

Introduction Key concepts in classical time series Quantum computing brief Quantum time series analysis and forecasting QTSA data encoding and analysis QTSA with variational quantum linear regression QTSA with variational quantum Fourier transforms QTSA with quantum neural networks QTSA with real data Summary and reflection

Quantum computing is modern magic Quantum machine learning turns data into magic

IBM quantum computer

Key Concepts in Quantum Time Series Analysis (QTSA) An Introduction and Preliminary Research Results

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Research

- Quantum computing
- Quantum machine learning
- Quantum time series analysis and anomaly detection
- Classical machine learning
- Data visualisation

Personal

- Recreational cycling
- Reading science and Sci-Fi
- Quantum challenges and hackathons





Classical TS Methods Key concepts in classical time series analysis



Analysis of the past Prediction of the future

- We are bombarded daily with volumes of time-based information, often in the form of data points in time, in other words - a *time series*
- Time series visualisations are used to inform experts, influence government policies and shape public opinion (e.g. about COVID)
- Time series analysis aims to *identify patterns* in collected historical data and to create *forecasts* of what data is likely to be collected in the future
- Sample applications include heart monitoring, weather forecasts, fault detection in rotating machinery, etc.
- Times series analysis and forecasting is an established and trusted discipline, with excellent tools and highly efficient methods
- Organisations that rely on time-based information are in the pursuit of more efficient or more effective time series analysis
- Quantum time series is a possible approach to time series analysis and forecasting



Key concepts in time series analysis

- As with any data set, time series needs some pre-processing for its effective use
- Time series must have an *index* a time-stamp sequencing the series
- It is often assumed that index is a key,
 i.e. *index values are unique*
- Time series needs to be *ordered* by its index
- Time series will also have some time-dependent attributes to be modelled
- Time series can be *univariate* or *multivariate*, depending on whether a single or multiple attributes are being investigated
- *Missing indeces* and their dependent attributes may need to be imputed (e.g. interpolated)
- A series can be defined over non-time entities, e.g. a landscape line or a DNA sequence

- Index needs to be of appropriate *granularity*, e.g. years, months, weeks, days, hours, etc.
- Attributes need to be *aggregated* to the required index granularity
- Time signal often shows *seasonality* in data, i.e. a regular repeating pattern
- With aggregation and smoothing seasonality can be removed and *trends* visually identified
- Majority of forecasting methods require *time-series to be stationary*, i.e. its mean, variance and auto-correlation are constant
- Time series analysis needs *data storage*



Neural Nets for Time Series Analysis

- The simplest neural networks, such as Multi-Layer Perceptrons (MLPs), map numeric inputs into numeric or categorical outputs via layers of "neurons", interconnected by weighed links, and calculating weighted sums with non-linearity
- The weights of neural links are trained within an optimisation process, such as gradient descent, by matching the calculated vs expected outputs
- Some types of deep neural networks can be trained for time series analysis, including: forecasting, classification and clustering, e.g.
 - Recurrent Neural Networks (RNN)
 - Long Short-Term Memory (LSTM) nets
 - Gated Recurrent Units (GRU) nets
- Unlike MLPs, networks such as RNN, LSTM and GRU are able to retain and rely on memory of the past training data
- Neural networks and RNNs are similar in their structure to quantum solutions (circuits)





Fundamental Quantum Concepts Approach, qubits and circuits, process and principles



Quantum Computing Approach and applications

- Quantum computing allows information processing to be accomplished by utilising the behaviour of matter and light on the atomic and subatomic scale
- Quantum computing aims at solving problems in many disciplines, e.g.
 - natural science, such as calculation of molecular energy or protein folding;
 - finance, such as portfolio optimisation, pricing of financial options or credit risk assessment;
 - optimisation, such as in vehicle routing or energy distribution using several quantum-enhanced optimisation techniques;
 - machine learning, featuring many general purpose algorithms, such as neural networks or kernel methods.

