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Quantum-enhanced machine learning: Implementing a quantum k-nearest neighbour algorithm

Bachelor Thesis

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Preface

Blah blah ...

Contents

Abstract	v
Nomenclature	vii
1 Introduction	1
1.1 Motivation	2
1.2 Research Question	2
2 Theoretical Foundations	3
2.1 Quantum Bits	3
2.1.1 Single Qubit Systems	3
2.1.2 Multiple Qubit Systems	5
2.2 Quantum Logic Gates	8
2.2.1 Single Qubit Gates	8
2.2.2 Multiple Qubit Gates	11
2.3 Classical Machine Learning	12
2.3.1 k-nearest Neighbour Algorithm	12
2.3.2 Algorithmic complexity	14
3 Methods	17
3.1 Liqui \rangle	17
3.2 IBM Quantum Experience	18
4 Literature Review: Quantum-enhanced Machine Learning	20
4.0.1 Quantum State Preparation Algorithms	20
4.0.2 Quantum k-nearest Neighbour Algorithm	24
5 Results and Discussion	28
5.1 Simulating the qubit-based kNN algorithm	28
5.2 Development of an amplitude-based kNN algorithm	31
6 Outlook	35
7 Conclusion	36
8 Personal reflection	37
References	38

Abstract

NEEDS MODIFICATION!

Quantum machine learning, the intersection of quantum computation and classical machine learning, bears the potential to provide more efficient ways to deal with big data through the use of quantum superpositions, entanglement and the resulting quantum parallelism. The proposed research will attempt to implement and simulate two quantum machine learning routines and use them to solve small machine learning problems. That will establish one of the earliest proof-of-concept studies in the field and demonstrate that quantum machine learning is already implementable on small-scale quantum computers. This is vital to show that an extrapolation to larger quantum computing devices will indeed lead to vast speed-ups of current machine learning algorithms.

Nomenclature

Symbols

\otimes	Tensor product	
i	Imaginary unit	$i = \sqrt{-1}$
\dagger	Hermitian conjugate	Complex conjugate transpose
$!$	Factorial	e.g. $3! = 3*2*1$

Indices

a	Ambient
air	Air

Acronyms and Abbreviations

RAM	Random-access memory
GB	Gigabyte
QML	Quantum machine learning
QC	Quantum computer
Prob	Probability
PM	Post-measurement
HD	Hamming distance
CM	Conditional measurement
CNOT	Controlled NOT gate
CCNOT	Controlled controlled NOT gate (Toffoli gate)
CU	Controlled U gate (where U can be any unitary quantum gate)

Chapter 1

Introduction

SOME MORE GENERAL INTRO TEXT HERE?

The ability to understand spoken language, to recognize faces and to distinguish types of fruit comes naturally to humans, even though these processes of pattern recognition and classification are inherently complex. Machine learning (ML), a subtopic of artificial intelligence, is concerned with the development of algorithms that perform these types of tasks, thus enabling computers to find and recognise patterns in data and classify unknown inputs based on previous training with labelled inputs. Such algorithms make the core of e.g. human speech recognition and recommendation engines as used by Amazon.

According to IBM (2016b), approximately 2.5 quintillion (10^{18}) bytes of digital data are created every day. This growing number implies that every area dealing with data will eventually require advanced algorithms that can make sense of data content, retrieve patterns and reveal correlations. However, most ML algorithms involve the execution of computationally expensive operations and doing so on large data sets inevitably takes a lot of time (Bekkerman, Bilenko, & Langford, 2011). Thus, it becomes increasingly important to find efficient ways of dealing with big data.

A promising solution is the use of quantum computation which has been researched intensively in the last few decades. Quantum computers (QCs) use quantum mechanical systems and their special properties to manipulate and process information in ways that are impossible to implement on classical computers. The quantum equivalent to a classical bit is called a quantum bit (qubit) and additionally to being in either state $|0\rangle$ or $|1\rangle$ it can be in their linear superposition.

This peculiar property gives rise to so-called quantum parallelism, which enables the execution of certain operations on many quantum states at the same time. Despite this advantage, the difficulty in quantum computation lies in the retrieval of the computed solution since a measurement of a qubit collapses it into a single classical bit and thereby destroys information about its previous superposition. Several quantum algorithms have been proposed that provide exponential speed-ups when compared to their classical counterparts with Shor's prime factorization algorithm being the most famous (Shor, 1994). Hence, quantum computation has the potential to vastly improve computational power, speed up the processing of big data and solve certain problems that are practically unsolvable on classical computers.

Considering these advantages, the combination of quantum computation and classical ML into the new field of quantum machine learning (QML) seems almost natural. There are currently two main ideas on how to merge quantum computation with ML, namely a) running the classical algorithm on a classical computer and outsourcing only the computationally intensive task to a QC or b) executing the quantum version of the entire algorithm on a QC. Current QML research mostly focusses on the latter approach by developing quantum algorithms that tap into the full potential of quantum parallelism.

1.1 Motivation

Classical ML is a very practical topic since it can be directly tested, verified and implemented on any commercial classical computer. So far, QML has been of almost entirely theoretical nature since the required computational resources are not in place yet. To yield reliable solutions QML algorithms often require a relatively large number of error-corrected qubits and some sort of quantum data storage such as the proposed quantum random access memory (qRAM) (Giovannetti, Lloyd, & Maccone, 2008). However, to date the maximum number of superconducting qubits reportedly used for calculation is nine, the D-Wave II quantum annealing device delivers 1152 qubits but can only solve a narrow class of problems and a qRAM has not been developed yet (O'Malley et al., 2016; D-Wave, 2015). Furthermore, qubit error-correction is still a very active research field and most of the described preliminary QCs deal with non error-corrected qubits with short lifetimes and are, thus, impractical for large QML implementations.

Until now there have been only few experimental verifications of QML algorithms that establish proof-of-concept. Li, Liu, Xu, and Du (2015) successfully distinguished a handwritten six from a nine using a quantum support vector machine on a four-qubit nuclear magnetic resonance test bench. In addition, Cai et al. (2015) were first to experimentally demonstrate quantum machine learning on a photonic QC and showed that the distance between two vectors and their inner product can indeed be computed quantum mechanically. Lastly, Ristè et al. (2015) solved a learning parity problem with five superconducting qubits and found that a quantum advantage can already be observed in non error-corrected systems.

Considering the gap between the number of proposed QML algorithms and the few experimental realisations, it remains important to find QML problems which can already be implemented on small-scale QCs. Hence, the purpose of this study is to provide proof-of-concept implementation of selected QML algorithms on small datasets. This is an important step in the attempt to shift QML from a purely theoretical research area to a more applied field such as classical ML.

1.2 Research Question

Don't know where this should go!

Matthias Troyer citation for this part:

There are many different ways of realising a QC such as using trapped ions, single photon sources or superconducting Josephson junctions, etc. Depending on the chosen substrate, different sets of quantum logic gates can be implemented and in order to run a quantum algorithm it has to be mapped to the available hardware. Thus, quantum algorithms have to be translated (compiled) into a series of gates consisting only of quantum gates from the available gate set. This is referred to as *quantum compilation*.

Finding optimal ways of compiling a given quantum algorithm as well as designing a high-level programming language or environment similar to that of classical computer code editors is called *quantum software engineering*.

In light of the theoretical nature of current QML research and the small number of experimental realizations, this research will address the following question:

How can a theoretically proposed k-nearest neighbour quantum machine learning algorithm be implemented on small-scale quantum computers?

The following sections will outline the steps required and the tools used in order to answer this research question.

Chapter 2

Theoretical Foundations

CHECK FOOTNOTE NUMBERS IN WHOLE DOCUMENT! INTRODUCE THE NOTION OF QUANTUM REGISTER SOMEWHERE!

2.1 Quantum Bits

2.1.1 Single Qubit Systems

Classical computers manipulate bits, whereas quantum computer's most fundamental unit is called a quantum bit, often abbreviated as qubit. Bits as well as qubits are binary entities, meaning they can only take the values 0 and 1.

A good example for a physical implementation of a qubit is the single electron of a hydrogen atom sketched in Fig. 2.1. Usually, the electron is found in its ground state which one can define as the $|0\rangle$ state of the qubit. Using a laser pulse the electron can be excited into the next highest valence shell which one can define as the $|1\rangle$ state of the qubit. After some time t the electron will decohere to its ground state ($|0\rangle$) which is called the longitudinal coherence or amplitude damping time and is an important parameter for measuring qubit lifetimes.

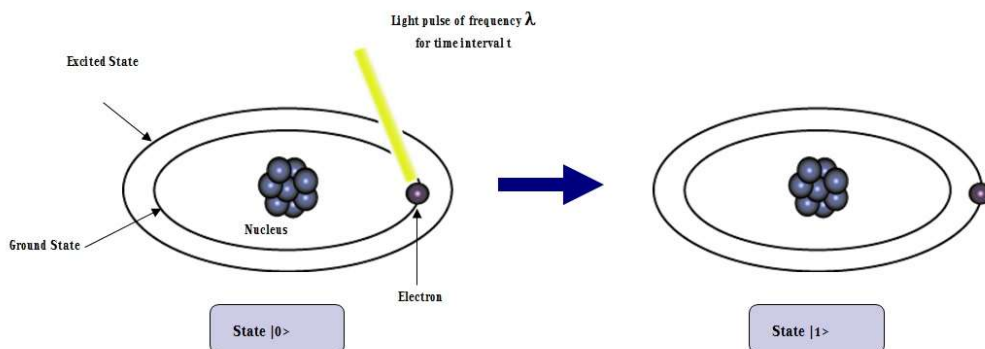


Figure 2.1: A simple example of a physical qubit using the electron of a hydrogen atom

¹Reprinted from RF Wireless World, n.d., Retrieved December 23, 2016, from <http://www.rfwireless-world.com/Terminology/Difference-between-Bit-and-Qubit.html>. Copyright 2012 by RF Wireless World. Reprinted with permission.

