# Hands-On Quantum Machine Learning With Python Volume 1: Get Started

### Dr. Frank Zickert



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Pre-Release 0.2, March 2021

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## 1. Introduction

Welcome to **Hands-On Quantum Machine Learning With Python**. This book is your comprehensive guide to get started with "Quantum Machine Learning" – the use of **quantum computing** for computation of **machine learning** algorithms.

**Hands-On Quantum Machine Learning With Python** strives to be the perfect balance between theory taught in a textbook and the actual hands-on knowledge you'll need to implement real-world solutions.

Inside this book, you will learn the basics of quantum computing and machine learning in a practical and applied manner. And you will learn to use state-of-the-art quantum machine learning algorithms.

By the time you finish this book, you'll be well equipped to apply quantum machine learning to your projects. You will be in the pole position to become a "Quantum Machine Learning Engineer" – the job to become the sexiest job of the 2020s.

### 1.1 Who This Book Is For

This book is for **developers**, **programmers**, **students**, and **researchers** who have at least some programming experience and who want to become proficient in quantum machine learning.

Don't worry if you're just getting started with quantum computing and machine learning. We will begin with the very basics. We don't assume prior knowledge of machine learning or quantum computing. You will not get left behind.

If you are already experienced in machine learning or quantum computing, the respective parts may be a repetition of concepts you're already familiar with. However, this may make learning the respective new topic easier and provide a slightly different angle to the known.

This book offers a practical, hands-on exploration of quantum machine learning. Rather than working through tons of theory, we will build up practical intuition about the core concepts. We will acquire the exact knowledge we need to solve practical examples with lots of code. Step by step, you will extend your knowledge and learn how to solve new problems.

Of course, we will do some math. Of course, we will cover a little physics. But I don't expect you to hold a degree in any of these two fields. We will go through all the concepts we need. While this includes some mathematical notation and formulae, we keep it at the minimum required to solve our practical problems.

The theoretical foundation of quantum machine learning may appear overwhelming at first sight. Be assured, when put into the right context and when explained conceptually, it is not harder than learning a new programming language. And this is what's inside **Hands-On Quantum Machine Learning With Python**.

Of course, we will write code. A lot of code, actually. If you know a little Python, great! If you don't know Python but another language, such as Java, Javascript, or PHP, you'll be fine, too. If you know programming concepts (such as if then else-constructs and loops) then learning the syntax is a piece of cake. If you're familiar with functional programming constructs, such as map, filter, and reduce, you're already well equipped. If not, don't worry, we will get you started with these constructs, too. We don't expect you to be a senior software developer. We will go through all the code. Line by line.

By the time you finish the first few chapters of this book, you will be proficient with doing the math, understanding the physics, and writing the code you need to graduate to the more advanced content.

This book is not just for beginners. There is a lot of advanced content in here, too. Many chapters of **Hands-On Quantum Machine Learning With Python** cover, explain, and apply quantum machine learning algorithms developed in the last two years. The insights this book provides can be directly applied in your job and research. The time you'll save by reading through **Hands-On Quantum Machine Learning With Python** will more than pay for itself.

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### 1.2 Book Organization

Machine learning and quantum computing rely on math, statistics, physics, and computer science. This a lot of theory. Covering it all upfront would be quite exhaustive and fill at least one book without any practical insight.

However, without at least some understanding of the underlying theoretical concepts, the code examples on their own do not provide many practical insights, either. While libraries free you from tedious implementation details, the code, even though short, does not explain the core concepts.

This book provides the theory needed to understand the code we're writing to solve a problem. We cover the theory when it applies and when we need the background to understand what we are doing. We will embed the theory into solving a practical problem and thus, directly see it in action.

As a result, the theory spreads among all the chapters. From simple to complex. You may skip certain examples if you like. But you should have a look at the theoretical concepts discussed in each chapter.

In this pre-release, we start with a **Variational Hybrid Quantum-Classical Algorithm** to solve a binary classification task. First, we have a detailed look at binary classification in chapter 2. Then, in chapter ??, we introduce the basic concept of the quantum bit, the quantum state, and how measurement affects it. Based on these concepts, we build our first **Parameterized Quantum Circuit** and use it to solve our binary classification task. Such a hybrid algorithm combines the quantum state preparation and measurement with classical optimization.

## 1.3 Why Should I Bother With Quantum Machine Learning?

In the recent past, we have witnessed how algorithms learned to drive cars and beat world champions in chess and Go. Machine learning is being applied to virtually every imaginable sector, from military to aerospace, from agriculture to manufacturing, and from finance to healthcare.

But these algorithms become increasingly hard to train because they consist of billions of parameters. Quantum computers promise to solve such problems intractable with current computing technologies. Their ability to compute multiple states simultaneously enables them to perform an indefinite number of superposed tasks in parallel. An ability that promises to improve and to expedite machine learning techniques. Unlike classical computers that are based on sequential information processing, quantum computing makes use of the properties of quantum physics. Superposition, entanglement, and interference. But rather than increasing the available computing capacity, it reduces the capacity needed to solve a problem.

But quantum computing requires us to change the way we think about computers. It requires a whole new set of algorithms. Algorithms that encode and use quantum information. This includes machine learning algorithms.

And it requires a new set of developers. Developers who understand machine learning and quantum computing. Developers capable to solve practical problems that have not been solved before. A rare type of developer. The ability to solve quantum machine learning problems today already sets you apart from all the others.

Quantum machine learning promises to be disruptive. Although this merger of machine learning and quantum computing, both areas of active research, is largely in the conceptual domain, there are already a number of examples where it is being applied to solve real-life problems. Google, Amazon, IBM, Microsoft, and a whole fleet of high-tech startups strive to be the first to build and sell quantum machine learning systems.

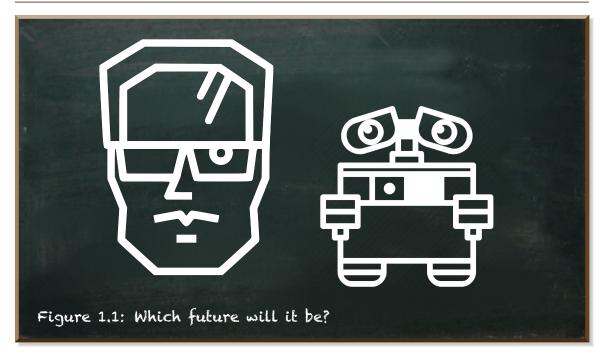
The opportunity to study a technology right at the moment when it is about to prove its supremacy is a unique opportunity. Don't miss it.

## 1.4 Quantum Machine Learning -Beyond The Hype

If there were two terms in computer science that I would describe as overly hyped and poorly understood, I would say machine learning and quantum computing.

That said, **Quantum Machine Learning** is the use of quantum computing for computation of machine learning algorithms. Could it be any worse?

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There are a lot of anecdotes on these two technologies. They start at machines that understand the natural language of us humans. And they end at the advent of the Artificial General Intelligence that either manifests as the Terminator-like apocalypse or the Wall-E-like utopia.

**Don't fall for the hype!** An unbiased and detailed look at a technology helps not to fall for the hype and the folklore. Let's start with machine learning.

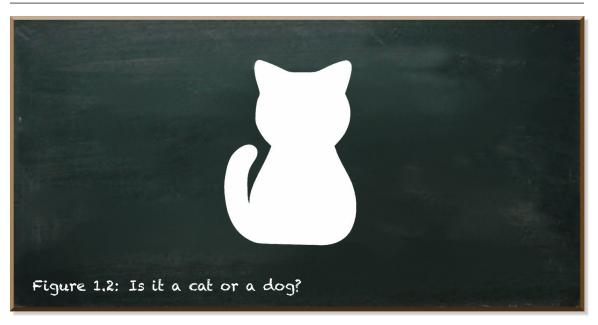
#### 1.4.1 What is Machine Learning?

#### "Machine learning is a thing-labeler, essentially"

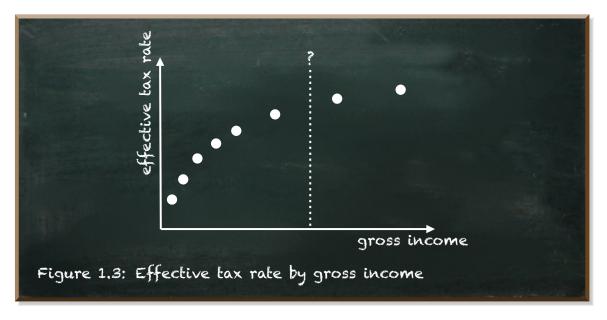
– Cassie Kozyrkov, Chief Decision Scientist at Google, source –

With machine learning, we aim to put a label onto a yet unlabeled thing. And there are three main ways of doing it: classification, regression, and segmentation.

In **classification**, we try to predict the discrete label of an instance. Given the input and a set of possible labels, which one is it? Here's a picture. Is it a cat or a dog?

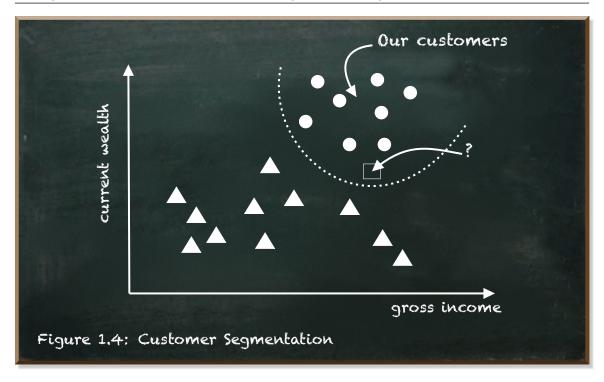


**Regression** is about finding a function to predict the relationship between some input and the dependent continuous output value. Given you know the income and the effective tax rates of your friends, can you estimate your tax rate given your income even though you don't know the actual calculation?



And **segmentation** is the process of partitioning the population into groups with similar characteristics who are thus likely to exhibit similar behavior. Given you produce an expensive product, such as yachts, and a population of potential customers, who do you want to try to sell to?

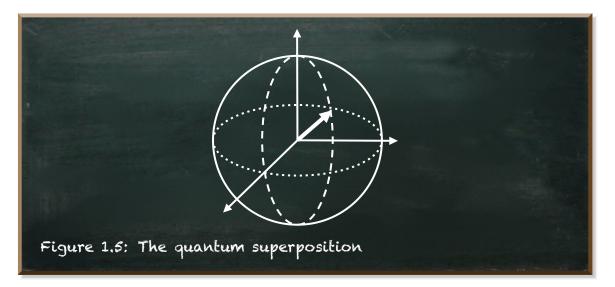
#### 1.4 Quantum Machine Learning - Beyond The Hype



### 1.4.2 What is Quantum Computing?

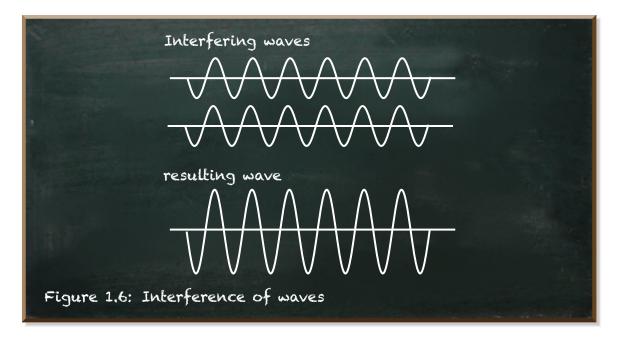
Quantum computing is a different form of computation. It uses three fundamental properties of quantum physics: superposition, interference, and entanglement.

**Superposition** refers to the quantum phenomenon where a quantum system can exist in multiple states concurrently.



Actually, the quantum system does not exist in multiple states concurrently. It exists in a complex linear combination of a state 0 and a state 1. It is a different kind of combination that is neither "or" nor is it "and". We will explore this state in depth in this book.

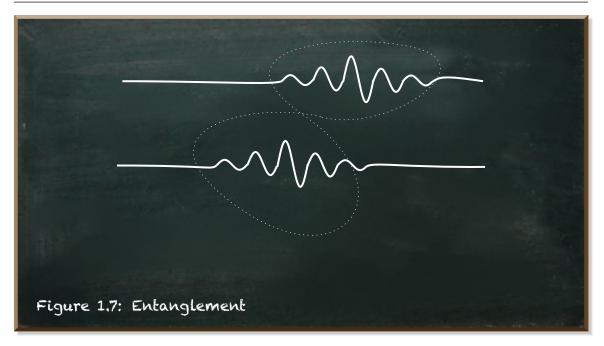
Quantum **interference** is what allows us to bias quantum systems toward the desired state. The idea is to create a pattern of interference where the paths leading to wrong answers interfere destructively and cancel out but the paths leading to the right answer reinforce each other.



**Entanglement** is an extremely strong correlation between quantum particles. Entangled particles remain perfectly correlated even if separated by great distances.

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#### 1.4 Quantum Machine Learning - Beyond The Hype



#### Do you see the Terminator already? No?

#### Maybe Wall-E? No again?

Maybe it helps to look at how these things work.

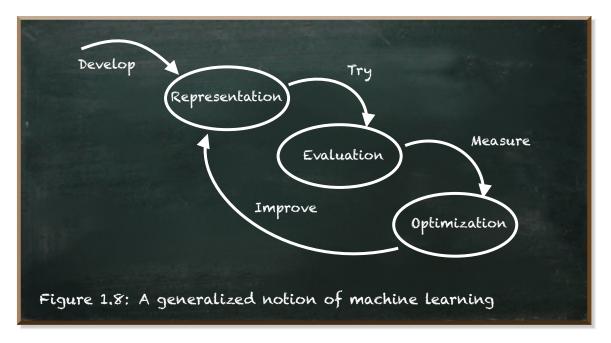
#### 1.4.3 How Does Machine Learning Work?

There are myriads of machine learning algorithms out there. But every one of these algorithms has three components:

- The **Representation** depicts the inner architecture the algorithm uses to represent the knowledge. It may consist of a set of rules, instances, decision trees, support vector machines, neural networks, and others.
- The **Evaluation** is a function to evaluate candidate algorithm parameterizations. Examples include accuracy, prediction and recall, squared error, posterior probability, cost, margin, entropy, and others.
- The **Optimization** describes the way of generating candidate algorithm parameterizations. It is known as the search process. For instance, combinatorial optimization, convex optimization, and constrained optimization.

The first step of machine learning is the development of the architecture, the representation. The architecture specifies the parameters whose values hold the representation of the knowledge. This step determines how suited the solution will be to solve a certain problem. More parameters are not always

better. If our problem can be solved by a linear function, trying to solve it with a solution that consists of millions of parameters is likely to fail. On the other hand, an architecture with very few parameters may be insufficient to solve complex problems such as natural language understanding.



Once we settled for the architecture to represent the knowledge, we train our machine learning algorithm with examples. Depending on the number of parameters, we need a lot of examples. The algorithm tries to predict the label of each example. We use the evaluation function to measure how the algorithm performed.

Finally, the optimizer adjusts the representation parameters in a way that promises better performance with regard to the measured evaluation. It may even involve changing the architecture of the representation.

Learning does not happen in giant leaps. Rather in tiny steps. In order to yield a good performance and depending on the complexity of the problem, it takes several iterations of this general process until the machine is able to put the correct label at a thing.

#### 1.4.4 What Tasks Are Quantum Computers Good At?

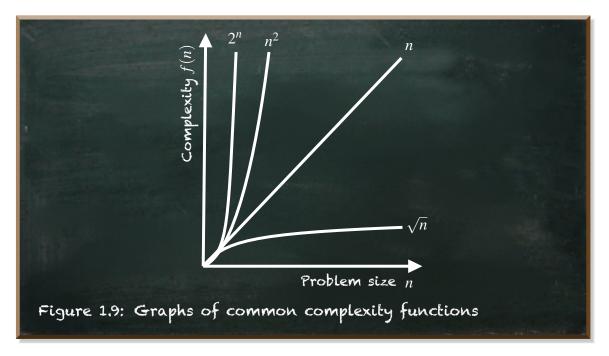
The world of quantum mechanics is different from the physics we experience in our everyday situations. So is the world of quantum computing different from classical (digital) computing. What makes quantum computing so powerful isn't its processing speed. In fact, it is rather slow. What makes quantum computing so powerful isn't its memory, either. In fact, it is absurdly tiny. We're talking about a few quantum bits.

What makes quantum computing so powerful is the algorithms it makes possible. These algorithms exhibit different complexity characteristics than their classical equivalents.

In order to understand what that means, let's have a brief look at complexity theory. Complexity theory is the study of the computational effort required to run an algorithm.

For instance, the computational effort of addition is  $\mathcal{O}(n)$ . This means that the effort of adding two numbers increases linearly with the size (digits) of the number. The computational effort of multiplication is  $\mathcal{O}(n^2)$ . The effort increases by the square of the number size. These algorithms are said to be solvable in polynomial time.

But these problems are comparably simple. The best algorithm solving the problem of factorization, that is finding the prime factors of an *n*-digit number, is  $\mathcal{O}(e^{n1/3})$ . It means that the effort increases exponentially with the number of digits.



The difference between  $\mathcal{O}(n^2)$  and  $\mathcal{O}(e^{n1/3})$  complexity must not be underestimated. While your smartphone is able to multiply numbers with 800 digits in a few seconds, the factorization of such numbers takes about 2,000 years

on a supercomputer.

A savvy quantum algorithm (such as Shor's algorithm) can use superposition to evaluate all possible factors of a number simultaneously. And rather than calculating the result, it uses interference to combine all possible answers in a way that yields a correct answer. This algorithm solves a factorization problem with  $\mathcal{O}((\log n)^2(\log \log n)(\log \log \log n))$  complexity. This is a polynomial complexity! So is multiplication.