- Quantum applications can demonstrate their advantage over classical solutions by relying on the following features of quantum systems:
 - True randomness of observable results (measurement of quantum states)
 - Pursuing alternative decisions concurrently (superposition of quantum states)
 - Controlling parallel choices with constraints (entanglement of quantum elements)
- An example where all three principles are applied – financial option price prediction



Quantum Machine Learning *Process of quantum problem-solving*

Qubit is the most important quantum tech concept. It is a unit of quantum information. It is also a device able to manipulate a single unit of such information.

Optimisation Algorithm



Quantum circuits are static - new data requires new circuit. However, it is possible to create "variational" circuits, which are templates with parametrised gates, e.g. P, Ry and Rz varying degrees of rotation, which can be optimised using some ML algorithm.

To find optimum circuit parameters, the circuit is repeatedly executed and its outputs measured. Outputs are then compared against the expected values using a cost function, so the optimiser could determine new values for the process parameters.

How qubits work In a simplified way!

Qubit is often "implemented" as a single elementary particle, e.g. electron or photon

Qubit represents a state of such a particle, e.g. an electron spin (<u>up</u> or <u>down</u>) or photon's linear polarisation (<u>horizontal</u> or <u>vertical</u>)

Qubits are in a state of *superposition* of some *basis states*, so the electron spin is not just <u>up</u> or <u>down</u> but a combination of these basis states, e.g. $\sqrt{3}$ 1

$$\frac{\sqrt{3}}{2} \times \underline{up} + \frac{1}{2} \times \underline{down}$$

When we *measure* the qubit, its state collapses probabilistically into one of the basis states <u>up</u> or <u>down</u>, measured as simple values, e.g.

- 0 / 1 for <u>up</u> or <u>down</u> for electrons, and
- 0 / 1 for <u>horizontal</u> or <u>vertical</u> for photons.

Mathematically a qubit state can be represented as a vector (a point) in space of all possible states.

The *qubit state space* has its own coordinate system, defined by the basis vectors, which are orthogonal unit vectors (of length=1), for example in 2D these could be vectors (1, 0) and (0, 1), denoted as |0> and |1>.



|0> and |1> are vectors, not values 0 and 1, which is what we observe on qubit measurement

Qubit measurement returns 0 or 1, but repeated measurements provide expectation values of observing 0 or 1

As we can see, any vector (a, b) is a (linear) combination of the basis vectors (1, 0) and (0, 1) – we call this *superposition*.

In reality, this is more complex as qubit states are described by two *complex numbers*, each with real and imaginary parts, making it 4 reals.

With a clever "projection" trick we can depict the qubit state in 3D (not 4D), e.g. as a *Bloch sphere*.



Experiments Data Encoding and Data Analysis



Ways of utilising time series data in quantum system computation

- Quantum systems have no memory!
- Quantum circuits take no data!
- The only way of obtaining and retaining information in a quantum system is via:
 - structure of a quantum circuit (as done in variational methods)
 - states of quantum computation (as done in adiabatic optimisation)
- In this presentation we will focus on the first option – the variational methods
- In variational time series analysis, the key concerns are:
 - data encoding strategy
 - circuit optimisation strategy

Schuld, Maria, and Francesco Petruccione. *Machine Learning with Quantum Computers. 2nd ed.* 2021 edition. Springer, 2021. https://link.springer.com/book/10.1007/978-3-030-83098-4.

There are many different quantum data encoding / state preparation methods:

- basis encoding, with qubits acting as bits in the encoded number (int) to be processed further in the circuit
- *angle encoding*, where qubit rotation (real) represents the value of data
- amplitude encoding, where each data point is encoded as expectation value of the measured circuit (real), usually no further data processing is present
- Others: QuAM, QRAM, Qsample, ...

We will explain these approaches by demonstration of:

- Quantum regression (function fitting)
- Quantum Fourier transform (function fitting)
- Quantum neural networks (pattern detect.)

