WiDS

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December 2022

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2.1 Postulates of Quantum Mechanics

Quantum mechanics on its own is definitely not sufficient for solving physical systems rather, it only provides the framework for solving these systems, these quantum mechanics postulates would help us in building the bridge between mathematical tools of quantum mechanics and the physical systems that we need to solve. These postulates were developed over years of trial and errors and more often that not, we can not guess the motivation behind these postulates but it is important to understand what each postulate has to convey.

2.1.1 Postulate 1 - State space

Associated to any physical isolated system is a complex vector space with inner product (that is, a Hilbert space) known as the state space of the system . The system is defined completely by its state vector which is a unit vector in the system's state space. Like I mentioned earlier, Quantum mechanics is not sufficient to define a state of a particle for example: Consider a photon, to define the state of a photon, you need the knowledge of Quantum mechanics coupled with quantum electrodynamics. In the qubit system, any state vector can be defined as $\alpha |0\rangle + \beta |1\rangle$ where α and β are any two complex numbers, for this state vector to be normalised that is $\langle\phi|\phi\rangle = 1$, $|\alpha|^2 + |\beta|^2 = 1$

2.1.2 Postulate 2 - Evolution

Evolution of any closed system (that is, a system which is left undisturbed) is defined by any unitary operation, in other words, if the state of a system at any time 't' is $|\psi\rangle$, and at any later time t_1 $|\psi_1\rangle$, then there exists a unitary matrix U such that $|\psi_1\rangle = U |\psi\rangle$

The above postulate is only helpful in discrete time intervals, for the continous case, we define the schrodinger equation which states that :

$i\hbar \frac{d|\psi\rangle}{dt} = H |\psi\rangle$ where H is the unitary operator known as the hamiltonian operator.

2.1.3 Postulate 3 - Measurement

Quantum measurements are described by the set of measurement operators M_m where the index 'm' refers to the different possible outcomes of measurement. If the system is in a state $|\psi\rangle$ just before the measurement, then the probability of the measurement 'm' occurring is given by $\langle\psi| M^\dagger M |\psi\rangle$ and the state immediately after the measurement is $\frac{M_m|\psi\rangle}{\sqrt{\langle\psi|M^\dagger M|\psi\rangle}}$

The set of measurement operators should satisfy the completeness relation that is $\sum_m M^\dagger M = I$ The completeness relation ensures that the sum of all probabilities of the possible outcomes is 1.

An important example of the measurement operators is in the qubit system where $M_0 = |0\rangle\langle 0|$ and $M_1 = |1\rangle\langle 1|$. It can be easily verified that they satisfy the completeness relation.

2.1.4 Distinguishing quantum states

An important application of Postulate 3 is to distinguish quantum states, physical states can easily be distinguished , for example: we can always figure whether a coin lands on heads or a tails but distinguishing quantum states is much more complex in quantum mechanics. We figure out that states which are not orthonormal to each other can't be measured. If the states are orthonormal then, we can define measurement operators as $|\psi_i\rangle\langle\psi_i|$, these need to satisfy the completeness relation, and if the state is $|\psi_i\rangle$ at that time, then probability of measuring 'i' at that time comes out to be one using our measurement operator.Hence, we conclude that states can be measured if they are orthonormal to each other an can't be measured if they are not.

2.1.5 Projective measurements

A projective measurement is described by an observable, M, a Hermitian operator on the state space of the system being observed. The observable has a spectral decomposition : M = $\sum mP_m$ where P_m is the projector onto the eigen space of M with the corresponding eigen value m, the probability of getting result 'm' is given by : p(m) = $\langle\psi| P_m |\psi\rangle$, given that the output of the measurement was 'm' then, the state of the quantum system immediately after the measurement is $\frac{P_m|\psi\rangle}{\sqrt{p(m)}}$

Projective measurements are just a special case of measurement operators that we discussed in postulate 2 , the only difference being that here, in addition to satisfying the completeness relation, they also satisfy that the set of M_m are orthogonal projectors that is, the M_m are hermitian and satisfy $M_m M_m' = \delta_m m' M_m$.