Quantum computing is powerful because it promises to solve certain types of mathematical calculations with reduced complexity.

Do you see the Terminator or Wall-E now? Not yet?

#### 1.4.5 The Case For Quantum Machine Learning

Quantum machine learning is the use of quantum computing for the computation of machine learning algorithms.

We have learned that machine learning algorithms contain three components: representation, evaluation, and optimization.

When we look at the representation, current machine learning algorithms, such as the Generative Pre-trained Transformer 3 (GPT-3) network, published in 2020, come to mind. GPT-3 produces human-like text. It has 175 billion parameters. The IBM Q quantum computer has 27 quantum bits. Even though quantum bits store a lot more information than a classical bit does (because it is not either 0 or 1), quantum computers are far away from advancing machine learning for their representation ability.

During the evaluation, the machine learning algorithm tries to predict the label of a thing. Classically, this involves measuring and transforming data points. For instance, neural networks rely on matrix multiplications. These are tasks classical computers are good at. However, if you have 175 billion parameters, then calculating the resulting prediction takes quite a lot of matrix multiplications.

Finally, the algorithm needs to improve the parameters in a meaningful way. The problem is to find a set of parameter values that result in better performance. With 175 billions of parameters, the number of combinations is endless.

Classical machine learning employs heuristics that exploit the structure of the problem to converge to a sufficient solution within a reasonable time. Despite the use of even advanced heuristics, training the GPT-3 would require 355 years to train on a single GPU (Graphics Processing Unit) and cost \$4.6 million. Just to get a feeling of what reasonable means in this context.

The main characteristic of quantum computing is the ability to compute multiple states concurrently. A quantum optimization algorithm can combine all possible candidates and yield those that promise good results. Therefore, quantum computing promises to be exponentially faster than classical computers in the optimization of the algorithm.

But this does not mean we only look at the optimization. Because the optimization builds upon running an evaluation. And the evaluation builds upon the representation. Thus, tapping the full potential of quantum computing to solve the machine learning optimization problem requires the evaluation and the representation to integrate with the quantum optimizer.

Having in mind what classical machine learning algorithms can do today, and if we expect quantum computing to reduce the complexity of training such algorithms by magnitudes, then the hype becomes understandable. Because we are "only" magnitudes away from things like Artificial General Intelligence.

But of course, building an Artificial General Intelligence requires more than the computation. It needs data. And it needs the algorithms.

The development of such algorithms is one of the current challenges in quantum machine learning. But there's another aspect to cope with in that challenge. That aspect is we are in the NISQ era.

### 1.5 Quantum Machine Learning In The NISQ Era

Quantum computing is a different form of computation. A form that, as we just learned, can change the complexity of solving problems making them tractable. But this different form of computation brings its own challenges.

Digital computers need to distinguish between two states: 0 and 1. The circuits need to tell the difference between high voltage and low voltage. Whenever there is a high voltage, it is 1 and if there is a lower voltage it is 0. This discretization means that errors must be relatively large to be noticeable and methods for detecting and correcting such errors can then be implemented.

Unlike digital computers, quantum computers need to be very precise. They keep a continuous quantum state. And quantum algorithms that base on precise manipulations of continuously varying parameters. In quantum computers, however, errors can be arbitrarily small and impossible to detect, but

still, their effects can build up to ruin a computation.

This fragile quantum state is very vulnerable to the noise coming from the environment around the quantum bit. Noise can arise from control electronics, heat, or impurities in the quantum computer's material itself, and can also cause serious computing errors that may be difficult to correct.

But to keep the promises quantum computers make, we need fault-tolerant devices. We need devices to compute Shor's algorithm for factoring. We need devices to execute all the other algorithms that have been developed in theory that solve problems intractable for digital computers.

But such devices require millions of quantum bits. This overhead is required for error correction since most of these sophisticated algorithms are extremely sensitive to noise.

Current quantum computers have up to 27 quantum bits. Even though IBM strives for a 1000-quantum bits computer by 2023, the quantum processors we expect in the near-term will have between 50 and 100 quantum bits. Even if they exceed these numbers, they remain relatively small and noisy. These computers can only execute short programs since the longer the program is the more noise-related output errors will occur.

Nevertheless, programs that run on devices beyond 50 quantum bits become extremely difficult to simulate on classical computers already. These devices can do things infeasible for a classical computer.

And this is the era we're about to enter. The era when we can build quantum computers that, while not being fault-tolerant, can do things classical computers can't. The era is described by the term "Noisy Intermediate-Scale Quantum" - NISQ.

Noisy because we don't have enough qubits to spare for error correction. And "Intermediate-Scale" because of the number of quantum bits is too small to compute sophisticated quantum algorithms, but large enough to show quantum advantage or even supremacy.

The current era of NISQ-devices requires a different set of algorithms, tools, and strategies.

For instance, **Variational Quantum-Classical Algorithms** have become a popular way to think about quantum algorithms for near-term quantum devices. In these algorithms, classical computers perform the overall machine learning task on information they acquire from running certain hard-to-compute calculations on a quantum computer.

The quantum algorithm produces information based on a set of parameters provided by the classical algorithm. Therefore, they are called **Parameter-ized Quantum Circuits (PQCs)**. They are relatively small, short-lived, and thus suited for NISQ-devices.

### 1.6 I learned Quantum Machine Learning The Hard Way

I did not have the fortune to take a quantum computing class in college. Not to speak of a class in quantum machine learning. At the time, it wouldn't have been much fun either. In the early 2000s, quantum computing was just about to take the step from a pure theory to be evaluated in research labs. It was a field for theoretical physicists and mathematicians.

At the time, I haven't even heard about it. Unfortunately. When I headed about quantum computing for the first time, I think it was around 2008, researchers had successfully entangled qubits and were able to control them. Of course, Star Trek-like transportation came to mind when I heard two particles that were physically apart could share a state so that it was possible to change the state of one particle by observing the other.

Yet, until around 2014, I did not pay much attention. I was too busy writing my doctoral dissertation about assessing the effort caused by the requirements in a software development project. When I returned to normal life, I was just right in time to experience the end of the second AI winter and the advent of practical machine learning. What had been theory thus far became reality now.

When I got into machine learning, the field was already quite evolved. Libraries such as Scikit-Learn, later Keras, TensorFlow, and PyTorch made the development of machine learning algorithms convenient. Even though my favorite books were published sometime later, there were already a lot of good books and learning material available.

My favorite books are: Hands-On Machine Learning with Scikit-Learn and TensorFlow by Aurélien Géron released 2017 and Deep Learning with Python by Francois Chollet released 2018.

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But the models we're developing today become increasingly hard to train. Open AI's GPT-3 model that uses deep learning to produce human-like text would require 355 years on a single GPU and cost \$4,600,000 to train. It is hard to believe that the upcoming milestones can be reached classically. This insight brought quantum computing back into my focus. Quantum computing promises to reduce the computational complexity of certain algorithms by magnitudes. It promises to solve tasks in a few seconds classical computers would need thousands of years for. It promises to prevent us from the next AI winter that would be caused by the inability to reach the next milestones of machine learning.



In 2018, I started to deep dive into quantum machine learning. Scientific papers and a few theoretical books were all I could find. And these did not cover quantum machine learning but quantum computing in general. I was happy about every little piece.

After reading these quantum computing publications, I was left scratching my head. Most of the papers are pretty heavy on math and assume you're familiar with a lot of physical jargon. I could not even find an appropriate starting point or some guidance on how to structure my learning efforts.

Frustrated with my failed attempts, I spent hours searching on Google. I hunted for quantum tutorials, only to come up empty-handed.

I could clearly see the potential value of quantum computing for machine learning. Yet, I couldn't see how all these parts of quantum computing fit together. Entry-level material was hard yo find. And practical guides were simply not existent. I wanted to get started, but I had nothing to show for my effort, except for a stack of quantum computing papers on my desk that I hardly understood.

Finally, I resorted to learning the theory first. I heard about Qiskit, the IBM quantum SDK for Python. At the time, its documentation was rather poor, especially if you were not familiar with all the physical jargon and its under-

lying theory. But it let me experience what some of these things like superposition, entanglement, and interference practice meant.

This practical knowledge enabled me to connect quantum computing with the algorithms I knew from machine learning. I found my way to quantum machine learning success through myriads of trial-and-error experiments, countless late nights, and a lot of endurance. I really believe that painstakingly working everything out in small pieces made an impact on how I understand quantum machine learning. Though, I would recommend not taking the same path.

My personal takeaways are:

- You don't need to cram all the theory before you start applying it
- You don't need to work through tons of equations
- You don't need to be a mathematician to master quantum machine learning
- You don't need to be a physicist to understand quantum machine learning
- You'll do great as a programmer, an engineer, a data scientist, or any other profession.
- But quantum machine learning is taught the wrong way

When I started studying the quantum part of quantum machine learning, I took a deep dive into the theory and into math. Because this is what most quantum computing resources focus on.

Of course, it is desirable to have an understanding of the underlying math and the theory. But more importantly, you need to have an understanding of what the concepts mean in practice. If you know what you can do and how you need to do it, you don't need to think about how it (physically) works all the time.

Don't get me wrong. In quantum machine learning, their and math are important. But if you don't use the theoretical knowledge and apply it to solve real-world tasks, then you'll have a hard time finding your space in the quantum machine learning world. You need to become a quantum machine learning practitioner from the very beginning. In contrast to the days when I started, today there are quite a few resources available. But most of them fall into one of the following categories

- Theoretical papers with lots of equations prove some quantum speedup of an algorithm. Yet, they don't show any code.
- Textbooks on quantum computing in general explain the concepts in an understandable manner. But they are short on showing how to use

them for a purpose.

• Blog posts show you an actual algorithm in code. But they don't relate the code to any underlying concept. You see it works. But you don't learn anything about why and how it works.

By no means do I want to say these resources are not worth reading. But none of these resources are useful to learn how to apply quantum machine learning. For someone just about to start with quantum machine learning, you would need to invest a lot of time and effort for little to no practical return.

There is a fundamental disconnect between theory and practice. There's a gap I want to help to fill with **Hands-On Quantum Machine Learning with Python** so you can learn in a more efficient-a better way.

This is the book I wish I had when I first started studying quantum machine learning. Inside this book, you'll find practical walkthroughs and hands-on tutorials with lots of code. The book introduces new theory just in time you need it to take the next step. You'll learn a lot of theory. But you're not left alone with it. We directly apply our newly acquired knowledge to solve an actual problem.

We will not only implement different quantum machine learning algorithms, such as Quantum Naïve Bayes, Quantum Bayesian Network, Variational Quantum Eigensolver, and Quantum Approximate Optimization Algorithms. But we also use them to solve actual problems taken from Kaggle.

By the time you finish this book, you'll know these algorithms, what they do, why you need them, how they work, and most importantly how to use them.

Hands-On Quantum Machine Learning With Python strives to be the perfect balance between theory taught in a textbook and the actual hands-on knowledge you'll need to implement real-world solutions.

This book is your comprehensive guide to get started with Quantum Machine Learning"–the use of quantum computing for machine learning tasks.

### 1.7 Quantum Machine Learning Is Taught The Wrong Way

The literature on quantum computing is full of physical jargon and formulae. Let's take the Variational Quantum Eigensolver (VQE) for instance.

VQE can help us to estimate the energy of the ground state of a given quantum mechanical system. This is the upper bound of the

lowest eigenvalue of a given Hamiltonian. It builds upon the variational principle that is described as:  $\langle \Psi \lambda | H | \Psi \lambda \rangle >= E_0$ 

The first and natural reaction-if you don't hold a degree in physics-is to put the article away.

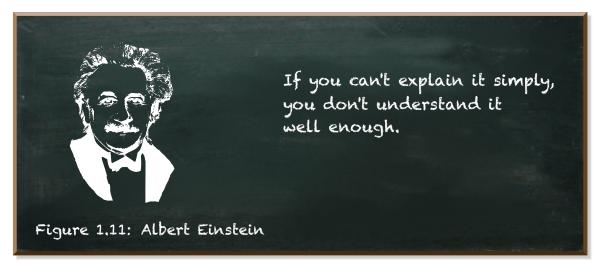
"Well, nice try. Maybe the whole topic is not for me", you think. "Maybe, quantum computing is beyond my reach".

Don't give up that fast. Most of the stuff in quantum computing was discovered by physicists and mathematicians. Of course, they build upon the knowledge of their peers when they share insights and teach their students. It is reasonable they use the terms they are familiar with.

You wouldn't use the vocabulary of a bartender to explain programming and machine learning either, would you? But maybe, we should.

It is reasonable to assume a certain kind of knowledge when we talk or write about something. But should we restrain students of other, nearby disciplines from learning the stuff? Why shouldn't we support a computer scientist or a software engineer in learning quantum computing?

I've got a clear opinion. I believe anyone sincerely interested in quantum computing should be able to learn it. There should be resources out there catering to the needs of the student, not to the convenience of the teacher. Of course, this requires a teacher able to explain the complex stuff in allegedly simple language.



I wouldn't dare to say I understood quantum computing well enough to explain it with the vocabulary bartenders use. But I'd give it a shot explaining it to a computer scientist and a software engineer. I don't see a reason to restrict this field to physicists, only. Of course, it is desirable to understand the underlying theory of quantum mechanics. Of course, it is desirable to be able to do the math. But, more importantly, you need to understand how to solve a certain problem.

In quantum computing, we use quantum superposition, entanglement, and interference to solve tasks. These are astonishing and maybe counterintuitive phenomena. But no matter how weird they may appear, quantum mechanical systems adhere to a certain set of physical laws. And these laws make the systems behave in certain ways. How deep do you have to know the physical laws? How much quantum math do you need?

I don't believe anyone (including me) really understands how a classical computer works. Yet, we all use them. We even program them! I learned how to code a classical computer because my teachers explained it to me in a way I was able to understand back then.

My high-school teacher explained the concepts of data types and algorithms in an applied way. He taught me how they work and what they are good for. Even though-or maybe because-we didn't go through electro-mechanical circuits and information theory, I was able to learn to program.

"Maybe quantum computing is different," you say? "Maybe, the stuff in there is too complex to learn without a degree in physics!"

The theoretical foundation of quantum machine learning may appear overwhelming at first sight. Be assured, when put into the right context and when explained conceptually, it is not harder than learning a new programming language. And this is what's inside Hands-On Quantum Machine Learning With Python.

In my post "Quantum Programming-For Non-Mathematicians", I showed how to calculate the joint probability of two probabilities with Qiskit-the quantum SDK of IBM. You don't need to know all the theory to follow it. In "Do You Struggle With The Quantum Superposition?", I give a hands-on introduction to quantum computing.

I truly believe developers, programmers, and students who have at least some programming experience can become proficient in quantum machine learning. Teaching QML the right way requires a different approach-a practical approach.

Rather than working through tons of theory, a good approach builds up practical intuition about the core concepts. I think it is best to acquire the exact theoretical knowledge we need to solve practical examples.

Step by step, we need to extend our knowledge and learn how to solve new

problems. Of course, we will need some math. Of course, we will need a little physics. But we should not expect the student to hold a degree in any of these two fields.

In a practical approach, we will write code. A lot of code, actually. Most machine learning and quantum computing libraries use Python. If you know a little Python, great! If you don't know Python but another language, such as Java, Javascript, or PHP, you'll be fine, too. It is more important to know programming concepts (such as if then else-constructs and loops) than it is to know the syntax. Once you have some experience in how things work, learning a different syntax is a piece of cake. The same is true for quantum computing. Once you know how to work with qubits, it doesn't really matter whether you use Qiskit (the IBM SDK) or Cirq (the Google SDK).

Quantum machine learning relies on math, statistics, physics, and computer science. This a lot of theory. Covering it all upfront would be quite exhaustive and fill at least one book without any practical insight. However, without at least some understanding of the underlying theoretical concepts, code examples on their own do not provide many practical insights, either. While libraries free you from tedious implementation details, the code, even though short, does not explain the core concepts.

An appropriate practical approach provides the theory needed to understand the code we write to solve a problem. We should cover the theory when it applies and when we need the background to understand what we are doing. We should embed the theory into solving a practical problem and thus, directly see it in action.

This is the approach we follow in the book Hands-on Quantum Machine Learning With Python.

This book is your comprehensive guide to get started with Quantum Machine Learning"–the use of quantum computing for machine learning tasks.

Hands-On Quantum Machine Learning With Python strives to be the perfect balance between theory taught in a textbook and the actual hands-on knowledge you'll need to implement real-world solutions. Inside this book, you will learn the basics of quantum computing and machine learning in a practical and applied manner. And you will learn to use state-of-the-art quantum machine learning algorithms. By the time you finish this book, you'll be well equipped to apply quantum machine learning to your projects. You will be in the pole position to become a "Quantum Machine Learning Engineer"-the job to become the sexiest job of the 2020s.

## 1.8 Configuring Your Quantum Machine Learning Workstation

Even though this book is about quantum machine learning, I don't expect you to have a quantum computer at your disposal. Thus, we will run most of the code examples in a simulated environment on your local machine. But we will need to compile and install some dependencies first.

We will use the following software stack:

- Unix-based operating system (not required but recommended)
- Python, including pip
- Jupyter (not required but recommended)

### 1.8.1 Python

For all examples inside **Hands-On Quantum Machine Learning With Python**, we use Python as our programming language. Python is easy to learn. Its simple syntax allows you to concentrate on learning quantum machine learning, rather than spending your time with the specificities of the language.

Most importantly, machine learning tools, such as PyTorch and Tensorflow, as well as quantum computing tools, such as Qiskit and Cirq, are available as Python SDKs.

### 1.8.2 Jupyter

Jupyter notebooks are a great way to run quantum machine learning experiments. They are a de facto standard in the machine-learning and quantum computing communities.