A classical non-probabilistic bit can only be in one of the two possible states at once. In contrast, qubits obey the laws of quantum mechanics, which gives rise to the powerful property that - besides being a definite 0 or 1 - they can also be in a superposition of the two states. Mathematically this is expressed as a linear combination of the states 0 and 1:

$$|\psi\rangle = \alpha |0\rangle + \beta |1\rangle \quad (2.1)$$

where α and β are complex coefficients ($\alpha, \beta \in \mathbb{C}$) and are often referred to as amplitudes. Any amplitude η can be further subdivided into a complex phase factor $e^{i\phi}$ and a non-negative real number e such that,

$$\eta = e^{i\phi} e \quad (2.2)$$

In Equ. 2.1, $|0\rangle$ is the Dirac notation for the qubit being in state 0 and it represents a two-dimensional vector in a complex 2-D vector space (called Hilbert space \mathcal{H}_2). $|0\rangle$ and $|1\rangle$ are the computational basis states and they constitute an orthonormal basis of \mathcal{H}_2 . For the sake of clarity, $|0\rangle$ and $|1\rangle$ can be thought of as the 2-D vectors shown below.

APPROXIMATELY EQUAL SIGN!

$$|0\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \quad |1\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix} \quad (2.3)$$

Subbing these vectors into Equ. 2.1 yields the vector representation of $|\psi\rangle$:

$$|\psi\rangle = \alpha \begin{pmatrix} 1 \\ 0 \end{pmatrix} + \beta \begin{pmatrix} 0 \\ 1 \end{pmatrix} = \begin{pmatrix} \alpha \\ \beta \end{pmatrix} \quad (2.4)$$

In the cases $\alpha = 1$ or $\beta = 1$ there is no quantum behaviour since the qubit is not in a superposition. However, if for example $\alpha = \beta = \frac{1}{\sqrt{2}}$ the qubit is in an equal quantum superposition which is impossible to achieve with a classical computer. This leads to another important qubit lifetime parameter - the transversal coherence or phase damping time. It is measured by preparing the equal superposition $\frac{|0\rangle + |1\rangle}{\sqrt{2}}$ and due to unavoidable interaction with the environment after some time t the quantum behaviour will be lost and the state will either be a definite $|0\rangle$ or $|1\rangle$. The process of losing quantum behaviour is called *decoherence*.

However, even though a qubit can be in a superposition of $|0\rangle$ and $|1\rangle$, when measured it will take the value $|0\rangle$ with a probability of

$$Prob(|0\rangle) = |\alpha|^2 \quad (2.5)$$

and $|1\rangle$ with a probability of

$$Prob(|1\rangle) = |\beta|^2 \quad (2.6)$$

The fact that the probability of measuring a particular state is equal the absolute value squared of the respective amplitude is called Born rule (citation). Since the total probability of measuring any value has to be 1, the following normalization condition must be satisfied:

$$|\alpha|^2 + |\beta|^2 = 1 \quad (2.7)$$

Therefore, a qubit is inherently probabilistic but when measured it collapses into a single classical bit (0 or 1). It follows that a measurement destroys information about the superposition of the

qubit (the values of α and β). This constitutes one of the main difficulties when designing quantum algorithms since only limited information can be obtained about the final states of the qubits in the quantum computer.

Similar to logic gates in a classical computer, a QC manipulates qubit by means of quantum logic gates which will be introduced in detail in Section 2.2. Generally, an arbitrary quantum logic gate U acting on a single qubit state is a linear transformation given by a 2x2 matrix whose action on $|\psi\rangle$ is defined as:

$$U|\psi\rangle = \begin{pmatrix} a & b \\ c & d \end{pmatrix} \begin{pmatrix} \alpha \\ \beta \end{pmatrix} = \begin{pmatrix} a * \alpha + b * \beta \\ c * \alpha + d * \beta \end{pmatrix} \quad (2.8)$$

Matrix U must be unitary which means that a) its determinant is equal to unity and b) its Hermitian conjugate U^\dagger must be equal to its inverse (see Equ. 2.9 and 2.10). All quantum logic gates must be unitary since this preserves the normalization of the qubit state it is acting on.

$$a) | \det(U) | = 1 \quad (2.9)$$

$$b) UU^\dagger = U^\dagger U = \mathbb{1} = UU^{-1} = U^{-1}U \quad (2.10)$$

Using spherical polar coordinates, a single qubit can be visualized on the so-called Bloch sphere by parameterising α and β in Equ. 2.1 as follows:

$$|q\rangle = \cos \frac{\theta}{2} |0\rangle + e^{i\phi} \sin \frac{\theta}{2} |1\rangle \quad (2.11)$$

The Bloch sphere has a radius of 1 and is therefore a unit sphere. The $|0\rangle$ qubit state is defined to lie along the positive z-axis (\hat{z}) and the $|1\rangle$ state is defined to lie along the negative z-axis ($-\hat{z}$) as labelled in Fig. 2.2. At this point, it is important to note that these two states are mutually orthogonal in \mathcal{H}_2 even though they are not orthogonal on the Bloch sphere.

Qubit states on the Bloch equator such as the \hat{x} and \hat{y} coordinate axes represent equal superpositions where $|0\rangle$ and $|1\rangle$ both have measurement probabilities equal to 0.5. The \hat{x} -axis for example represents the equal superposition $|q\rangle = \frac{1}{\sqrt{2}}|0\rangle + \frac{1}{\sqrt{2}}|1\rangle$. As illustrated in Fig. 2.2 any arbitrary 2-D qubit state $|\psi\rangle$ can be decomposed into the polar angles θ and ϕ and visualized as a vector on the Bloch sphere. Such an object is called the Bloch vector of the qubit state $|\psi\rangle$. The Bloch sphere will be the main visualization tool for qubit manipulations in this thesis.

2.1.2 Multiple Qubit Systems

A classical computer with one bit of memory is not particularly useful and equally a QC with one qubit is rather useless. In order to be able to perform large and complicated computations many individual qubits need to be combined to create a large QC. When moving from single to multi qubit systems a new mathematical tool, the so-called tensor product (symbol \otimes), is needed. A tensor product of two qubits is written as:

$$|\psi\rangle \otimes |\psi\rangle = |0\rangle \otimes |0\rangle = |00\rangle \quad (2.12)$$

²Reprinted from Wikipedia, n.d., Retrieved September 7, 2016, from https://en.wikipedia.org/wiki/Bloch_Sphere. Copyright 2012 by Glosser.ca. Reprinted with permission.

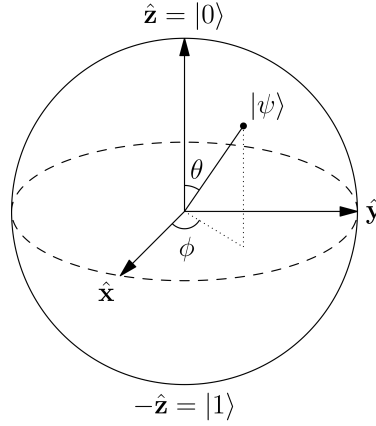


Figure 2.2: An arbitrary two-dimensional qubit $|\psi\rangle$ visualized on the Bloch sphere.²

whereby the last expression omits the \otimes symbol which is the shorthand form of a tensor product between two qubits.

In vector notation a tensor product of two vectors (red and green) is defined as shown below:

$$|00\rangle = |0\rangle \otimes |0\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \otimes \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} 1 * \begin{pmatrix} 1 \\ 0 \end{pmatrix} \\ 0 * \begin{pmatrix} 1 \\ 0 \end{pmatrix} \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix} \quad (2.13)$$

The last expression in Equ. 2.13 shows that the two-qubit state $|00\rangle$ is no longer two but four-dimensional. Hence, it lives in a four-dimensional Hilbert space \mathcal{H}_4 . A quantum gate acting on multiple qubits can therefore not have the same dimensions as a single-qubit gate (Equ. 2.8) which demands for a new gate formalism for multi qubit systems.

Consider wanting to apply an arbitrary single-qubit gate U (Equ. 2.8) to the first qubit and leaving the second qubit unchanged, essentially applying the identity matrix $\mathbb{1}$ to it. To do this, one defines the tensor product of two matrices as follows,

$$U \otimes \mathbb{1} = \begin{pmatrix} a & b \\ c & d \end{pmatrix} \otimes \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} = \begin{pmatrix} a * \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} & b * \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \\ c * \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} & d * \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \end{pmatrix} = \begin{pmatrix} a & 0 & b & 0 \\ 0 & a & 0 & b \\ c & 0 & d & 0 \\ 0 & c & 0 & d \end{pmatrix} \quad (2.14)$$

Thus, the result of the tensor product $U \otimes \mathbb{1}$ is a unitary 4x4 matrix which can now be used to linearly transform the 4x1 vector representing the $|00\rangle$ state in Equ. 2.13:

$$U \otimes \mathbb{1} |00\rangle = \begin{pmatrix} a & 0 & b & 0 \\ 0 & a & 0 & b \\ c & 0 & d & 0 \\ 0 & c & 0 & d \end{pmatrix} \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix} = \begin{pmatrix} a \\ 0 \\ c \\ 0 \end{pmatrix} \quad (2.15)$$

One can also first perform the single qubit operations on the respective qubits followed by the tensor product of the two resulting vectors:

$$(U \otimes \mathbb{1})(|0\rangle \otimes |0\rangle) = U|0\rangle \otimes \mathbb{1}|0\rangle = \begin{pmatrix} a & b \\ c & d \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} \otimes \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} a \\ c \end{pmatrix} \otimes \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} a \\ 0 \\ c \\ 0 \end{pmatrix} \quad (2.16)$$

This formalism can be extended to any number of qubits and the use of tensor products leads to an exponential increase in the dimensionality of the Hilbert space. Hence, n qubits live in a 2^n -dimensional Hilbert space ($\mathcal{H}_2^{\otimes n}$) and can store the content of 2^n classical bits. As an example, only 33 qubits can store the equivalent of $2^{33} = 8,589,934,592$ bits (= 1 gigabyte) which clearly bears the potential for enormous speed-ups in computations as will be demonstrated later.