2.1.6 POVM measurements

The postulate 3 that we discussed earlier has 2 aspects to it. First , it tells us about the respective probabilities of different outcomes of a particular measurement and second, it tells us about the state of the system after the measurement has taken place. However for a lot of cases, the state of the system post measurement is of little interest while the main interest is the probabilities of the measurements. In these systems where we measure the system only once, we use the mathematical tool of POVM which stands for 'Positive Operator Valued Measure'.

Suppose we define $E_m = M^\dagger M$, then from postulate 3 and elementary linear algebra, E_m is a positive operator such that $\sum_m E_m = I$ and $p_m = \langle\psi| E_m |\psi\rangle$.

Thus, the set of operators E_m are sufficient to measure the probabilities of the different measurement outcomes. The complete set of E_m is known as a POVM.

2.1.7 Phase

Phase is an important aspect of quantum mechanics. Consider a vector :$|\psi\rangle = e^{i^\theta} |\psi\rangle$, then $|\psi\rangle$ is said to be equal upto a global phase factor $'\theta'$ with respect to $|\psi\rangle$. However it can be shown that this phase factor has no impact on the statistics of measurement as for any particular outcome 'm' $\langle\psi| e^{-i\theta} M^\dagger M e^{i\theta} |\psi\rangle = \langle\psi| M^\dagger M |\psi\rangle$ .The other kind of phase is the relative phase consider $\frac{|0\rangle+|1\rangle}{\sqrt{2}}$ and $\frac{|0\rangle-|1\rangle}{\sqrt{2}}$, these two have the same amplitudes for the corresponding amplitudes but the qubit $|1\rangle$ has a relative phase factor of '-1'

2.1.8 Postulate 4 - Composite systems

The composite of many physical systems can be described as the tensor of several states , for example, consider states $|\psi_1\rangle, |\psi_2\rangle \ldots |\psi_n\rangle$ then the composite system can be defined as $|\psi_1\rangle \otimes |\psi_2\rangle \otimes \ldots |\psi_n\rangle$

3 Quantum Circuits

3.1 Quantum Algorithms

Many intriguing problems are practically hard to solve on a traditional computer due to the astronomical resources needed to do so, not because they are intractable in theory.

real-world examples of the issue The amazing potential of quantum computers is the creation of new algorithms that make it possible to solve issues that would otherwise require enormous amounts of computing power to solve.

3.2 Single qubit operations

Any single qubit is a vector of the form $|\psi\rangle$ = a$|0\rangle$ + b$|1\rangle$ where $|a|^2+|b|^2 = 1$

There are some major single qubit gates which are used to implement quantum circuits: The hadamard gate (H) : $\frac{1}{\sqrt{2}}\begin{bmatrix}1 & 1\\1 & -1\end{bmatrix}$

The Pauli-X gate (X) : $\begin{bmatrix}0 & 1\\1 & 0\end{bmatrix}$

The Pauli-Y gate (Y) : $\begin{bmatrix}0 & -i\\i & 0\end{bmatrix}$

The Pauli-Z gate (Z) : $\begin{bmatrix}1 & 0\\0 & -1\end{bmatrix}$

The Phase gate (S) : $\begin{bmatrix}1 & 0\\0 & i\end{bmatrix}$

The $\pi/8$ gate (T) : $\begin{bmatrix}1 & 0\\0 & i\end{bmatrix}$

4 Introduction to Quantum Machine learning

Machine learning algorithms learn a desired input-output relation from examples in order to interpret new inputs. This is important for tasks such as image and speech recognition or strategy optimisation, with growing applications in the IT industry. In the last couple of years, researchers investigated if quantum computing can help to improve classical machine learning algorithms. Ideas range from running computationally costly algorithms or their subroutines efficiently on a quantum computer to the translation of stochastic methods into the language of quantum theory. This contribution gives a systematic overview of the emerging field of quantum machine learning.