A notebook is a file format (.ipynb). The Jupyter Notebook app lets you edit your file in the browser while running the Python code in interactive Python kernels. The kernel keeps the state in memory until it is terminated or restarted. This state contains the variables defined during the evaluation of code.

A notebook allows you to break up long experiments into smaller pieces you can execute independently. You don't need to rerun all the code every time you make a change. But you can interact with it.

#### 1.8.3 Libraries and Packages

We will use the following libraries and packages:

- Scikit-learn
- PyTorch or Tensorflow
- Qiskit or Cirq

Scikit-learn is the most useful library for machine learning in Python. It contains a range of supervised and unsupervised learning algorithms. Scikitlearn builds upon a range of other very useful libraries, such as:

- NumPy: Work with n-dimensional arrays
- SciPy: Fundamental library for scientific computing
- Matplotlib: Comprehensive 2D/3D plotting
- IPython: Enhanced interactive console
- Sympy: Symbolic mathematics
- Pandas: Data structures and analysis

PyTorch and Tensorflow are the major libraries when it comes to deep neural networks. Qiskit is IBM's quantum computing SDK and Cirq is Google's.

#### 1.8.4 Virtual Environment

Like most programming languages, Python has its own package installer. This is pip. It installs packages from the Python Package Index (PyPI) and other indexes.

By default, it installs the packages in the same base directory that is shared among all your Python projects. It makes an installed package available to all your projects. This seems to be good because you don't need to install the same packages over and over again.

However, if any two of your projects require different versions of a package, you'll be in trouble. Because there is no differentiation between versions. You would need to uninstall one version and install another whenever you switch working on either one of the projects.

This is where virtual environments come into play. Their purpose is to create an isolated environment for each of your Python projects. It's no surprise, using Python virtual environments is the best practice.

#### 1.8.5 Configuring Ubuntu For Quantum Machine Learning with Python

In this section, we go through the installation on Ubuntu Linux. An Ubuntu Linux environment is highly recommended when working with quantum machine learning and Python because all the tools you need can be installed and configured easily.

Other Linux distributions (such as Debian) or MacOS (that also builds upon Unix) are also ok. But there are a few more aspects to consider.

All the code should work on Windows, too. However, the configuration of a Windows working environment can be a challenge on its own. Fortunately, there is a way out. So, if you have a Windows operating system, have a look at the next section **??** before you continue with the following instructions.

We accomplish all steps by using the Linux terminal. To start, open up your command line and update the apt-get package manager.

```
$ sudo apt-get update
$ sudo apt-get upgrade
$ sudo apt-get install -y build-essential wget python3-dev \
    libreadline-gplv2-dev libncursesw5-dev libssl-dev \
    libsqlite3-dev tk-dev libgdbm-dev libc6-dev libbz2-dev \
    libffi-dev
```

The next step downloads and installs Python 3.8.5 (the latest stable release at the time of writing).

```
$ mkdir /tmp/Python38
$ cd /tmp/Python38
$ wget https://www.python.org/ftp/python/3.8.5/Python-3.8.5.tar.xz
$ tar xvf Python-3.8.5.tar.xz
$ cd /tmp/Python38/Python-3.8.5
$ ./configure
$ sudo make altinstall
```

If you want to have this Python version as the default, run

```
$ sudo ln -s /usr/local/bin/python3.8 /usr/bin/python
```

Python is ready to work. Let's now install and update the Python package manager pip:

```
$ wget https://bootstrap.pypa.io/get-pip.py && python get-pip.py
$ pip install --upgrade pip
```

You might restart your machine to recognize pip as a command.

As mentioned, we install all the Python packages in a virtual environment. So, we need to install virtualenv:

\$ sudo apt-get install python3-venv

To create a virtual environment, go to your project directory and run venv. The following parameter (here env) specifies the name of your environment

```
$ python -m venv env
```

You'll need to activate your environment before you can start installing or using packages.

```
$ source env/bin/activate
```

When you're done working on this project, you can leave your virtual environment by running the command deactivate. If you want to reenter, simply call source env/bin/activate again.

We're now ready to install the packages we need.

Install Jupyter:

```
$ pip install jupyter notebook jupyterlab --upgrade
```

Install PyTorch:

\$ pip install torch

Install TensorFlow

\$ pip install tensorflow

Install **Qiskit** 

\$ pip install qiskit

If you don't install Qiskit in the virtual environment, you should add the -- user flag. Otherwise, the installation might fail due to missing permissions.

Install Cirq

\$ pip install cirq

Install further dependencies required of Qiskit and Scikit-Learn. If you don't use a virtual environment, use the --user flag here, too.

\$ pip install numpy scipy matplotlib ipython pandas sympy nose seaborn

 $In stall {\small \ \ Scikit-Learn, with the --user flag if you're not using a virtual environment.}$ 

\$ pip install scikit-learn

Install drawing libraries:

\$ pip install pylatexenc ipywidgets

You're now ready to start. Open up JupyterLab with

\$ jupyter lab

### 1.8.6 How To Setup JupyterLab For Quantum Computing – On Windows

If you're a Python developer, there's no way around a Unix-based operating system. Python is a language to write software that's usually supposed to run at a server. And most servers run some kind of Linux.



Consequently, the default configuration in Python caters to the specificities of a Unix-based system. While Python works on Windows, too, it requires a lot more attention to get all the configuration details right. Starting from the path separator that is not a slash but a backslash (\) to the different charset (windows-1252), to different commands (e.g. del /s /q instead of rm), Windows differs in quite a few aspects.

While Linux is great for developing, you may prefer Windows in other situations. Maybe you don't even have a choice. Your working computer simply runs Windows. Full stop.

Fortunately, there's a solution - at least if you're running Windows 10. Windows 10 contains WSL2, the Windows Subsystem for Linux. It lets you run a

full Ubuntu Linux inside Windows. Windows 10 must be updated to version 2004 and Intel's virtualization technology must be enabled in BIOS settings.

In the first step, we need to activate the Windows Subsystem for Linux optional feature. Open PowerShell as Administrator and run the following command:

```
dism.exe /online /enable-feature /featurename:Microsoft-Windows-
Subsystem-Linux /all /norestart
```

In the next step, we update the subsystem to WSL2. Download the latest kernel update for your system from https://aka.ms/wsl2kernel and install the MSI package.

Now, we enable the Virtual machine platform and set WSL2 as the default version.

```
dism.exe /online /enable-feature /featurename:
    VirtualMachinePlatform /all /norestart
wsl --set-default-version 2
```

Finally, we can install a Linux distribution as if it was a normal program. Open the Microsoft store, search for "Ubuntu 20.04 LTS", and install the program. Once the installation finishes, you can start Ubuntu from your start menu. On the first start, you need to create a new Unix user and specify a password.

You can proceed with the installation of the libraries and packages as described in the previous section **1.8.5**.

## 2. Binary Classification

### 2.1 Predicting Survival On The Titanic

The sinking of the Titanic is one of the most infamous shipwrecks in history.

On April 15, 1912, the Titanic sank after colliding with an iceberg. Being considered unsinkable, there weren't enough lifeboats for everyone on board. 1502 out of 2224 passengers and crew members died that night.

Of course, the 722 survivors must have had some luck. But it seems as if certain groups of people had better chances to survive than others.

Therefore, the sinking of the Titanic has also become a famous starting point for anyone interested in machine learning.

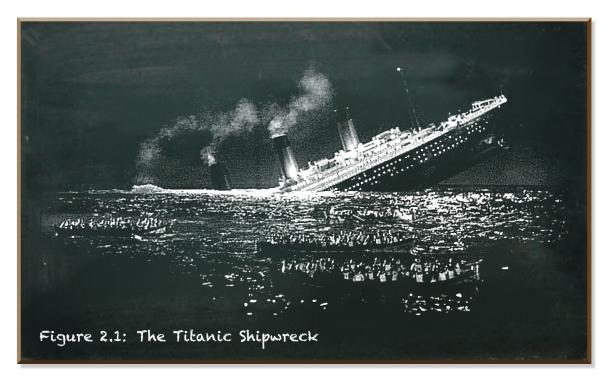
If you have some experience with machine learning, you'll probably know the legendary Titanic ML competition provided by Kaggle.

If you don't know Kaggle yet, Kaggle is among the world's largest data science communities. It offers many interesting datasets and therefore, it is a good place to get started.

The problem to be solved is simple. Use machine learning to create a model that, given the passenger data, predicts which passengers survived the Titanic shipwreck.

### 2.2 Get the Dataset

In order to get the dataset, you'll need to create a Kaggle account (it's free) and join the competition. Even though Kaggle is all about competitions, you don't need to take part in them actively by uploading your solution.



When you join a competition, you need to accept and abide by the rules that govern how many submissions you can make per day, the maximum team size, and other competition-specific details.

You'll find the competition data in the Data tab at the top of the competition page. Then, scroll down to find the list of files.

There are three files in the data:

- train.csv
- test.csv
- gender\_submission.csv

The file train.csv contains the data of a subset of the Titanic's passengers. This file is supposed to serve your algorithm as basis to learn whether a passenger survived or not.

The file test.csv contains the data of another subset of passengers. It serves to determine how good your algorithm performs.

The gender\_submission.csv file is an example that shows how you should structure your predictions if you plan to submit them to Kaggle. Since we're here to start learning and not yet be ready to compete, we'll skip this file.

Download the files train.csv and test.csv.

#### 2.3 Look at the data

The first thing we need to do is to load the data. We use Pandas for that. It is renowned in the machine learning community for data processing. It offers a variety of useful functions, such as a function to load .csv-files: read\_csv.

Listing 2.1: Load the data from the csv-files

```
1 import pandas as pd
2
3 train = pd.read_csv('./data/train.csv')
4 test = pd.read_csv('./data/test.csv')
```

We loaded our data into train and test. These are Pandas DataFrames.

A DataFrame keeps the data in a two-dimensional structure with labels. Such as a database table or a spreadsheet. It provides a lot of useful attributes and functions out of the box.

For instance, the DataFrame's attribute shape provides a tuple of two integers that denote the number of rows and the number of columns.

Let's have a look:

Listing 2.2: The shapes of the Titanic datasets

```
1 print('train has {} rows and {} columns'.format(*train.shape))
2 print('test has {} rows and {} columns'.format(*test.shape))
```

train has 891 rows and 12 columns test has 418 rows and 11 columns

We can see we have 891 training and 418 testing entries. More interestingly, the train dataset has one more column than the test dataset.

The DataFrame's info() method shows some more detailed information. Have a look at the train dataset.

Listing 2.3: The structure of the train dataset

1 train.info()

```
<class 'pandas.core.frame.DataFrame'>
RangeIndex: 891 entries, 0 to 890
Data columns (total 12 columns):
                 Non-Null Count Dtype
 #
    Column
    _____
                 _____
                                 ____
 0
    PassengerId 891 non-null
                                 int64
    Survived
                891 non-null
                                 int64
 1
 2
    Pclass
                                 int64
                 891 non-null
 3
    Name
                 891 non-null
                                 object
 4
    Sex
                 891 non-null
                                 object
                                 float64
 5
    Age
                 714 non-null
    SibSp
 6
                 891 non-null
                                 int64
 7
    Parch
                 891 non-null
                                 int64
 8
    Ticket
                 891 non-null
                                 object
 9
    Fare
                 891 non-null
                                 float64
 10 Cabin
                 204 non-null
                                 object
 11 Embarked
                 889 non-null
                                 object
dtypes: float64(2), int64(5), object(5)
memory usage: 83.7+ KB
```

The info method returns a list of the columns: their index, their names, how many entries have actual values (are not null), and the type of values.

Let's have a look at the test dataset, too.

Listing 2.4: The structure of the test dataset

1 test.info()

```
<class 'pandas.core.frame.DataFrame'>
RangeIndex: 418 entries, 0 to 417
Data columns (total 11 columns):
 #
                 Non-Null Count Dtype
    Column
    _____
                                ____
 0
    PassengerId 418 non-null
                                 int64
    Pclass
                 418 non-null
                                 int64
 1
 2
    Name
                418 non-null
                                 object
                418 non-null
 3
    Sex
                                 object
                                 float64
 4
    Age
                332 non-null
 5
    SibSp
               418 non-null
                                 int64
 6
    Parch
                418 non-null
                                 int64
 7
                418 non-null
    Ticket
                                 object
 8
                417 non-null
                                 float64
    Fare
 9
    Cabin
                91 non-null
                                 object
 10 Embarked 418 non-null
                                 object
dtypes: float64(2), int64(4), object(5)
memory usage: 36.0+ KB
```

When comparing both info, we can see the test dataset misses the column Survived that indicates whether a passenger survived or died.

As Kaggle notes, they use the test dataset to evaluate the submissions. If they provided the correct answer, it wouldn't be much of a competition anymore, would it? It is our task to predict the correct label.

Since we do not plan to submit our predictions to Kaggle to get an evaluation of how our algorithm performed, the test dataset is quite useless for us.

So, we concentrate on the train dataset.

The info output is quite abstract. Wouldn't it be good to see some actual data? No problem. That's what the head-method is for.

The head method shows the column heads and the first five rows. With this impression, let's go through the columns. You can read an explanation on the Kaggle page, too.

Listing 2.5: Look at the data

1 train.head()

	PassengerId	Survived	Pclass	Name	Sex	Age	SibSp	Parch	Ticket	Fare	Cabin	Embarked
0	1	0	3	Braund, Mr. Owen Harris	male	22.0	1	0	A/5 21171	7.2500	NaN	S
1	2	1	1	Cumings, Mrs. John Bradley (Florence Briggs Th	female	38.0	1	0	PC 17599	71.2833	C85	С
2	3	1	3	Heikkinen, Miss. Laina	female	26.0	0	0	STON/O2. 3101282	7.9250	NaN	S
3	4	1	1	Futrelle, Mrs. Jacques Heath (Lily May Peel)	female	35.0	1	0	113803	53.1000	C123	S
4	5	0	3	Allen, Mr. William Henry	male	35.0	0	0	373450	8.0500	NaN	S

Each column represents one feature of our data. The PassengerId is a consecutive number identifying each row. Survived is the indicator on whether the passenger survived (0 = No, 1 = Yes). Pclass is the ticket class (1 = 1st, 2 = 2nd, 3 = 3rd). Then we have self-explanatory Name, Sex, and Age.

SibSp denotes the number of this passenger's siblings or spouses aboard the Titanic. Parch denotes the number of this passenger's parents or children aboard the Titanic.

Then, there are the Fare the passenger paid, the Cabin number and the port of embarkation (embarked) (C = Cherbourg, Q = Queenstown, S = Southampton).

# 2.4 Data Preparation and Cleaning

Our data has different types. There is numerical data, such as the Age, SibSp, Parch, and the Fare. There is categorial data. Some of the categories are represented by numbers (Survived, Pclass). Some are represented by text (Sex and Embarked). And there is textual data (Name, Ticket, and Cabin).

This is quite a mess. For a computer. Furthermore, when having another look at the result of train.info(), you can see that the counts vary for different columns. While we have 891 values for most columns, we only have 714 for Age, 204 for Cabin, and 889 for Embarked.

Before we can feed our data into any machine learning algorithm, we need to clean up.

### 2.4.1 Missing Values

Most machine learning algorithms don't work well with missing values. There are three options of how we can fix this:

- Get rid of the corresponding rows (removing the passengers from consideration)
- Get rid of the whole column (remove the whole feature for all passengers)
- Fill the missing values (for example with zero, the mean, or the median)

Listing 2.6: Cope with missing values

```
<class 'pandas.core.frame.DataFrame'>
Int64Index: 889 entries, 0 to 890
Data columns (total 11 columns):
    Column Non-Null Count Dtype
 #
    _____
                 _____
                                 ____
____
    PassengerId 889 non-null
 0
                                int64
    Survived 889 non-null int64
 1
                889 non-null int64
 2
    Pclass
               889 non-null object
889 non-null object
889 non-null float64
 3
    Name
 4
    Sex
 5
    Age
                                float64
               889 non-null int64
889 non-null int64
 6
    SibSp
 7
    Parch
 8
    Ticket
                889 non-null object
 9
    Fare
                889 non-null
                                 float64
 10 Embarked
                889 non-null
                                 object
dtypes: float64(2), int64(5), object(4)
memory usage: 83.3+ KB
```

We can accomplish these things easily using DataFrame's dropna(), drop(), and fillna() methods. There is no one best option in general. But you should carefully consider the specific context.

There are only two passengers whose port of embarkation we don't know.

40

These account for less than 1% of our data. If we completely disregard these two passengers, we won't see completely different results. Thus, we drop these rows (line 3) with the dropna-method.

The dropna-method takes the column ("Embarked") as named parameter subset. This parameter specifies the columns that determine whether to remove the row (passenger). If at least one value of these columns is missing, the row gets removed.

The situation is different with regard to the Cabin. We only have this information for 204 out of 991 passengers. It is questionable if this is enough to draw any information from. We don't know why these values miss. Even if we found the Cabin to be highly correlated with the survival of a passenger, we wouldn't know whether this correlation can be generalized to all passengers or whether there is a selection bias meaning that the fact that we know the Cabin depends on some other aspect.

We drop the whole column with the method drop. We provide the column (Cabin) we want to remove as positioned argument. The value 1 we provide as named argument axis specifies that we want to remove the whole column.

Next, we know the Age of 714 passengers. Removing all the passengers from consideration whose Age we don't know doesn't seem to be an option because they account for about 22% of our data, quite a significant portion. Removing the whole column doesn't seem to be a good option either. First, we know the Age of most of the passengers and intuition suggest that the Age might be important for someone's chance to survive.

We fill the missing values with the fillna method (line 13). Since we want to fill only the missing values in the Age column, we call this function on this column and not the whole DataFrame. We provide as argument the value we want to set. This is the mean age of all passengers we calculated before (line 12).