Lastly, when considering multi qubit systems one will find composite states that can or cannot be factorized. Consider for example the last expression in Equ. 2.16 which can be reexpressed as follows,

$$\begin{pmatrix} a \\ 0 \\ c \\ 0 \end{pmatrix} = a \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix} + 0 \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix} + c \begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \end{pmatrix} + 0 \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix} = a|00\rangle + 0|01\rangle + c|10\rangle + 0|11\rangle \quad (2.17)$$

This can be factorized into the following tensor product:

$$a|00\rangle + c|10\rangle = (a|0\rangle + c|1\rangle) \otimes |0\rangle \quad (2.18)$$

In contrast, consider the following state:

$$|\phi\rangle = \frac{|00\rangle + |11\rangle}{\sqrt{2}} \quad (2.19)$$

It is straightforward to see that there is no way to factorize the state $|\phi\rangle$ into a tensor product of two states. Now imagine, two people Andy and Beatrice are given two electrons prepared in the quantum state $|\phi\rangle$. Andy keeps the first electron in the lab and Beatrice takes the second electron to her house. Andy gets interested in measuring if his electron is in the $|0\rangle$ or $|1\rangle$ state and performs a measurement. He finds the electron to be in the $|1\rangle$ state. From Equ. 2.19 and knowing that measurement collapses a superposition the post-measurement (PM) state $|\phi\rangle_{PM}$ is given by:

$$|\phi\rangle_{PM} = |11\rangle \quad (2.20)$$

Looking at this expression tells Andy that Beatrice's electron must be in state $|1\rangle$ as well without having measured her electron! Even more suprising is the fact that the second electron was nowhere close to Andy and he was still able to determine its state.

Non-local correlations between qubit measurement outcomes is a peculiar quantum property of non-factorising quantum states and is called *entanglement*. It is an integral part of quantum computation and Section 2.2.2 will give a concrete example of how to create such a state in a QC.

2.2 Quantum Logic Gates

In order to perform quantum computations, tools, analogous to the classical logic gates, are needed for qubit manipulation. Quantum logic gates are square matrices that can be visualized as rotations on the Bloch sphere. The following subsections will introduce the major single and multi qubit logic gates.

2.2.1 Single Qubit Gates

Qubit Flip (X) Gate

The quantum equivalent of the classical NOT logic gate is called X gate and is given by the 1st Pauli matrix:

$$\sigma_1 = X = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad (2.21)$$

The action of a quantum gate on the arbitrary qubit state $|\psi\rangle$ (Equ. 2.4) can be analysed using the gate's matrix and the qubit's vector representation. Applying some straightforward linear algebra yields:

$$X \otimes |\psi\rangle = X \otimes (\alpha |0\rangle + \beta |1\rangle) = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} \alpha \\ \beta \end{pmatrix} = \begin{pmatrix} \beta \\ \alpha \end{pmatrix} = \beta |0\rangle + \alpha |1\rangle \quad (2.22)$$

Thus, applying the X gate to qubit state $|\psi\rangle$ swaps the amplitudes of $|0\rangle$ and $|1\rangle$. More specifically, applying X to the $|0\rangle$ state results in the $|1\rangle$ state,

$$X \otimes |0\rangle = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} 0 \\ 1 \end{pmatrix} = |1\rangle \quad (2.23)$$

In terms of the example with the electron of a hydrogen atom shown in Fig. 2.1 an X gate can be implemented by exciting the electron from the ground state ($|0\rangle$) into the next highest electron valence shell ($|1\rangle$) using a controlled laser pulse.

The $|0\rangle$ state is recovered when applying X again to the $|1\rangle$ state,

$$X \otimes |1\rangle = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} 0 \\ 1 \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \end{pmatrix} = |0\rangle \quad (2.24)$$

On the Bloch sphere, the X gate corresponds to an anti-clockwise π rotation around the x-axis as shown in Fig. 2.3.

From Equ. 2.22, 2.23 and 2.24 it follows that X is its own inverse as well as its own Hermitian conjugate:

$$X X = X X^\dagger = \mathbb{1} \quad (2.25)$$

$$X = X^{-1} = X^\dagger \quad (2.26)$$

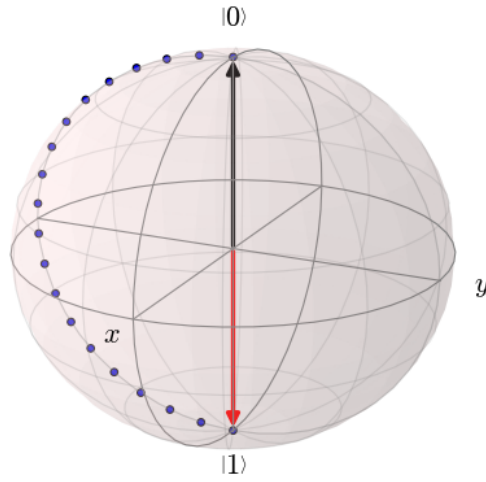
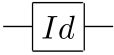
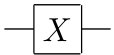
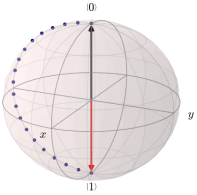
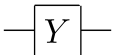
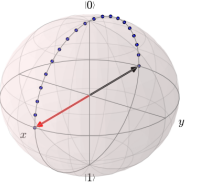
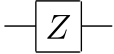
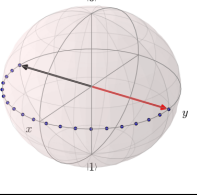
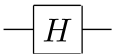
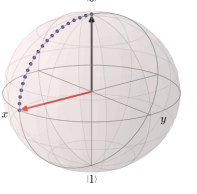
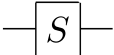
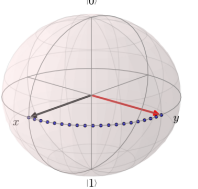
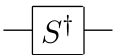
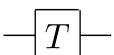
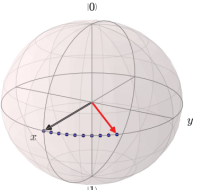
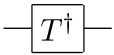



Figure 2.3: Visualization of the X gate on the Bloch sphere. Initial state (black) transformed to final state (red).

The action, circuit & matrix representation and Bloch sphere visualization for the most important single-qubit quantum logic gates are summarised in Table 2.1 below.

Table 2.1: Table of major single-qubit quantum logic gates.

Gate	Name	Circuit representation	Matrix	Description	Rotation	Bloch sphere
\mathbb{I}	Identity		$\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$	Idle or waiting gate	-	-
X	Qubit flip		$\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$	Swaps amplitudes of $ 0\rangle$ and $ 1\rangle$	π rotation around \hat{x}	
Y	Qubit & phase flip		$\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$	Swaps amplitudes and introduces phase	π rotation around \hat{y}	
Z	Phase flip		$\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$	Adds a negative sign to the $ 1\rangle$ state	π rotation around \hat{z}	
H	Hadamard		$\begin{pmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} \end{pmatrix}$	Creates equal superpositions	$\frac{\pi}{2}$ rotation around \hat{y} and π rotation around \hat{x}	
S	$\frac{\pi}{2}$ rotation gate		$\begin{pmatrix} 1 & 0 \\ 0 & i \end{pmatrix}$	\sqrt{Z}	$\frac{\pi}{2}$ rotation around \hat{z}	
S^\dagger	$-\frac{\pi}{2}$ rotation gate		$\begin{pmatrix} 1 & 0 \\ 0 & -i \end{pmatrix}$	Adjoint of S	$-\frac{\pi}{2}$ rotation around \hat{z}	
T	$\frac{\pi}{4}$ rotation gate		$\begin{pmatrix} 1 & 0 \\ 0 & e^{i\pi/4} \end{pmatrix}$	\sqrt{S}	$\frac{\pi}{4}$ rotation around \hat{z}	
T^\dagger	$-\frac{\pi}{4}$ rotation gate		$\begin{pmatrix} 1 & 0 \\ 0 & e^{-i\pi/4} \end{pmatrix}$	Adjoint of T	$-\frac{\pi}{4}$ rotation around \hat{z}	
ZM	Z-basis measurement		-	Measurement in standard basis	Collapses the state	-

2.2.2 Multiple Qubit Gates

Controlled NOT Gate

The most important two-qubit quantum gate is the controlled NOT or CNOT gate given by the following 4x4 matrix:

$$CNOT = \begin{pmatrix} \mathbb{1} & 0 \\ 0 & X \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix} \quad (2.27)$$

The CNOT gate takes two qubits, a control and a target qubit, as input. If and only if the control qubit is in the $|1\rangle$ state, the NOT (X) gate is applied to the target qubit. In equations, the CNOT will always be followed by parantheses containing the control (c) qubit followed by the target (t) qubit: CNOT(c,t). The input-output relation (truth table) for the CNOT gate is given in Table 2.2 below.

Table 2.2: CNOT truth table with first qubit as control, second qubit as target.

