Quantum Bayes AI

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Abstract
Quantum Bayesian AI (Q-B) is an emerging field that lever the computational gains available in Quantum computing. The promise is an exponential speed-up in many Bayesian algorithms. Our goal is to apply these methods directly to statistical and machine learning problems. We provide a duality between classical and quantum probability for calculating of posterior quantities of interest. Our framework unifies MCMC, Deep Learning and Quantum Learning calculations from the viewpoint from von Neumann’s principle of quantum measurement. Quantum embeddings and neural gates are also an important part of data encoding and feature selection. There is a natural duality with well-known kernel methods in statistical learning. We illustrate the behaviour of quantum algorithms on two simple classification algorithms. Finally, we conclude with directions for future research.

Key Words: Quantum Bayes, Quantum Deep Learning, Quantum Feature Extraction, Machine Learning, Quantum Algorithms, Quantum Embedding, Quantum Learning, Quantum Sensing, Quantum Entanglement, Quantum Encryption, Quantum MNIST.

1 Introduction
Quantum computers are devices that harness quantum mechanics to perform computations in ways that classical computers cannot. Quantum computing promises an exponential speed-up for Bayesian computation. Our goal is to provide a review of existing quantum algorithms with an emphasis on their applicability in Bayesian Learning. We view quantum embeddings as kernel methods and as such as central to modern day machine learning problems. Quantum state measurement is based on an idea of [Von Neumann](1932) where the state of a physical system is used to measure quantities of interest. Simulating the quantum system has counterparts in Bayesian learning such as MCMC simulation and Deep Learning. For recent reviews of quantum computing and its promise for big data analytics, see [Wang](2022); [Hidary](2021) and [Schuld and Killoran](2019); [Schuld](2021).

Von Neumann’s principle of quantum measurement is central to the initial data encoding problem. [Feynman](1986), in a seminal paper, discusses the implications of quantum physics for mechanical

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computational methods. From a statistical viewpoint, Smith (1984) and Breiman (2001) provide a framework for Bayesian computation and black box neural networks for data science in the 21st century. Whilst the quantum mechanics underlying the construction of a quantum computer is still in its infancy, there are many algorithms that are available for speed-up of existing methods. In a recent experiment, Google AI showed quantum supremacy in a stylized experiment.

Quantum embedding is an important part of the data encoding process and the type of functions that are easy to evaluate with quantum simulation. First, we create a density matrix of states of size $2^b \times 2^b$ from a $b$ Qubit computer. This will form the equivalent of the kernel space that is commonplace in learning methods. Machine learning methods essentially use linear algebra algorithms on this augmented feature space and quantum computers are directly applicable to such storage and calculations as they typically provide an exponential speed up in such algorithms, e.g. principal components, matrix inversion, Fourier transforms, inverse problem to a name a few.

The rest of the paper is outlined as follows. Section 1.1 provides a discussion of computability of functions (Church, Turing) and its implementation in prediction and learning. Section 1.2 provides a review of important quantum algorithms. Section 2 provides a review of quantum probability (Wang (2011)) and simulation. Von Neumann's approach to quantum measurement is also described with particular emphasis on MCMC simulation, Deep Learning and Quantum Simulation. Our goal is to provide a unified overview of such methods as they pertain to quantum encoding. This provides a unifying view for quantum implementation of machine learning algorithms and provides an avenue for determining extensions. Section 3 describes quantum Bayes AI methods including quantum embedding. Section 4 describes quantum machine learning methods. Section 5 provides an example to quantum MNIST. Finally, Section 6 concludes with directions for future research.

Much of the gains from quantum computing will be in regard to computability and representation of multivariate functions. Deep learning achieves this via a superposition of semi-affine functions whereas quantum computers use the Bloch sphere and a variety of quantum embeddings.

### 1.1 Computability of Functions

The central question is simply the speed and computability of functions. Church (1936) defines the so-called $\lambda$-calculus where $\lambda$ denotes a function. Turing (1937) famously wrote about computability of functions (a.k.a. predictive rules). The promise of quantum computation and physical measurement by simulation relies on the simple observation that it only takes a few dozen Qubits to be able to calculate a large superposition of functions. Compositions of functions (as opposes to additive structures) such as deep learners are also naturally computable. Computer languages such as Haskell are directly designed to perform such calculations. Polson and Sokolov (2020) provide a discussion of symbolic differentiation and manipulation for deep learning. Gradients are also easily computed using quantum simulation.

