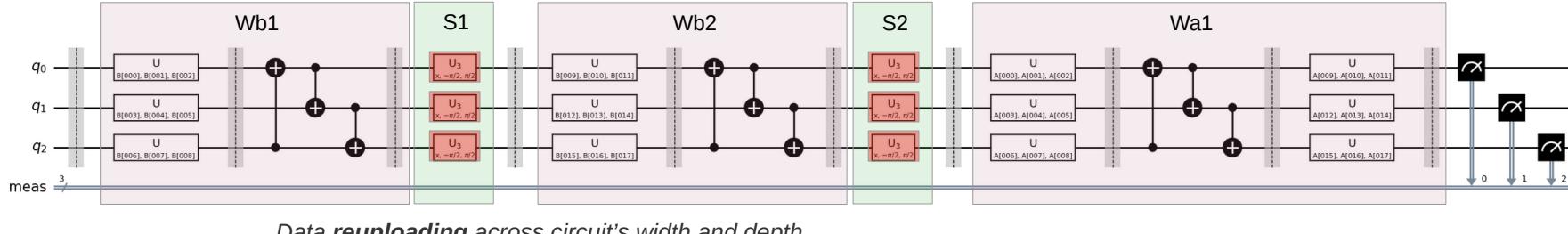
# Ansatz design and training

## 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**!*



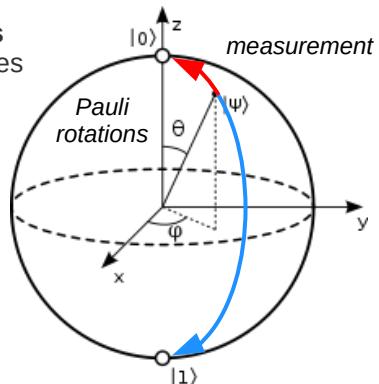
## **feature maps vary in:** structure and function (!!?)

## **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-Leibnner 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 (QPPUs)

# Commonly used measurements and interpretation

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

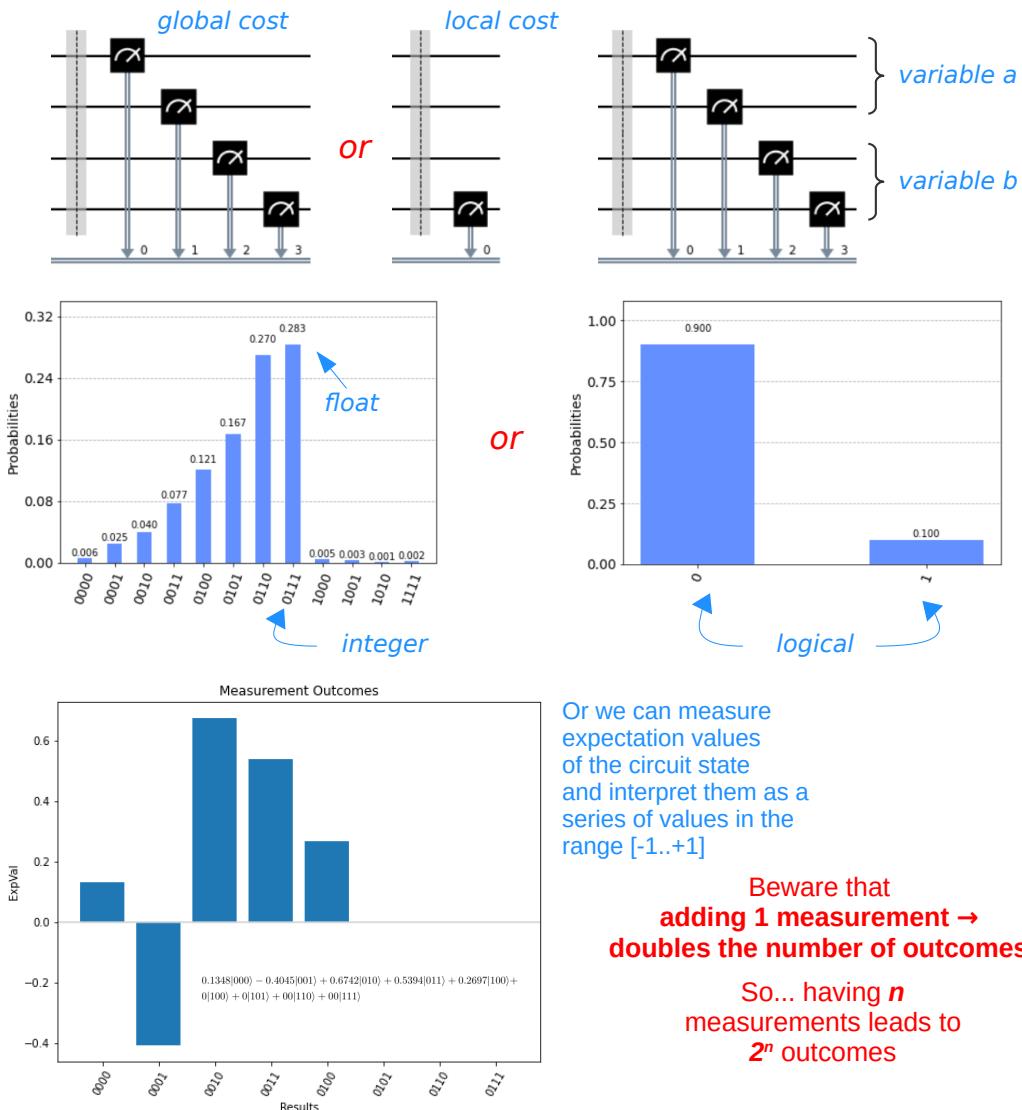
- all qubits (global cost / measurement)
- a few selected qubits (local cost / measurement)
- groups of qubits (each as a variable value)

And received in many different formats, e.g.

