Secrets revealed in this session:

To gain experience to evaluate design and implementation options for the development of quantum estimation models

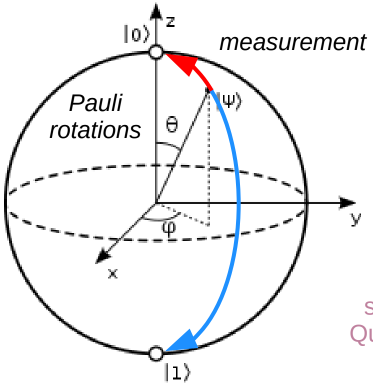
- *QML process*
- *Quantum estimation*
- *Linear models*
- *Data preparation and partitioning*
- *Fixing the random seed*
- *Model creation and training*
- *Chasing the performance targets*
- *Scoring the model*
- *Never trust your luck!*
- *Don’t get cocky*
- *Avoiding barren plateaus*
- *Model diagnostics - residual analysis*
- *Barriers to quantum estimation*

Quantum Machine Learning

Quantum Estimators

Jacob L. Cybulski

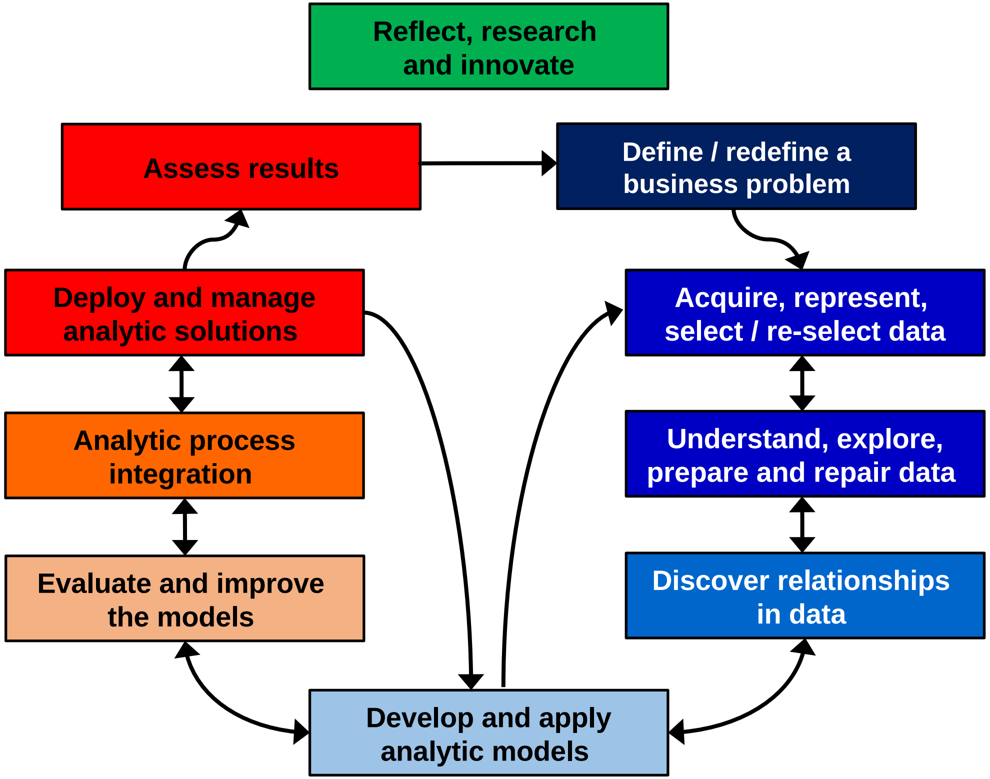
Enquanted, Melbourne, Australia



We will assume some knowledge of Quantum Computing ML and Python

11-12 October 2025, QPoland, Fundacja Quantum AI

Process of quantum model development



Define a business problem – Formulate a business problem and specify requirements for its solution in terms of decisions to be turned into business actions.

Understand and prepare data – Select a data sample. Explore and understand attributes characteristics. Deal with missing values and outliers. Clean, transform, convert and select attributes. Reduce data dimensionality if needed.

Discover relationships in data – Explore, visualise and understand relationships between data features. Determine targets, labels and their predictors.

Create analytic models – Evaluate alternative quantum models and algorithms to suit the problem and data. Study the models' characteristics, their strengths and weaknesses. Select and build the most promising.

Evaluate and improve the models – Validate and test the model for its ability to predict or explain. Evaluate the model training and test performance. Tune the model to optimise its performance. Interpret and report results.

Analytic process integration – Integrate pre-processing, exploratory and predictive analytic elements and visualisations into a complete analytic process.

Deploy, manage and assess analytic solutions – Embed the final quantum model and classical analytic process in a business application. Apply the process to live data. Use the results to support business decisions and actions. Measure and assess the model performance on real data. Reflect, research and innovate.

Classical estimation / Quantum estimation

Estimation models (or estimators) in machine learning are used to predict continuous numerical outputs (or targets), in contrast to classification models, which predict discrete labels. Such models are able to estimate quantities based on input features.