The fundamental problem is to reconstruct input-output representations. We first represent them using quantum 0–1 interaction terms. We represent it as a mixture (data augmentation of 0–1s) using quantum embedding, then simulate the solution to Schrodinger’s equation to provide the von Neumann measurement of the quantity of interest. Turing showed that you can represent an n dim function (boolean) $\{0,1\}^n \rightarrow \{0,1\}$. In $\lambda$-calculus and evaluate it as a composite function. Kolmogorov-Arnold theory discusses the representation of multivariate functions. Qubit activation allows you to represent Boolean functions and compute them quickly.

### 1.2 Quantum Algorithms

There are many quantum algorithms which include Grover’s algorithm, quantum Bayesian Shor’s factorization algorithm which has implications in cryptography and quantum versions of standard machine learning algorithms.
Quantum Cryptography: Shor’s Algorithm Shor’s quantum factoring algorithm has implications in cryptography and the strong Church-Turing thesis, see Wang and Liu (2022) for further discussion. For classical computer, finding all price factors of a given number is known to be $O(\exp(n^{1/3}\log^{2/3} n))$. Shor (1994) showed theoretically that quantum computer can factorize any number in $O(n^2 \log n \log \log n)$ operations. This has implications for Quantum Encryption.

Harrow (2020) shows how to use classical computers for data pre-processing and quantum computers for sampling and optimisation required to build a predictive model. This paper addresses the problem of loading a dataset onto a quantum computer. Computationally, this task is very expensive, however a pre-processing technique can be used to reduce the size of the training data set required by a quantum computer. Practically, also shows how the Grover algorithm can be used to solve several computational problems that arise in machine learning using a reduced data set. The problem is formulated as the following minimization problem

$$
\arg\min_{y \in Y} \sum_{x \in X} f(x, y)
$$

Here $Y$ indexes the set of candidate models, $X$ is the training data set and $f$ is a loss function.

Grover’s Algorithm As input for Grover’s algorithm, suppose we have a function

$$
f: \{0, 1, \ldots, N - 1\} \rightarrow \{0, 1\}.
$$

In the “unstructured database” analogy, the domain represent indices to a database, and $f(x) = 1$ if and only if the data that $x$ points satisfy the search criterion. We additionally assume that only one index satisfies $f(x^*) = 1$, and we call this index $x^*$. Our goal is to identify $x^*$.

Harrow’s Algorithm. This applies Grover’s algorithm to the fundamental estimator of Bayesian Machine learning, the MAP estimator, via the optimisation problem,

$$
\arg\min_{y \in Y} \sum_{x \in X} f(x, y) + \lambda \phi(y)
$$

where $\phi(y)$ is a regularisation penalty and $f(\cdot, \cdot)$ is an empirical loss function. See Peng et al. (2020) for further discussion.

Quantum Monte Carlo: Annealing and Tunneling This allows a speed up of traditional Monte Carlo algorithms based on the notion of quantum tunneling. As with all quantum measurement there is a preparation of states, denoted by $|\psi\rangle$, then a quantum device is used for evolution of states allowing the application of unitary transformation $U$. See Wang (2011, 2016, 2022) for further discussion and algorithmic details. Quantum annealing utilizes the physical process of a quantum system whose lowest energy, or equivalently, a ground state of the dynamic system, gives a solution to the posed Monte Carlo problem via the solution of the Schrödinger equation.

There are many applications of quantum algorithms. One area of application is in quantum sensing.

Quantum Sensing Degen et al. (2017) Quantum Sensing is an advanced sensor technology that improves the accuracy of how we measure, navigate, study, explore, see, and interact with the world around us by sensing changes in motion, and electric and magnetic fields. The analyzed data is collected at the atomic level.

2 Classical Learning

Supervised statistical learning given data as a sequence of input-output pairs. The goal is to determine a predictive rule for new input cases or to describe with statistical uncertainty is described by predictive distribution $p(y \mid x)$ of future observations.
How does one achieve such a goal given the empirical data of \(N\) input-output pairs \((y_i, x_i)_{i=1}^{N}\). We need to formulate an input-output map, \(y = f(x)\), the question is how to construct \(f\)?