4.1 Classical Machine Learning

In the theory of machine learning, the term learning can be categorized as supervised, unsupervised and reinforcement learning.

1. Supervised Learning - In supervised learning, a computer is given examples of correct input-output relations and has to infer a mapping therefrom. Probably the most important task is pattern classification, where vectors of input data have to be assigned to different classes. This is something that we do in our everyday lives where we identify faces from different angles and light conditions as well.

2. Unsupervised Learning - For a long time, machine learning did not include unsupervised learning, which refers to the process of identifying patterns in data without the use of examples or past knowledge. Data clustering, or creating subgroups from a dataset, is a common job used to condense a big quantity of information into a small number of stereotypes.

3. Reinforcement Learning - This is a form of learning in which an agent ie usually a computer program that acts as a player in a game is either rewarded or punished based on the strategy it uses to win, a reward leads to reinforcement of the strategy while a punishment leads to adaptation of the strategy

4.2 Quantum Machine learning

The ability of quantum states to be in superposition of several states can lead to much faster computations since operations on many states can be done in the same time, Quantum gates are usually expressed as unitary matrices.

Quantum algorithms are created in quantum machine learning in order to utilise the effectiveness of quantum computing to tackle common machine learning challenges.

Typically, this is accomplished by making expensive classical algorithms or their time-consuming subroutines compatible with a hypothetical quantum computer. It is anticipated that such devices would soon be widely accessible for applications and be able to assist in processing the expanding amounts of global information. The new discipline also contains methodologies that work the other way around, notably well-proven machine learning techniques that can aid in extending and enhancing quantum information theory.

5 Implementation

The main of implementation is s the natural representation of quantum models as a Fourier-type sum

$$f_\theta(x) = \sum c_w(\theta)e^{iwx}$$

We use the nomenclature partial Fourier series to indicate the fact that only a subset of the Fourier coefficients are nonzero. The Fourier series formalism allows us to study quantum models using the rich techniques developed in Fourier analysis.

5.1 Quantum Models as partial fourier series

We define a (univariate) quantum model f_θ(x) as the expectation value of some observable with respect to a state prepared via a parametrised quantum circuit, i.e

$$f_\theta(x) = \left\langle U \middle| U^\dagger(x,\theta)MU(x,\theta)\right\rangle |U\rangle$$

The overall quantum circuit has the form:

$$U(x) = W^(l+1)S(x)W^lS(x).....W$$

The encoding strategy is very natural, since the physical control parameters of quantum dynamics usually enter as time evolutions of Hamiltonians – the most prominent example being Pauli rotations. This model includes "parallel encodings" that repeat the encoding on different subsystems, as well as "data reuploading", where the encoding is repeated multiple times in sequence. With a small amount of classical pre-processing this model includes even many quantum machine learning algorithms that are not based on the principles of parametrised circuits Our goal is to write f as a partial Fourier series