Classical estimation models include:

- ***Linear Regression Models***
  (Ordinary Least Squares Regression, Ridge and Lasso Regression)
- ***Non-Linear Regression Models***
  (Polynomial Regression, Support Vector Regression)
- ***Bayesian Models***
  (Bayesian Regression, Gaussian Processes)
- ***Neural Networks***
  (Feedforward Neural Networks, Recurrent Neural Networks)
- ***Time Series Forecasting Models***
- ***Ensemble Models***
- ***Etc.***

Quantum estimation models adopt the principles of quantum mechanics to enhance the precision, efficiency, or computational power of estimation tasks. These models are especially useful in situations where classical estimation methods face limitations, such as:

- *high-dimensional data*
- *noisy environments, or*
- *highly complex calculations.*

Applications of classical and quantum estimators:

- ***Finance:***
  Risk assessment, stock price prediction.
- ***Healthcare:***
  Disease progression estimation, drug effectiveness.
- ***Retail:***
  Demand forecasting, inventory optimization.
- ***Autonomous Vehicles:***
  Estimating distances, speeds.
- ***Energy:***
  Power consumption prediction.
- ***Etc.***

Quantum models capable of estimation tasks:

- ***Quantum Neural Networks (QNNs):***
  speedups for high-dimensional data.
- ***Quantum Kernel Methods:***
  encoding data into quantum Hilbert space.

Quantum model dev.

training, validation and testing

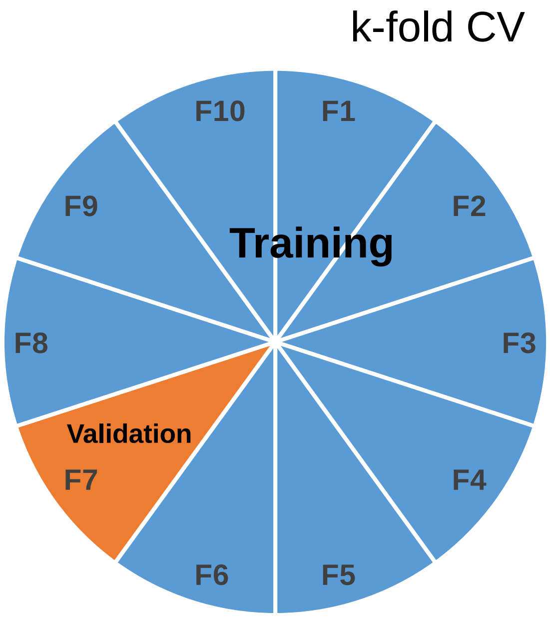
While developing a quantum model we need to test its capacity to learn. This can be done by applying the model to data used in its training, with the objective to test its ability to recall what it learnt.

To assess the model's performance on new data we need to apply it to data not used in training.

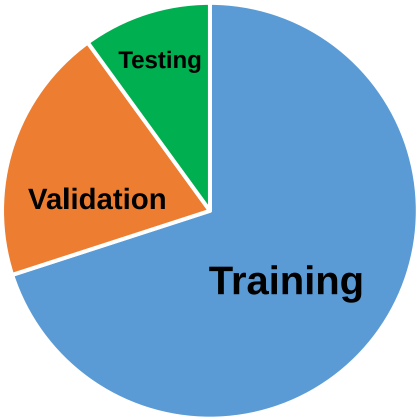
Commonly adopted approach is known as *holdout testing*, where we randomly split data into three partitions - one to be used for model *training*, one for its *validation* while improving the model, and one for *honest testing* on data never used before.

Holdout testing validates and test the model once only, assuming all data partitions as representative of the population, which may not be true.

Cross-validation (CV) is a more appropriate testing method, which repeatedly trains and validates a model using different data samples (folds), then averaging the performance obtained from all runs.



As training a quantum model may be extremely slow, cross-validation may not be feasible.