The machine learning problem then is to find a good predictor rule from a training dataset if input-output pairs \((y_i, x_i)_{i=1}^{N}\) of observed data. The goal is to predict at a new high dimensional \(x_i = (x_{i1}, \ldots, x_{ip})\). To achieve good generalisability we need to be able to perform nonlinear dimension reduction and to find a suitable set of features/factors. Hence, machine learning algorithms rely on interpolation. Gaussian processes and deep learners provide two classes of interpolators that have been shown to do well in many fields of application. We will provide quantum speed-ups of Gaussian processes and a framework for quantum deep learning. An area of future research, is whether quantum representations provide other useful classes of interpolators.

Given a set of \((output, input)\) pairs \((y_i, x_i)_{i=1}^{N}\), the goal is simply to find a mapping (a.k.a. data transformation), denoted by \(\hat{f}\), where

\[ y_i = f(x_i) \]

and then to find a generalised prediction rule, that holds \(\forall x \in \mathcal{X}\), denoted by

\[ \hat{y}(x) = \hat{f}(x) \]

Here \(\hat{f}\) is estimated from the "training" dataset.

Bayesian predictive calculations start with a probabilistic model and map (a.k.a. data generating process), denoted by \(p(y|x)\). Under predictive mean squared error (MSE), the optimal rule is then given by the predictive mean

\[ \hat{y}(x) = E(y | x) = \sum_{y \in \mathcal{Y}} y \ p(y|x) \]

The use of latent (hidden) variables, denoted by \(z\), is also an important feature of Bayesian thinking. They can be viewed as "extending the art of the conversation", see [Lindley (1990)]. In quantum computing they can be viewed as states of a physical system. With latent variables, \(z\), we can write, the optimal predictive rule as

\[ \hat{y}(x) = E[E(y | x, z)] . \]

This is simply the law of total probability. The key insight is that it is easier to assess the inner expectations, the caveat being that we need to evaluate large sums which are tailored made for quantum computers. This includes the case of classification, where we need to evaluate classification probabilities \(p(y = 1 | x)\) via expectations of an indicator functions.

The predictive distribution is given by

\[ p(y|x) = \frac{p(x|y)p(y)}{p(x)} \]

The introduction of latent states, \(z\), allows the posterior to be broken into simpler parts

\[ p(y|x) = \sum_{z \in \mathcal{Z}} p(y|z, x) p(z|x) \]

Again we require enumeration over the latent states \(z\). These expectations can be calculated via von Neumann’s quantum measurement simulation as a state of a system. This is similar to the view of a particle filter where the researcher simulates a stochastic process whose marginals over time as realisations of the sequence of posterior distributions that one wishes to calculate.

3 Quantum Bayes AI

We begin with a basic review of classical and quantum probability to contrast the two approaches.
**Classical Probability.** In a simple coin tossing experiment, \( y \) takes one of two values \( \{0, 1\} \) with probability \( p_1, p_0 \) where \( p_1 = 1 - p_0 \). Here \( p_0, p_1 > 0 \) and \( \|p\|_1 = 1 \).

**Quantum Probability.** Quantum probability generalises this to the complex plane with the \( L^2 \)-norm for its complex coefficients. One can view this as a data transformation to the Bloch sphere which is shown in Figure 1.

![Figure 1: Bloch sphere](image)

**Qubit** Like a bit is a basic unit of information in traditional computing, the qubit is a basic quantum unit and it encodes a two-state quantum system, such as spin of the electron (up/down). We can measure a qubit (the simplest quantum system) and obtain either 0 with probability \( \|a_0\|^2 \) or 1 with probability \( \|a_1\|^2 \). Using Dirac’s notation, besides states \(|0\rangle \) and \(|1\rangle\), a qubit can also take states as their super-positions, which are linear combinations of the form

\[
|\psi\rangle = a_0|0\rangle + a_1|1\rangle
\]

where \( a_0, a_1 \in \mathbb{C} \) are called amplitudes such that \( \|a_0\|^2 + \|a_1\|^2 = 1 \). The notation \(|+\rangle = \frac{1}{2}|0\rangle + \frac{1}{2}|1\rangle\) is used for the halfway state generated by superposition.

Qubits can evaluate boolean functions quickly particularly deep learning representations based on superposition of affine functions. In general, a system of \( b \) qubits has \( 2^b \) computational basis states of the form \(|x_1 x_2 \ldots x_b\rangle\) where \( x_j = 0, 1 \) and \( 1 \leq j \leq b \) that generate a \( 2^b \)-dim complex vector space and a superposition state that is based on \( 2^b \)-amplitudes. Hence, we only need a system of a few dozen 'qubits' to provide a significant increase in computational speed as \( 2^{52} \approx 10^{16} \). A system with \( b = 500 \) qubits would have the ability to model more than the number of atoms in the universe.