- as counts of outcomes (repeated measurements)
- as probabilities of outcomes (e.g.  $P(|0111\rangle)$ )
- 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.

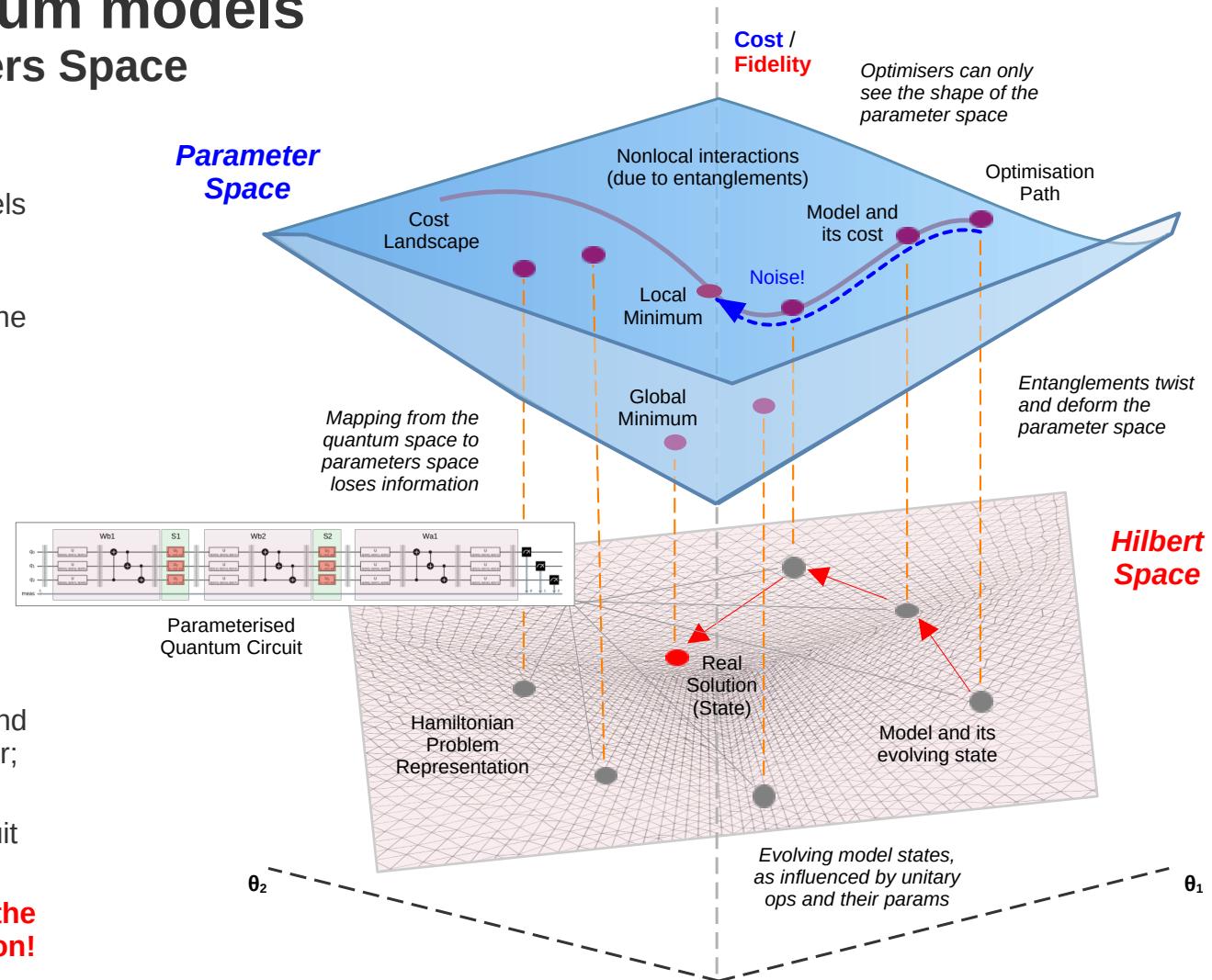
- as a probability distribution (as is)
- as a series of values (via expvals)
- as a binary outcome:  
single qubit measurement or parity of kets
- as an integer:  
most probable ket in multi-qubit measurement
- as a continuous variable:  
probability of the selected ket (e.g.  $|0^n\rangle$ )