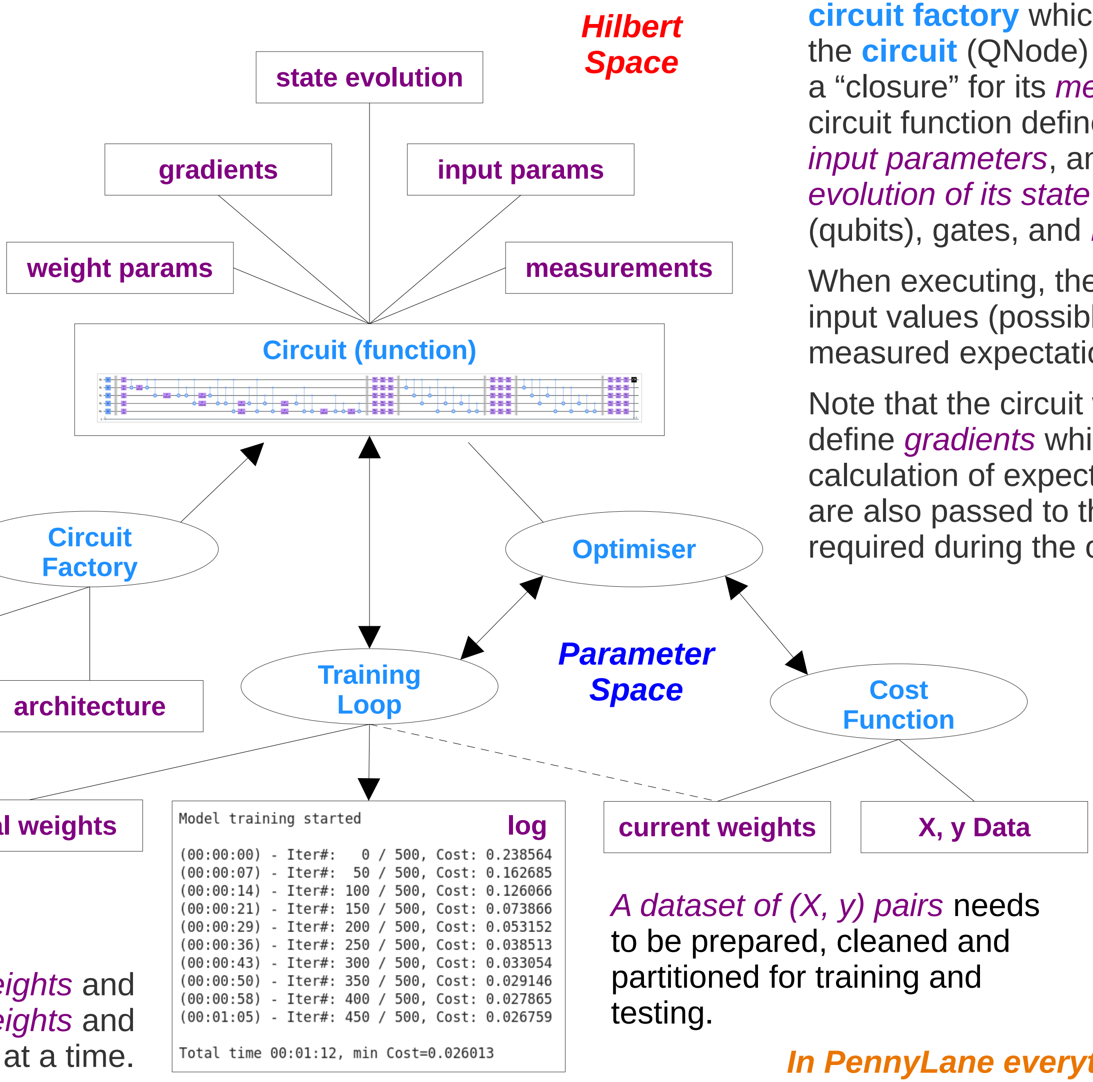


As quantum models are sensitive to their initialisation, once the model is developed, we retest it with differently initialised weights, in the process also resampling data partitions.

Note: as we develop the model we freeze data partitions by setting a *random seed*, to ensure performance changes are due to our actions and not differences in data partitions.

Training a
PennyLane model

Optimiser provides a function ***step_and_cost*** which executes a step in a training loop. Starting with some model *initial weights*, it is called iteratively to perform a *forward* step to execute the **circuit** using the *current weights* and *data*, the **cost function** is then applied to the results producing the model's cost. Then a *backward* step is taken to improve the model weights, which are returned with the calculated cost.



The purpose of the **training loop** is to manage and improve the circuit weights and collect the costs of intermediate models to the *log*.

The loop starts with the model's *initial weights* and then passes the **cost function**, *current weights* and *input data* to the **optimiser** one step at a time.

In PennyLane the PQC is written as a **circuit factory** which is a function building the **circuit** (QNode) *architecture* and creating a "closure" for its *meta-parameters*. The circuit function defines its *weight parameters*, *input parameters*, and most importantly the *evolution of its state*, by means of wires (qubits), gates, and *measurements*.

When executing, the circuit takes weight and input values (possibly in batches) and returns measured expectation values.

Note that the circuit weight parameters also define *gradients* which are used in the calculation of expectation values, and which are also passed to the **optimiser** whenever required during the optimisation process.

For the circuit to be executable it needs to become a QNode, associated with a quantum device (e.g. "default.qubit"), and optionally interfaced with some gradient package (e.g. "torch") and a differentiation method (e.g. "adjoint").

A dataset of (X, y) pairs needs to be prepared, cleaned and partitioned for training and testing.

In PennyLane everything is a function!

Quantum model performance:
Scoring your quantum model

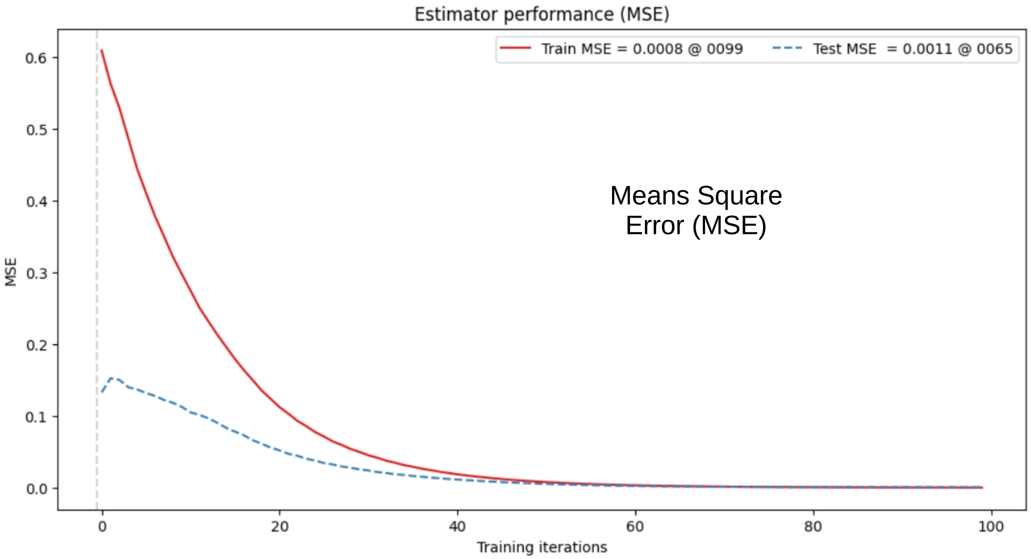
In model training we rely on the specific loss / cost function, e.g. MSE or MAE, to guide the optimiser.