Variational quantum linear regression Function Fitting

We are trying to find *a* and *b* to satisfy a linear equation

We will encode a normalised vector y as a quantum state $|y\rangle$

We will identify *a* and *b* in the optimisation process, which considers a sequence of states:

The optimisation will search for such a and b, and thus $|\phi\rangle$ to minimise the cost function C_p which tries to maximise the similarity of $|y\rangle$ and $|\phi\rangle$

What's remaining is to create a quantum circuit able to calculate $\langle y | \phi \rangle$ based on pairs *a* and *b*, so that the cost function could drive the optimisation process

 $\vec{y} = a \vec{x} + b$

 $|y\rangle = \frac{1}{C_u}\overrightarrow{y} = \frac{1}{C_u}(a\overrightarrow{x} + b)$ $|\phi\rangle = \frac{1}{C_{\phi}}(a\overrightarrow{x} + b)$ $|\phi_0\rangle, |\phi_1\rangle, ..., |\phi_n\rangle$ Starting with $|\phi_0\rangle = |\phi\rangle (a_0, b_0)$ $C_n = (1 - \langle y | \phi \rangle)^2$ Can be adapted for fitting higher order polynomials

 $\langle y|\phi\rangle$

The required circuit will be built into the cost function. It will rely on the *amplitude encoding* of sample data, which ensures that measured expectation values of the composite qubit states corresponds to data values

We encode normalised ax+b in qubits q₀ and q₁, and normalised y in qubits q₂ and q₃. These encoded values act as constraints on the calculation. The Hadamard gate H allows measuring the expectation value, which implies the value of the inner product of interest (for explanation, see ref: Qiskit 2020)

Bravo-Prieto, Carlos, Ryan LaRose, Marco Cerezo, Yigit Subasi, Lukasz Cincio, and Patrick J. Coles. "Variational Quantum Linear Solver." *ArXiv Preprint* ArXiv:1909.05820, 2019.

Qiskit. "Variational Quantum Regression", in *Learn Quantum Computation Using Qiskit. Textbook*, 2020. https://qiskit.org/textbook/ch-demos/variational-quantum-regression.html

Experiment R1: Target - Line Fit

data: samples train=16, samples valid=0 x0=[0.5, 0.5], max iter=200

R2:

R2:

R2:

R2:

BFGS

BEGS

COBYLA

COBYLA

Powell

Powell

Nelder-Mead

Nelder-Mead

trust-constr R2:

Here data is only 16 points



v = a * x + b

regardless of their hyper-parameters!

Linear

Regression

Experiment R2: Target - Poly3 Fit

data: samples train=16, samples valid=0 x0=[random, ...], max iter=200

0.0412

-4.4545

-1.0734

-1.8532

-1.2052

-0.8519

MAPE: 3.573

MAPE: 9.554

MAPE: 6.3691

MAPE: 3,9021

R2:

R2:

R2:

R2: Nelder-Mead MAPE: 7.1835

R2:

trust-constr MAPE: 5.9791





Here data is only 16 points This data fitting was surprisingly slow! Different optimisers give vastly different results!

Classical

Classical

BEGS

BEGS

COBYLA

COBYLA

Powell

Powell

Nelder-Mead

trust-constr R2:

Linear

Regression

Experiment R3: Target - Poly3 Fit

data: samples train=16, samples valid=0 x0=[random, ...], max iter=200

Classical

Classical

BEGS

BFGS

COBYLA

COBYLA

Powell

Powell

Nelder-Mead

trust-constr R2:

Here data is only 16 points

R2:

R2:

R2:

R2:

R2:



Higher Order

Poly Fit

Experiment R4: Target_Trig_trend

data: samples_train=32, samples_valid=0
x0=[random, ...], max iter=200



Linear

Regression

Experiment R5: Target_Trig_trend

data: samples_train=32, samples_valid=0
x0=[random, ...], max_iter=200



Higher Order

Poly Fit

Variational quantum linear regression Reflections

- Variational quantum regression can only be used to fit linear data (with some noise)
- Its training convergence is highly sensitive to the optimisation strategy and the optimiser's hyper-parameters
- While the approach taken can be easily adapted to fitting higher order polynomials, only certain types of functions fit successfully (mainly those appearing in publications)
- As compared with classical methods of linear/polynomial fitting, experiments with variational quantum regression indicate the adopted quantum regression approach is not promising
- It is worth noting that other, more recent methods such as QSVT (Quantum Singular Value Decomposition), can assist fitting any function (or data) with higher-order polynomials