**Quantum Entanglement.** Quantum entanglement is the physical phenomenon that occurs when a group of particles are generated, interact, or share spatial proximity in a way such that the quantum state of each particle of the group cannot be described independently of the state of the others, including when the particles are separated by a large distance. The topic of quantum entanglement is at the heart of the disparity between classical and quantum physics: entanglement is a primary feature of quantum mechanics lacking in classical mechanics.

**Quantum Von Neumann Measurement.** The idea is to 'measure' the ensemble sum via the simulation of the physical system. A quantum state is completely described by density operators. A vector \(|\psi\rangle \in \mathbb{H}\) corresponds to a density operator \( \rho = |\psi\rangle \langle \psi| \) the projection onto \(|\psi\rangle\). An ensemble state \( \rho_k \) with probability \( p_k \) of being in vector \(|\psi_k\rangle\) has density operator

\[
\rho_k = \sum_{k=1}^{K} p_k |\psi_k\rangle \langle \psi_k|
\]
Suppose that $\rho$ is generated by a $b$-qubit state, creating a $2^b \times 2^b$-Hermitian density matrix.

**Quantum Features.** From a data analytic and Bayesian learning perspective, one can think of the mapping $\rho : x \rightarrow \rho(x)$ as a fixed feature map providing a data encoding from $X$ to density matrices. This quantum embedding is the equivalent of feature selection in machine learning (see Hoadley, 2000, Bhadra et al 2022, Polson, Sokolov, Xu (2022)) and is an important part of which class of functions that can be represented by quantum neural networks. The corresponding quantum kernel is

\[ k(x, x') = \text{tr}(\rho(x)\rho(x')) \]

with the space of functions, for weight operator $W$ being of the form

\[ f_W(x) = \text{tr}(\rho(x)W) \]

For example, Kernel ridge regression $y = f_W(x) + \epsilon$ will be straightforward to calculate using quantum simulation and von Neumann measurement.

Specifically, if $|\psi(t)\rangle$ is the state of the quantum system, then $|\psi(t_1)\rangle$ and $|\psi(t_2)\rangle$ are related by

\[ |\psi(t_2)\rangle = U(t_1, t_2)|\psi(t_1)\rangle \quad \text{with} \quad U(t_1, t_2) = e^{iH(t_2 - t_1)} \]

where $U$ is a unitary operator and $H$ is a Hamiltonian. In practice this operator has to be discretized in simulation via Trotter’s (1959) formula. The Trotter’s formula approximates $e^{-iH\delta}$ by $U_\delta$, which requires only the evaluation of each $e^{-iH_l\delta/2}$, where

\[ U_\delta = [e^{-iH_1\delta/2}, \ldots, e^{-iH_L\delta/2}][e^{-iH_1\delta/2}, \ldots, e^{-iH_L\delta/2}] \]

see also Wang (2011).

With a quantum state prepared in a physical state, $\rho$, the observable $Y$ with values in $\{y_1, \ldots, y_M\}$ has a probability distribution

\[ p_\rho(Y = y) = \text{tr}(\rho Q_{y}) = \sum_{j=1}^{M} y_j p_\rho(Y = y_j) \]

The equivalence between everything can be thought of as an iterative map (a.k.a. stochastic simulation)

### 3.1 General Paradigm

This allows us to construct a general paradigm for quantum measurement in machine learning.

**Quantum Simulation** Here the initial complex state is subject to a unitary transformation

\[ |\psi(t)\rangle = U^t|\psi(0)\rangle \]

where $U = e^{-iH}$ is a unitary operator with $UU^\dagger = 1$ and $H$ is the Hamiltonian of the system.

In continuous-time we can argue as follows. The heat equation simulation is to solve Schrödinger’s equation

\[ i\frac{\partial |\psi(t)\rangle}{\partial t} = H|\psi(0)\rangle \]

starting from initial state $|\psi(0)\rangle$ with solution

\[ |\psi(t)\rangle = e^{-iHt}|\psi(0)\rangle \]

The numerical evaluation of $e^{-iHt}$ is needed and this requires discretization using Trotter’s formula (Trotter, 1959).
MCMC Simulation Here the initial probabilistic state $p^{(0)}$ is subject to a stochastic transition matrix, $P$, that is time reversible and the evolution of the system is given by

$$p^{(t)} = P^t p^{(0)}$$

In continuous-time $P$ can be generated by the infinitesimal generator (which takes the place of the Hamiltonian in the quantum system)

Deep Learning Here the initial state $x^{(0)}$ is subject to an iterate map (with $t$-layers)

$$x^{(t)} = F^t x^{(0)}$$

where the map $F$ is a composition of ridge functions (see Polson, Sokolov and Xu, 2022).