Input	Output
00	00
01	01
10	11
11	10

To demonstrate the usefulness of the CNOT gate consider starting with two unentangled qubits both in the $|0\rangle$ state,

$$|\phi\rangle = |0\rangle \otimes |0\rangle = |00\rangle \quad (2.28)$$

Applying the H gate onto the first qubit yields the following (still unentangled) state:

$$(H \otimes \mathbb{1})|\phi\rangle = (H \otimes \mathbb{1})|00\rangle = \frac{1}{\sqrt{2}}|00\rangle + \frac{1}{\sqrt{2}}|10\rangle \quad (2.29)$$

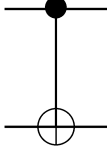
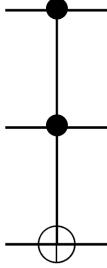
Now consider applying the CNOT to this state whereby the control qubit is coloured **red** and the target qubit **green**.

$$CNOT(\text{red}, \text{green}) \otimes \left(\frac{1}{\sqrt{2}}|\text{red}0\rangle + \frac{1}{\sqrt{2}}|\text{red}1\rangle \right) = \frac{1}{\sqrt{2}}|\text{red}0\rangle + \frac{1}{\sqrt{2}}(\mathbb{1} \otimes X)|\text{red}1\rangle = \frac{1}{\sqrt{2}}|\text{red}0\rangle + \frac{1}{\sqrt{2}}|\text{red}1\rangle \quad (2.30)$$

The last expression in Equ. 2.30 was used as an example (Equ. 2.19) for entanglement in Section 2.1.2 and it is one of the famous Bell states which are a set of four maximally entangled states (CITATION). Thus, this example demonstrates how the CNOT gate is crucial for the generation of entangled states since it applies the X gate to a qubit depending on the state of a second qubit.

The three most important multi qubit quantum gates CNOT, Toffoli and nCNOT are characterised in Table 2.3.

Table 2.3: Table of major multi-qubit quantum logic gates where c_j stands for the j^{th} control qubit and $\mathbb{1}_k$ for the $k \times k$ identity matrix.

Gate	Name	Circuit representation	Matrix	Description
CNOT	Controlled NOT		$\begin{pmatrix} \mathbb{1} & 0 \\ 0 & X \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix}$	$\text{CNOT}(c_1, \text{target})$
Toffoli	Controlled controlled NOT		$\begin{pmatrix} \mathbb{1}_6 & 0 \\ 0 & X \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \end{pmatrix}$	$\text{CCNOT}(c_1, c_2, \text{target})$
nCNOT	n-controlled NOT	-	$\begin{pmatrix} \mathbb{1}_{2^n-2} & 0 \\ 0 & X \end{pmatrix}$	$\text{nCNOT}(c_1, \dots, c_n, \text{target})$

2.3 Classical Machine Learning

Machine learning can be subdivided into three major fields.

Supervised ML

- Based on *input* and *output* data

"I know how to classify this data but I need the algorithm to do the computations for me."

Unsupervised ML

- Based on *input* data only

"I have no clue how to classify this data, can the algorithm create a classifier for me?"

Reinforcement learning

- Based on *input* data only

"I have no clue how to classify this data, can the algorithm classify this data and I'll give it a reward if it's correct or I'll punish it if it's not."

This thesis is focussing on quantum-enhancements in the field of supervised machine learning only.

2.3.1 k-nearest Neighbour Algorithm

Understanding the quantum version of the distance weighted k -nearest neighbour (kNN) algorithm as proposed by Schuld, Sinayskiy, and Petruccione (2014) requires prior knowledge of the classical

version of the algorithm that will be introduced in this subsection.

Imagine working for a search engine company and you are given the task of classifying unknown pictures of fruits as either apples or bananas. To train your classification algorithm you are given 5 different pictures of apples and 5 different pictures of bananas. This will be called the *training data set* D_T . The pictures in D_T may be taken from different angles, in varying light settings and include different coloured apples and bananas. Two examples of such pictures are shown in Fig. 2.4.



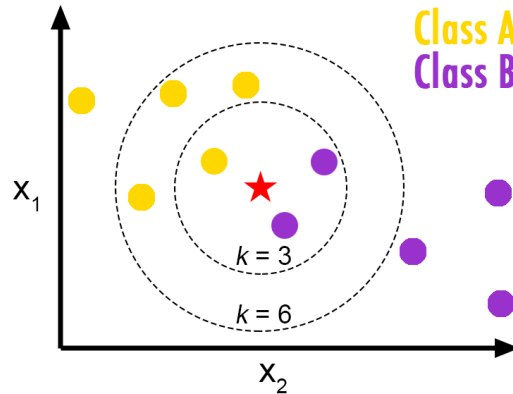
Figure 2.4: Pictures of apple and banana from training data set D_T .³

Most of the time, using the full pixel representation of each picture for classification does not lead to optimal results. Therefore, the next step is to select a certain number of characteristic *features* extracted from the pictures in the training set that can be used to differentiate apples from bananas. Such a feature might be the RGB value of the most frequent pixel colour since bananas and apples have different colour spectra. Using a measure of the curvature of the main object in the picture is another possibility since an apple is almost spherical whereas a banana looks more like a bend line.

By selecting and extracting features, the dimensionality of the training data set is drastically reduced from a few thousand pixels to a handful of features. The m extracted features for the j^{th} picture are stored in the m -dimensional *feature vector* \vec{v}_j . Mathematically, the training data set D_T consists of ten feature vectors $\vec{v}_0, \vec{v}_1, \dots, \vec{v}_{10}$ that are each assigned to either class A (apple) or B (banana). The training vectors are visualized as yellow and purple circles in Fig. 2.5.

Given a new picture of either a banana or an apple, you first extract the same m features from it and store it in the input vector \vec{x} . From many algorithms you decide to use the kNN algorithm since it is a non-parametric classifier meaning it makes no prior assumption about the class of the new picture. Given a new unclassified input vector \vec{x} (red star in Fig. 2.5), the algorithm considers the k nearest neighbours within the training set (using a predefined measure of distance) and classifies \vec{x} , based on a majority vote, as either A or B . Thereby, k is a positive integer, usually chosen to be small and its value determines the classification outcome. Namely, in the case $k = 3$ in Fig. 2.5, vector \vec{x} will be classified as class B (purple) but in the case $k = 6$ it will be labelled class A (yellow).

³Reprinted from Pixabay, Retrieved December 24, 2016, from <https://pixabay.com/en/apple-red-fruit-frisch-vitamins-1632016/> and <https://pixabay.com/en/banana-fruit-yellow-1504956/>. Creative Commons Licence 2016 by Pixabay. Reprinted with permission.

Figure 2.5: Visualization of a kNN classifier⁴

In the case of $k = 10$, \vec{x} would simply be assigned to the class with the most members. In this case, the training vectors should be given distance-dependent weights (such as $\frac{1}{distance}$) to increase the influence of closer vectors over more distant ones.

2.3.2 Algorithmic complexity

Big-O Notation

In the fields of computer science and quantum information, the so-called Big-O notation, first described by Bachmann (1894), is often used to describe how the runtime of an algorithm depends on variables such as the desired accuracy, the number of input vectors or their size.

⁴Reprinted from GitHub, Burton de Wilde, Retrieved September 13, 2016, from <http://bdewilde.github.io/blog/blogger/2012/10/26/classification-of-hand-written-digits-3/>. Copyright 2012 by Burton de Wilde. Reprinted with permission.

Definition of Big-O

For any monotonic functions $t(n)$ and $g(n)$ defined on a subset of the real numbers (\mathbb{R}), one says that $t(n) = \mathcal{O}(g(n))$ if and only if when there exists constants $c \geq 0$ and $n_0 \geq 0$ such that

$$|f(n)| \leq c * |g(n)| \quad \text{for all } n \geq n_0 \quad (2.31)$$

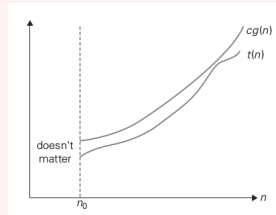


Figure 2.6: Visualization of $c * g(n)$ being an upper asymptotic bound of $t(n)$ ⁵

This implies that the function $f(n)$ does not grow at a faster rate than $g(n)$, or in other words that some constant multiple of the function $g(n)$ is an upper asymptotic bound for the function $f(n)$, for all $n \rightarrow \infty$.

⁵Reprinted from Anany Levitin and Soumen Mukherjee. Introduction to the Design & Analysis of Algorithms. Reading, MA: Addison-Wesley, 2003. Copyright 2012 by Levitin & Mukherjee.

Fig. 2.7 provides a good visual comparison between common algorithmic complexity classes regarding their relation to the input size n . It can be seen that the best possible algorithmic time complexity is constant time, $\mathcal{O}(1)$, that is being independent of the size of the input data e.g. determining if a binary number is even or odd. An algorithm is still considered excellent if it runs in logarithmic time $\mathcal{O}(\log(n))$. Linear search algorithms for example are linear in time expressed as $\mathcal{O}(n)$. More complex sort algorithms like "bubble sort" have a higher time complexity and often run in quadratic time ($\mathcal{O}(n^2)$). Furthermore, algorithms with complexity $\mathcal{O}(n^c)$ are said to run in polynomial time for some $c > 2$. If an algorithm has time complexity $\mathcal{O}((\log(n))^c)$ for some $c \geq 1$ it is called polylogarithmic. The highest complexity classes are exponential $\mathcal{O}(c^n)$ with $c \geq 1$ and factorial time $\mathcal{O}(n!)$. For example, solving the travelling salesman problem using brute-force search runs in factorial time.

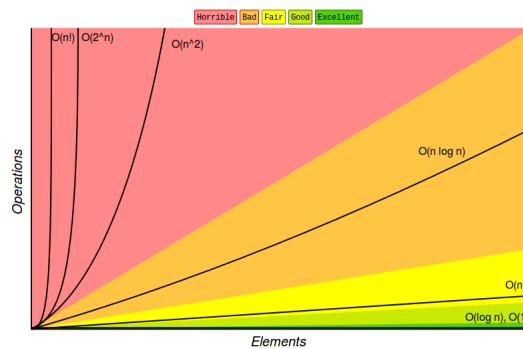


Figure 2.7: Overview of algorithmic complexity classes⁶

⁶Reprinted from Big-O Cheatsheet, Retrieved December 28, 2016, from <http://bigocheatsheet.com/>. Copyright

Chapter 3

Methods

More general text here!