# Working with quantum models

## Hilbert Space vs Parameters Space

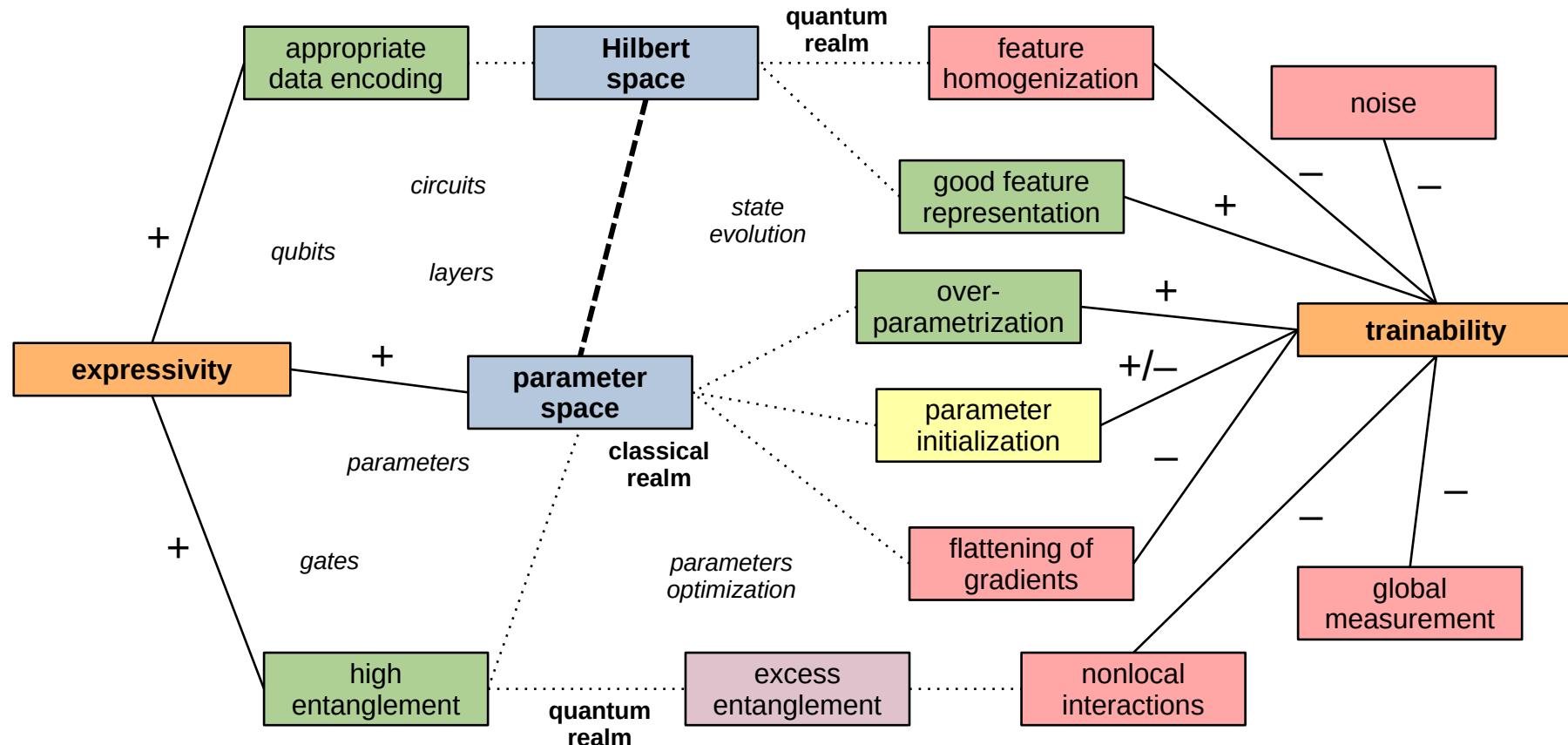
- **Hilbert state space** (dim = the number of qubits) is the quantum realm where the models and their states evolve in response to unitary operations as defined by the circuit gates;
- **Data encoding** brings in classical data into the Hilbert space as unique and correlated quantum states during the 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.



# 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):

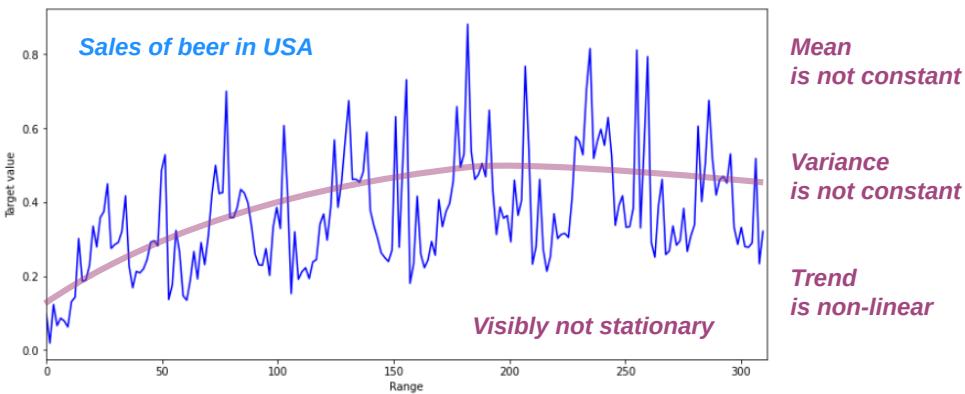
- Add ML 0.8.3 package to Qiskit 1.4.4 (Python 3.11)
- Create a few simple models to fit samples of data
- Learn to initialise model weights
- Learn the interaction b|n data encoding and ansatz
- Understand how observables / measurements work
- Explore the impact of ansatz structure on performance
-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