Variational quantum Fourier transforms

We consider a quantum model of the following form, which takes 1D data

The circuit consists of *n* layers, each with encoding block $S_n(x)$, which is a Pauli rotation gate, and a trainable block $W_n(\theta_n)$

We can now rewrite $f\theta$ as as a Fourier-like sum of "frequency" components.

Th components are determined by $S_n(x)$ "frequencies" and $W_n(\theta_n)$ coefficients

Re-uploading of $S_n(x)$ allows to vary the "frequencies" by accumulating rotations $W_n(\theta_n)$.

$$f_{\theta} = \left\langle 0 | U^{\dagger}(x,\theta) M U(x,\theta) | 0 \right\rangle$$

where M is a measurement observable, $U(x, \theta)$ is a variational quantum circuit that encodes data and depends on params θ

$$S_n(x) = e^{inx}$$

$$f_{\theta}(x) = \sum_{n \in \Omega} W_n(\theta_n) S_n(x)$$

Schuld, Maria, Ryan Sweke, and Johannes Jakob Meyer. "The Effect of Data Encoding on the Expressive Power of Variational Quantum Machine Learning Models." *Physical Review A* 103, no. 3 (March 24, 2021)

Pérez-Salinas, Adrián, Alba Cervera-Lierta, Elies Gil-Fuster, and José I. Latorre. "Data Re-Uploading for a Universal Quantum Classifier." Quantum 4 (Feb 6, 2020): 226.

PennyLane. "Quantum models as Fourier series", 2021. https://pennylane.ai/qml/demos/tutorial_expressivity_fourier_series.html

The circuit is structured as a *series* of $W_n(\theta_n) S_n(x)$ layers over a single qubit, with data repeatedly re-uploaded

Alternatively, $S_n(x)$ blocks can be arranged in *parallel*, with $W_{a/b}(\theta)$ blocks before and after, over multiple qubits

The circuit parameters can then be trained by the ML optimiser of choice



Experiment F1: Fit for Sin function

sin(): samples_train=50, samples_valid=20
layers=1, optimizer=L_BFGS_B(maxiter=16)





Serial Model

Experiment F2: Fit for Sin function

v 2 0, w 2 1, w 2 2

sin(): samples_train=50, samples_valid=20
layers=5, optimizer=L_BFGS_B(maxiter=16)

w 1 0, w 1 1, w 1 2



U

3 0, w 3 1, w 3

U

40, w41, w

Serial Model

U

w 5 0, w 5 1, w 5

Experiment F5: Fit for Sin function

sin(): samples_train=50, samples_valid=20
qubits=5, layers=2, interpretation=parity, optimizer=L BFGS B(maxiter=15)



Parallel Model

Experiment F7: Fit for 2-Sins function

Serial Model

2-sins(): samples_train=50, samples_valid=20 layers=15, optimizer=NELDER_MEAD()



Experiment F8: Fit for 2-Sins function

Parallel Model

2-sins(): samples_train=50, samples_valid=20 qubits=5, layers=2, optimizer=COBYLA()



Quantum Fourier transforms Reflection

- Serial quantum Fourier transforms work amazingly well with a single qubit curve fitting
- With increased depth of a serial circuit, the performance decreases
- This is where the parallel quantum Fourier transform steps in and improves the outcome
- However, in both cases the more model parameters, the worse was the outcome (volatility of the objective function)
- Any deviation from a sine function, severely degrades the fit of both approaches
- The hypothesis that the parallel model could improve if we were to adopt the serial model's data re-uploading proved to be incorrect
- Worth noting that COBYLA and NELDER_MEAD optimisation excels in its task, L_BFGS_B is painfully slow, even though it provides good results (when finally completes)