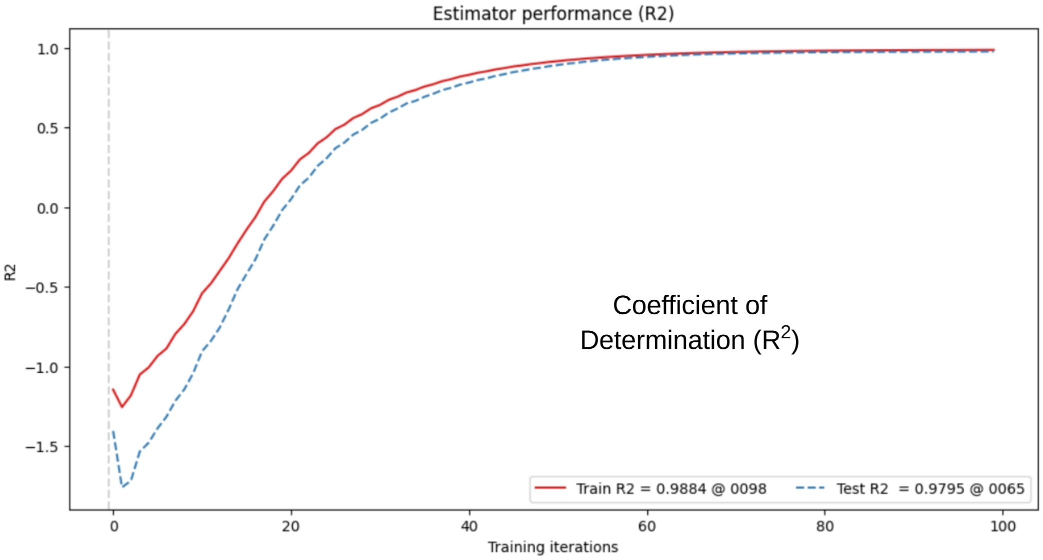
During training, the costs and the model parameters for all optimisation steps are saved for later use.

The lowest cost indicates the optimum model training parameters. However, the model performing best in training may not be the most generalisable.

So we can use all saved model parameters, to reconstruct the intermediate models and apply them to either training, validation or test data.

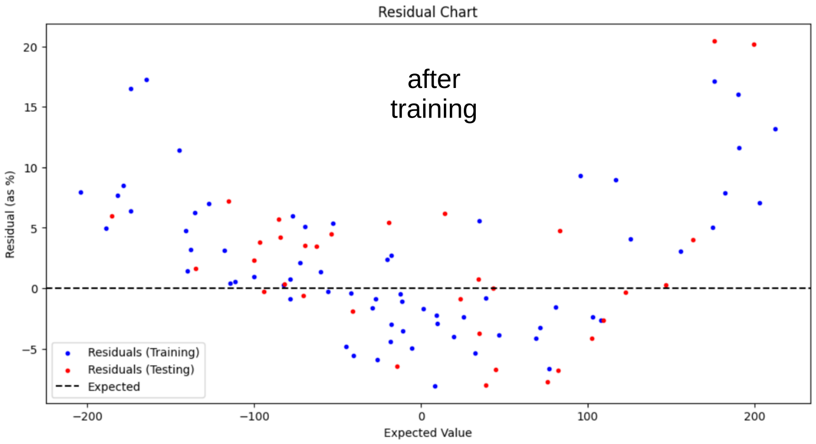
This allows calculation of other performance scores useful in further analysis to determine the parameters of the model that is optimum for the population (and future data) and most suitable for its final deployment.