Great. We now have 889 rows, 10 columns, and no missing data anymore.

## 2.4.2 Identifiers

The goal of machine learning is to create an algorithm that is able to predict data. Or, as we said before: to put a label on a thing. While we use already labeled data when building our algorithm, the goal is to predict labels we don't know yet.

We don't tell our algorithm how it can decide which label to select. Rather, we tell the algorithm, "here is the data, figure it out yourself". That being said,

a savvy algorithm may be able to memorize all the data you provide it with. This is referred to as overfitting. The result is an algorithm performing well on known data, but poorly on unknown data.

If our goal was to only predict labels we know already, the best thing we could do is to memorize all passengers and whether they survived. But if we want to create an algorithm that performs well even on unknown data, we need to prevent memorization.

We have not even started building our algorithm. Yet, the bare features we provide our algorithm with affect whether the algorithm will be able to memorize data. Because we have potential identifiers in our data.

When looking at the first five entries of the dataset, three columns appear suspicious: the PassengerId, the Name, and the Ticket.

The PassengerId is a subsequent number. There should be no connection between how big the number is and whether a passenger survived.

Neither should the name of a passenger or the number on a ticket be a decisive factor for survival. Rather, these are data identifying single passengers. Let's validate this assumption.

Let's have a look at how many unique values are in these columns.

Listing 2.7: Unique values in columns

1 print('There are {} different (unique) PassengerIds in the data'.format( train["PassengerId"].nunique()))

- 2 print('There are {} different (unique) names in the data'.format(train["
   Name"].nunique()))
- 3 print('There are {} different (unique) ticket numbers in the data'.format
   (train["Ticket"].nunique()))

```
There are 889 different (unique) PassengerIds in the data
There are 889 different (unique) names in the data
There are 680 different (unique) ticket numbers in the data
```

Name and PassengerId are perfect identifiers. Each of the 889 rows in our dataset has a unique value.

And there are 680 different Ticket numbers. A possible explanation for the Ticket not to be a perfect identifier may be family tickets. Yet, a prediction

based on this data appears to support memorization rather than learning transferable insights.

We remove these columns.

Listing 2.8: Remove identifying data

```
1 train = train.drop("PassengerId", axis=1)
2 train = train.drop("Name", axis=1)
3 train = train.drop("Ticket", axis=1)
4
5 train.info()
```

```
<class 'pandas.core.frame.DataFrame'>
Int64Index: 889 entries, 0 to 890
Data columns (total 8 columns):
 #
    Column Non-Null Count Dtype
            _____ ____
    _____
___
    Survived 889 non-null
                            int64
 0
   Pclass 889 non-null
                           int64
 1
    Sex 889 non-null object
2
 3
            889 non-null
    Age
                           float64
    SibSp 889 non-null
 4
                           int64
 5
   Parch
            889 non-null
                           int64
 6
    Fare
             889 non-null
                            float64
 7
    Embarked 889 non-null
                            object
dtypes: float64(2), int64(4), object(2)
memory usage: 62.5+ KB
```

### 2.4.3 Handling Text and Categorical Attributes

As we will see throughout this book, all the algorithms, both classic and quantum algorithms, work with numbers. Nothing but numbers. If we want to use textual data, we need to translate it into numbers.

Scikit-Learn provides a transformer for this task called LabelEncoder.

Listing 2.9: Transforming textual data into numbers

```
1 from sklearn.preprocessing import LabelEncoder
2 le = LabelEncoder()
3
4 for col in ['Sex', 'Embarked']:
5 le.fit(train[col])
6 train[col] = le.transform(train[col])
7
8 train.head()
```

	Survived	Pclass	Sex	Age	SibSp	Parch	Fare	Embarked
0	0	3	1	22.0	1	0	7.2500	2
1	1	1	0	38.0	1	0	71.2833	0
2	1	3	0	26.0	0	0	7.9250	2
3	1	1	0	35.0	1	0	53.1000	2
4	0	3	1	35.0	0	0	8.0500	2

First, we import the LabelEncoder (line 1) and initialize an instance (line 2). We loop through the columns with textual data (Sex and Embarked) (line 4). For each column, we need to fit the encoder to the data in the column (line 5) before we can transform the values (line 6).

Finally, let's have another look at our DataFrame. You can see that both, Sex and Embarked are now numbers (int64). In our case, Ø denotes male and 1 denotes female passengers. But when you run the transformation again you may yield different assignments.

#### 2.4.4 Feature Scaling

Machine learning algorithms only work with numbers. Moreover, they usually work with numbers with identical scales. If numbers have different scales, the algorithm may consider those with higher scales to be more important.

Even though all our data is numerical, it is not yet uniformly scaled. The values of most of the columns range between 0 and 3. But Age and Fare have far bigger scales.

The max method returns the maximum value in a column. As we can see, the oldest passenger was 80 years old and the highest fare was about 512.

```
44
```

Listing 2.10: The maximum values

1 print('The maximum age is {}'.format(train["Age"].max()))
2 print('The maximum fare is {}'.format(train["Fare"].max()))

```
The maximum age is 80.0
The maximum fare is 512.3292
```

A common way to cope with data of different scales is min-max-scaling (also known as normalization). This process shifts and rescales values so that they end up ranging from 0 to 1. It subtracts the minimum value from each value and divides it by the maximum minus the minimum value.

Scikit-Learn provides the MinMaxScaler transformer to do this for us.

Listing 2.11: Normalization of the data.

The minimum value is 0.0 and the maximum value is 1.0

Again, we first import the transformer (line 1) and initialize it (line 3). Then, we fit the transformer to our data (line 4) and transform it (line 5).

As a result, all the data in our dataset range between 0.0 and 1.0.

The scaler returns a Numpy-array rather than a Pandas DataFrame.

## 2.4.5 Training and Testing

We already mentioned the goal of building an algorithm that does not only perform well on data it already knows but one that also predicts the labels of yet unknown data.

That's why it is important to separate the data into a training and a testing set. We use the training set to build our algorithm. And we use the testing set to validate its performance.

Even though Kaggle provides a testing set, we skipped it for not including the Survived column. We would need to ask Kaggle every time we wanted to validate it. To keep things simple and be able to do the validation on our own, we rather spare some rows from the Kaggle training set for testing.

Separating a test set is quite simple. Scikit-learn provides a useful method for that, too. This is train\_test\_split.

Further, we need to separate the input data from the resulting label we want to predict.

Listing 2.12: Separating input from labels and training from testing sets

We have 711 training and 178 testing rows There are 7 input columns

We separate the input columns from the labels with Python array indices (lines 3-4). The first column (position Ø) contains the Survived flag we want to predict. The other columns contain the data we use as input.

train\_test\_split separates the training from the testing data set. The parameter test\_size = 0.2 (= 20%) specifies the portion we want the testing set to

have.

We can see our training data set consists of 711 entries. Accordingly, our testing set consists of 178 entries. We have input 7 columns and a single column output.

Let's save our prepared data so that we can use it in the future without needing to repeat all these steps.

Listing 2.13: Save the data to the filesystem

```
import numpy as np
with open('data/train.npy', 'wb') as f:
np.save(f, train_input)
np.save(f, train_labels)
with open('data/test.npy', 'wb') as f:
np.save(f, test_input)
np.save(f, test_labels)
```

## 2.5 Baseline

Now, we have our input data and the resulting labels. And we have it separated into a training and a testing set. The only thing left is our algorithm.

Our algorithm should predict whether a passenger survived the Titanic shipwreck. This is a classification task since there are distinct outcome values. Specifically, it is a binary classification task because there are exactly two possible predictions (survived or died).

Before we develop a quantum machine learning algorithm, let's implement the simplest algorithm we can imagine. A classifier that guesses.

Listing 2.14: A random classifier

```
1 import random
2 random.seed(a=None, version=2)
3 
4 def classify(passenger):
5 return random.randint(0, 1)
```

We import the random number generator (line 1) and initialize it (line 2).

Our classifier is a function that takes passenger data as input and returns either 0 or 1 as output. Similar to our data, 0 indicates the passenger died and 1 the passenger survived.

In order to use the classifier, we write a Python function that runs our classifier for each item in the training set.

Listing 2.15: The classification runner

```
1 def run(f_classify, x):
2 return list(map(f_classify, x))
```

This function takes the classifier-function as the first argument (we can replace the classifier later) and the input data (as x) as the second parameter (line 1).

It uses Python's map function to call the classifier with each item in x and return an array of the results.

Let's run it.

Listing 2.16: Run the classifier

```
1 result = run(classify, train_input)
```

```
[0, 1, 0, \ldots 0, 1, 1]
```

When we run the classifier with our train\_input we receive a list of predictions.

Since our goal is to predict the actual result correctly, we need to evaluate whether the prediction matches the actual result.

Let's have a look at the accuracy of our predictions.

Listing 2.17: Evaluate the classifier

```
1 def evaluate(predictions, actual):
2 correct = list(filter(
3 lambda item: item[0] == item[1],
4 list(zip(predictions,actual))
5 ))
6 return '{} correct predictions out of {}. Accuracy {:.0f} %' \
.format(len(correct), len(actual), 100*len(correct)/len(actual))
8 print(evaluate(run(classify, train_input), train_labels))
```

378 correct predictions out of 711. Accuracy 53 %

We define another function evaluate. It takes the predictions of our algorithm and the actual results as parameters (line 1).

The term list(zip(predictions, actual)) (line 4) creates a list of 2-item lists. The 2-item lists are pairs of a prediction and the corresponding actual result.

We filter these items from the list where the prediction matches the actual result (lambda item: item[0] == item[1]) (line 3). These are the correct predictions. The length of the list of correct predictions divided by the total number of passengers is our Accuracy.

Great! We are already correct in half of the cases (more or less). This is not a surprise when guessing one out of two possible labels.

But maybe we can do even better? I mean without any effort. We know that more people died than survived. What if we always predicted the death of a passenger?

Listing 2.18: Always predict a passenger died

```
1 def predict_death(item):
2   return 0
3 
4  print(evaluate(run(predict_death, train_input), train_labels))
```

442 correct predictions out of 711. Accuracy 62 %

We're up to an accuracy of 61% of our predictions. Not too bad, is it? This value, that is the ratio between the two possible actual values is the prevalence.

Let's consider a different task for a moment. Let's say you're a doctor and your task is to predict whether a patient has cancer. Only 1% of your patients actually have cancer. If you predicted no-cancer all the time, your accuracy would be astonishing 99%! But you would falsely diagnose the patients that actually have cancer. And for the resulting lack of treatment, they're going to die.

Maybe the accuracy of the predictions alone is not a good measure to evaluate the performance of our algorithm.

## 2.6 Classifier Evaluation and Measures

As we mentioned in section 1.4.3, the evaluation is one main part of every machine learning algorithm. It may seem trivial at first sight. Yet, deciding on the right measure is a very important step. When you optimize your algorithm towards better performance, you will inevitably optimize towards better scores in your evaluation function.

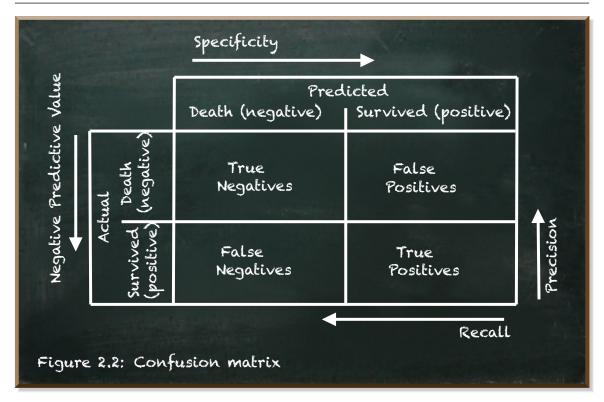
We will get to know more sophisticated evaluation functions in this book. But right now, we keep it simple. A better way to evaluate the performance of a classifier is to look at the confusion matrix.

The general idea is to compare the predictions with the actual values. In binary classification, there are two possible actual values: true or false. And there are two possible predictions: true or false.

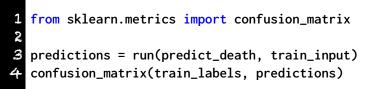
There are four possibilities:

- **True Negatives** (TN): a passenger who died was correctly predicted
- False Positives (FP): a passenger who died was wrongly predicted to survive
- False Negatives (FN): a passenger who survived was wrongly predicted to die
- True Positive (TP): a passenger who survived was correctly predicted

Let's have a look at the confusion matrix of the predict death classifier.



Listing 2.19: Confustion matrix of the predict death classifier



```
array([[442, 0],
[269, 0]])
```

Scikit-Learn provides the confusion\_matrix method that we import (line 1). It takes the actual values as first and the predictions as the second parameter (line 3).

It returns a two-dimensional array. In the first row, it shows the true negatives (TN) and the false positives (FP). In the second row, it shows the false negatives (FN) and the true positives (TP). We can define the accuracy we measured thus far as:

$$Accuracy = \frac{\sum TruePositives + \sum TrueNegatives}{TotalPopulation}$$
(2.1)

It does not care whether there is a systematic error, such as the algorithm's inability to correctly predict a passenger who survived (true positives) as long as it performs well at correctly predicting passengers who die (true negatives).

The confusion matrix offers us more detailed measures of our classifier performance. These are:

- precision
- recall
- specificity
- negative predictive value (NPV)

The precision is the "accuracy of the positive predictions". It only looks at the positive predictions, these are predictions that the passenger survived.

$$Precision = \frac{\sum TruePositives}{\sum AllPredictedPositives}$$
(2.2)

Let's have a look at the code:

Listing 2.20: The precision score

The precision score of the predict\_death classifier is 0.0

Scikit-Learn provides a function to calculate the precision\_score. It takes the list of actual values and the list of predicted values as input.

Since we did not have a single positive prediction, our precision is not defined. Scikit-Learn interprets this as a score of 0.0.

The recall is the "accuracy of the actual positives". It only looks at the actual positives.

$$Recall = \frac{\sum TruePositives}{\sum AllActualPositives}$$
(2.3)

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In Python, it is:

Listing 2.21: The recall score

```
1 from sklearn.metrics import recall_score
2 print('The recall score of the predict_death classifier is {}'.format(
        recall_score(train_labels, predictions)))
```

The recall score of the predict\_death classifier is  $0.0\,$ 

This time, even though recall is defined (the number of actual positives is greater than 0), the score is 0.0 again, because our classifier did not predict a single survival correctly. Not a surprise when it always predicts death.

The specificity is the "accuracy of the actual negatives". It only looks at actual negatives (deaths).

$$Specificity = \frac{\sum TrueNegatives}{\sum AllActualNegatives}$$
(2.4)

And the 'negative predictive value' (NPV) is the "accuracy of the negative predictions".

$$NegativePredictiveValue(NPV) = \frac{\sum TrueNegatives}{\sum AllPredictedNegatives}$$
(2.5)

These two functions are not provided out of the box. But with the values we get from the confusion matrix, we can calculate them easily:

Listing 2.22: The specificity and the npv

```
1 def specificity(matrix):

    return matrix[0][0]/(matrix[0][0]+matrix[0][1]) if (matrix[0][0]+matrix

    [0][1] > 0) else 0

3 def npv(matrix):

    return matrix[0][0]/(matrix[0][0]+matrix[1][0]) if (matrix[0][0]+matrix

    [1][0] > 0) else 0

6 cm = confusion_matrix(train_labels, predictions)

7 print('The specificity score of the predict_death classifier is {:.2f}'.

    format(specificity(cm)))

10 print('The npv score of the predict_death classifier is {:.2f}'.format(

    npv(cm)))
```

The specificity score of the predict\_death classifier is 1.00 The npv score of the predict\_death classifier is 0.62

The function specificity takes the confusion matrix as a parameter (line 1). It divides the true negatives (matrix[0][0]) by the sum of the true negatives and the false positives (matrix[0][1]) (line 2).

The function npv takes the confusion matrix as a parameter (line 4) and divides the true negatives by the sum of the true negatives and the false negatives (matrix[1][0]).

 $These four scores \, provide \, a \, more \, detailed \, view \, of \, the \, performance \, of \, our \, classifiers.$ 

Let's calculate these scores for our random classifier as well:

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Listing 2.23: The scores of the random classifier

```
1 random_predictions = run(classify, train_input)
2 random_cm = confusion_matrix(train_labels, random_predictions)
3 
4 print('The precision score of the random classifier is {:.2f}'.format(
        precision_score(train_labels, random_predictions)))
5 print('The recall score of the random classifier is {:.2f}'.format(
        recall_score(train_labels, random_predictions)))
6 print('The specificity score of the random classifier is {:.2f}'.format(
        specificity(random_cm)))
7 print('The npv score of the random classifier is {:.2f}'.format(npv(
        random_cm)))
```

The precision score of the random classifier is 0.34 The recall score of the random classifier is 0.45 The specificity score of the random classifier is 0.47 The npv score of the random classifier is 0.59

While the predict death classifier exhibits a complete absence of precision and recall, it has perfect specificity and reaches an NPV score that matches the percentage of negatives in our test dataset (the prevalence).

The random classifier yields more balanced scores. You'll get a little bit different scores every time you run the classifier. But the values seem to stay in certain ranges. While the precision of this classifier is usually below 0.4 the npv is above 0.6.

The confusion matrix and related measures give you a lot of information. But sometimes, you need a more concise metric. In fact, the evaluation function in a machine learning algorithm must return a single measure it can optimize.

And this single measure should unmask a classifier that does not really add any value.