Quantum Pattern Matching

- A typical QNN consists of two main components, i.e. a feature map and an ansatz (also called variational model)
- The feature encodes the input data and prepares the quantum system state, using as many features as there are qubits
- The ansatz consists of several layers and, similarly to a classical NN, is responsible for inter-linking the layers - this is accomplished by trainable Pauli rotation gates and entanglement blocks
- Finally, the qubit states are measured and interpreted as QNN output

Abbas, Amira, David Sutter, Christa Zoufal, Aurelien Lucchi, Alessio Figalli, and Stefan Woerner. "The Power of Quantum Neural Networks." Nature Computational Science 1, no. 6 (June 2021): 403–9. https://doi.org/10.1038/s43588-021-00084-1.

> Schreiber, Amelie. "Quantum Neural Networks for FinTech." Medium, May 8, 2020. https://towardsdatascience.com/quantum-neural-networks-for-fintech-dddc6ac68dbf.

- In contrast to function / data fitting, QNNs are able to perform pattern matching, i.e. work with a sequence of values themselves rather than with the mapping between an index and values
- In the following experiments, we will adopt a sliding window approach to structuring the time series
- However, the standard QNN model does not lean itself to time series analysis, i.e.
 - You are limited to the TS window of size equal to the number of qubits



In Qiskit

VOR Model

Quantum neural networks Sliding windows / Serial model

- Experiments show that typical QNN (VQR) do not perform well with time series data
- The solution is to extend the Fourier quantum model into the multi-qubit QNN
- This required creation of a custom quantum circuit, which consists of encoding blocks $S_n(x)$ and trainable ansatz blocks $W_n(\theta_n)$
- The Fourier parallel model simply replicated the Sn(x) blocks, which limited the TS window size to the number of qubits, and which was tested to perform quite poorly

- An alternative was to adapt the Fourier serial model and distribute the TS window data across the encoding blocks Sn(xk), where each block would hold as many data points as there are qubits (k)
- Should the last block Sn(xk) be only partially filled with TS data, then the identity gates are used to make the complete block
- The circuit is then trained by optimising the parameters of trainable blocks Wn(θn)



Experiment N1: Forecast for 2 Sins

2_sins(): samples_train=70, samples_valid=30

Data: wind=7, horizon=1

MLPRegressor: hidden_layer_sizes=(150,100,50), random_state=2022, max_iter=850, activation = 'relu', solver = 'adam', shuffle=True

Sliding Window

sklearn MLPRegressor



Experiment N2: Forecast for 2 Sins

sin(): samples_train=70, samples_valid=30
Data: wind=7, horizon=1 Prep: fmap=ZZFeatureMap(q=7, lays=1), ansatz=EfficientSU2(q=7, lays=2, ent="full", su2_gates=['ry', 'rz'])
VQR: observable='ZZZZZZZZ', COBYLA()

Sliding Window VOR



Experiment N3: Forecast for 2 Sins

Sliding Window

Parallel Model

2 sins(): samples train=70, samples valid=30

Data: wind=7. horizon=1

swindow parallel model+NNR+CircuitQNN: interpret=parity, qubits=7, ans layers=3, optimizer=COBYLA()



Minimum objective function value: (399, 0.28848159138111823)

R2 for pred vs training data: Fake R2 for mean vs training data: MAPE for pred vs training data:

R2 for pred vs validation data: Fake R2 for mean vs validation data: MAPE for pred vs validation data:

0.22890923678220454 -0.44818249358929796 1.7365546202086017

0.022659435706280873 -0.331291369357034743.4162479029701087



R. R. R. R. R. R. Ra Ro Ro R. _ R. _ R. R. R. R. R. _ R. _ R. R. _ R. _ R R. _ R. _ R R. _ R. _ F R_i R_i R₂ R. R. R. R. R. R. R_i R, R_j R. R. R. R. _ R. _ F R_x R_y R_y R_y R. R. R. Re Re Re Re By By Re By Re B₂ B₂ B₂ Re By Re Ro Re Re Re By By R. R. R. R. R. R. Ra Ro Ra Ra Ra Ra R. R. R. Ra Ro Ro R. R. R. R. R. R. R. _ R. _ R. _ R. _ R. By Re Re $B_{\rm f}=B_{\rm f}=B_{\rm f}$ $B_{\rm f} = B_{\rm f} = E_{\rm f}$ Be _ Be _ Be $B_{\rm f} \equiv B_{\rm f} \equiv B_{\rm f}$ Ba Be Be Be Br Br

Experiment N7: Forecast for 2 Sins

0.8

0.7

06

([u]X)J

0.4

0.3

0.2

0.1

2_sins(): samples_train=70, samples_valid=30

Data: wind=7, horizon=1

swindow_serial_model + NNR+CircuitQNN: interpret=parity, qubits=3, layers=3, optimizer=COBYLA()



R2 for pred vs training data: Fake R2 for mean vs training data: MAPE for pred vs training data:

R2 for pred vs validation data: Fake R2 for mean vs validation data: MAPE for pred vs validation data: 0.4216243799816321 -0.15692687936155725 0.2766545159136265

0.594852151990251 -0.18588781421017253 0.2256624176380796

The sliding window serial model demonstrated good prediction of both seasonality and the signal amplitude.

25

50

75

The model does not re-upload data, however, it overloads TS data points.



Index n

100

125

This model can handle TS windows longer than the number of qubits available!

150

```
The model prediction significantly improved, well above the classical MLP!
```

175

200

Sliding Window Serial Model



y, qubits=3, layers=3, optimizer=COBYLA() Original function vs fit and predictions

Quantum neural networks Reflection

- QNNs are a promising approach to QTS forecasting.
- Unlike other QTS methods, QNNs are capable not only of data fitting but also pattern matching and prediction.
- However, the standard QNN model consisting of a feature map and a trainable ansatz, demonstrate poor performance when trained with more complex data.
- The proposed model for QTS forecasting, extends the single-qubit quantum Fourier serial model to work in a multi-qubit settings and more complex data.
- The model relies on the TS data continuity to reduce the need for re-uploading its input data, and instead overloads the qubits with blocks encoding the entire TS window of data points.
- The proposed model not only is able to encode more data than the number of its qubits, but the preliminary experiments also demonstrated the performance exceeding that of the classical MLP.



Other researchers in QNNs proposed quantum models of RNNs and LSTM! Bausch, Johannes. "Recurrent Quantum Neural Networks." Advances in Neural Information Processing Systems 33 (2020): 1368–79.

Chen, Samuel Yen-Chi, Shinjae Yoo, and Yao-Lung L. Fang. "Quantum Long Short-Term Memory." In ICASSP 2022-2022 IEEE International Conference on Acoustics, Speech and Signal Processing (ICASSP), 8622–26. IEEE, 2022.

Working with world data

- Our QTSA research features real-world applications. For example, our work involved records of beer sales in USA.
- The preliminary experiments indicate that more work is required to make the proposed model practical.
- The future work will include:
 - Adoption of different circuit measurement strategies and interpretation of results.
 - Inclusion of non-linearities to mimic NN activation functions.
 - Dealing with larger TS horizons and nonstationary TS
 - Most importantly: Exploration of avenues for QTSA to demonstrate real quantum advantage, e.g. in TS anomaly detection, adoption of stochastic TS analysis, etc.







Bird-view of Quantum Time Series Analysis Summary, reflections and questions

TS processing requires data storage Variational quantum regression is too simplistic QNNs with data re-uploading and overloading are key

Quantum systems have no memory



Quantum Fourier transforms are promising Variational quantum models effectively simulate memory

QC creates opportunities for TSA Quantum neural nets suggest the solution to QTSA