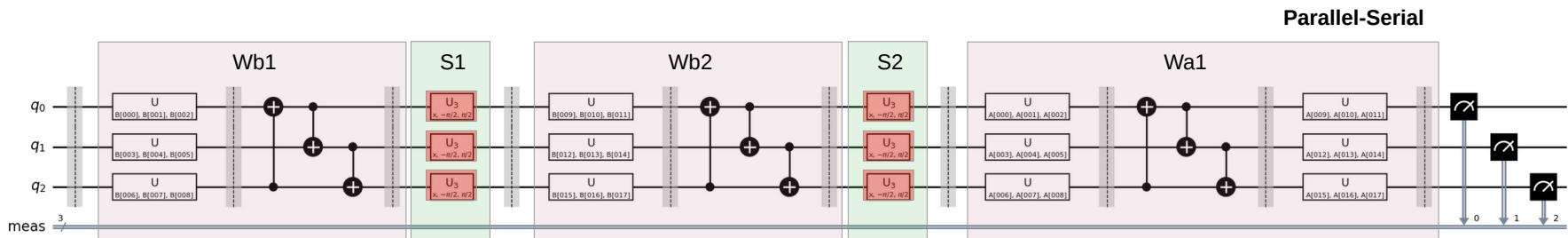
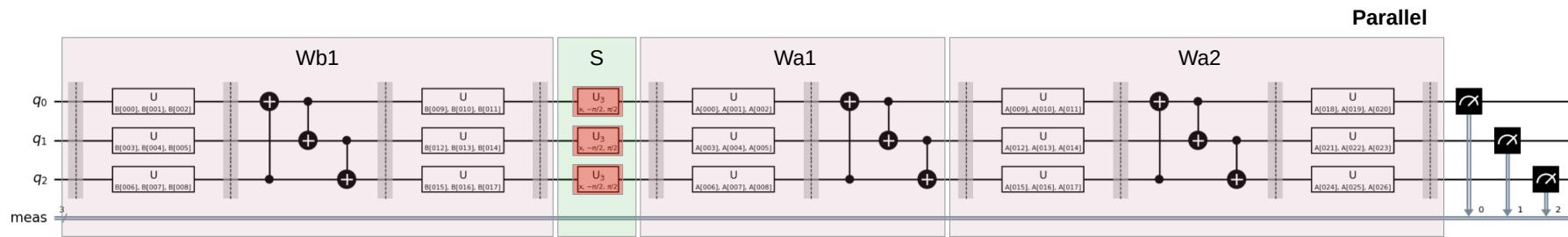
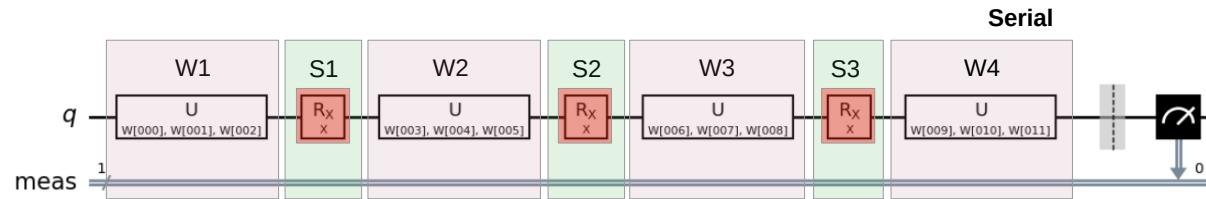
- Time series (TS) analysis aims to *identify patterns* in historical time data and to *create forecasts* of what data is likely to be collected in the future
- *Many TS applications*, including heart monitoring, weather forecasts, machine condition monitoring, etc.
- Time series can be *univariate*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



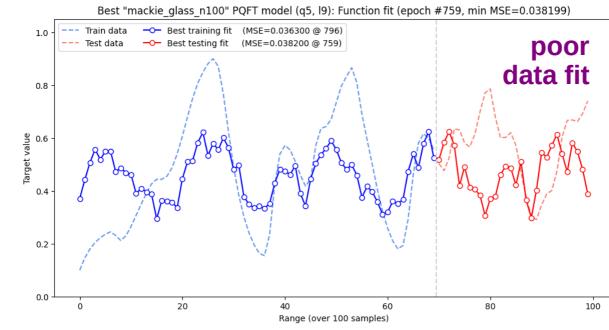
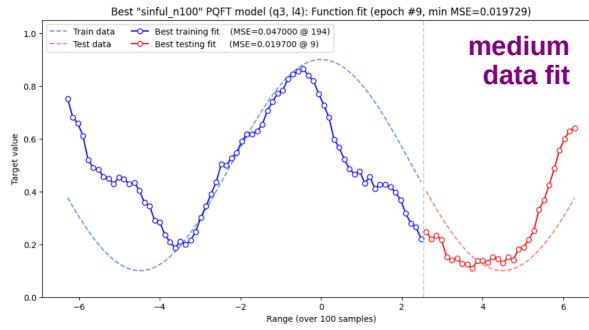
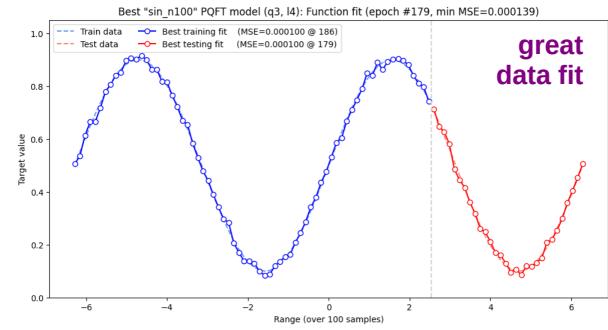
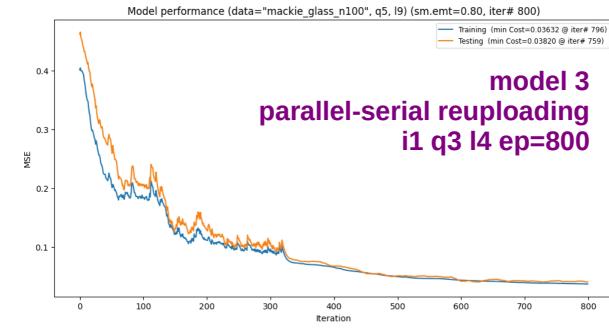
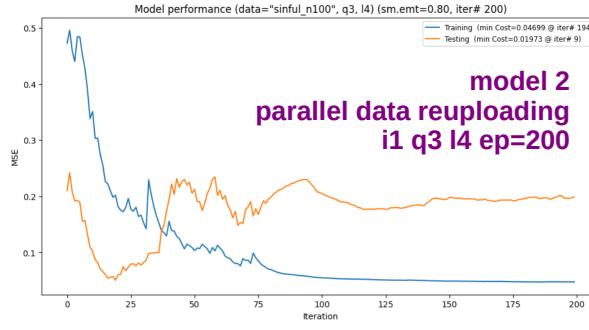
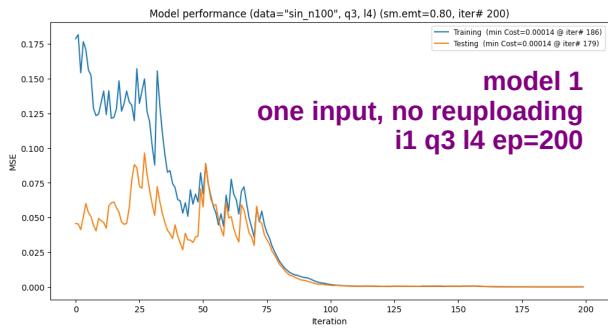
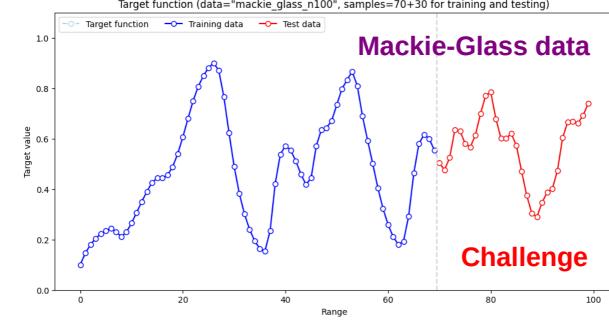
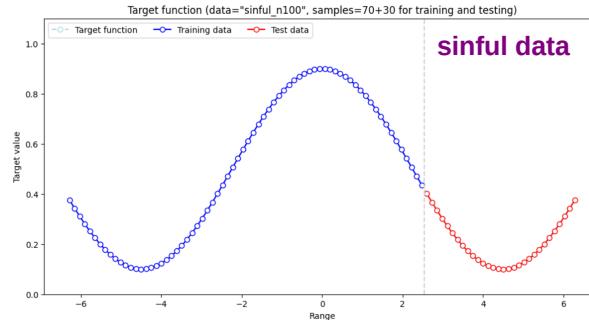
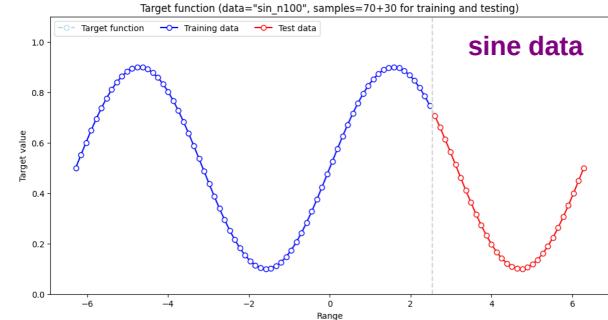
Quantum time series analysis is hard!