# 2.7 Unmask the Hypocrite Classifier

Even though the predict death classifier does not add any insight, it outperforms the random classifier with regard to overall accuracy. It exploits the prevalence, the ratio between the two possible values, not being 0.5. The confusion matrix reveals more details on certain areas. It shows the predict death classifier lacks any recall, the accuracy of predicting actual positives. This is no surprise, since it always predicts death.

But having a whole set of metrics makes it difficult to measure real progress. How do we recognize that one classifier is better than another? How do we even identify a classifier that adds no value at all? How do we identify such a hypocrite classifier?

Let's write a generalized hypocrite classifier and see how we can unmask it.

Listing 2.24: A hypocrite classifier

```
1 def hypocrite(passenger, weight):
2 return round(min(1,max(0,weight*0.5+random.uniform(0, 1))))
```

The hypocrite classifier takes the passenger data and a weight. The weight is a number between -1 and 1. It denotes the classifier's tendency to predict death (negative values) or survival (positive values).

The formula weight\*0.5+random.uniform(0, 1) generates numbers between -0.5 and 1.5. The min and max functions ensure the result to be between 0 and 1. The round function returns either 0 (death) or 1 (survival).

Depending on the weight, the chances to return the one or the other prediction differs.

If weight is -1, it returns -1\*0.5+random.uniform(0, 1), a number between -0.5 and 0.5. A number almost always rounding to 0 (predicted death).

If weight is 0, the formula returns -1\*0+random.uniform(0, 1). This is our random classifier.

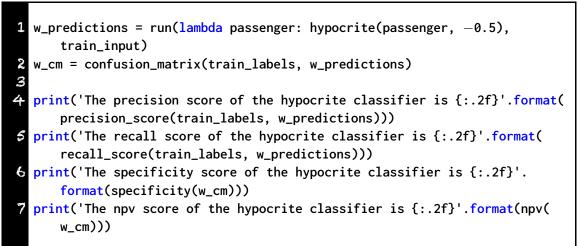
If weight is 1, it returns 1\*0.5+random.uniform(0, 1), a number that is always greater than 0.5 and thus, rounding to 1(predicted survival).

We can choose the tendency from -1 to 1. -1 always predicts death, 0 is completely random, 1 always predicts survival.

Let's have a look at how the predictions vary. We pass the weight as a hyperparameter. Try different values, if you like.

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Listing 2.25: The scores of the hypocrite classifier



The precision score of the hypocrite classifier is 0.35 The recall score of the hypocrite classifier is 0.25 The specificity score of the hypocrite classifier is 0.73 The npv score of the hypocrite classifier is 0.61

If you run the hypocrite classifier a few times, you may get a feeling for its performance. But let's create a visualization of it.

The following code runs the hypocrite classifier for different values of weight.

Listing 2.26: Run the hypocrite classifiers

```
1 import numpy as np
 2
 3 # number of steps to consider between -1 and 1
 4567
   cnt_steps = 40
   # a list of the step numbers [0, 1, ..., 38, 39]
   steps = np.arange(0, cnt_steps, 1).tolist()
 8
 9 # list of the weights at every step [-1, -0.95, \dots 0.9, 0.95, 1.0]
10 weights = list(map(
11
     lambda weight: round(weight, 2),
12
     np.arange(-1, 1+2/(cnt_steps-1), 2/(cnt_steps-1)).tolist()
13))
14
15 # list of predictions at every step
16 l_predictions = list(map(
17
     lambda step: run(
18
        lambda passenger: hypocrite(passenger, weights[step]),
19
       train_input
20
     ),
21
     steps
22 ))
23
24 # list of confusion matrices at every stee
25 l_cm = list(map(
26
     lambda step: confusion_matrix(train_labels, l_predictions[step]),
27
     steps
28))
```

The range of allowed weights is between -1 and 1. We divide this range into 40 (cnt\_steps) steps (line 4). We create lists of the indices (steps=[0, 1, ..., 38, 39], line 7) and of the weights at every step (weights=[-1, -0.95, ... 0.9, 0.95, 1.0], lines 10-13). We run the hypocrite classifier for every step (lines 17-19) and put the results into 1\_predictions (line 16). Based on the predictions and the actual results, we calculate the confustion matrix for every step (line 26) and store them in 1\_cm (line 25).

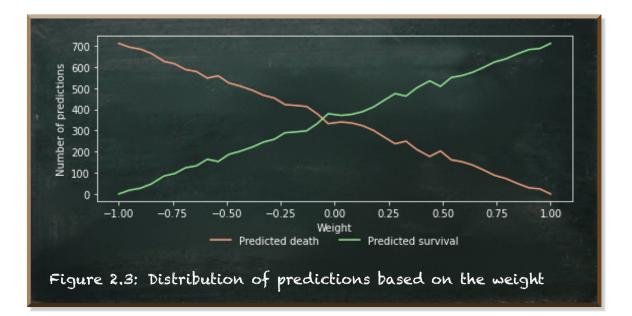
The next piece of code takes care of rendering the two graphs.

The green graph depicts the number of predicted survivals at a step. The red graph depicts the number of predicted deaths.

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Listing 2.27: Plot the distribution of predictions

```
1 import matplotlib.pyplot as plt
 2 import matplotlib
 3
 4
   # create a graph for the number of predicted deaths
 5
   deaths, = plt.plot(
6
7
8
9
10)
      weights, # point at x-axis
      list(map(lambda cur: l_cm[cur][0][0]+l_cm[cur][1][0], steps)),
      'lightsalmon', # color of the graph
      label='Predicted death'
11
12 # create a graph for the number of predicted survivals
13 survivals, = plt.plot(
14
     weights, # point at x-axis
15
      list(map(lambda cur: l_cm[cur][0][1]+l_cm[cur][1][1], steps)),
16
      'lightgreen', # color of the graph
17
      label='Predicted survival'
18)
19
20 plt.legend(handles=[deaths, survivals],loc='upper center',
21
      bbox_to_anchor=(0.5, -0.15), framealpha=0.0, ncol=2)
22 plt.xlabel("Weight")
23 plt.ylabel("Number of predictions")
24 plt.show()
```



We can see that the hypocrite classifier generates the expected tendency in its predictions. At weight=-1, it always predicts death, at weight=0 it is 50:50, and at weight=1 it always predicts survival.

Let's see how the different hypocrite classifiers perform at the four metrics depending on the weight.

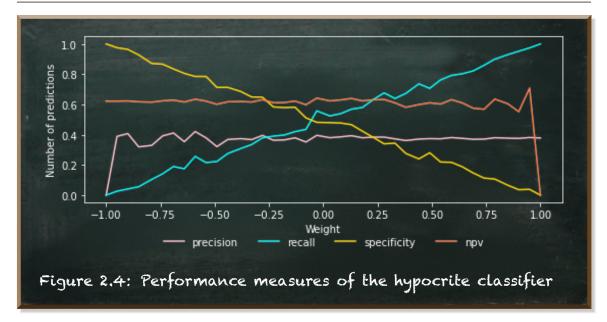
Listing 2.28

<pre>l_precision = list(map(lambda step: precision_score(train_labels,</pre>
<pre>l_predictions[step]),steps))</pre>
<pre>l_recall = list(map(lambda step: recall_score(train_labels, l_predictions</pre>
[step]),steps))
<pre>l_specificity = list(map(lambda step: specificity(l_cm[step]),steps))</pre>
<pre>l_npv = list(map(lambda step: npv(l_cm[step]),steps))</pre>

In these four lines, we calculate the four metrics at each step. Let's visualize them.

Listing 2.29: Plot the performance measures

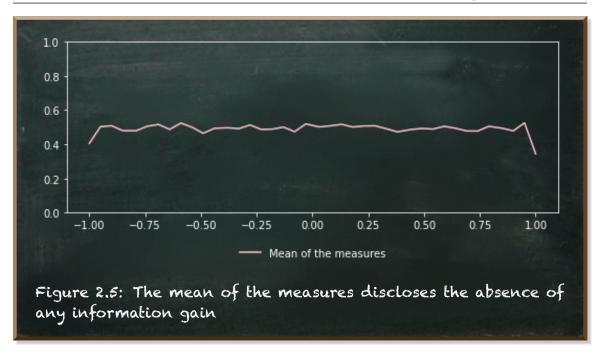
```
1 m_precision, = plt.plot(weights, l_precision, 'pink', label="precision")
 2 m_recall, = plt.plot(weights, l_recall, 'cyan', label="recall")
 3 m_specificity, = plt.plot(weights, l_specificity, 'gold', label="
       specificity")
   m_npv, = plt.plot(weights, l_npv, 'coral', label="npv")
4567890
   plt.legend(
     handles=[m_precision, m_recall, m_specificity, m_npv],
     loc='upper center',
     bbox_to_anchor=(0.5, -0.15),
     framealpha=0.0,
11
     ncol=4)
12
13 plt.xlabel("Weight")
14 plt.ylabel("Number of predictions")
15 plt.show()
```



These graphs show some interesting characteristics. specificity and recall are directly related to the classifier's tendency either towards predicting death (higher specificity) or towards predicting survival (higher recall).

Except for the edge cases where all predictions are death or all are survival, the values for precision and npv seem to be horizontal lines. In fact, precision relates to the prevalance of 39% survivals in our data and npv to the prevalance of 61% deaths.

Listing 2.30: Calculating the mean of the measures



When looking at the mean of all four measures, we see an almost flat line. Its drops at the edges are due to precision and npv being 0 there because there are no predicted survivals (left edge) respectively no predicted deaths (right edge) to calculate some measures.

This line indicates the overall level of information provided by all hypocrite classifiers is equal. And the level is about 0.5. That is the baseline for a binary classifier for there are only two possible outcomes.

Even though specific types of hypocrite classifiers are able to trick a single measure (like accuracy, recall, precision, Or npv) by exploiting the prevalence, when looking at all complementary measures at once, we can unmask the hypocrite classifier.

However, this does not imply that the mean of these measures is the best measure to evaluate the performance of your classifier with. Depending on your task at hand, you may, for instance, favor precision over recall. Rather, the implication is that you should look at the overall level of information provided by the classifier, too. You should not let yourself be dazzled by the classifier's performance at a single measure.

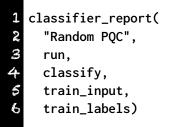
Finally, let's create a resuable function that calculates the measures for us and displays the results.

Listing 2.31: A reusable function to unmask the hypocrite classifier

```
1 def classifier_report(name, run, classify, input, labels):
 2
      cr_predictions = run(classify, input)
34567890
      cr_cm = confusion_matrix(labels, cr_predictions)
      cr_precision = precision_score(labels, cr_predictions)
      cr_recall = recall_score(labels, cr_predictions)
      cr_specificity = specificity(cr_cm)
      cr_npv = npv(cr_cm)
      cr_level = 0.25*(cr_precision + cr_recall + cr_specificity + cr_npv)
11
     print('The precision score of the {} classifier is {:.2f}'.format(name,
        cr_precision))
12
     print('The recall score of the {} classifier is {:.2f}'.format(name,
       cr_recall))
13
     print('The specificity score of the {} classifier is {:.2f}'.format(
       name, cr_specificity))
14
      print('The npv score of the {} classifier is {:.2f}'.format(name,
       cr_npv))
15
      print('The information level is: {:.2f}'.format(cr_level))
```

Let's use this function to get a report of our random classifier.

Listing 2.32: The report of the random classifier



The precision score of the Random PQC classifier is 0.36 The recall score of the Random PQC classifier is 0.47 The specificity score of the Random PQC classifier is 0.48 The npv score of the Random PQC classifier is 0.60 The information level is: 0.48

Listing 2.33

# 3. The Qubit and the Quantum States

In this chapter, we start with the very basics of quantum computing. The quantum bit. And we will write our first quantum circuit. A quantum circuit is a sequence of quantum bit transformations. The quantum program. Let's start with the basics.

## 3.1 Exploring the Quantum States

The world of quantum mechanics is... different. A quantum system can be in a state of superposition. A popular notion of superposition is that the system is in different states concurrently unless you measure it.

For instance, the spin of a particle is not up **or** down but it is up **and** down at the same time. But when you look at it, you find it either up **or** down.

Or, let's say you flip a quantum coin. In the air, it has both values heads **and** tails. If and only if you catch it and look at it, it decides for a value. Once landed, it is a normal coin with heads up **or** tails up.

Another notion of superposition is that the system is truly random and therefore distinguishes from the systems we know. Tossing a (normal) coin, for instance, seems random, because whenever you do it, the conditions are slightly different. And even tiny differences can change the outcome from heads to tails. The coin is sensitive dependent to initial conditions.

If we were able to measure all conditions precisely, we could tell the outcome. In classic mechanics, there is no randomness. Things in our everyday world, such as the coin, seem random. But they are not. If measured with infinite precision, randomness would disappear. By contrast, a quantum system is truly random.

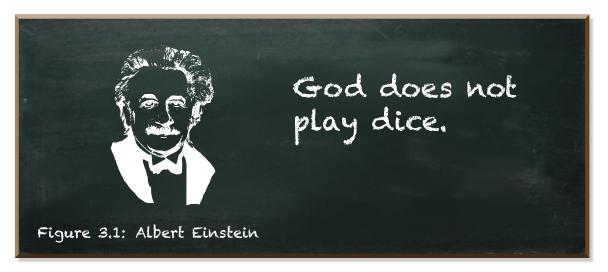
Maybe you wonder: Ok, it's random. Where's the big deal?

The big thing is the consequences. In a classic system, a system sensitive dependent to initial conditions, the answer to a question is already determined before we ask it.

Rather than watching the baseball match tonight, you spend the evening with your friends. When you return home, even though you don't know the results, the match is over and there is a definite result. There could be different results, but you simply don't know the result until you look at it.

Contrarily, in a quantum system, the answer to a question is not determined up until the time you ask it. And since it is not determined yet, you still can change the probabilities of measuring distinct states.

If you have doubts, good! Not even Einstein liked this notion. It led him to his famous statement of God does not play dice.



Many physicists, including Einstein, proposed the quantum state, though hidden, to be a well-defined state. This is known as the hidden variable theory.

There are statistically distinct behaviors between a system following the hidden variable theory and a quantum system following the superposition principle. And experiments showed that the quantum mechanical predictions were correct.

For now, let's accept the quantum state is something different. Later in this

book, we will have a closer look at it. And its consequences. But this requires a little more theory and math.

We turn to the quantum computer. Let's say you have a quantum bit. We call it qubit. Unless you observe its value, it is in a superposition state of 0 and 1. Once you observe its value, you'll get 0 or 1.

The chances of a qubit to result in either one value don't need to be 50:50. It can be 25:75, 67:33, or even 100:0. It can be any weighted probability distribution.

The probability distribution a qubit has when observed depends on its state. The quantum state.

In quantum mechanics, we use vectors to describe the quantum state. A popular way of representing quantum state vectors is the **Dirac** notation's "ket"-construct that looks like  $|\psi\rangle$ . In Python, we don't have vectors. But we have arrays. Luckily, their structures are similar.

Let's have a look. We start with the simplest case. Let's say, we have a qubit that, when observed, always has the value  $\emptyset$ . If you argued this qubit must have the value  $\emptyset$  even before it is observed, you wouldn't be completely wrong. Yet, you'd be imprecise. Before it is observed, this qubit has the probability of 1 (= 100%) to have the value  $\emptyset$  when observed.

These are the equivalent representations (ket, vector, array) of a qubit that always results in 0 when observed:

$$|0
angle = egin{bmatrix} 1 \\ 0 \end{bmatrix}$$
 and in Python [1, 0].

Accordingly, the following representations depict a qubit that always results in 1 when observed:

$$|1\rangle = \begin{bmatrix} 0\\1\end{bmatrix}$$
 and in Python [0, 1].

Ok, enough with the theory for now. Let's have a look at the code of such a qubit.

If you haven't configured your workstation yet, have a look at the brief explanation of how to set up the working environment (section 1.8).

Now, open the Jupyter notebook and test whether Qiskit works.

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Listing 3.1

1 import qiskit 2 qiskit.\_\_qiskit\_version\_\_

```
{'qiskit-terra': '0.16.4',
  'qiskit-aer': '0.7.4',
  'qiskit-ignis': '0.5.2',
  'qiskit-ibmq-provider': '0.11.1',
  'qiskit-aqua': '0.8.2',
  'qiskit': '0.23.5'}
```

If you get a response like this, Qiskit works. Great! We're ready to create our first qubit.

Listing 3.2: The first qubit

```
1 from qiskit import QuantumCircuit
2
3 # Create a quantum circuit with one qubit
4 qc = QuantumCircuit(1)
5
6 # Define initial_state as |1>
7 initial_state = [0,1]
8
9 # Apply initialization operation to the qubit at position 0
10 qc.initialize(initial_state, 0)
```

The fundamental unit of Qiskit is the quantum circuit. A quantum circuit is a model for quantum computation. The program, if you will. Our circuit consists of a single one qubit (line 4).

We define [0,1] as the initial\_state of our qubit (line 7) and initialize the first and only qubit (at position 0 of the array) of our quantum circuit with it (line 10).

Remember [0,1]? This is the equivalent to  $|1\rangle = \begin{bmatrix} 0 \\ 1 \end{bmatrix}$ . And in plain English, it is a qubit resulting in the value 1 when observed.

This is it. It's now time to boot our quantum computer. In case you don't

have one, no problem. We can simulate it. (In case you have one: "Cool, let me know").

```
Listing 3.3: Prepare the simulation backend
```

```
1 from qiskit import execute, Aer
2 
3 # Tell Qiskit how to simulate our circuit
4 backend = Aer.get_backend('statevector_simulator')
5 
6 # Do the simulation, returning the result
7 result = execute(qc,backend).result()
```

Qiskit provides the Aer package (that we import at line 1). It provides different backends for simulating quantum circuits. The most common backend is the statevector\_simulator (line 4).