All the calculations and plots for this thesis are done in the programming language Python which has a very intuitive syntax and comes with large libraries for scientific computing and plotting.

For the implementation of the quantum kNN algorithm there are two fundamentally different ways: Running it a) by simulating a QC or b) by actually executing it on a real QC. The required tools for both possibilities will be explained in the following subsections.

3.1 Liqui| \rangle

Classical computers can be used to simulate the behaviour of small quantum computers. Such simulations are associated with exponential computational costs thereby limiting the number of simulated qubits. Since current state-of-the-art quantum technology uses around ten qubits, a classical computer can still be used for simulation.

For the quantum computing simulations in this thesis the quantum simulation toolsuite Liqui| \rangle developed by Microsoft Research will be used. Liqui| \rangle is based on the functional programming language F# and allows for simulation of up to 30 qubits (Research, 2016). It comes with a large palette of predefined single and multi qubit quantum logic gates and allows for custom-defined quantum gates such as nCNOT and rotation gates controlled by n qubits which is crucial for some of the work done in this thesis. A short piece of example code from Liqui| \rangle written in F# is shown in Fig. 3.1.

```

275 [<LQD>] //defines that function can be called from the command line
276 let __LiquidCodeExample() = //define function name
277
278     show "This is a simple example of a Liqui|> function"
279
280     //initialize state vector (Dirac ket) with two qubits
281     let k = Ket(2)
282     //create qubit list from ket k
283     let qs = k.Qubits
284
285     //apply Hadamard to first qubit in qubit list qs
286     H [qs.[0]]
287     //apply CNOT with control qs.[0] and target qs.[1]
288     CNOT [qs.[0];qs.[1]]
289     //measure the first qubit
290     M [qs.[0]]
291     //measure the second qubit
292     M [qs.[1]]
293
294     show "Measurement result for first qubit: %i" qs.[0].Bit.v
295     show "Measurement result for second qubit: %i" qs.[1].Bit.v

```

Figure 3.1: F# code snippet from Microsoft's quantum simulation toolsuite Liqui|>

A Lenovo ThinkPad T450 containing an Intel i5 processor with 2 cores and 8GB random-access memory (RAM) is used for all quantum simulations in this thesis.

3.2 IBM Quantum Experience

Earlier this year IBM has enabled public cloud access to their experimental quantum processor containing five non error-corrected superconducting qubits located at the IBM Quantum Lab at the Thomas J Watson Research Center in Yorktown Heights, New York (IBM, 2016a). Instead of only simulating on classical hardware, this opens up the possibility of executing the QML algorithm on actual quantum hardware.

The so-called IBM Quantum Experience provides the user with access to the "Quantum Composer" which is the main tool for algorithm design. The quantum composer shown in Fig. 3.2 consists of 5 horizontal lines, one for each qubit, and enables the user to choose from a universal gate set (bottom of Fig. 3.2) consisting of 10 quantum logic gates. Additionally, there are two different measurement types: a) A measurement in the standard z-basis ($|0\rangle$ / $|1\rangle$) resulting in a probability distribution over all possible states and b) a Bloch measurement that visually projects the state onto the Bloch sphere. The user can compose an algorithm by applying up to 40 quantum logic and measurement gates to the five qubits by means of drag-and-drop.

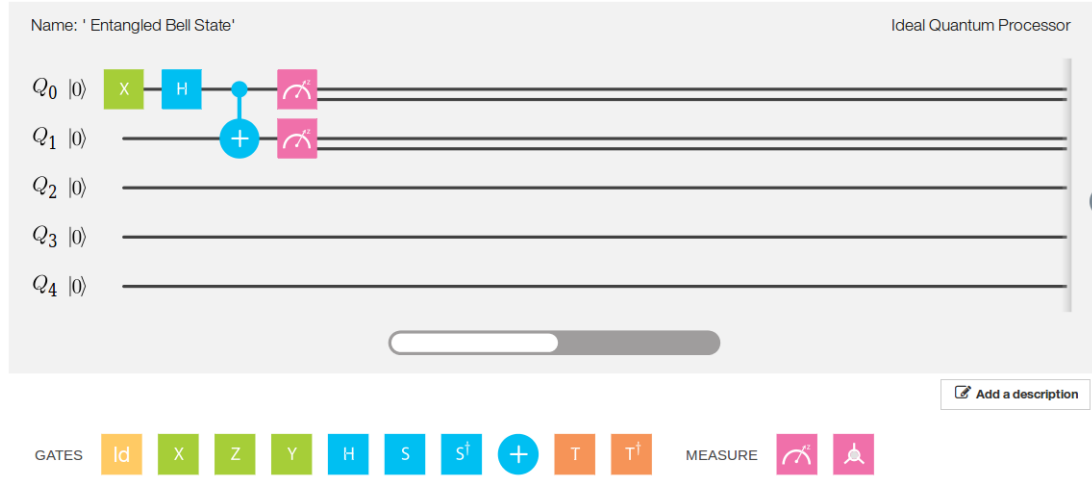


Figure 3.2: Screenshot showing IBM Quantum Composer

By spending limited user coins the gate sequence of a composed algorithm is then sent to IBM's QC in New York and depending on the waiting queue and the availability of the QC the results will be sent back via mail within a few minutes or days. IBM Quantum Experience also allows for free quantum simulations under ideal or real conditions which provides a great tool for experimentation without spending user coins.

The main limitation of the IBM Quantum Experience are the qubit decoherence times since they restrict the maximum number of possible operations before the qubits lose their quantum behaviour and their quantum information. Thus, the number of quantum gates is currently limited to only 40 which essentially means 39 logic gates and 1 measurement gate. According to the qubit calibration results shown in Fig. 3.3, the amplitude damping times of the five qubits range from $52.3 \mu\text{s}$ to $81.5 \mu\text{s}$. Furthermore, the phase damping times range from $60.9 \mu\text{s}$ to $112.4 \mu\text{s}$. Currently, the implementation of a single qubit quantum logic gate takes 130ns and applying a CNOT gate takes 500ns (Bishop, 2016).

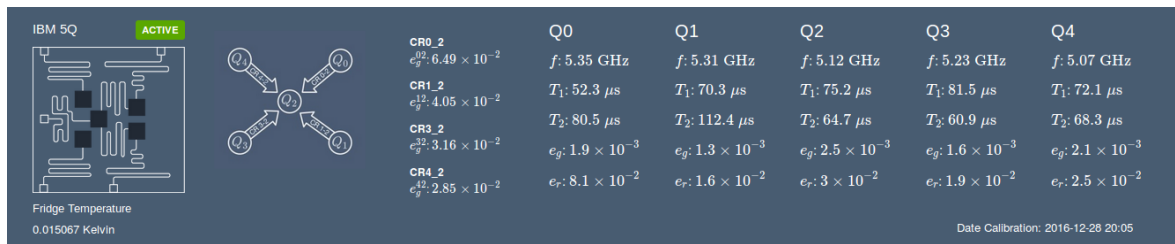


Figure 3.3: Screenshot of IBM QC calibration results (28. December 2016 - 20:05)

Chapter 4

Literature Review: Quantum-enhanced Machine Learning

Classical machine learning takes classical data as input and learns from it using classical algorithms executed on classical computers - this will be referred to as C/C (classical data with classical algorithm). One enters the field of quantum machine learning when either quantum data or quantum algorithms are combined with ideas from classical machine learning. Thus, quantum machine learning can be subdivided into three different subfields: 1) C/Q - classical data with quantum algorithm, 2) Q/C - quantum data with classical algorithm and 3) Q/Q - quantum data with quantum algorithm.

Quantum data includes any data describing a quantum mechanical system such as e.g. the Hamiltonian of a system or the state vector of a certain quantum state. A *quantum algorithm* is any algorithm that can only be executed on a quantum computer.

C/Q is the topic of this thesis

Analogously, Q/C is the subfield where quantum data is being processed using a classical machine learning algorithm. Examples for Q/C:

used genetic algorithms to reduce digital and experimental errors in quantum gates

A tantamount task is then to find a model (a.k.a. effective) Hamiltonian of the system and to determine properties of the present noise sources. By computing likelihood functions in an adaptation of Bayesian inference, Wiebe et al. found that quantum Hamiltonian learning can be performed using realistic resources such as depolarizing noise.

Q/Q would include learning a model Hamiltonian of a system implemented in a lab using a quantum learning algorithm.

4.0.1 Quantum State Preparation Algorithms

Quantum state preparation is the process of preparing a quantum state that accurately represents a vector containing classical (normalized) data. There are two fundamentally different ways of preparing a quantum state representing the classical example vector v :

$$v = \begin{pmatrix} 0.6 \\ 0.4 \end{pmatrix} \quad (4.1)$$

Encoding classical data into qubits

The most straightforward type of quantum state preparation does not make use of quantum superpositions but only uses the definite $|0\rangle$ or $|1\rangle$ states to store binary information in a multi qubit system as outlined in the example below.

Multiply vector v by ten such that the normalized entries can easily be represented in binary,

$$\begin{pmatrix} 0.6 \\ 0.4 \end{pmatrix} * 10 = \begin{pmatrix} 6 \\ 4 \end{pmatrix} \quad (4.2)$$

Convert each entry to binary,

$$\begin{pmatrix} 6 \\ 4 \end{pmatrix} \rightarrow \begin{pmatrix} 0110 \\ 0100 \end{pmatrix} \quad (4.3)$$

Rewrite the 2-D vector as a 1-D bit string,

$$\begin{pmatrix} 0110 \\ 0100 \end{pmatrix} \rightarrow n = 01100100 \quad (4.4)$$

For g bits initialize g qubits in the $|0\rangle$ state & apply the X gate to the respective qubits:

$$n = 01100100 \rightarrow |n\rangle = (\mathbb{1} \otimes X \otimes X \otimes \mathbb{1} \otimes \mathbb{1} \otimes X \otimes \mathbb{1} \otimes \mathbb{1}) |00000000\rangle = |01100100\rangle \quad (4.5)$$

When encoding classical data into qubit states, a k -dimensional probability vector requires $4k$ classical bits which are encoded one-to-one into $4k$ qubits. Thus, the number of qubits increases linearly with the size of the classical data vector. Due to this one-to-one correspondence between classical bits and qubits there is no data compression improvement compared to classical data storage. Only slight (up to quadratic) speed-ups are possible through clever quantum algorithm design (CITATION).