Hence, from the von Neumann measurement viewpoint, all there methods can be though of as symbolic manipulation of linear operators leading to the physical evaluation of the quantity of interest. The main advantage of quantum systems is the exponential speed up as you can directly calculate the sums need for Bayesian learning, Expectations and Predictive rules which we discuss in Section 3. Deep learners have the advantage of representing multivariate functions.

3.2 Quantum Data Encoding

As data grows in scale and complexity and algorithms such as deep learning become more elaborate, computational techniques become ever more important.

Quantum Superposition An intrinsic difference exists between bit representation in classical and quantum systems. All classical algorithms prevent the simultaneous occurrence of their states. The quantum system allows for simultaneous occurrence of their states. The computational basis takes the form $|x_1, x_2, \ldots, x_b\rangle$, where $x_j = 0, 1, j = 1, \ldots, b$. Any quantum superposition state is a linear combination of $2^b$ possible base states whose complex coefficients are called amplitudes. A $b$-qubit state $|\psi\rangle$ may take a superposition state of the form

$$|\psi\rangle = \sum_{x_1, x_2, \ldots, x_b} \alpha_{x_1, x_2, \ldots, x_b} |x_1, x_2, \ldots, x_b\rangle, \text{ s.t. } \sum_{x_1, x_2, \ldots, x_b} |\alpha_{x_1, x_2, \ldots, x_b}|^2 = 1.$$

Quantum Gates and Circuits. There are many gates and circuits that can be used to transform quantum probabilities on the Bloch sphere. For example, one of the simplest gate is a quantum NOT gate maps $|0\rangle$ to $|1\rangle$ and $|1\rangle$ to $|0\rangle$ and transforms $|\psi\rangle = \alpha_0|0\rangle + \alpha_1|1\rangle$ into $|\psi\rangle = \alpha_0|1\rangle + \alpha_1|0\rangle$. The quantum NOT gate can be represented by the Pauli gate matrix

$$
\begin{pmatrix}
1 & 0 \\
0 & 1
\end{pmatrix},
$$

which has the property of being a unitary operator in $\mathbb{C}^2$. Figure 2 shows other quantum gates.
Figure 2: Quantum Gates

Another useful data Encoding gate is the rotational gate. Here the encoding gate $U_\rho(x)$ transforms data samples $x = (x_1, \ldots, x_n) \in \mathbb{R}^n$ into a quantum state

$$|x\rangle = U_\rho(x) |0\rangle = R_z(x_1) \otimes R_x(x_2) \otimes \ldots \otimes R_x(x_n) |0\rangle^{O \times n},$$

where

$$R_x(x) = e^{-i\phi x/2} = \begin{pmatrix} \cos(\phi/2) & -i \sin(\phi/2) \\ -i \sin(\phi/2) & \cos(\phi/2) \end{pmatrix}.$$

We will discuss the application of these later in the our discussion of Quantum Neural Networks. Now we describe quantum entanglement.

### 4 Quantum Machine Learning

Schuld (2021) makes an important observation that, though quantum models maps data into a high-dimensional feature space, they can be trained and selected in a low-dimensional subspace. With the density matrices $\rho(x)$ given by some embedding as feature vectors, quantum machine learning models are linear in the feature space. And borrowing ideas from classical machine learning kernel theory, similar results can be derived from the quantum kernel $k(x, x') = \text{tr}(\rho(x')\rho(x))$. For example, the optimal models that minimise the cost is linear expansion in terms of quantum kernel functions:

$$f(x) = \sum_{m=1}^M \alpha_m \text{tr}(\rho(x^m)\rho(x))$$

where $x^m, m = 1, \ldots, M$ are training data. Hence, searching for the optimal model based on a given dataset is essentially an $M$-dimensional optimisation problem. Furthermore, by choosing a convex loss function, this helps avoid the barren plateaus in variational training and guarantees the optimality.