The execute-function (that we import at line 1, too) runs our quantum circuit (qc) at the specified backend. It returns a job-object that has a useful method job.result(). This returns the result object once our program completes it.

Let's have a look at our qubit in action.

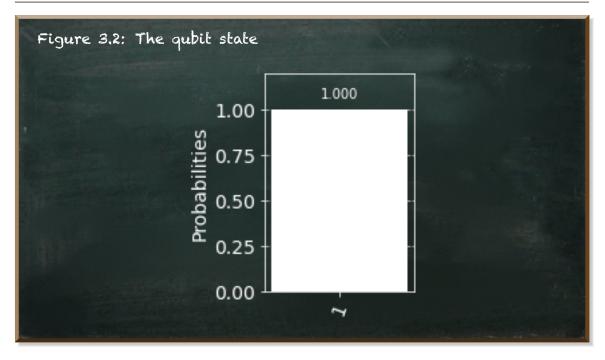
Qiskit uses Matplotlib to provide useful visualizations. A simple histogram will do. The result object provides the get\_counts method to obtain the histogram data of an executed circuit (line 5).

The method plot\_histogram returns a Matplotlib figure that Jupyter draws automatically (line 8).

We see we have a 100% chance of observing the value 1.

Listing 3.4: The measured qubit

```
1 from qiskit.visualization import plot_histogram
2 import matplotlib.pyplot as plt
3
4 # get the probability distribution
5 counts = result.get_counts()
6
7 # Show the histogram
8 plot_histogram(counts)
```



Now, let's move on to a more advanced case. Say, we want our qubit to result in either 0 or 1 with the same probability (50:50).

In quantum mechanics, there is the fundamental principle superposition. It says any two (or more) quantum states can be added together ("superposed") and the result will be another valid quantum state.

Wait! We already know two quantum states,  $|0\rangle$  and  $|1\rangle$ . Why don't we add them?  $|0\rangle$  and  $|1\rangle$  are vectors. Adding two vectors is straight forward.

A vector is a geometric object that has a magnitude (or length) and a direction. Usually, they are represented by straight arrows, starting at one point on a coordinate axis and ending at a different point.

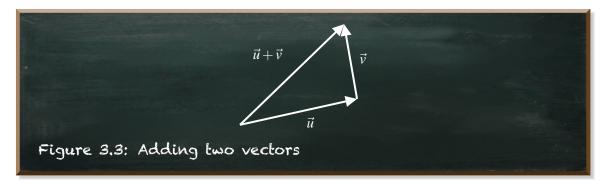
You can add two vectors by placing one vector with its tail at the other vector's head. The straight line between the yet unconnected tail and the yet unconnected tail is the sum of both vectors. Have a look at the figure 3.3.

Mathematically, it is as easy.

Let 
$$\vec{u} = \begin{bmatrix} u_1 \\ u_2 \end{bmatrix}$$
 and  $\vec{v} = \begin{bmatrix} v_1 \\ v_2 \end{bmatrix}$  be two vectors.

The sum of  $\vec{u}$  and  $\vec{v}$  is:

$$\vec{u} + \vec{v} = \begin{bmatrix} u_1 + v_1 \\ u_2 + v_2 \end{bmatrix}$$
(3.1)



Accordingly, our superposed state should be  $\psi^*$ :

$$|\psi\rangle = \underbrace{|0\rangle + |1\rangle}_{superposition} = \begin{bmatrix} 1+0\\0+1 \end{bmatrix} = \begin{bmatrix} 1\\1 \end{bmatrix}$$
 (3.2)

 $\psi$  ("psi") is a common symbol used for the state of a quantum system.

We have a computer in our hands. Why don't we try it?

Listing 3.5: First attempt to superpose two states

```
1 # Define state |psi>
initial_state = [1, 1]
3 # Redefine the quantum circuit
qc = QuantumCircuit(1)
6 # Initialise the 0th qubit in the state `initial_state`
qc.initialize(initial_state, 0)
9 # execute the qc
11 results = execute(qc,backend).result().get_counts()
12 # plot the results
14 plot_histogram(results)
```

QiskitError: 'Sum of amplitudes-squared does not equal one.'

It didn't quite work. It tells us: QiskitError: 'Sum of amplitudes—squared does not equal one.'.

The amplitudes are the values in our array. They are proportional to probabilities. And all the probabilities should add up to exactly 1 (100%). We need to add weights to the quantum states  $|0\rangle$  and  $|1\rangle$ . Let's call them  $\alpha$  and  $\beta$ .

We weight  $|0\rangle$  with  $\alpha$  and  $|1\rangle$  with  $\beta$ . Like this:

$$|\psi
angle = lpha |0
angle + eta |1
angle = egin{bmatrix} 1 \cdot lpha + 0 \cdot eta \ 0 \cdot lpha + 1 \cdot eta \end{bmatrix} = egin{bmatrix} lpha \ eta \end{bmatrix}$$

Amplitudes are proportional to probabilities. We need to normalize them so that:

$$\alpha^2 + \beta^2 = 1 \tag{3.3}$$

If both states  $|0\rangle$  and  $|1\rangle$  should have the same weight, then

$$\alpha = \beta$$

And therefore, we can solve our equation to  $\alpha$ :

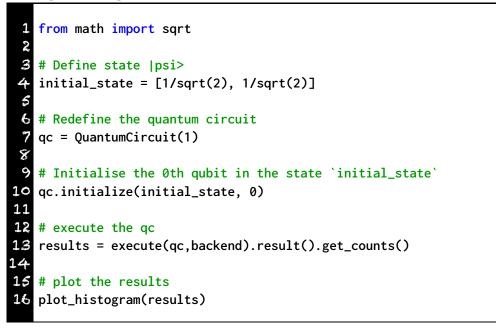
$$\alpha^2 + \alpha^2 = 1 \Leftrightarrow 2 \cdot \alpha^2 = 1 \Leftrightarrow \alpha^2 = \frac{1}{2} \Leftrightarrow \alpha = \frac{1}{\sqrt{2}}$$

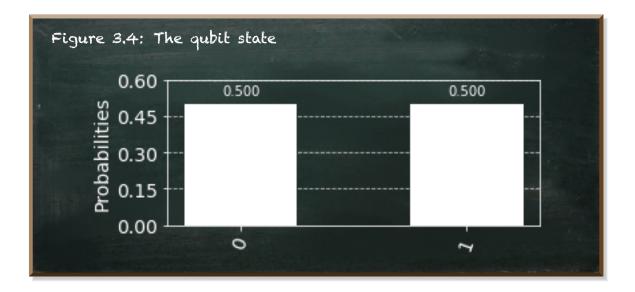
And we insert the value for both  $\alpha$  and  $\beta$  (both are equal). Let's try this quantum state:

$$|\psi\rangle = \frac{1}{\sqrt{2}}|0
angle + \frac{1}{\sqrt{2}}|1
angle = \begin{bmatrix} \frac{1}{\sqrt{2}}\\ \frac{1}{\sqrt{2}} \end{bmatrix}$$

The corresponding array in Python is: [1/sqrt(2), 1/sqrt(2)]. Don't forget to import sqrt.

Listing 3.6: Weighted initial state





What is the state of qubit that has a 25 chance of resulting in 0 and 75 of resulting in 1?

The solution is solving the following equation system.

**Equation 3.4**. This is the definition of a qubit in superposition. This qubit, when observed, has the probability of  $\alpha^2$  to result in 0 and  $\beta^2$  to result in 1.

$$|\psi\rangle = \alpha|0\rangle + \beta|1\rangle = \begin{bmatrix} \alpha \\ \beta \end{bmatrix}$$
 (3.4)

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**Equation 3.5**. This is the required normalization. It requires the sum of the squared amplitudes ( $\alpha$  and  $\beta$ ) to equal 1.

$$\alpha^2 + \beta^2 = 1 \tag{3.5}$$

Let's regard the probabilities 25% and 75% as fractions and equate them to  $\alpha^2$  and  $\beta^2$ , respectively.

$$\alpha^2 = \frac{1}{4} \Leftrightarrow \alpha = \frac{1}{2} \tag{3.6}$$

and

$$\beta^2 = \frac{3}{4} \Leftrightarrow \beta = \frac{\sqrt{3}}{2} \tag{3.7}$$

Now, we insert 3.6 and 3.7 into equation 3.4:

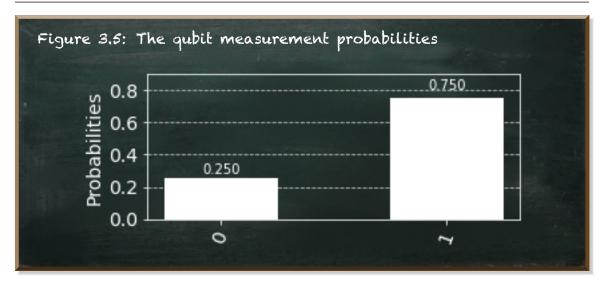
$$|\psi\rangle = \frac{1}{2}|0\rangle + \frac{\sqrt{3}}{2}|1\rangle = \begin{bmatrix} \frac{1}{2}\\ \frac{\sqrt{3}}{2} \end{bmatrix}$$

In Python, the array [1/2, sqrt(3)/2] represents the vector  $\begin{vmatrix} \frac{1}{2} \\ \frac{\sqrt{3}}{2} \end{vmatrix}$ 

Now, let's open our Jupyter notebook and test our calculation.

Listing 3.7: The qubit with a probability of 0.25 to result in 0

```
1 from qiskit import QuantumCircuit, execute, Aer
12 from qiskit.visualization import plot_histogram
3 from math import sqrt
4
5 qc = QuantumCircuit(1)
6 initial_state = [1/2, sqrt(3)/2] # Here, we insert the state
7 qc.initialize(initial_state, 0)
8 backend = Aer.get_backend('statevector_simulator')
9 result = execute(qc,backend).result()
10 counts = result.get_counts()
11 plot_histogram(counts)
```



Phew. In this chapter, we introduced quite a few terms and equations just to scratch on the surface of quantum mechanics. But the actual source code is pretty neat, isn't it?

We introduced the notion of the quantum state. In particular, the state of a binary quantum system. The quantum bit or qubit.

Until we observe a qubit, it is in superposition. Contrary to a classical bit that can be either 0 or 1, a qubit is in a superposition of both states. But once you observe it, there are distinct probabilities of measuring 0 or 1.

This means that multiple measurements made on multiple qubits in identical states will not always give the same result. The equivalent representations of a quantum bit that, when observed, has the probability of  $\alpha^2$  to result in 0 and  $\beta^2$  to result in 1 are:

 $|\psi\rangle = \alpha|0\rangle + \beta|1\rangle = \begin{bmatrix} \alpha \\ \beta \end{bmatrix}$ , with  $\alpha^2 + \beta^2 = 1$ . In Python the array [alpha, beta] denotes this state.

# 3.2 Visual Exploration Of The Qubit State

The qubit is a two-dimensional quantum system. Each dimension is denoted by a standard basis vector:

$$|0
angle = egin{bmatrix} 1 \\ 0 \end{bmatrix}$$
 in Python [1, 0] and

$$|1\rangle = \begin{bmatrix} 0\\1 \end{bmatrix}$$
, in Python [0, 1].

The state of the qubit is represented by the superposition of both dimensions. This is the qubit state vector  $|\psi\rangle$  ("psi").

$$|\psi\rangle = \alpha|0\rangle + \beta|1\rangle = \begin{bmatrix} \alpha \\ \beta \end{bmatrix}$$
 (3.8)

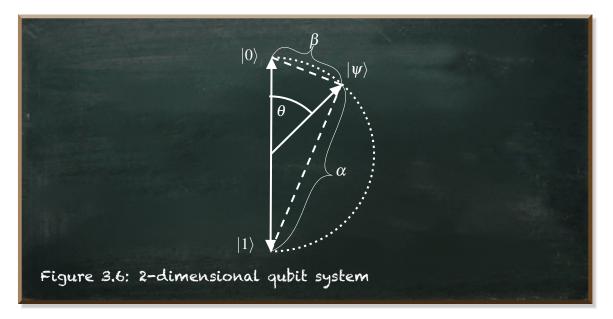
In Python,  $|\psi
angle$  is the array [alpha, beta].

But  $|\psi\rangle$  must be normalized by:

$$\alpha^2 + \beta^2 = 1 \tag{3.9}$$

Although normalizing the qubit state vector is not a difficult task, doing the math over and over again is quite cumbersome.

But maybe, there's another way. An easy way. Let's first have a look at a graphical representation of the qubit state  $|\psi\rangle$  in the following figure 5.12.



In this representation, both dimensions reside at the vertical axis but in opposite directions. The top and the bottom of the system correspond to the standard basis vectors  $|0\rangle$  and  $|1\rangle$ , respectively.

When there are two dimensions, the usual way is to put the two dimensions orthogonal to each other. While using one axis to

represent both dimensions is rather an unusual representation for a two-dimensional system, it is well suited for a quantum system. But more on this later.

Let's have a look at the arbitrary qubit state vector  $|\psi\rangle$  in this figure 5.12.

Since qubit state vectors are normalized,  $|\psi\rangle$  originates in the center and has the magnitude (length) of  $\frac{1}{2}$ . Due to this equal magnitude, all state vectors end at the pointed circle. So does  $|\psi\rangle$ .

The angle between the state vector  $|0\rangle$  and  $|\psi\rangle$ , named  $\theta$  ("theta"), controls the proximities of the vector head to the top and the bottom of the system (dashed lines).

These proximities represent the probabilities of

- $\alpha^2$  of measuring  $|\psi\rangle$  as 0
- and  $\beta^2$  of measuring it as 1.
- The proximities  $\alpha$  and  $\beta$  are at the opposite sides of the state's probability  $(|\psi\rangle)$  they describe.  $\alpha$  is the proximity (or distance) to  $|1\rangle$  because with increasing distance to  $|1\rangle$  the probability of measuring '0' increases.

Thus, by controlling the proximities, the angle  $\theta$  also controls the probabilities of measuring the qubit in either state 0 or 1.

Rather than specifying the relation between  $\alpha$  and  $\beta$  and then coping with normalizing their values, we can specify the angle  $\theta$  and use the required normalization to derive  $\alpha$  and  $\beta$  from it.

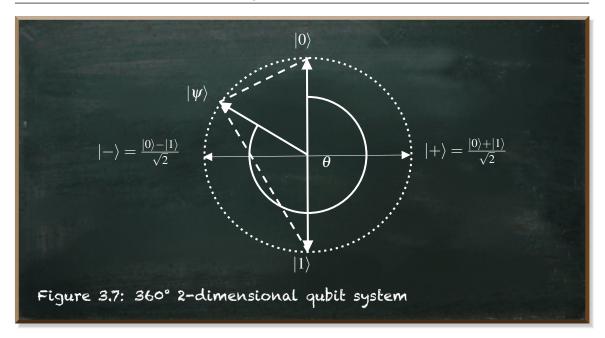
We can deduct the values of  $\alpha$  and  $\beta$  and thus the state  $|\psi\rangle$ :

$$|\psi\rangle = \cos\frac{\theta}{2}|0\rangle + \sin\frac{\theta}{2}|1\rangle = \begin{bmatrix}\cos\frac{\theta}{2}\\\sin\frac{\theta}{2}\end{bmatrix}$$
 (3.10)

In Python the two-field array [cos(theta/2), sin(theta/2)] denotes this state.

There's one problem left. For  $\theta \in \mathbb{R}$ , what if  $\pi < \theta < 2\pi$ ? Or in plain English, what if the  $\theta$  denotes a vector pointing to the left side of the vertical axis?

Figure 11.9 shows this situation.



Mathematically, we don't have a problem. Since we square  $\alpha$  and  $\beta$ , their signs (+ or -) are irrelevant for the resulting probabilities.

But what does it mean? How can either  $\alpha^2$  or  $\beta^2$  be negative, as the figure indicates? The answer is *i*. *i* is a complex number whose square is negative:  $i^2 = -1$ .

And if  $\alpha$  and  $\beta$  are complex numbers ( $\alpha, \beta \in \mathbb{C}$ ), their squares can be negative.

This entails a lot of consequences. And it raises a lot of questions. We will unravel them one by one in the following sections. For now, we interpret all vectors on the left-hand side of the vertical axis to have a negative value for  $\beta^2$  ( $\beta^2 < 0$ ).

While such a value lets us distinguish the qubit state vectors on both sides of the vertical axis, it does not matter for the resulting probabilities.

For instance, the state  $|\psi\rangle = \frac{|0\rangle + |1\rangle}{\sqrt{2}}$  yields the same probability of measuring 0 or 1. It resides at the horizontal axis. And so does  $|\psi\rangle = \frac{|0\rangle - |1\rangle}{\sqrt{2}}$ 

Although these states share the same probabilities, they are different. And the angle  $\theta$  differentiates between them.

 $heta=rac{\pi}{2}$  specifies  $|\psi
angle=rac{|0
angle+|1
angle}{\sqrt{2}}$  that is also known as |+
angle.

And  $\theta = \frac{3}{2}\pi$  or  $\theta = -\frac{\pi}{2}$  specifies  $|\psi\rangle = \frac{|0\rangle - |1\rangle}{\sqrt{2}}$  that is also known as  $|-\rangle$ .

One of the consequences mentioned above of  $\alpha^2$  or  $\beta^2$  being negative is that our normalization rule needs some adjustments.