- 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



# Data and some results



Approach to quantum TS modelling is data dependent!

# Qiskit circuit creation

```
##### 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
```

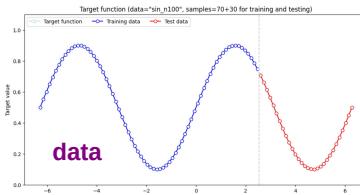
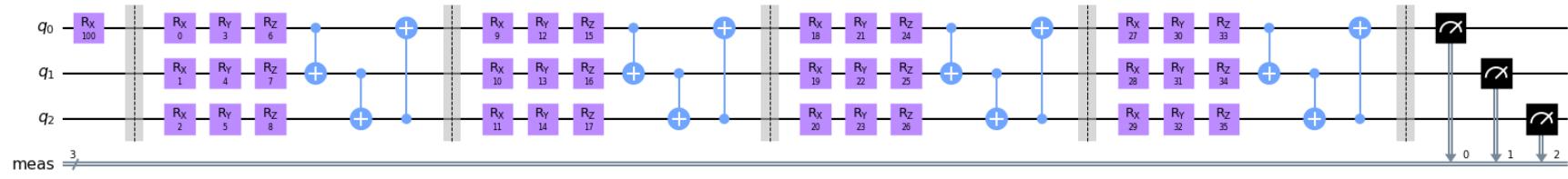
##### Model settings for models with 1 input

```
inputs_no = 1      # Number of inputs
qubits_no = 3       # Number of qubits
layers_no = 4       # Number of layers
epochs = 200        # Training epochs
shots = 1000        # Ignored
print_fract = 0.1   # Frequency of printing
weights_scaler = 1.00 # Scale factor for weights
```

model circuit

and its  
meta-params

2



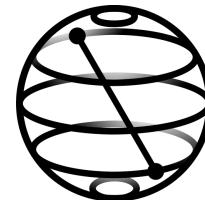
Sample data needs to be prepared, cleaned and split into training and test partitions.