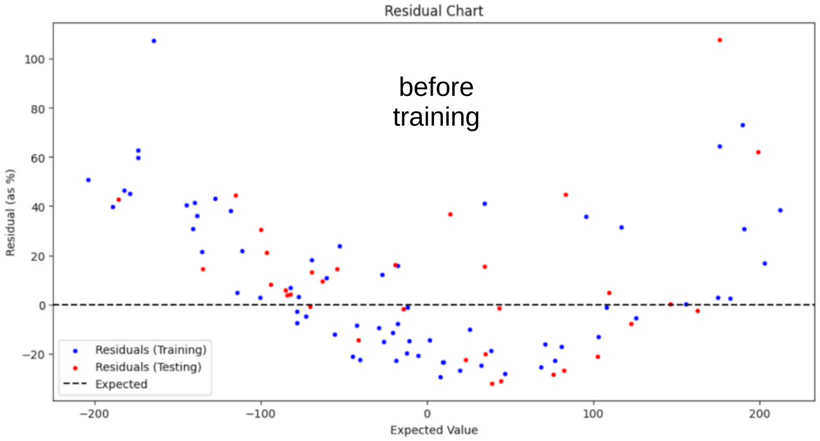


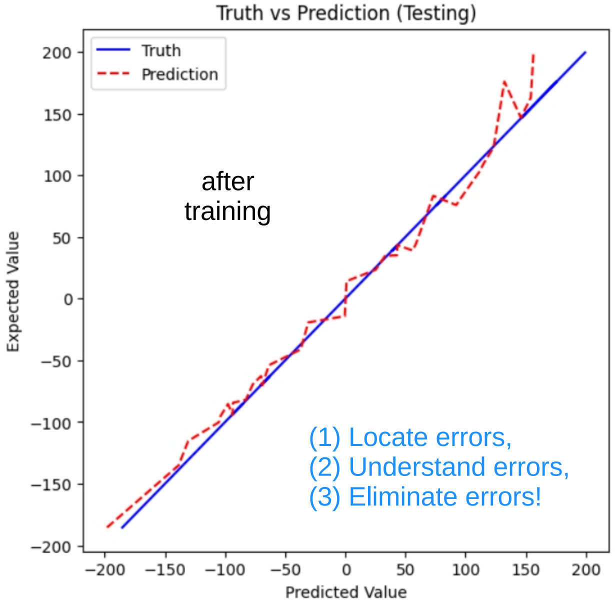


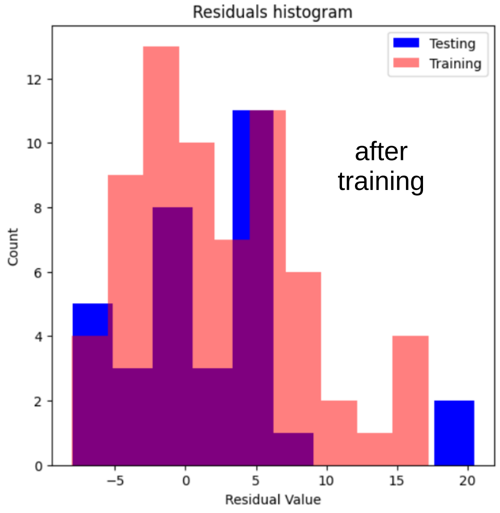
Diagnostic charts

Performance is not enough!









- The purpose of diagnostic charts is to better understand the accuracy (or precision) of the model and errors it makes.
- The residual scatter plot (left) gives an overview of the errors produced before and after training. However, the plot does not give an intuition of the severity of the problem.
- The severity of the errors (and their location) is better reflected in a histogram of residuals (upper-right), where the residual values are aggregated.
- The truth vs prediction chart (middle-up) allows to see how and where the prediction deviates from the expectation.

Can the model still learn? Example

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

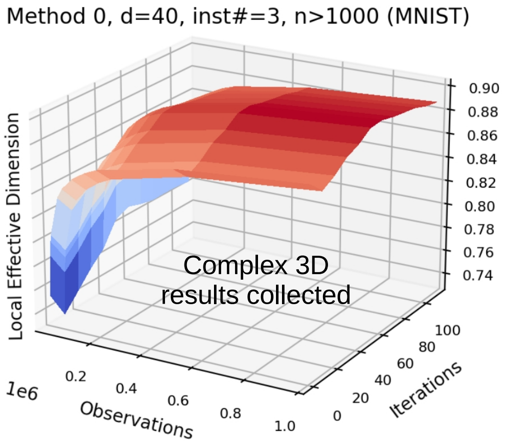
Global Effective Dimension (GED):