#### 4.1 Quantum Kernels

Quantum kernel, the inner product of two feature vectors $\rho(x')$ and $\rho(x)$, depends on the underlying data-encoding $\phi(x)$:

$$k(x, x') = \text{tr}(\rho(x')\rho(x)) = |\langle \phi(x')| \phi(x) \rangle|^2.$$

The simple amplitude encoding is defined as

$$\phi(x) = |x\rangle \langle x| = \sum_{i,j=1}^N x_i x_j^* |i\rangle \langle j|$$
where $x$ is normalized such that $\|x\|^2 = \sum_i x_i^2 = 1$ and $i, j$ are computational basis. The induced kernel is $k(x, x') = |\langle x'|x \rangle|^2 = |x^\dagger x'|^2$.

Other interesting and common strategies including: basic encoding $\phi(x) = |\langle i'_x i_x \rangle|^2$ which gives the Kronecker kernel $k(x, x') = \delta_{x,x'}$ where the input binary string $x$ is represented by the integer $i_x = \sum_{k=0}^{n-1} 2^k x_k$, and coherent state encoding which gives a Gaussian kernel. There is resemblance between quantum kernels and classical machine learning kernels, and many of them have Fourier representation.

### 4.2 Quantum Models

A quantum model is defined as the expectation of the measurement $\mathcal{M}$ under the density matrix $\rho(x)$,

$$f(x) = \text{tr}(\rho(x)\mathcal{M})$$

and the measurement $\mathcal{M}$ can always be expressed as a linear combination of $\rho(x^k)$ where $x^k$ are from the data domain. More specifically, there exist $\{x^k, k = 1, 2, \ldots\}$, such that

$$\text{tr}(\rho(x)\mathcal{M}) = \text{tr}(\rho(x)\mathcal{M}_{exp})$$

for all $x$, where $\mathcal{M}_{exp} := \sum_k \gamma_k \rho(x^k)$. More importantly, this indicates that any quantum model can be represented as

$$f(x) = \text{tr} \left( \rho(x) \left( \sum_k \gamma_k \rho(x^k) \right) \right) = \sum_k \gamma_k k(x^k, x)$$

### 4.3 Optimizing Quantum Models

The representor theorem states that the optimal quantum models which minimize the regularized empirical risk,

$$\frac{1}{M} \sum_{m=1}^{M} L(y^m, f(x^m)) + \gamma \|f\|_F^2$$

admits a representation of the form

$$f(x) = \sum_{m=1}^{M} \alpha_m k(x^m, x)$$

Here $x^m$ are training samples and $F$ is the reproducing kernel Hilbert space (RKHS) corresponding the encoding. Hence, the optimisation over the regularized empirical risk is the same as finding the optimal measurement $\mathcal{M}$. The vectorized $\mathcal{M}_{opt}$ is the familiar form

$$|\mathcal{M}_{opt}\rangle = \sum_m y^m \left( \sum_{m'} |\rho(x^{m'})\rangle \langle \rho(x^{m'})| \right)^{-1} |\rho(x^m)\rangle,$$

This is analogous to the ordinary least square result for regression coefficients as quantum models are linear in feature space.
4.4 Quantum FFT

The quantum Fourier transform is naturally calculated in a quantum measurement system as it is already expressed in rotational form.

The QFT takes a “position” state \( |x\rangle \) to the corresponding momentum state \( |p\rangle \) and is defined as follows

\[
\text{QFT}_q(x) = \frac{1}{\sqrt{q}} \sum_{p=0}^{q-1} \exp(i px/q) |p\rangle,
\]

where \( q \) is the dimension of the systems Hilbert space. See Weinstein et al. (2001) for further discussion.

In terms of gates, the two but QFT corresponds to the unitary operator

\[
\text{QFT}_4 = \frac{1}{2} \begin{pmatrix}
1 & -1 & 1 & 1 \\
1 & i & -1 & -i \\
1 & -1 & 1 & -1 \\
1 & -i & -1 & i
\end{pmatrix}
\]

Then we can simulate system forward in an iterative manner as described in our general paradigm.

4.5 Quantum Linear Regression

In a high dimensional regression setting, we need to calculate \( \hat{\beta} = X^T y \) where \( X^T \) is the Moore-Penrose pseudo-inverse of \( X \). The singular decomposition can be computed as \( X^T = V \Sigma^{-1} U^T \) and hence represented as a quantum state, see Schuld et al. (2016). Then we need to calculate

\[
\bar{\beta} = \sum_{k=1}^{K} \sigma_k^{-1} v_k u_k^T y
\]

The optimal prediction rule under MSE, is given by

\[
\hat{y}(x) = \sum_{k=1}^{K} \sigma_k^{-1} x^T v_k u_k^T y
\]

We need to calculate a set of inner products with is easily computable using a quantum computer which are naturally designed to calculate inner products. See Harrow et al. (2009) for further discussion.