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(model.num_parameters - inputs_no)
```

create model circuit  
calculate initial weights

4

# 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),
)
```

```
### 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
)

    ## 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)
```

```
Model training started
training log
(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
```

5 estimator

6 regressor

7 training loop



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

##### 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}, +\n'
                  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.

callback function

8

# Quantum model performance: Scoring your quantum model

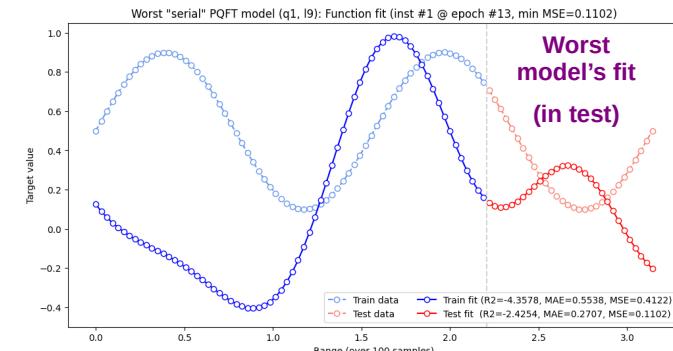
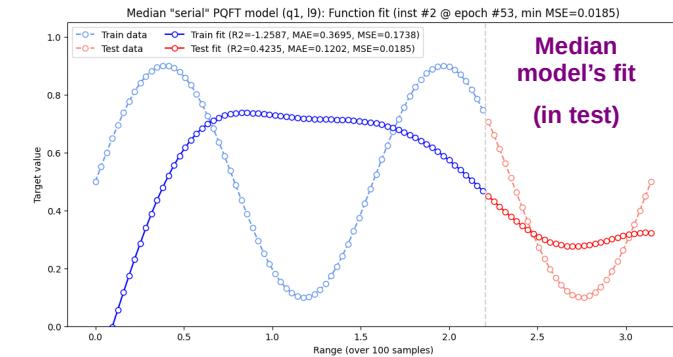
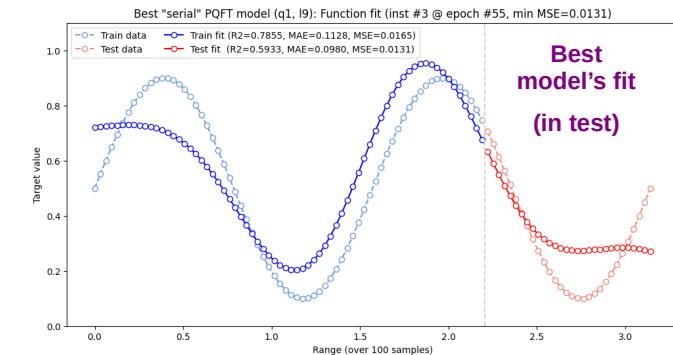
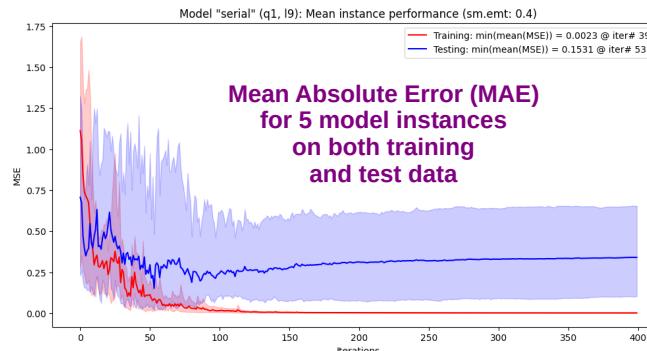
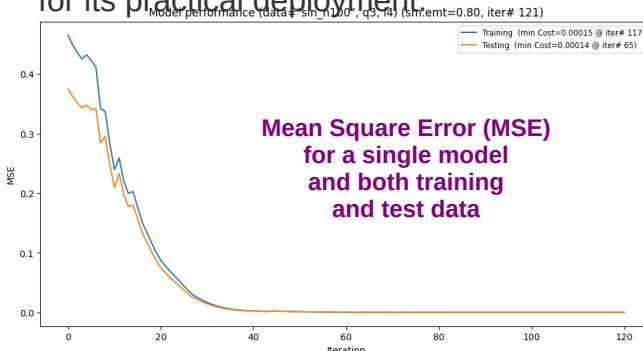
Quantum model training relies on the training data and a loss function to guide the optimiser, e.g. L2Loss (MSE cost), however, other performance metrics may also be needed, e.g. MSE, MAE or  $R^2$ , calculated for training, validation and test data.

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).