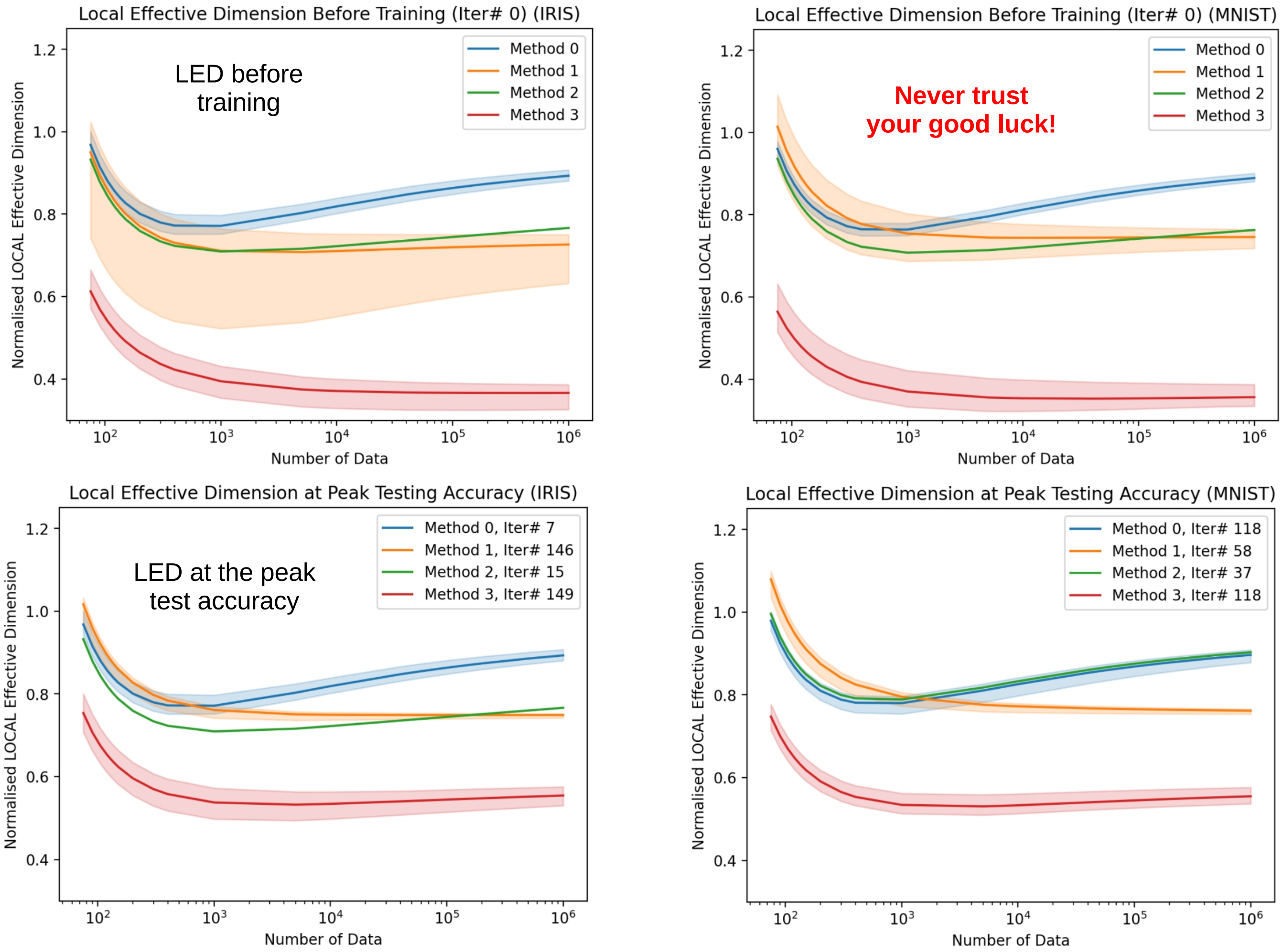
A static, probabilistic measure of the model complexity as the geometry of its entire parameter space.

Local Effective Dimension (LED):

Dynamic geometric measure of the model complexity in training, derived from GED, but affected by data distribution and optimisation algorithm

The study investigated how GED and LED correlated with **barren plateaus (BP)**.





This study used **two** different datasets - IRIS and MNIST, investigated **four** approaches to dealing with BPs, each required a **unique** quantum model, however, each model had **ten** runs **randomly initiated**.

Jacob L. Cybulski and Sebastian Zając (2024): "The Art of Data Encoding and Decoding for Quantum Time Series Analysis." 8th Intl Conf on *Quantum Techniques in Machine Learning*, University of Melbourne, Melbourne, Australia, 25-29 Nov 2024.

Compare models: quantum vs classical

QAE *CAE*

The experiments show:

The larger the QAE latent space, the better learning
(the accepted idea that reducing latent space helps abstraction is wrong)

There is an optimum depth for the QAE model.

PennyLane "minimum" hybrid models outperformed Qiskit models in training, but not in validation.

Within the limit of 1000 epochs, QAE matched CAE.

In general, QML models on simple tasks (such as DL AE) *do not outperform the classical models* – so to gain quantum advantage you need to pick the application very carefully.

USA beer sales (IRI) **Varying the latent space:** DL CAE model in PyTorch @ 1000 epochs

	Experiments		Training									Validation
	Lat	Tr	TR2	TMSE	TRMSE	TMAE	TMAPE	VR2	VMSE	VRMSE	VMAE	VMAPE
Run												
0	8	0	0.9621	0.0087	0.0925	0.0716	0.0615	0.7475	0.0478	0.2105	0.1583	0.1444
1	7	1	0.9636	0.0086	0.0925	0.0683	0.0607	0.7491	0.0463	0.2016	0.1614	0.1431
2	6	2	0.9631	0.0081	0.0911	0.0708	0.0604	0.7547	0.0466	0.2133	0.1554	0.1443
3	5	3	0.9592	0.0085	0.0925	0.0710	0.0624	0.7468	0.0455	0.2133	0.1633	0.1467
4	4	4	0.9609	0.0088	0.0941	0.0713	0.0618	0.7668	0.0445	0.2120	0.1604	0.1445
5	3	5	0.9625	0.0092	0.0973	0.0701	0.0646	0.7461	0.0453	0.2146	0.1677	0.1464
6	2	6	0.9515	0.0121	0.1096	0.0815	0.0697	0.7144	0.0516	0.2264	0.1694	0.1504
7	1	7	0.8575	0.0321	0.1788	0.1274	0.1098	0.4706	0.0937	0.3012	0.2217	0.1859