4.6 Quantum Gaussian Process Q-GP

A quantum algorithm for Gaussian process regression was introduced in Zhao et al. (2019). The GP predictor is

\[
\hat{f}_* = k_*^T (K + \sigma^2 I_n)^{-1} y,
\]

depending on whether the goal is to compute the mean or variance, we choose \( |b\rangle = |y\rangle \) or \( |b\rangle = |k_*\rangle \), where \( k_* = k(x_*, x_*) \) is the covariance of the target point with itself, with the corresponding formula for the predictive variance. The quantum GP algorithm simulates \( K + \sigma^2 I_n \) as a Hamiltonian acting on an input state \( |b\rangle \). Then performs quantum phase estimation to extract estimates of the eigenvalues of \( K_n^2 I_n \) and stores them as a weighted superposition and then creates the desired prediction. Schuld (2021) show how to provide estimates of

\[
k_*^T (K + \sigma^2 I_n)^{-1} y \quad \text{and} \quad k_*^T (K + \sigma^2 I_n)^{-1} k_*,
\]

written as two inner products.
4.7 Quantum Stochastic Gradient Descent (Q-SGD)

Gradients are much easier to calculate in quantum systems. This is due to the following property of unitary transformations. To implement the gradient descent, we approximate the derivative of the loss function by taking the symmetric difference,

\[
\frac{df}{dx}(x) = \frac{f(x + \epsilon) - f(x - \epsilon)}{2\epsilon} + O(\epsilon^2). \tag{1}
\]

However the gradient can be analytically calculated when we use the following unitary operators

\[
\exp(i \theta \Sigma) \tag{2}
\]

where \( \Sigma \) is a generalized Pauli acting on a few qubits, that is, \( \Sigma \) is a tensor product of operators from the set \( \{\sigma_x, \sigma_y, \sigma_z\} \) acting on a few qubits. The derivative with respect to \( \theta \) gives an operator whose norm is bounded by 1. Therefore, the gradient of the loss function with respect to \( \vec{\theta} \) is bounded by \( L \), the number of parameters.

For this function the gradient is the generalised Pauli operator \( \Sigma_k \)

\[
\frac{d\text{loss}(\vec{\theta}, z)}{d\theta_k} = 2 \text{Im} \left( \langle z, 1 | U | z, 1 \rangle \right) \tag{3}
\]

Note that \( Y_{n+1} \) and \( \Sigma_k \) are both unitary operators. Define the unitary operator

\[
\mathcal{U}(\vec{\theta}) = U_1^1 ... U_L^1 Y_{n+1} U_{n+1} ... U_k^1 \Sigma_k U_k ... U_1 \tag{4}
\]

No we can express the gradient as

\[
\frac{d\text{loss}(\vec{\theta}, z)}{d\theta_k} = 2 \text{Im} \left( \langle z, 1 | \mathcal{U} | z, 1 \rangle \right). \tag{5}
\]

Here, we can think of \( \mathcal{U}(\vec{\theta}) \) as a quantum circuit composed of \( 2L + 2 \) unitaries each of which depends on only a few qubits. The quantum device allows \( \mathcal{U}(\vec{\theta}) \) to act on \( |z, 1\rangle \). Using an auxiliary qubit we can measure the right-hand side of (5). We start with

\[
|z, 1\rangle \frac{1}{\sqrt{2}} \left( |0\rangle + |1\rangle \right) \tag{6}
\]

and act with \( i \mathcal{U}(\vec{\theta}) \) conditioned on the auxiliary qubit being 1. This leads to

\[
\frac{1}{\sqrt{2}} \left( |z, 1\rangle + i \mathcal{U}(\vec{\theta}) |z, 1\rangle |0\rangle \right) \tag{7}
\]

Performing a Hadamard on the auxiliary qubit gives

\[
\frac{1}{2} \left( |z, 1\rangle + i \mathcal{U}(\vec{\theta}) |z, 1\rangle |0\rangle \right) + \frac{1}{2} \left( |z, 1\rangle - i \mathcal{U}(\vec{\theta}) |z, 1\rangle |1\rangle \right). \tag{8}
\]