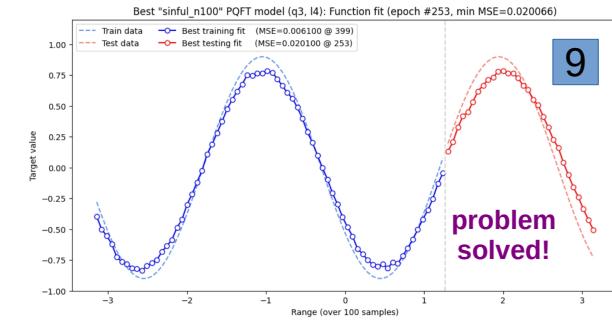
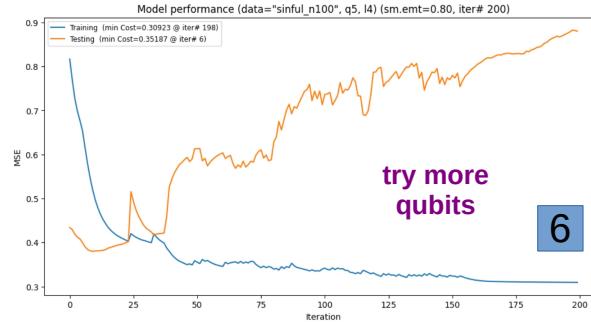
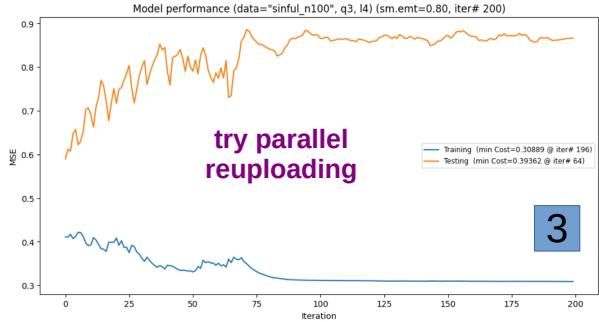
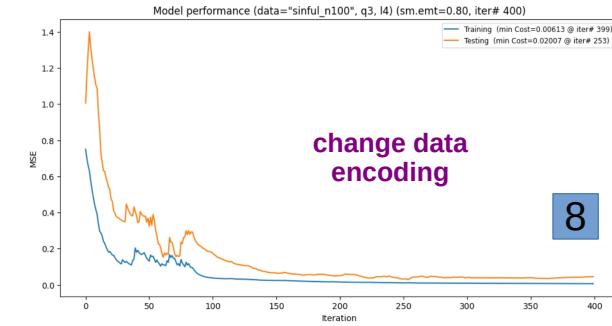
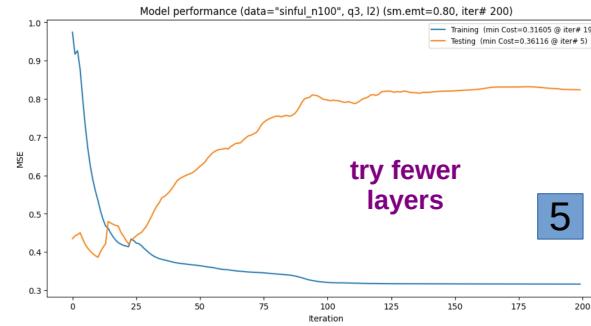
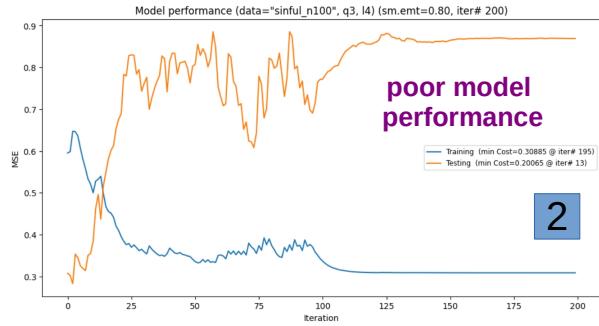
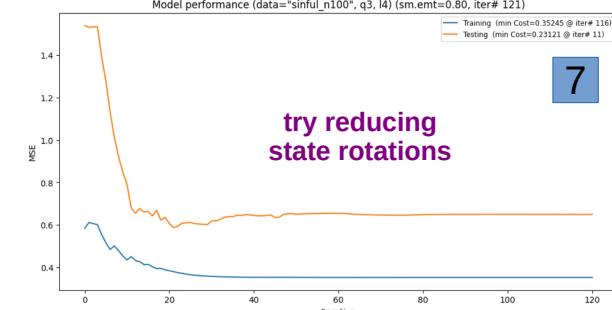
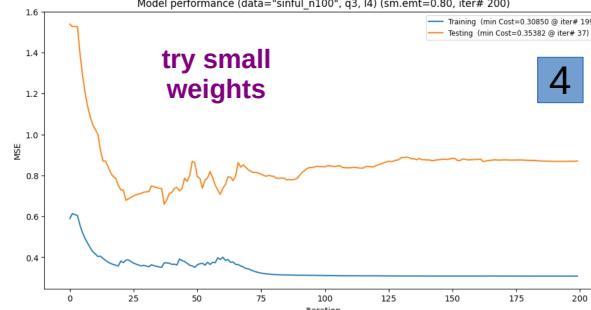
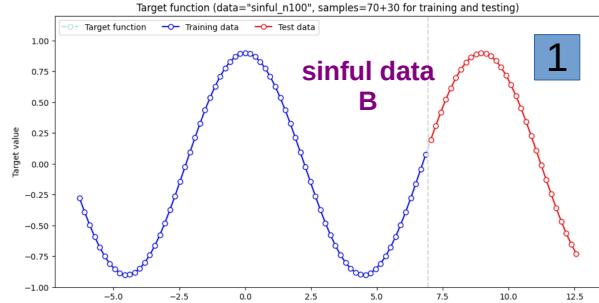
However, as a quantum model performance is highly sensitive to its initialisation, it is also advisable to run multiple, differently initialised, instances of the same model. Subsequently we can analyse a distribution of their performance results, e.g. here we present 5 instances of the same model with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

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

In this way, our performance assessment is not subject to our luck or the lack thereof, and most importantly we can provide an honest and unbiased reporting on the model's fitness for its practical deployment.