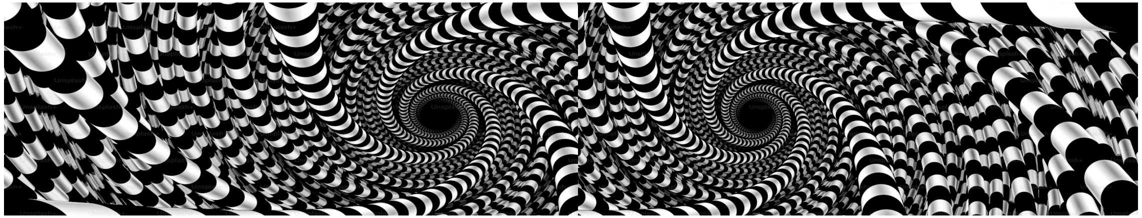
Varying the circuit depth: quantum model in PennyLane + PyTorch @ 1000 epochs

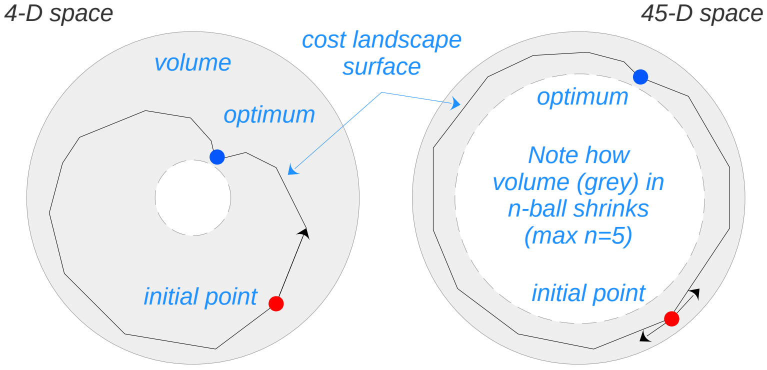
	Experiments				Training									Validation
	Lay	Lat	Tr	Xtr	TR2	TMSE	TRMSE	TMAE	TMAPE	VR2	VMSE	VRMSE	VMAE	VMAPE
Run														
8	1	5	3	0	0.7663	0.0449	0.2112	0.1508	0.1285	0.1460	0.1019	0.3154	0.2192	0.2081
9	2	5	3	0	0.9635	0.0084	0.0910	0.0703	0.0652	0.6278	0.0475	0.2169	0.1656	0.1598
10	3	5	3	0	0.9589	0.0093	0.0953	0.0693	0.0631	0.6926	0.0400	0.1994	0.1470	0.1397
11	4	5	3	0	0.9644	0.0081	0.0885	0.0656	0.0592	0.6890	0.0413	0.2028	0.1545	0.1457
12	5	5	3	0	0.9572	0.0096	0.0971	0.0693	0.0624	0.7198	0.0386	0.1962	0.1474	0.1374
13	6	5	3	0	0.9528	0.0104	0.1015	0.0722	0.0642	0.6915	0.0408	0.2016	0.1531	0.1445
14	7	5	3	0	0.9499	0.0111	0.1052	0.0747	0.0659	0.6866	0.0412	0.2027	0.1502	0.1404
15	8	5	3	0	0.9525	0.0106	0.1027	0.0728	0.0649	0.7073	0.0400	0.1999	0.1503	0.1411

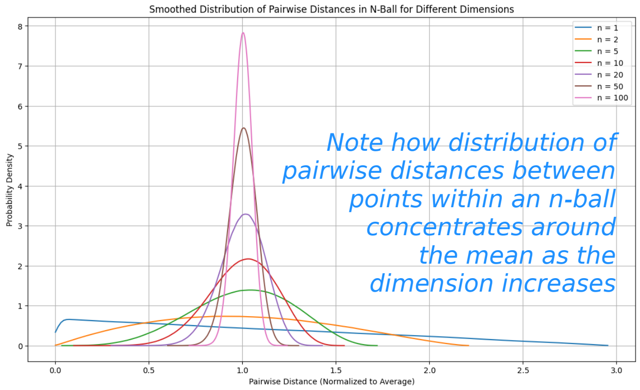
Varying the latent space: quantum model in PennyLane + PyTorch @ 1000 epochs

	Experiments				Training									Validation
	Lay	Lat	Tr	Xtr	TR2	TMSE	TRMSE	TMAE	TMAPE	VR2	VMSE	VRMSE	VMAE	VMAPE
Run														
0	3	8	0	1	0.9732	0.0062	0.0770	0.0581	0.0541	0.7139	0.0417	0.2034	0.1545	0.1478
1	3	7	1	1	0.9736	0.0061	0.0764	0.0579	0.0545	0.7350	0.0373	0.1928	0.1467	0.1460
2	3	6	2	1	0.9667	0.0076	0.0864	0.0643	0.0602	0.6953	0.0438	0.2083	0.1518	0.1463
3	3	5	3	1	0.9540	0.0103	0.1003	0.0731	0.0653	0.6770	0.0455	0.2126	0.1620	0.1499
4	3	4	4	1	0.9244	0.0160	0.1221	0.0879	0.0765	0.6189	0.0499	0.2211	0.1688	0.1593
5	3	3	5	1	0.9056	0.0194	0.1346	0.0980	0.0866	0.6106	0.0553	0.2332	0.1765	0.1642
6	3	2	6	1	0.8435	0.0309	0.1703	0.1205	0.1035	0.4838	0.0653	0.2533	0.1814	0.1662
7	3	1	7	1	0.7197	0.0522	0.2284	0.1521	0.1263	0.2278	0.0895	0.2991	0.2136	0.1878

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 parameters)

- Pairwise distances between uniformly distributed points in high-D space become (almost) identical, the surface of such a space is almost flat (all n-ball points are near its surface).
- In a quantum model with a high-D parameter space, the cost landscape is also 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 optimum.
- Selecting the optimisation initial point far from the optimum (e.g. random) makes it even more difficult!