Now measure the auxiliary qubit. The probability to get 0 is

\[
\frac{1}{2} - \frac{1}{2} \text{Im} \left( \langle z, 1 | \mathcal{U}(\vec{\theta}) | z, 1 \rangle \right) \tag{9}
\]

Thus, by making repeated measurements we can get a good estimate of the imaginary part becomes an estimate of the \( k \)’th component of the gradient.
We demonstrate an application of a quantum neural network to the problem of image classification. It is assumed that input is an image that is represented as a sequence of \( n \) elements \( z = (z_1, \ldots, z_n) \), with each \( z_i \) being +1 or -1. The output \( l(z) \) is also binary and takes values +1 and -1. The basic building block of a quantum neural network is a unitary operator \( U_a(\theta) \).

We assume that this operator acts on a subset of the qbits and is defined by parameter \( \theta \). Then the neural network is a composition of those unitary operators.

\[
U(\theta) = U_L(\theta_L)U_{L-1}(\theta_{L-1}) \ldots U_1(\theta_1).
\]

Assume our output (readout) bit is 1, then the corresponding input \( z \), we construct a computational basis

\[
|z, 1\rangle = |z_1, \ldots, z_n, 1\rangle.
\]

Applying our neural network to the input \( z \) gives the state

\[
U(\theta)|z, 1\rangle.
\]

Then on the readout qubit, we measure a Pauli operator \( \sigma \) which give us +1 or -1. The goal is that this outcome matches the true label of the data (e.g. image). Given that the outcome is uncertain, we can use multiple copies of the outputs and then average them out.

**Quantum Empirical Loss.** Then to train a quantum model, we use the following loss function

\[
\text{loss}(\vec{\theta}, z) = 1 - l(z) \langle z, 1|U(\vec{\theta})^\dagger Y_{n+1}U(\vec{\theta})|z, 1\rangle.
\]

**Quantum TensorFlow: MNIST** Now we illustrate how to use Tensorflow-Quantum [Broughton et al., 2021] to demonstrate the quantum computing. We will demonstrate how quantum computing works for the problem of binary classification. Our framework described above has a binary readout bit, and we train a model to discriminate between digits 3 and 6 in the MNIST dataset.

To represent the image as a sequence of +1 and -1 elements, we downscale MNIST data set so that each image is 4×4 and fits into a quantum computer.

```python
x_train_small = tf.image.resize(x_train, (4,4)).numpy()
x_test_small = tf.image.resize(x_test, (4,4)).numpy()
```

Since, we introduce each pixel with a qbit, we make the data set binary. We do it by simply “thresholding” the pixel values.

```python
THRESHOLD = 0.5
x_train_bin = np.array(x_train_nocon > THRESHOLD, dtype=np.float32)
x_test_bin = np.array(x_test_small > THRESHOLD, dtype=np.float32)
```

Figure 5 shows the original image of digit 6 and compares it with the downscale image as well as binary image.
Then we “flatten” the image into a vector and rotate each +1 qbit using an X gate. We use the cirq library that allows to write, manipulate, and optimize quantum circuits, and then running them on a simulated quantum computer.

```python
values = np.ndarray.flatten(image)
qubits = cirq.GridQubit.rect(4, 4)
circuit = cirq.Circuit()
for i, value in enumerate(values):
    if value:
        circuit.append(cirq.X(qubits[i]))

Then we convert each image to TensorFlow Quantum circuits

x_train_tfcirc = tfq.convert_to_tensor(x_train_circ)

The figure below shows an example of a single quantum circuit layer.

![Quantum Circuit Layer](image)

Figure 4: Example of a Layer of a Quantum Neural Network

The resulting model predicts the label of an image rather well. In fact, the accuracy is comparable to the accuracy of a classical neural network.
6 Discussion

Whilst quantum hardware in its infancy, the theoretical and quantum algorithms are well-developed. Our goal is to show how to apply these to machine learning and AI. In many cases, quantum von Neumann measurement provide an exponential speedup in computations. We outline a unified framework for quantum machine learning algorithms. We embed regression and classification methods, Bayesian learning, MCMC simulations [Hammersley and Handscomb (1964)] and deep learning into quantum measurement systems. As with ML algorithms, quantum ML uses kernel methods and feature extraction. Again storage and calculations of inner products and matrix inversions provide exponential increases in speed.

Harnessing the power of quantum computing is one of the challenges in the 21st century.

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