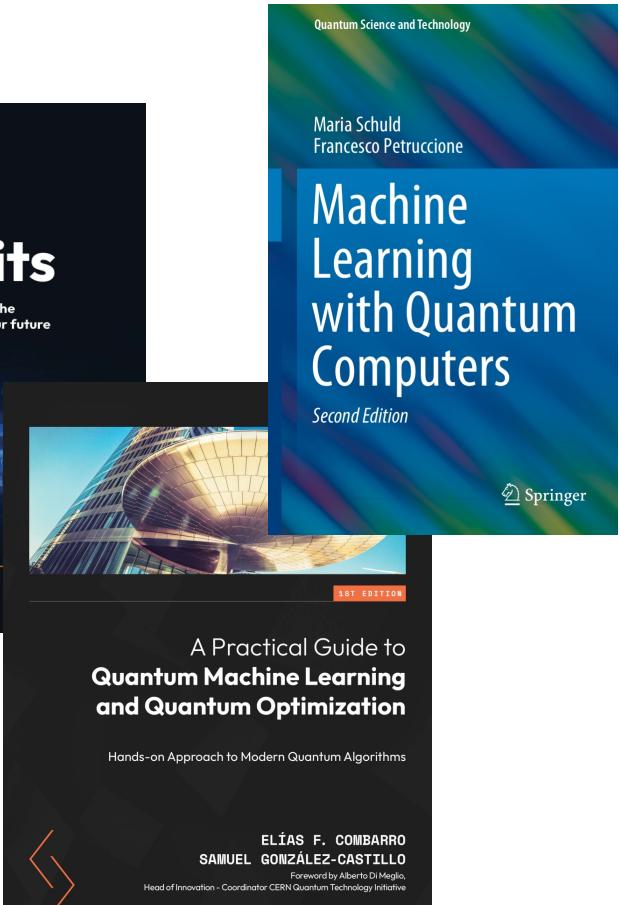
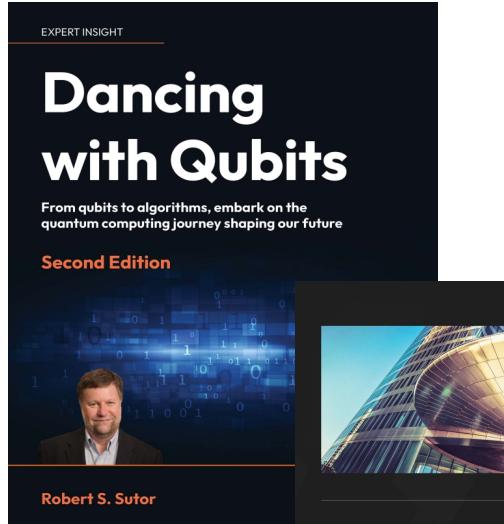


# In search of solution!



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

# Recommended reading on QML with Qiskit



[ph] 19 Jun 2024

Quantum computing with Qiskit

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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. Lastly, we discuss some of the ecosystem of tools and plugins that extend Qiskit for various tasks. Lastly, we discuss some of the ecosystem of tools and plugins that extend Qiskit for various tasks.

## I. INTRODUCTION

## II. DESIGN PHILOSOPHY

Quantum computing is progressing at a rapid pace, and robust software tools such as Qiskit are becoming increasingly important as a means of facilitating research, education, and to run computationally interesting problems on quantum computers. For example, Qiskit was

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

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(Dated: Friday 13<sup>th</sup> June, 2025)*

## 1. INTRODUCTION

The convergence of quantum computing and machine learning promises a significant 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 tools that bridge the gap between theoretical QML algorithms and their practical implementation on

merging quantum and classical computation, and simulators. Qiskit Modeler [1] is an end-to-end workflow designed with the Qiskit framework [2] that addresses this need by providing a comprehensive and user-friendly platform for exploring the exciting landscape of QML. Qiskit Modeler integrates such primitives as quantum circuit design, simulation, and execution to enable users to quickly and easily experiment with quantum kernels to establish methods such as quantum kernels for Support Vector Machines, or explore new, fully quantum approaches. Its integration with Python and reliance on widely used libraries like NumPy [2] and sk-learn [3] makes it accessible to a wide range of users, from engineers to the life sciences. It also includes [3] a detailed API reference and a rich set of tutorials designed to help users learn how to use Qiskit Modeler to its full potential.

Qiskit ML is freely distributed under the Apache 2.0 license, encouraging community participation and open collaboration. Moreover, it sets itself apart from other platforms like PennyLane [5] in its approach to quantum hardware usage. Specifically, Qiskit ML's architecture is deliberately designed to handle quantum hardware workloads, while also allowing experimentation with

one-art classical simulators and models of emulated noise from near-term devices. Moreover, it is to be modular and extensible, making the development of new quantum algorithms or building upon ones straightforward. Supported by extensive online resources and tutorials, Qiskit ML stands at the forefront of QML research, helping students, scientists, and developers worldwide investigate the application of quantum computing for machine learning.

This section outlines the role of Qiskit ML within broader computing software stacks, as illustrated in Figure 1. Qiskit ML sits at the application level, providing a suite of tools and algorithms that leverage the power of quantum computing for machine learning tasks. It serves as a bridge between high-level machine learning concepts and the underlying quantum hardware or simulators. The design of Qiskit ML prioritizes extensibility, modularity, and an intuitive user interface, leading to rapid prototyping and deployment. The high-level API for prototyping of new and existing QML protocols and high-level structure includes Quantum Neural Networks (QNN), Variational Quantum Circuits (VQC), Quantum Kernel Estimation (QKE), and a module for Support Vector Machines, among other QML applications. These are provided through workflows shown in the Unified Modelling Language (UML) diagram in Figure 2.

It is summarised in Table I. Embedded within the wider Qiskit ecosystem, Qiskit predominantly depends on Qiskit's primitives. It interfaces with classical machine learning frameworks such as scikit-learn and Python numerical-core libraries like NumPy, enabling a continuous integration of classical and quantum machine learning techniques. Additionally, the models follow SciPy's structural foundation, and there is functionality for integrating neural networks with PyTorch to support the design, training, and inference of hybrid quantum-classical models.

We begin by discussing how Qiskit's scope, 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 circuit, for example Fermion to qubit mapping [34, 62]. Circuits at this level can be quite abstract, for example specifying the action of a single operator or a sequence of 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-

Release News: Qiskit SDK v2.1  
here!

technical release summary for Qiskit SDK v2.1, including updates on top new features, breaking changes, and our ongoing efforts to make Qiskit the world's most performant quantum SDK.



# Thank you!

## Any questions?

Available resources, see:  
ironfrown (Jacob L. Cybulski, Enquanted)  
[https://github.com/ironfrown/qml\\_abc\\_lab](https://github.com/ironfrown/qml_abc_lab)



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