Qubit-based quantum state preparation becomes slightly more complicated when aiming to achieve a quantum memory state $|M\rangle$ in an equal superposition of l binary patterns l^j of the form

$$|M\rangle = \frac{1}{\sqrt{l}} \sum_{j=1}^l |l^j\rangle \text{ where } |l^j\rangle = |l_1^j, l_2^j, \dots, l_n^j\rangle \text{ and } l_k^j \in \{0, 1\} \quad (4.6)$$

Preparing this quantum state is a requirement for the later used qubit-encoded kNN quantum algorithm by Schuld et al. (2014). Trugenberger (2001) describe a quantum routine that can efficiently prepare such a state as will be explained in detail below.

First, Trugenberger (2001) defines the new unitary quantum gate S^j ,

$$S^j = \begin{pmatrix} \sqrt{\frac{j-1}{j}} & \frac{1}{\sqrt{j}} \\ -\frac{1}{\sqrt{j}} & \sqrt{\frac{j-1}{j}} \end{pmatrix} \quad (4.7)$$

and introduces its controlled version CS^j :

$$CS^j = \begin{pmatrix} \mathbb{1} & 0 \\ 0 & S^j \end{pmatrix} \quad (4.8)$$

The initial quantum state is given in Equ. 4.9 and consists of three registers; the first being the pattern register containing the first pattern l^1 , the second register u is a utility register initialized in state $|01\rangle$ and the third register m represents the memory register initialized with n zeros in which all patterns l^j will be loaded one after the other.

$$|\Psi_0^1\rangle = |l^1; u; m\rangle = |l_1^1, l_1^1, \dots, l_n^1; 01; 0_1, \dots, 0_n\rangle \quad (4.9)$$

The routine will use the second utility qubit u_2 to separate the initial state into two terms whereby $u_2 = |0\rangle$ flags the already stored patterns and $u_2 = |1\rangle$ indicates the processing term. In order to store a pattern l^j in the memory register one has to perform the following operations:

Step 1: Using u_2 as one of the control qubits for the CCNOT gate, copy the pattern l^j into the memory register of the processing term ($u_2 = |1\rangle$):

$$|\Psi_1^j\rangle = \prod_{r=1}^n CCNOT(l_r^j, u_2, m_r) |\Psi_0^j\rangle \quad (4.10)$$

Step 2: If the qubits in the pattern and memory register are identical (true only for the processing term) then overwrite all qubits in the memory register with ones:

$$|\Psi_2^j\rangle = \prod_{r=1}^n X(m_r) CNOT(l_r^j, m_r) |\Psi_1^j\rangle \quad (4.11)$$

Step 3: Apply a nCNOT gate controlled by all n qubits in the m register and flip u_2 if and only if all n qubits are ones (true only for the processing term):

$$|\Psi_3^j\rangle = nCNOT(m_1, m_2, \dots, m_n, u_2) |\Psi_2^j\rangle \quad (4.12)$$

Step 4: Using the previously defined CS^j operation, with control u_1 and target u_2 , the new pattern is transferred from the processing term into the term containing the already stored patterns ($u_2 = |0\rangle$):

$$|\Psi_4^j\rangle = CS^{l+1-j}(u_1, u_2) |\Psi_3^j\rangle \quad (4.13)$$

Step 5 & 6: In Step 2 & 3 all qubits in the memory register were overwritten with ones and these steps can be undone by applying their inverse operations:

$$|\Psi_5^j\rangle = nCNOT(m_1, m_2, \dots, m_n, u_2) |\Psi_4^j\rangle \quad (4.14)$$

$$|\Psi_6^j\rangle = \prod_{r=n}^1 CNOT(l_r^j, m_r) X(m_r) |\Psi_5^j\rangle \quad (4.15)$$

The resulting state is now given by the following equation:

$$|\Psi_6^j\rangle = \frac{1}{\sqrt{l}} \sum_{w=1}^j |l^j; 00; l^w\rangle + \sqrt{\frac{l-j}{l}} |l^j; 01; l^j\rangle \quad (4.16)$$

Step 7: Finally, by applying the inverse operation of Step 1 the memory register of the processing term is restored to zeros only:

$$|\Psi_7^j\rangle = \prod_{r=n}^1 CCNOT(l_r^j, u_2, m_r) |\Psi_6^j\rangle \quad (4.17)$$

At the end of Step 7 the next pattern can be loaded into the first register and by applying Steps 1-7 again the pattern gets added to the memory register. After repeating this procedure l times the memory register m will be in the desired state $|M\rangle$ defined by Equ. 4.6.

Encoding classical data into amplitudes

A more sophisticated way of representing the classical vector v (Equ. 4.1) as a quantum state makes use of the large number of available amplitudes in a multi qubit system. The general idea is demonstrated in Equ. 4.18 below.

$$\begin{pmatrix} 0.6 \\ 0.4 \end{pmatrix} \rightarrow |n\rangle = \sqrt{0.6}|0\rangle + \sqrt{0.4}|1\rangle \quad (4.18)$$

Using amplitude-based quantum state preparation, a k -dimensional probability vector is encoded into only $\log_2(k)$ qubits since the number of amplitudes grows exponentially with the number of qubits. This type of quantum data storage makes exponential compression of classical data possible. Since a quantum gate acts on all amplitudes in the superposition at once there is the possibility of exponential speed-ups in quantum algorithms compared to their classical counterparts. Compared to the one-to-one correspondence in qubit-encoded state preparation, amplitude-encoding requires a much smaller number of qubits that grows logarithmically with the size of the classical data vector. However, initializing an arbitrary amplitude distribution is still an active field of research and requires the implementation of non-trivial quantum algorithms.

For the case when the classical data vectors represent discrete probability distributions which are efficiently integrable on a classical computer, Grover and Rudolph (2002) developed a quantum routine to initialize the corresponding amplitude distribution. Additionally, Soklakov and Schack (2006) proposed a quantum algorithm for the more general case that includes initializing amplitude distributions for classical data vectors representing non-efficiently integrable probability distributions.

4.0.2 Quantum k-nearest Neighbour Algorithm

The quantum distance-weighted kNN algorithm outlined in this section was proposed by Schuld et al. (2014) and is based on classical data being encoded into qubits rather than amplitudes. The first step is to prepare an equal superposition $|T\rangle$ over N training vectors \vec{v} of length n with binary entries v_1, v_2, \dots, v_n each assigned to a class c as follows,

$$|T\rangle = \frac{1}{\sqrt{N}} \sum_{p=1}^N |v_1^p, v_2^p, \dots, v_n^p, c^p\rangle \quad (4.19)$$

The unknown vector \vec{x} of length n and binary entries x_1, x_2, \dots, x_n needs to be classified and is added to the training superposition resulting in the initial state $|\psi_0\rangle$:

$$|\psi_0\rangle = \frac{1}{\sqrt{N}} \sum_{p=1}^N |x_1, x_2, \dots, x_n; v_1^p, v_2^p, \dots, v_n^p; c^p\rangle \quad (4.20)$$

An ancilla qubit initially in state $|0\rangle$ is added to the state such that the superposition is now described by,

$$|\psi_1\rangle = \frac{1}{\sqrt{N}} \sum_{p=1}^N |x_1, x_2, \dots, x_n; v_1^p, v_2^p, \dots, v_n^p; c^p\rangle \otimes |0\rangle \quad (4.21)$$

The state now consists of four registers: 1) input(x) register, 2) training(v) register, 3) class(c) register and 4) ancilla($|0\rangle$) register. Next, the ancilla register is put into an equal superposition by applying an H gate to it,

$$\begin{aligned}
|\psi_2\rangle &= \frac{1}{\sqrt{N}} \sum_{p=1}^N |x_1, x_2, \dots, x_n; v_1^p, v_2^p, \dots, v_n^p; c^p\rangle \otimes H|0\rangle \\
&= \frac{1}{\sqrt{N}} \sum_{p=1}^N |x_1, x_2, \dots, x_n; v_1^p, v_2^p, \dots, v_n^p; c^p\rangle \otimes \frac{(|0\rangle + |1\rangle)}{\sqrt{2}}
\end{aligned} \tag{4.22}$$

The main step in any kNN algorithm is calculating some measure of distance between each training vector \vec{v} and the input vector \vec{x} which in this quantum algorithm is taken to be the Hamming distance defined in the red box below.

Hamming distance (CITATION?)

Hamming distance (HD) is the number of differing characters when comparing two equally long binary patterns p_0 and p_1 .