We need to change the normalization equation 3.9 to:

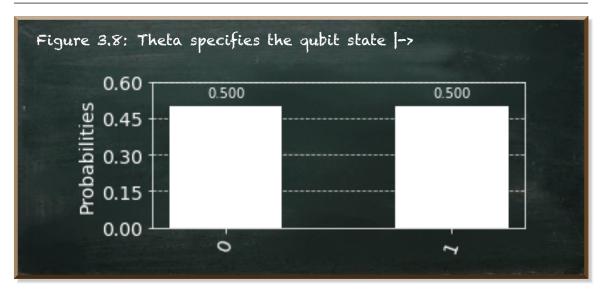
$$|\alpha|^2 + |\beta|^2 = 1 \tag{3.11}$$

This section contained a lot of formulae. The important takeaway is we can specify quantum states that yield certain probabilities of measuring 0 and 1 by an angle  $\theta$ . It saves us doing the normalization manually.

Let's have a look.

```
Listing 3.8: Using theta to specify the quantum state vector
```

```
1 from math import pi, cos, sin
 2 from qiskit import QuantumCircuit, Aer, execute
 3 from giskit.visualization import plot_histogram
4
5 def get_state (theta):
 6
7
     """returns a valid state vector"""
     return [cos(theta/2), sin(theta/2)]
 8
 9 # play with the values for theta to get a feeling
10 theta = -pi/2 # affects the probabilities
11
12
13 # create, initialize, and execute the quantum circuit
14 qc = QuantumCircuit(1)
15 qc.initialize(get_state(theta), 0)
16 backend = Aer.get_backend('statevector_simulator')
17 result = execute(qc,backend).result()
18 counts = result.get_counts()
19
20 # Show the histogram
21 plot_histogram(counts)
```



In this piece of code, we introduced the function getState (line 5). It takes theta as a parameter and returns the array [cos(theta/2), sin(theta/2)]. This is the vector we specified in the equation 3.10.

### 3.3 Derive The Proof Of The Theta-Formula

In the last section **??**, we introduced the formula: **3.10**:

$$|\psi\rangle = \cos\frac{\theta}{2}|0\rangle + \sin\frac{\theta}{2}|1\rangle = \begin{bmatrix}\cos\frac{\theta}{2}\\\sin\frac{\theta}{2}\end{bmatrix}$$

The structure of this formula derives directly from the definition of the qubit superposition state.

$$|\psi\rangle = \alpha|0\rangle + \beta|1\rangle = \begin{bmatrix} lpha \\ eta \end{bmatrix}$$
 (3.12)

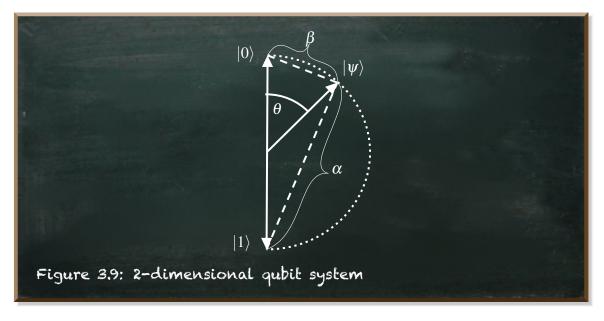
To prove equation 3.10, we need to prove the following two terms

$$\alpha = \cos\frac{\theta}{2} \tag{3.13}$$

and

$$\beta = \sin\frac{\theta}{2} \tag{3.14}$$

Let's have a look at our graphical definition of  $\alpha$  and  $\beta$ . We already saw this figure 5.12 in section 3.2.



 $\alpha$  and  $\beta$  describe the proximity to the top and the bottom of the system, respectively.  $\theta$  is the angle between the standard basis vector:  $|0\rangle = \begin{bmatrix} 1\\0 \end{bmatrix}$  and the qubit state vector  $|\psi\rangle$  it represents.

Any valid qubit state vector must be normalized:

$$\alpha^2 + \beta^2 = 1 \tag{3.15}$$

This implies all qubit state vectors have the same magnitude (length). Since they all originate in the center, they form a circle with the radius of their magnitude (that is half of the circle diameter).

#### In such a situation, Thales' theorem states, if

- A, B, and C are distinct points on a circle (condition 1)
- where the line AC is a diameter (condition 2)
- then the angle  $\angle ABC$  (the angle at point B) is a right angle.

In our case, the heads of  $|0\rangle$ ,  $|1\rangle$ , and  $|\psi\rangle$  represent the points A, B, and C, respectively (satisfy condition 1). The line between  $|0\rangle$  and  $|1\rangle$  is the diameter (satisfy condition 2). Therefore, the angle at the head of  $|\psi\rangle$  is a right angle.

Now, the **Pythagorean theorem** states the area of the square whose side is opposite the right angle (hypotenuse, *c*) is equal to the sum of the areas of the

squares on the other two sides (legs *a*, *b*).

$$c^2 = a^2 + b^2 \tag{3.16}$$

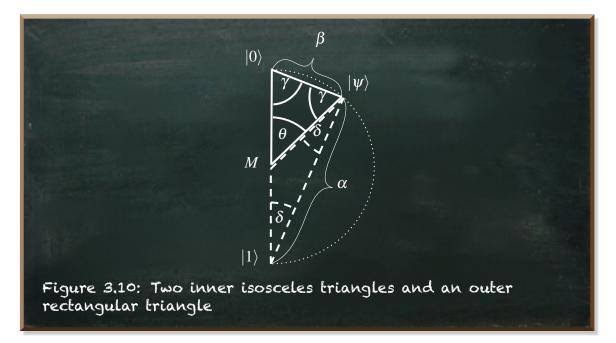
When looking at figure 3.9, again, we can see that  $\alpha$  and  $\beta$  are the two legs of the rectangular triangle and the diameter of the circle is the hypotenuse. Therefore, we can insert the normalization equation 3.15

$$c = \sqrt{\alpha^2 + \beta^2} = \sqrt{1} = 1 \tag{3.17}$$

The diameter *c* is two times the radius, thus two times the magnitude of any vector  $|\psi\rangle$ . The length of  $|\psi\rangle$  is thus  $\frac{c}{2} = \frac{1}{2}$ .

Since all qubit state vectors have the same length, including  $|0\rangle$  and  $|1\rangle$ , there are two isosceles triangles ( $\Delta M |0\rangle |\psi\rangle$  and  $\Delta M |\psi\rangle |1\rangle$ ).

Have a look at the following figure 3.10.



You can see the two isosceles triangles. The angles in isosceles triangles at the equal legs are equal, as denoted by  $\gamma$  and  $\delta$ .

Further, the sum of all three angles in a triangle is 180°. Therefore,

 $\theta + 2\gamma = 180^{\circ} \tag{3.18}$ 

Let's solve this after  $\gamma$ 

$$\gamma = \frac{180^{\circ} - \theta}{2} = 90^{\circ} - \frac{\theta}{2}$$
(3.19)

In a rectangular triangle (the outer one), trigonometric identity says the sine of an angle is the length of the opposite leg divided by the length of the hypotenuse. In our case, this means:

$$\sin\gamma = \frac{\alpha}{1} = \alpha \tag{3.20}$$

Now, we insert equation 3.19:

$$\sin\left(90^{o} - \frac{\theta}{2}\right) = \alpha \tag{3.21}$$

With  $sin(90^{\circ} - x) = \cos x$ , we can see:

$$\alpha = \cos \frac{\theta}{2}$$

This is the first equation 3.13 to prove.

The further proof works accordingly and is straight forward. At the center (*M*), the (unnamed) angle inside the dashed triangle is  $180^{o} - \theta$ .

$$(180^{\circ} - \theta) + 2\delta = 180^{\circ} \Leftrightarrow \delta = \frac{\theta}{2}$$
 (3.22)

Again, we use the trigonometric identity. This time it implies:

$$\sin \delta = \frac{\beta}{1} = \beta \tag{3.23}$$

Finally, we insert 3.22:

$$\sin\frac{\theta}{2} = \beta \tag{3.24}$$

This is the second equation to prove.

# 3.4 Exploring The Observer Effect

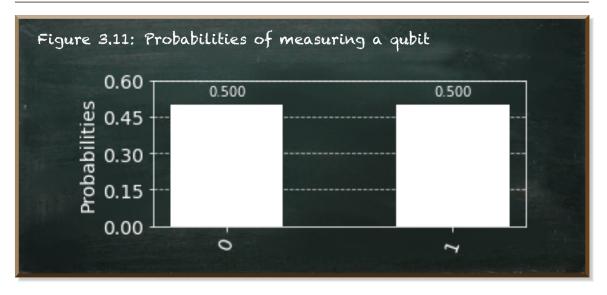
A qubit is a two-level quantum system that is in superposition of the quantum states  $|0\rangle$  and  $|1\rangle$  unless you observe it. Once you observe it, there are distinct probabilities of measuring 0 or 1. In physics, this is known as the observer effect. It says the mere observation of a phenomenon inevitably changes that phenomenon itself. For instance, if you're measuring the temperature in your room, you're taking away a little bit of the energy to heat up the mercury in the thermometer. This loss of energy cools down the rest of your room. In the world we experience, the effects of observation are often negligible.

But in the sub-atomic world of quantum-mechanics, these effects matter. They matter a lot. The mere observation of a quantum bit changes its state from a superposition of the states  $|0\rangle$  and  $|1\rangle$  to either one value. Thus, even the observation is a manipulation of the system we need to consider when developing a quantum circuit.

Let's revisit the quantum circuit from section **??**. Here's the code and the result if you run it:

Listing 3.9: A circuit without measurement

```
1 from giskit import QuantumCircuit, execute, Aer
 2 from qiskit.visualization import plot_histogram
 3 from math import sqrt
 4
 5 # Create a quantum circuit with one qubit
 6 qc = QuantumCircuit(1)
 7
 % # Define state |Psi>
 9 initial_state = [1/sqrt(2), 1/sqrt(2)]
10
11 # Apply initialization operation to the qubit at position 0
12 qc.initialize(initial_state, 0)
13
14 # Tell Qiskit how to simulate our circuit
15 backend = Aer.get_backend('statevector_simulator')
16
17 # Do the simulation, returning the result
18 result = execute(qc,backend).result()
19
20 # Get the data and display histogram
21 counts = result.get_counts()
22 plot_histogram(counts)
```



Our circuit consists of a single one qubit (line 6). It has the initial state [1/sqrt (2), 1/sqrt(2)] (line 9) that we initialize our quantum circuit with (line 12).

Here are the Dirac and the vector notation of this state:

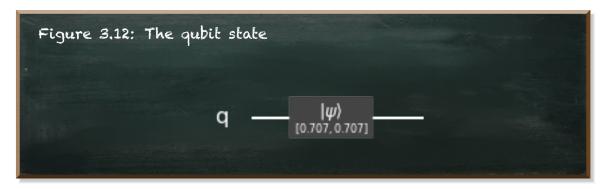
$$|\psi\rangle = \frac{1}{\sqrt{2}}|0\rangle + \frac{1}{\sqrt{2}}|1\rangle = \begin{bmatrix} \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \end{bmatrix}$$

We add a simulation backend (line 15), execute the circuit and obtain the result (line 18). The result object provides the get\_counts function that provides the probabilities for the resulting (observed) state our qubit.

Let's have a look at our circuit. The QuantumCircuit provides the draw function that renders an image of the circuit diagram. Provide output=text as named parameter to get an ASCII art version of the image.

Listing 3.10: Draw the circuit

```
1 qc.draw(output='text')
```



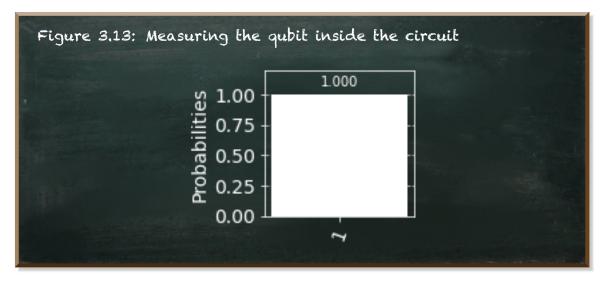
This drawing shows the inputs on the left, outputs on the right, and operations in between.

What we see here is our single qubit (q) and its initialization values ( $\frac{1}{\sqrt{2}}$  = 0.707). These values are both, the input and the output of our circuit. When we execute this circuit, our result-function evaluates the quantum bit in the superposition state of  $|0\rangle$  and  $|1\rangle$ . Thus, we have a 50:50 chance to catch our qubit in either one state.

Let's see what happens if we observe our qubit as part of the circuit.

Listing 3.11: Circuit with measurement

```
1 qc = QuantumCircuit(1)
2 qc.initialize(initial_state, 0)
3 
4 # observe the qubit
5 qc.measure_all()
6 
7 # Do the simulation, returning the result
8 result = execute(qc,backend).result()
9 counts = result.get_counts()
10 plot_histogram(counts)
```

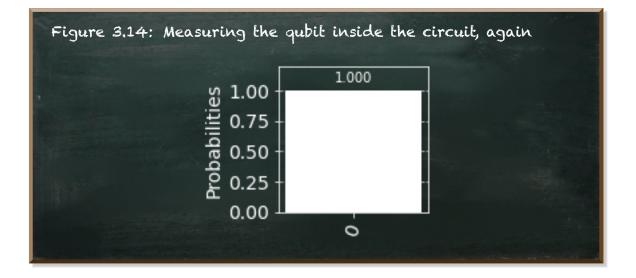


"Whoa?!"

We get a 100% probability of resulting state 1. That can't be true. Let's rerun the code... (I know, doing the same things and expecting different results is a sign of insanity)

Listing 3.12: Circuit with measurement

```
1 qc = QuantumCircuit(1)
2 qc.initialize(initial_state, 0)
3 qc.measure_all()
4 result = execute(qc,backend).result()
5 counts = result.get_counts()
6 plot_histogram(counts)
```

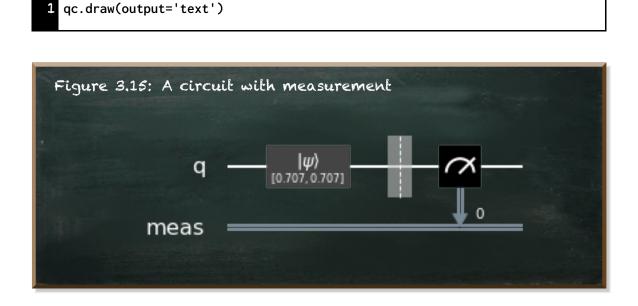


Again. 100% probability of measuring ... wait ... it's state 0.

No matter how often you run this code, you'll always get 100% probability of either 0 or 1. In fact, if you reran the code many, many times and counted the results, you'd see a 50:50 distribution.

Sounds suspicious? Yes, you're right. Let's have a look at our circuit.

Listing 3.13: A circuit with measurement



Our circuit now contains a measurement. That is an observation. It pulls our qubit out of a superposition state and lets it collapse into either 0 **or** 1. When we obtain the result afterwards, there's nothing quantumic anymore. It is a distinct value. And this is the output (to the right) of the circuit.

Whether we observe a 0 or a 1 is now part of our quantum circuit.

The small number at the bottom measurement line does not depict a qubit's value. It is the measurement's index. It starts counting at 0. The next measurements will have the numbers 1, 2, etc.

Sometimes, we refer to measurement as collapsing the state of the qubit. This notion emphasizes the effect a measurement has. Unlike classical programming, where you can inspect, print, and show values of your bits as often as you like, in quantum programming, it has an effect on your results. If we constantly measured our qubit to keep track of its value, we would keep it in a well-defined state, either 0 or 1. Such a qubit wouldn't be different from a classical bit. Our computation could be easily replaced by a classical computation. In a quantum computation, we must allow the qubits to explore more complex states. Measurements are therefore only used when we need to extract an output. This means that we often place the all measurements at the end of our quantum circuit.

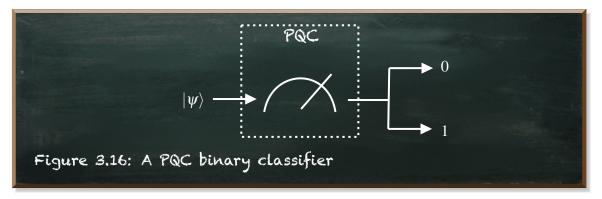
In this section, we had a look at the simplest quantum circuit. We initialize a single qubit and observe it. But it effectively demonstrates the observer effect in quantum computing. It is something we need to keep in mind, when we start manipulating our qubits.

## 3.5 Parameterized Quantum Circuit

In chapter 2, we created different hypocrite classifiers. These are classifiers solely building upon chance when predicting the label of a thing. While such a classifier can yield seemingly good performance in a single measure, such as "precision", it does not reach an average far beyond 0.5 four the four measures that directly result from the confusion matrix (precision, recall, specificity, and NPV).

In this section, we use a quantum circuit as to solve our binary classification task. This quantum circuit is a **Parameterized Quantum Circuit** (PQC). A PQC is a quantum circuit that takes all data it needs as input paramters. Therefore it has its name "parameterized". It predicts the label of the thing based on these parameters.

The following image 3.16 depicts the simple PQC we are about to build in this section.



This PQC takes a single quantum state ( $\psi$ ) as its input. It measures the state and provides its prediction as output.

We created such a quantum circuit in the last section 3.4, already.

Here's the source code.

Listing 3.14: A simple PQC binary classifier

```
1 qc = QuantumCircuit(1)
2 initial_state = [1/sqrt(2), 1/sqrt(2)]
3 qc.initialize(initial_state, 0)
4 qc.measure_all()
```

In fact, this circuit outputs either 0 or 1, each with a probability of 50%. It sounds a lot like the random classifier we created in section 2.5.

Let's wrap this circuit into a function we can use with the run and evaluate functions we created in that section to see whether it behaves similarly.