$$f(x) = \sum c_n e^{inx}$$

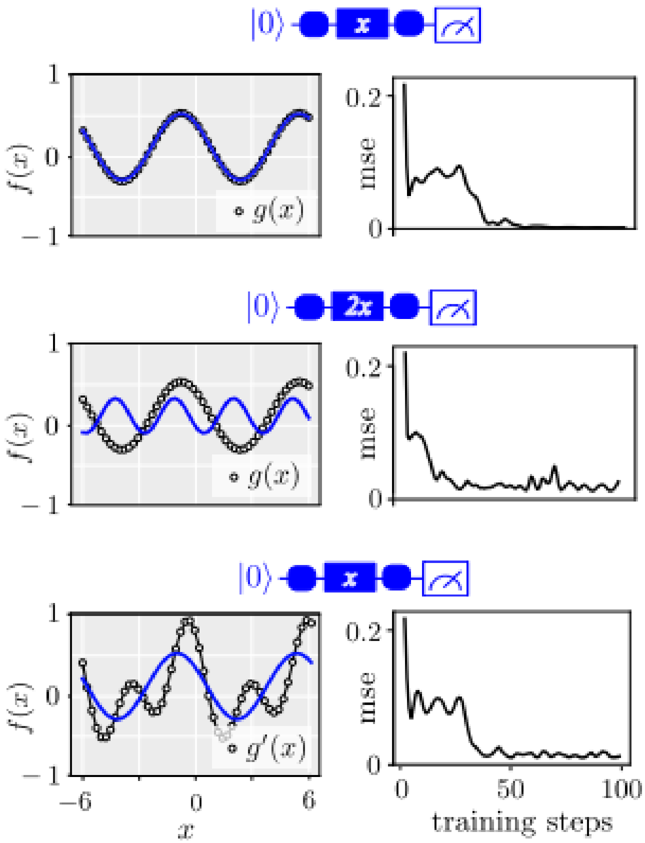
, After several manipulations we are able to express f(x) as

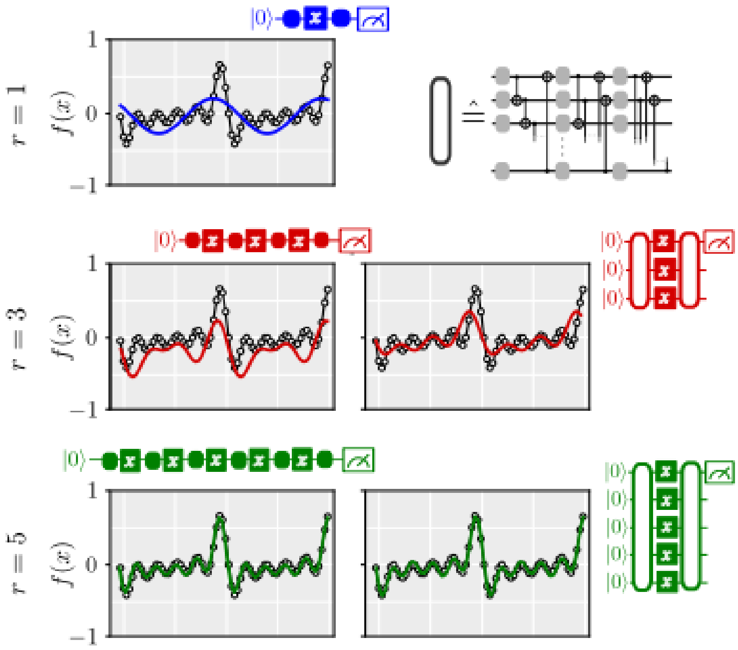
$$f(x) = \sum_{w \epsilon \omega} c_w e^{iwx}$$

where the coefficients are obtained by summing over all $a_{k,j}$ contributing to the same frequency. For both integer or non-integer frequencies, the expressivity of a quantum model is determined by two different properties: the frequency spectrum of the quantum model, including its size and degree, and the expressivity of the coefficients controlled by the model

5.2 Fitting Fourier series with serial Pauli-rotation encoding

First we will reproduce the following figures from the paper. These show how quantum models that use Pauli rotations as data-encoding gates can only fit Fourier series up to a certain degree. The degree corresponds to the number of times that the Pauli gate gets repeated in the quantum model. Let us consider circuits where the encoding gate gets repeated sequentially (as in Figure 2a of the paper). For simplicity we will only look at single-qubit circuits





We now move on to defining a target function- As a "ground truth" against which the quantum model must be consistent, we first define a (classical) goal function. The target function is built as a certain degree of Fourier series.