Example:

$p_0 = \quad 0 \quad 0 \quad 1$

$p_1 = \quad 1 \quad 0 \quad 1$

HD = 1 + 0 + 0 = 1

Given quantum state $|\psi_2\rangle$ the HD between the input and each training register can be calculated by applying $CNOT(x_s, v_s^p)$ gates to all qubits in the first and second register using the input vector qubits x_s as controls and the training vector qubits v_s^p as targets. This will change the qubits in the second register according to the rules specified in Equ. 4.23.

$$d_s^p = \begin{cases} 0, & \text{if } |v_s^p\rangle = |x_s\rangle \\ 1, & \text{otherwise} \end{cases} \tag{4.23}$$

The sum of the qubits in the second register now represents the total HD between each training register and the input. Applying an X gate to each qubit in the second register reverses the HD such that small HDs become large and vice versa. This is crucial since training vectors close to the input should get larger weights than more distant vectors. The quantum state is now given by,

$$\begin{aligned}
|\psi_3\rangle &= \prod_{s=1}^n X(v_s^p) CNOT(x_s, v_s^p) |\psi_2\rangle \\
&= \frac{1}{\sqrt{N}} \sum_{p=1}^N |x_1, x_2, \dots, x_n; d_1^p, d_2^p, \dots, d_n^p; c^p\rangle \otimes \frac{(|0\rangle + |1\rangle)}{\sqrt{2}}
\end{aligned} \tag{4.24}$$

By applying the unitary operator U defined by,

$$U = e^{-i\frac{\pi}{2n}K} \tag{4.25}$$

where

$$K = \mathbb{1} \otimes \sum_s \left(\frac{\sigma_z + 1}{2} \right)_{d_s} \otimes \mathbb{1} \otimes (\sigma_z)_c \quad (4.26)$$

the sum over the second register is computed. As a result, the total reverse HD, denoted $d_H(\vec{x}, \vec{v}^p)$, between the p th training vector \vec{v}^p and the input vector \vec{x} is written into the complex phase of the p th term in the superposition. The ancilla register is now separating the superposition into two terms due to a sign difference in the amplitudes (negative sign when ancilla is $|1\rangle$). The result is given by,

$$\begin{aligned} |\psi_4\rangle &= U |\psi_3\rangle \\ &= \frac{1}{\sqrt{2N}} \sum_p^N e^{i \frac{\pi}{2n} d_H(\vec{x}, \vec{v}^p)} |x_1, x_2, \dots, x_n; d_1^p, d_2^p, \dots, d_n^p; c^p; 0\rangle \\ &\quad + e^{-i \frac{\pi}{2n} d_H(\vec{x}, \vec{v}^p)} |x_1, x_2, \dots, x_n; d_1^p, d_2^p, \dots, d_n^p; c^p; 1\rangle \end{aligned} \quad (4.27)$$

Applying an H gate to the ancilla register transfers the $d_H(\vec{x}, \vec{v}^p)$ from the phases into the amplitudes such that the new quantum state is described by,

$$\begin{aligned} |\psi_5\rangle &= (\mathbb{1} \otimes \mathbb{1} \otimes \mathbb{1} \otimes H) |\psi_4\rangle \\ &= \frac{1}{\sqrt{N}} \sum_p^N \cos\left[\frac{\pi}{2n} d_H(\vec{x}, \vec{v}^p)\right] |x_1, x_2, \dots, x_n; d_1^p, d_2^p, \dots, d_n^p; c^p; 0\rangle \\ &\quad + \sin\left[\frac{\pi}{2n} d_H(\vec{x}, \vec{v}^p)\right] |x_1, x_2, \dots, x_n; d_1^p, d_2^p, \dots, d_n^p; c^p; 1\rangle \end{aligned} \quad (4.28)$$

At this point the ancilla qubit is measured along the standard basis and all previous steps have to be repeated until the ancilla is measured in the $|0\rangle$ state. Since it is conditioned on a particular outcome, this type of measurement is called *conditional measurement* (CM). The probability of a successful CM is given by the square of the absolute value of the amplitude and is dependent on the average reverse HD between all training vectors and the input vector:

$$Prob(|a\rangle = |0\rangle) = \sum_p^N \cos^2\left[\frac{\pi}{2n} d_H(\vec{x}, \vec{v}^p)\right] \quad (4.29)$$

Finally, to classify the input vector \vec{x} the class register is measured along the standard basis. The probability of measuring a specific class c is then given by the following expression:

$$Prob(c) = \frac{1}{N Prob(|a\rangle = |0\rangle)} \sum_{l \in c} \cos^2\left[\frac{\pi}{2n} d_H(\vec{x}, \vec{v}^l)\right] \quad (4.30)$$

From Equ. 4.30 it is evident that the probability of measuring a certain class c is dependent on the average total reverse HD between all training vectors belonging to class c and the input vector \vec{x} . Since the total reverse HD represent distance-dependent weights it gets clear why this is the quantum equivalent to a classical distance-weighted kNN algorithm.

In order to obtain a full picture of the probability distribution over the different classes a sufficient number of copies of $|\psi_5\rangle$ needs to be prepared and after successful CM on the ancilla qubit the class qubit needs to be measured.

Algorithmic complexity

According to Schuld et al. (2014), the preparation of the superposition has a complexity of $\mathcal{O}(Pn)$ where P is the number of training vectors and n is the length of the feature vectors. The algorithm has to be repeated T times in order to get a statistically precise picture of the results. Hence, the total quantum kNN algorithm has an algorithmic complexity of $\mathcal{O}(TPn)$.

Chapter 5

Results and Discussion

Some more general text Why are some parts simulating and some parts using IBM?

5.1 Simulating the qubit-based kNN algorithm

The computer used for the Liqui|⟩ quantum simulations in this thesis only provides 8GB of RAM, thereby limiting the maximum number of simulated qubits to 24. Unfortunately, real-world machine learning problems usually involve large datasets that would require much more qubits such that a small artificial dataset needs to be constructed. For this reason, the classification of 9-bit, little-endian RGB colour codes into the classes *red* and *blue* will be considered. A 9-bit RGB colour code uses three bits to encode the content of each RGB colour; red, green and blue. Three binary bits b_0, b_1, b_2 can encode any of the numbers 0-7 according to the formula,

$$b_0 * 2^0 + b_1 * 2^1 + b_2 * 2^2 \text{ where } b_0, b_1, b_2 \in \{0, 1\} \quad (5.1)$$

For example, the 9-bit RGB code 111 100 100 can be written in roman numerals as 7,1,1 (full red, little green, little blue) and represents this red tone.

Since the class qubit $|c\rangle$ can only take binary values, class red is defined as $|c\rangle = |0\rangle$ and class blue is defined as $|c\rangle = |1\rangle$. The training set consists of 3 randomly chosen red and blue tones listed in Table 5.1.

The quantum classifier will then be tested on four new colour tones (two red, two blue) listed in Table 5.1. Note that all training colours are either pure red colours (without green or blue

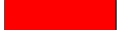





Colour	Binary 9-bit RGB string	Class
	111 000 000	red ($ 0\rangle$)
	101 000 000	red ($ 0\rangle$)
	110 000 000	red ($ 0\rangle$)
	000 000 111	blue ($ 1\rangle$)
	000 000 101	blue ($ 1\rangle$)
	000 000 100	blue ($ 1\rangle$)

Table 5.1: Training data set of six 9-bit RGB colour codes





Colour	Binary 9-bit RGB string	Expected classification outcome
	100 000 000	red ($ 0\rangle$)
	110 100 000	red ($ 0\rangle$)
	000 000 110	blue ($ 1\rangle$)
	000 100 111	blue ($ 1\rangle$)

Table 5.2: Input data set containing 9-bit RGB colour codes that require classification

content) or pure blue colours (without green or red content). The input colours, however, also include colours with additional green content testing how the classifier reacts in cases that are not included in the training set.

The first step towards the classification of RGB colour codes using the qubit-based kNN algorithm proposed by Schuld et al. (2014) as described in detail in Section 4.0.2 is preparing the initial superposition over all six 9-bit RGB training patterns t^j :

$$|T\rangle = \frac{1}{\sqrt{6}} \sum_{j=1}^N |t_1^j, t_2^j, \dots, t_9^j; c^j\rangle \quad (5.2)$$

This can be done using the quantum state preparation algorithm by Trugenberger (2001) outlined in Section 4.0.1. In this case, the seven steps (see blue box in Section 4.0.1) of the state preparation algorithm have to be repeated six times in order to load the six RGB training patterns t^j into the memory register m defined in Equ. 4.9. Afterwards, the state is given by,

$$|\phi_0\rangle = \frac{1}{\sqrt{6}} \sum_{j=1}^6 |t_1^6, t_2^6, \dots, t_9^6; u_1 = 0, u_2 = 0; t_1^j, t_2^j, \dots, t_9^j\rangle \quad (5.3)$$

Equ. 5.3 shows that the first register still contains the last stored RGB colour code t^6 , the second register consists of the utility qubits $|u_1\rangle$ and $|u_2\rangle$ that are both in the $|0\rangle$ state and the last register is in an equal superposition over all six RGB training colours. Thus, besides the missing class qubit $|c\rangle$ the last register is in the desired superposition defined in Equ. 5.2.