There exist well-known causes of BPs and there are 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)

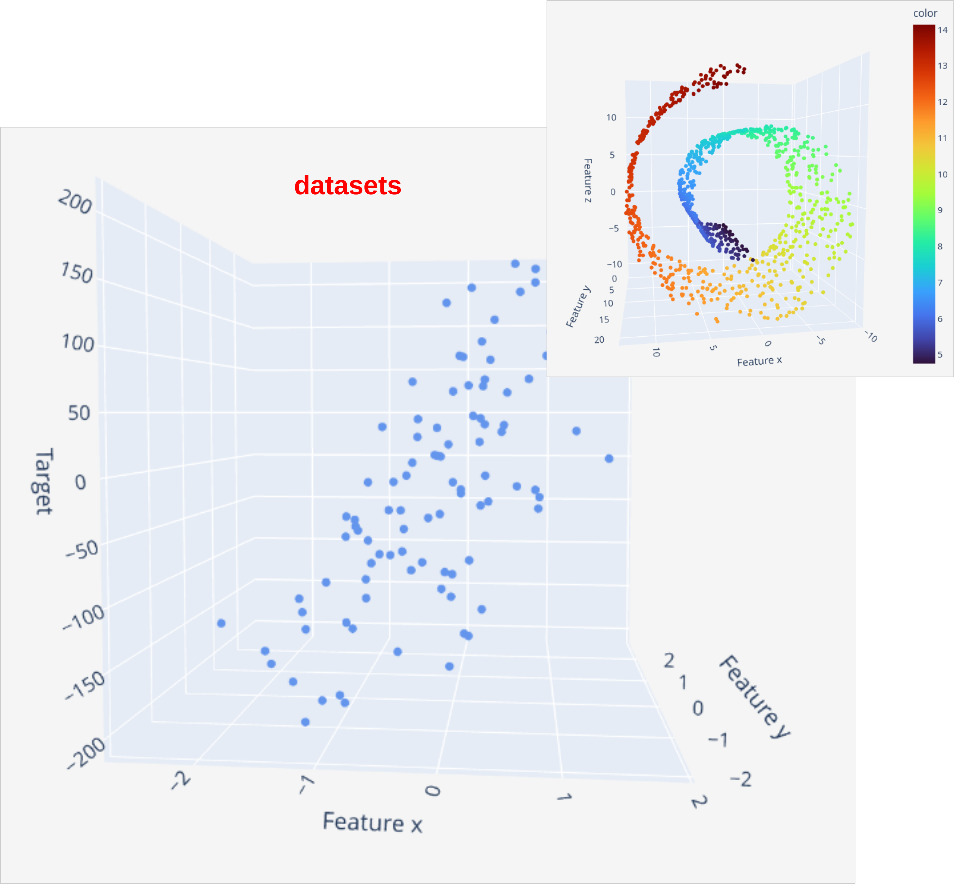
Barriers to quantum estimation

Problems	**Possible Solutions**
In VQA training • Quick forward step (quantum) • Slow backward step (classical)	• Use parameter-shift rules (quantum native gradients) • Use hardware-efficient differentiation • Use quantum kernels, where training is one-shot linear algebra • Use quantum annealing for training • Train using quantum Gibbs sampling (Bolzmann Machines) • Adopt time-evolution based gradients (with Trotterisation) • Use adaptive Trotterisation (to balance precision vs circuit depth)
Precision of continuous results = number of shots	• More shots, more precision (more slow) • Continuous-variable quantum computing (e.g. photonics) • Analogue quantum computing (e.g. neutral atoms, photonic systems, quantum annealing) • Superconducting resonators • Hadamard test / Iterative phase estimation
Quantum noise	• Train models with simulated noise • Apply error correction and error mitigation techniques

Isaac De Vlugt. *Differentiation on quantum hardware, PennyLane Tutorial*. Sep 12, 2023.

PennyLane Demo

Functions within functions...



PennyLane Demo:

- Explore the synthetic data
- Investigate data preprocessing tasks
- Learn how to encode data
- Check the clever cost function enclosure
- Look at the model as a function factory
- Learn how to calculate the model shape
- Produce the circuit and its plot
- Train the model
- Score the model and plot scores
- Perform analysis of residuals

Key takeaways:

- Quantum modelling is an engineering task
- There is more to success than a clever model
- Data encoding is (again) crucial to performance
- Experiment with the ansatz parameters
- A default optimiser may be the best afterall, however, design experiments to test it!
- More training does not give better results
- When the model converged it is time for its scoring
- Estimation needs residual analysis

Thank you!

Any questions?

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