We also allow for a hyperparameter scaling, which we will also use in the quantum model, to rescale the data. The scaling of the quantum model and the target function must match, as demonstrated, for the quantum model to learn the classical model in the experiment below. This is a crucial finding for the development of quantum machine learning models. The weights will then need to be optimised to fit the actual data. The quantum model learns to suit the ground truth precisely with the starting settings and enough training steps. This is to be expected given that the degree of the ground truth Fourier series and the number of Pauli-rotation-encoding gates are both 1.

The fit will appear much less precise if the degree of the ground truth is higher than the quantum model's number of layers. Additionally, the data must be scaled correctly because fitting will fail even with sufficient encoding repetitions if one of the models changes the scaling parameter, which effectively scales the frequencies.

6 Fitting Fourier series with parallel Pauli-rotation encoding

Our next task is to repeat the function-fitting experiment for a circuit where the Pauli rotation gate gets repeated r times on different qubits, using a single layer L=1

As shown in the paper, we expect similar results to the serial model: a Fourier series of degree r can only be fitted if there are at least r repetitions of the encoding gate in the quantum model. However, in practice this experiment is a bit harder, since the dimension of the trainable unitaries W grows quickly with the number of qubits.

In the paper, the investigations are made with the assumption that the purple trainable blocks W are arbitrary unitaries. We could use the ArbitraryUnitary template, but since this template requires a number of parameters that grows exponentially with the number of qubits ($4 * *L - 1$ to be precise), this quickly becomes cumbersome to train. The alternative is PennyLane's StronglyEntanglingLayers layer structure, which, as its name implies, has a user-defined number of levels (which we will refer to as "ansatz layers" to avoid confusion). The model is trained in the same way as before, however it might take much longer this time. The default number of steps is 25, however you should raise it if necessary. Depending on your choices, small models with up to six qubits typically converge after no more than a few hundred steps.

6.1 Sampling Fourier coefficients

Since the expressivity of quantum models also depends on the Fourier coefficients the model can create, it is likely that even with enough repetitions of the data-encoding Pauli rotation, the quantum model cannot fit the circuit when we utilise the trainable ansatz above.

The Fourier coefficients from quantum models were taken as samples from a model family that was defined by an ansatz for the trainable circuit block. A function that numerically calculates the Fourier coefficients of a periodic function f with period 2π is required for this. A quantum model has to be defined right now. This could be any model, one of the aforementioned quantum models, one that makes use of a qubit or continuous-variable circuit. We will slightly modify the parallel qubit model() from above and apply the BasicEntanglerLayers ansatz this time. When experimenting with various quantum models, we discover that some quantum models produce distinct coefficient distributions from others. While StronglyEntanglingLayers will have a non-zero variance for all supported coefficients, BasicEntanglingLayers (with the default Pauli-X rotation) appears to have a structure that forces the even Fourier coefficients to zero.

Also we observe how, with increasing orders of the coefficients, the variance of the distribution reduces; this is a result of a Fourier series convergent phenomenon.

6.2 Conclusion

The paper raises a number of intriguing topics that are still open. First, can the framework created here aid in our understanding and quantification of the generalisation potential of quantum models, and hence meaningfully aid in the selection of models? Can one, in particular, compute useful contemporary generalisation measures [40] and use these for the creation of model-selection rules utilising the representation of a quantum model as a partial Fourier series? Second, we have demonstrated our universality finding using trainable circuit blocks with exponential depth (which provides a reasonable notion of asymptotic universality with respect to circuit depth). In actuality

however one is interested in depth-restricted trainable circuit blocks. Can one demonstrate the universality of such quantum models using trainable circuit blocks with constant, logarithmic, or polynomial depths? Our toolbox needs to be improved in order to comprehend how the design of the trainable circuit blocks affects the pool of Fourier coefficients that may be accessed in order to respond to this query. Finally, it's not yet apparent which specific applications quantum models would be well suited for or where they might have an advantage over more established methods like neural networks. Therefore, another question is if one may suggest natural applications for quantum machine learning using knowledge of the function class expressed by quantum models, as developed in our study.

7 References

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