In the next step of the quantum kNN the yet unclassified 9-bit RGB input pattern x and an ancilla qubit $|a\rangle$ initialized in state $|0\rangle$ are added to the training superposition $|T\rangle$ to result in the full initial state $|\psi_0\rangle$:

$$|\psi_0\rangle = \frac{1}{\sqrt{6}} \sum_{j=1}^6 |x_1, x_2, \dots, x_9; t_1^j, t_2^j, \dots, t_9^j; c^j; 0\rangle \quad (5.4)$$

The trick now is to realize that Equ. 5.3 and 5.4 contain the same number of qubits. Firstly, each of them has nine qubits in the first register. Secondly, Equ. 5.3 has two utility qubits that are balanced by the ancilla and the class qubit in Equ. 5.4. Lastly, there are again nine qubits in the third register in Equ. 5.3 and the second register in Equ. 5.4. Thus, $|\psi_0\rangle$ and $|\phi\rangle$ both contain $9 + 9 + 2 = 20$ qubits. Since $|\phi\rangle$ is the current state of the qubits in the simulation, one simply needs to redefine the utility qubits such that the first one becomes the class qubit $|u_1\rangle = |c^j\rangle$ and the second utility qubit becomes the ancilla $|u_2\rangle = |a\rangle$. Since u_1 and u_2 are currently both in the $|0\rangle$ state the quantum state is now in the state,

$$|\phi_1\rangle = \frac{1}{\sqrt{6}} \sum_{j=1}^6 |t_1^j, t_2^j, \dots, t_9^j; c^j = 0; a = 0; t_1^j, t_2^j, \dots, t_9^j\rangle \quad (5.5)$$

Equ. 5.5 shows a quantum state with four registers as desired but the first register still contains the last training colour code. It can simply be overwritten with the desired input pattern by comparing the two patterns and flipping qubits at positions where the patterns do not match up. For example, if the last training pattern was 000 000 100 and the input pattern is 000 000 110 one simply needs to flip the 8th qubit through the application of an X gate. The state is now given by,

$$|\phi_1\rangle = \frac{1}{\sqrt{6}} \sum_{j=1}^6 |x_1, x_2, \dots, x_9; 0; 0; t_1^j, t_2^j, \dots, t_9^j\rangle \quad (5.6)$$

5.2 Development of an amplitude-based kNN algorithm

IBM doesn't allow for qubit based kNN due to restriction in qubit number

need for a new algorithm based on amplitudes

$$\frac{1}{\sqrt{2M}} \sum_{m=1}^M (|0\rangle |\Psi_{\tilde{x}}(\star)\rangle + |1\rangle |\Psi_{x^m}\rangle) |y^m(A \text{ or } B)\rangle |m\rangle \quad (5.7)$$

where

$$|\Psi_{\tilde{x}}(\star)\rangle = \sum_{i=1}^N \tilde{x}_i |i\rangle \quad |\Psi_{x^m}\rangle = \sum_{i=1}^N x_i^m |i\rangle \quad (5.8)$$

$$e.g. \quad \begin{pmatrix} 0.6 \\ 0.4 \end{pmatrix} \rightarrow |n\rangle = \sqrt{0.6} |0\rangle + \sqrt{0.4} |1\rangle \quad (5.9)$$

Applying the **Hadamard gate** interferes the input and the training vectors:

$$\frac{1}{2\sqrt{M}} \sum_{m=1}^M (|0\rangle [|\Psi_{\tilde{x}}\rangle + |\Psi_{x^m}\rangle] + |1\rangle [|\Psi_{\tilde{x}}\rangle - |\Psi_{x^m}\rangle]) |y^m(A \text{ or } B)\rangle |m\rangle \quad (5.10)$$

→ Perform **conditional measurement** on ancilla qubit.

Successful if $|0\rangle$ state is measured.

After successful conditional measurement, the state is proportional to

$$\frac{1}{2\sqrt{M}} \sum_{m=1}^M \sum_{i=1}^N (\tilde{x}_i + x_i^m) |0\rangle |i\rangle |y^m(A \text{ or } B)\rangle |m\rangle \quad (5.11)$$

Probability to measure class B:

$$p(|y^m\rangle = |1(B)\rangle) = \sum_{m|y^m=1(B)} 1 - \frac{1}{4M} |\tilde{x} - x^m|^2 \quad (5.12)$$

Hereby, the advantages of the quantum version are the parallel computation of the distances between each training vector and the input vector as well as contracting distance computation and distance weighting into one computational step.

The quantum advantage of the algorithm is the simultaneous computation of the HD between the input vector and each training vector which is impossible to do classically. For example, if the training set contains 1,000,000 vectors with 10 entries each, the quantum algorithm performs all 1,000,000 distance computations with the application of only 10 X and 10 CNOT gates. In contrast, the classical algorithm would need to perform 1,000,000 individual computations in order to be able to apply distance-dependent weights to each training vector.

Diffusion matrix from quantum random walks

Initialization of amplitude distribution is non-trivial

Need for a simpler way - using diffusion matrix from quantum random walks

For the simplest case, consider the entries in the classical probability vector v to be normal distributed, e.g.

CHECK THE ORDER!

$$v = \begin{pmatrix} 0.064180 \\ 0.146860 \\ 0.146770 \\ 0.341590 \\ 0.026840 \\ 0.063590 \\ 0.061700 \\ 0.148470 \end{pmatrix} \quad (5.13)$$

The goal is to encode this classical data into a quantum memory state $|M\rangle$ of the form,

$$\begin{aligned} |M\rangle = & 0.064180 |000\rangle + 0.146860 |100\rangle + 0.146770 |010\rangle + 0.341590 |001\rangle \\ & + 0.026840 |110\rangle + 0.063590 |011\rangle + 0.061700 |101\rangle + 0.148470 |111\rangle \end{aligned} \quad (5.14)$$

Furthermore, a useful tool of visualizing the HDs between binary patterns made from three qubits is a 3-D cube as shown in Fig. 5.1. On the cube, adjacent qubit patterns have a HD of 1 and the HD increases by 1 for every additional corner. For example, the qubit state $|000\rangle$ is adjacent to $|100\rangle$ since they only differ in one qubit ($HD = 1$). Moving one more corner yields the state $|101\rangle$ or $|110\rangle$ which both have a HD of 2 compared to $|000\rangle$.

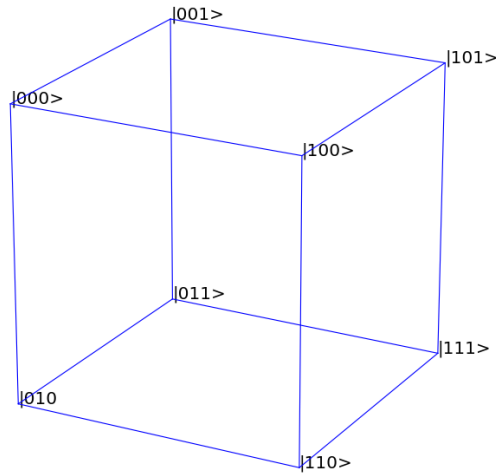


Figure 5.1: Visualizing Hamming distances on a 3-D cube

This way of visualizing HDs can be extended to the 16 binary patterns made by four qubits that can be visualized on a 4-D cube, also called tesseract, as illustrated in Fig. 5.2.

The idea of a coin operator C can be borrowed from the theory of quantum random walks to initialize a gaussian distribution centered around a chosen binary qubit pattern. For this purpose, the coin operator is defined as,

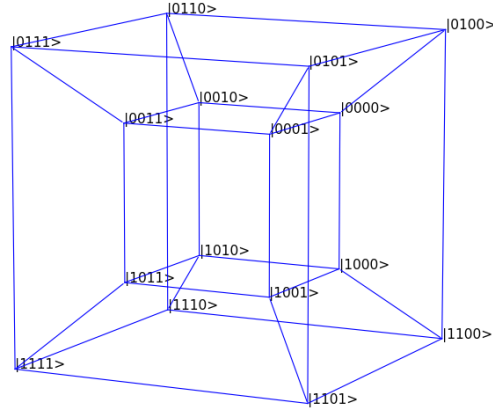


Figure 5.2: Visualizing Hamming distances on a 4-D cube (tesseract)

$$C = \begin{pmatrix} \sqrt{\delta} & 1 - \sqrt{\delta} \\ 1 - \sqrt{\delta} & -\sqrt{\delta} \end{pmatrix} \quad (5.15)$$

where $0 \leq \delta \leq 1$.

IBM implementation problems

Complexity analysis of actual implementation with IBM QC

Controlled U Gate

Often there is a need for applying certain quantum gates in a controlled manner. Thus a controlled U (CU) gate is required whereby U can be any unitary single-qubit gate. The CU gate is defined as:

$$CU = \begin{pmatrix} \mathbb{1} & 0 \\ 0 & U \end{pmatrix} \quad (5.16)$$

It is important to note that the CNOT gate is essentially a CU gate in the case of $U = X$.

Most of the time the CU gate cannot be implemented directly and has to be realized through larger quantum circuits consisting of CNOT and single-qubit gates. Nielsen and Chuang (2010) describe such a decomposition as shown in Fig. 5.3.

The idea is that when the control qubit is $|0\rangle$ the gate combination ABC is applied to the target qubit and has to equal the identity gate:

$$ABC = \mathbb{1} \quad (5.17)$$

³Reprinted from Michael A. Nielsen and Isaac L. Chuang. Quantum Computation and Quantum Information. Cambridge University Press, 2000. Copyright 2010 by Nielsen & Chuang.

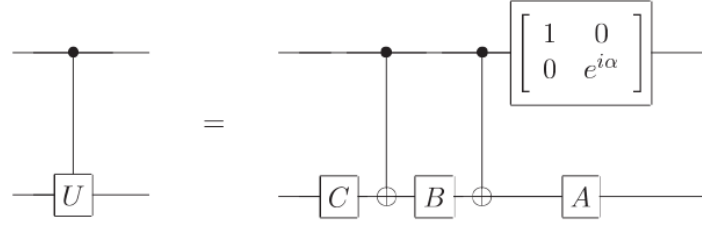


Figure 5.3: Circuit decomposition for a controlled-U operation for single-qubit gate U .³

If and only if the control qubit is $|1\rangle$ then the gate sequence $e^{i\alpha}AXBXC$ is applied to the target. Since the goal is to apply the unitary U to the target qubit the following equation must be satisfied,

$$e^{i\alpha}AXBXC = U \quad (5.18)$$

In order to find the matrices A, B, C and the additional parameter α the following equation has to be solved:

$$U = \begin{pmatrix} e^{i(\alpha - \frac{\beta}{2} - \frac{\delta}{2})} \cos \frac{\gamma}{2} & -e^{i(\alpha - \frac{\beta}{2} + \frac{\delta}{2})} \sin \frac{\gamma}{2} \\ e^{i(\alpha + \frac{\beta}{2} - \frac{\delta}{2})} \sin \frac{\gamma}{2} & e^{i(\alpha + \frac{\beta}{2} + \frac{\delta}{2})} \cos \frac{\gamma}{2} \end{pmatrix} \quad (5.19)$$

Chapter 6

Outlook

Chapter 7

Conclusion

Chapter 8

Personal reflection

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