Listing 3.15: The parameterized quantum circuit classifier

```
1 from qiskit import execute, Aer, QuantumCircuit
 2 from math import sqrt
 3 from sklearn.metrics import recall_score, precision_score,
       confusion_matrix
45678910
    def pqc_classify(backend, passenger_state):
      """backend -- a giskit backend to run the guantum circuit at
      passenger_state -- a valid quantum state vector"""
      # Create a quantum circuit with one qubit
      qc = QuantumCircuit(1)
11
12
13
      # Define state |Psi> and initialize the circuit
      qc.initialize(passenger_state, 0)
14
15
      # Measure the qubit
16
      qc.measure_all()
17
18
      # run the quantum circuit
19
      result=execute(qc,backend).result()
20
21
      # get the counts, these are either {'0': 1} or {'1': 1}
22
      counts=result.get_counts(qc)
23
24
      # get the bit 0 or 1
25
      return int(list(map(lambda item: item[0], counts.items()))[0])
```

The first difference to notice is the function takes two parameters instead of one (line 5). The first parameter is a Qiskit backend. Since the classifier will run a lot of times in a row, it makes sense to reuse all we can. And we can reuse the backend.

The second parameter differs from the classifiers thus far. It does not take the passenger data, but a quantum state vector (passenger\_state) as input. This is not a problem right now, since all the hypocrite classifiers we developed so far ignored the data anyway.

The function creates a quantum circuit with one qubit (line 12), initializes it with the passenger\_state (line 15), measures the qubit (line 18), executes the quantum circuit (line 21) and retrieves the counts from the result (line 24). All these steps did not change.

But how we return the counts is new (line 27). counts is a Python dictionary. It contains the measurement result (either 0 or 1) as a key and the probability as the associated value. Since our quantum circuit measures the qubit, it collapsed to a finite value. Thus, the measurement probability is always 1. Consequently, counts is either {'0': 1} or {'1': 1}.

All we're interested in here is the key. And this is what we return.

We start (from inner to outer) with the term counts.items(). It transforms the Python dictionary into a list of tuples, like [('0', 1)]. Since we only have one key in the dictionary, there is only one tuple in the list. The important point is to get the tuple rather than the dictionary's key-value construct because we can access a tuple's elements thorugh the index.

This is what we do in the function lambda: item: item[0]. It takes a tuple and returns its first element. We do this for every item in the list (even though there is only one item) by using list(map(...)). From this list, we take the first (and only) item (either '0' or '1') and transform it into a number (int(...)).

Before we can run it, we need to load the prepared passenger data.

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Listing 3.16: Load the data

```
1 import numpy as np
2
3 with open('data/train.npy', 'rb') as f:
4 train_input = np.load(f)
5 train_labels = np.load(f)
6
7 with open('data/test.npy', 'rb') as f:
8 test_input = np.load(f)
9 test_labels = np.load(f)
```

The following code runs the pqc\_classifier with the initial state with a probability of 0.5 to measure 0 or 1, respectively (line 5).

Further, we create a backend (line 2) and provide it as a parameter to be reused (line 8).

Listing 3.17: The scores of the random quantum classifier

```
1 # Tell Qiskit how to simulate our circuit
2 backend = Aer.get_backend('statevector_simulator')
3 # Specify the quantum state that results in either 0 or 1
initial_state = [1/sqrt(2), 1/sqrt(2)]
6 7 classifier_report("Random PQC",
1 ambda passenger: pqc_classify(backend, initial_state),
1 train_input,
1 train_labels)
```

```
The precision score of the Random PQC classifier is 0.35
The recall score of the Random PQC classifier is 0.46
The specificity score of the Random PQC classifier is 0.46
The npv score of the Random PQC classifier is 0.57
The information level is: 0.46
```

When we run the pqc\_classify classifier with the initial state, we can see that it yields the same scores as the random classifier did.

But how these two classifiers create the results is completely different.

The classic "random" classifier uses the function random and initializes it, as depicted by the following code snippet.

Listing 3.18: Initialization of classical (pseudo-)random

```
1 import random
2 random.seed(a=None, version=2)
```

We provide None as the randomness source (a). This implies the function takes a value from the operating system. It appears random, but it is not. If we knew the value it gets from the operating system or if we specified a distinct value ourselves, we could reproduce the exact predictions.

That's why Python's random-function generates pseudo-random (see Pythondocs) numbers.

By contrast, the PQC generates truly random results (when being run on a real quantum computer). This is in accordance with one of the interpretations of the quantum state of superposition. we discussed in section (??).

Nevertheless, we have not used anything quantumic yet which would make us see the difference between classical pseudo-random and quantumic truly random.

# 3.6 Variational Hybrid Quantum-Classical Algorithm

The PQC binary classifer we created in the previous section 3.5 is as good as the random classifier. Or as poor as. Because it does not provide any increase in the information level.

This is going to change now. So far, we always feed the PQC with the same initial state:  $|\psi\rangle = \begin{bmatrix} \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \end{bmatrix}$ , with the corresponding array in Python: [1/sqrt(2), 1/sqrt(2)].

This state does not take into account the passenger data at all. It is a hypocrite classifier, such as the classifiers we build in section 2.7. Hypocrite classifiers solely use chance when predicting the label of a thing. While such a classifier can yield seemingly good performance in a single measures, such as "precision", it does not reach an average above 0.5 for the four measures

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that directly result from the confusion matrix (precision, recall, specificity, and NPV). It does not provide any information gain.

In order to improve our classifier, we need to use the passenger data. Even though we prepared the passenger data into normalized numerical data, it does not fit the quantum state vector we need to feed into our PQC. We need to pre-process our passenger data to be computable by a quantum computer.

In fact, we also need to post-process it. We implicitly post-processed the results as part of the return statement, as shown in the following snippet.

Listing 3.19

```
1 def pqc_classify(backend, passenger_state):
2  # ...
3 
4  # get the bit 0 or 1
5  return int(list(map(lambda item: item[0], counts.items()))[0])
```

Since we have a binary classification task, our prediction is in fact 0 or 1. Our post-processing is limited to transforming the output format. But in any other setting, post-processing may involve translation from the output of the quantum circuit into a useable prediction.

Altogether, we wrap the PQC into a process of classical pre- and postprocessing. This is an algorithm with an outer structure running at a classical computer and an inner component running on a quantum computer. It is a **Variational Hybrid Quantum-Classical Algorithm** and it is a popular approach for near-term quantum devices.

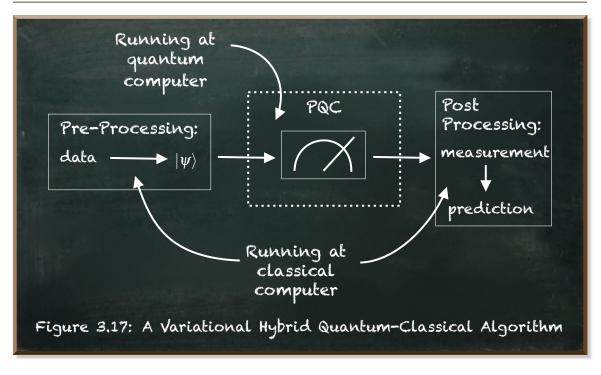
Figure 3.17 shows the overall architecture of our simple Variational Hybrid Quantum-Classical Algorithm.

The data is pre-processed on a classical computer to determine a set of parameters for the PQC. In our simple case, this is the quantum state vector  $|\psi\rangle$ .

The quantum hardware uses the intitial quantum state, works with it and performs measurements. All its calculations are parameterized. So, they are relatively small and short-lived. In our case, we only measure the quantum state. We do not use any further parameters beyond  $|\psi\rangle$ .

Finally, the measurement outcomes are post-processed by the classical computer to generate a prediction.

The overall algorithm consists of a closed loop between the classical and

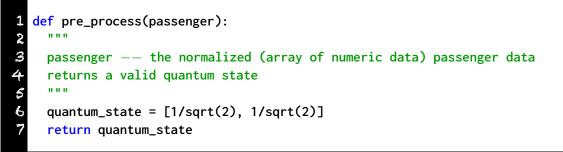


quantum components.

Let's separate our code thus far into the three parts:

- Pre-processing
- PQC
- Post-processing

Listing 3.20: Pre-processing template



The function pre\_process takes the passenger data as an array of numeric data.

It returns a valid quantum state vector. In this first version, it returns the balanced state of measuring 0 or 1 with equal probabilities.

Listing 3.21: The parameterized quantum circuit

```
1 def pgc(backend, guantum_state):
 2
      .....
3456789011
      backend -- a giskit backend to run the guantum circuit at
      quantum_state -- a valid quantum state vector
      returns the counts of the measurement
      ....
      # Create a quantum circuit with one qubit
      qc = QuantumCircuit(1)
      # Define state |Psi> and initialize the circuit
12
      qc.initialize(quantum_state, 0)
13
14
15
16
17
18
      # Measure the gubit
      qc.measure_all()
      # run the guantum circuit
      result=execute(gc,backend).result()
19
20
      # get the counts, these are either {'0': 1} or {'1': 1}
21
      counts=result.get_counts(qc)
22
23
      return counts
```

The function pqc is the PQC. It takes a quantum backend and a valid quantum\_state as input parameters.

It prepares and runs the quantum circuit before it returns the counts of its measurements.

Listing 3.22: Post-processing

```
1 def post_process(counts):
2 """
3 counts -- the result of the quantum circuit execution
4 returns the prediction
5 """
6 return int(list(map(lambda item: item[0], counts.items()))[0])
```

The function post\_process takes the counts as input and returns the prediction (see section 3.5 for the detailed explanation of how to transform the counts dictionary into the prediction).

Let's put it all together.

Listing 3.23: The scores of the random quantum classifier

```
1 # Tell Qiskit how to simulate our circuit
backend = Aer.get_backend('statevector_simulator')
3 4 classifier_report(
5 "Variational",
1 ambda passenger: post_process(pqc(backend, pre_process(passenger))),
7 train_input,
8 train_labels)
```

```
The precision score of the Variational classifier is 0.43
The recall score of the Variational classifier is 0.54
The specificity score of the Variational classifier is 0.51
The npv score of the Variational classifier is 0.62
The information level is: 0.52
```

We first create the statevector\_simulator backend we can reuse for all our predictions (line 2).

We use the classifier\_report wrapping function we developed in section 2.7.

Besides an arbitrary name it uses in the output (line 5) the main input is the classifier we provide (line 6).

We provide an anonymous (lambda) function (a function without a name) as our classifier. It takes a single parameter passenger and runs (from inner to outer) the pre\_process function with the passenger as parameter. We put the result alongside the backend into the pqc function whose result we put into the post\_process function.

When we run the pqc classifier with the initial state, we can see that it yields the same scores as the random classifier.

Now, it's finally time to build a real classifier. One that uses the actual passenger data to predict whether the passenger survived the Titanic shipwreck or not.

Let's start at the end. The current post-processing already returns either 0 or 1. This fits our required output, since 0 represents the passenger died and 1 represents the passenger survived. The current PQC measures the provided quantum state vector and returns the counts. We could leave it unchanged, if we provided as input a vector whose probability corresponds to the passenger's actual probability to survive.

The passenger data consists of an array of seven features. We already transformed all features into numbers between 0 and 1 (section 2.4).

Thus, it is the task of the pre-processing to translate these seven numbers into a quantum state vector whose probability corresponds to the passenger's actual probability to survive.

Finding such a probability is the innate objective of any machine learning algorithm.

Our data consists of seven features. The main assumption is these features determine or at least affected whether a passenger survived or not. If that wasn't the case, we wouldn't be able to predict anything reliably. Let's assume the features determine survival.

The question then is, **how do these seven features determine survival?** Is one feature more important than another? Is there a direct relationship between a feature and survival? Are there any interdependencies between the features, such as if A then B indicates survival. But if not A, then B is irrelevant but C is important.

But before we use sophisticated tools (such as neural networks) that are able to discover complex structures of how the features determine the outcome, we start simple.

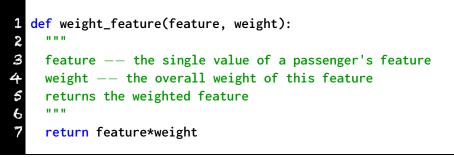
We assume all features are independent from each other and each features contributes more or less to the survival or death of the passenger.

Therefore, we say the overall probability of survival P(survival) is the sum of each feature's value F times the feature's weight  $\mu_F$  ("mu").

$$P(survival) = \sum (F \cdot \mu_F)$$
(3.25)

Let's have a look at what this means in Python.

Listing 3.24: weight a passenger's feature



The weight\_feature function calculates and returns the term  $F \cdot \mu_F$ . This function calculates how much a passenger's feature, the age for instance, contributes to this passenger's overall probability to survive. The higher the weighted value, the higher the probability.

Next, we need to add all the weighted features to calculate the overall probability.

Listing 3.25: Calculate the overall probability

The function get\_overall\_probability takes two parameters. First, the list of a passenger's feature values. This is a passenger's data. Second, the list of the feature weights.

We construct a list of tuples for each feature (line 10) containing the feature and its weight. Python's zip-function takes two separate lists and creates the respective tuple for each two elements in the lists.

We reduce this list of (feature, weight) into a single number (line 8). We call the weight\_feature-function for each of the tuples and add up the results (line 9), starting with the value 0 (line 11).

Now, we need to calculate the weights of the features. These are similar across all passengers. We build the weights upon the correlation coefficients.

The correlation coefficient is a measure of the relationship between two variables. Each variable is a list of values. It denotes how much the value in one list increases as the value of the other list increases. The correlation coefficient can take values between -1 and 1.

- A correlation coefficient of 1 means that for every **increase** in one variable, there is a proportional **increase** in the other.
- A correlation coefficient of –1 means that for every **increase** in one variable, there is a proportional **decrease** in the other.
- A correlation coefficient of 0 means that the two variables are not linearly related.

We calculate the correlation coefficient for each feature in our dataset in relation to the list of labels. In the following code, we thus separate our dataset into a list of the columns (line 4).

The term list(map(lambda passenger: passenger[i], train\_input transforms each passenger's data into its value at the position i. And we do this for i in range(0,7). It means we do this for each column.

Listing 3.26: Calculate the correlation coefficients

```
1 from scipy.stats import spearmanr

2 # separate the training data into a list of the columns

4 columns = [list(map(lambda passenger: passenger[i], train_input)) for i

5 in range(0,7)]

5 # calculate the correlation coefficient for each column

5 correlations = list(map(lambda col: spearmanr(col, train_labels)[0],

5 columns))

6 correlations
```

```
[-0.3197157323427042,
-0.578307132534222,
-0.07119068845990383,
0.09087327268445101,
0.13761444319293503,
0.31592964952566327,
-0.1745346616390969]
```

There are different types of correlation coefficients. The most frequently used are the Pearson and Spearman correlation methods.

The Pearson correlation is best suited for linear continuous variables whereas the Spearman correlation also works for monotonic ordinal variables. Since we have some categorial data (Plass, Sex, and Embarked), we use the Spearman method to calculate the correlation coefficient.

Scipy provides the function spearmanr for us. We call this function for each column and the train\_labels (line 7). The function returns two values, the correlation coefficient and the p-value. We're only interested in the first (at index 0).

The correlation coefficients range from -0.58 to 0.32.

Let's put this all together in the pre-processing.

Listing 3.27: The weighting pre-processing

```
1 from math import pi, sin, cos
 2
 3 def get_state (theta):
456789011
      """returns a valid state vector from angle theta"""
      return [cos(theta/2), sin(theta/2)]
   def pre_process_weighted(passenger):
      passenger —— the normalized (array of numeric data) passenger data
      returns a valid quantum state
      .....
12
13
      # caluclate the overall probability
14
15
      mu = get_overall_probability(passenger, correlations)
16
      # theta between 0 (|0>) and pi (|1>)
17
      quantum_state = get_state((1-mu)*pi)
18
19
      return quantum_state
```

We use the function get\_state from section 3.2. It takes the angle theta and returns a valid quantum state. An angle of 0 denotes the state  $|0\rangle$  that is the probability of 100% of measuring 0. An angle of  $\pi$  denotes the state  $|1\rangle$  that is the probability of 100% of measuring 1.

Accordingly, we multiply the overall probability we calculate at line 14 with

pi to specify an angle up to  $\pi$  (line 17). Since the correlation coefficients are between -1 and 1 and most of our coefficients are negative, a value of  $\mu$  towards -1 implies the passenger actually died. Thus, we reverse the angles by calculating (1-mu)\*pi.

Now, we're ready to run the classifier. Let's feed it into the classifier\_report wrapping function.

Listing 3.28: Run the PQC with the weighted pre-processing

```
backend = Aer.get_backend('statevector_simulator')
classifier_report("Variational",
    lambda passenger: post_process(pqc(backend, pre_process_weighted(
        passenger))),
    train_input,
    train_labels)
```

```
The precision score of the Variational classifier is 0.77
The recall score of the Variational classifier is 0.61
The specificity score of the Variational classifier is 0.88
The npv score of the Variational classifier is 0.77
The information level is: 0.76
```

We achieve an overall information level of about 0.73 to 0.77. Not too bad, is it? But before we're start to party, we need to test our classifier. We "trained" the classifier with the training data. So it has seen the data before we just used.

Let's run the classifier with the test dataset.

Listing 3.29: Test the PQC-based classifier on data it has not seen before

```
1 classifier_report("Variational-Test",
2 lambda passenger: post_process(pqc(backend, pre_process_weighted(
        passenger))),
3 test_input,
4 test_labels)
```

```
The precision score of the Variational-Test classifier is 0.60
The recall score of the Variational-Test classifier is 0.55
The specificity score of the Variational-Test classifier is 0.85
The npv score of the Variational-Test classifier is 0.82
The information level is: 0.70
```

The overall information level is somewhere between 0.66 and 0.71. This is only a little bit lower than the value we get when running it on the training data. The algorithm seems to generalize (to a certain extent).

Most importantly, in comparison to the hypocrite classifiers, we see a significant increase in the information level. This classifier provides some actual insights. Not too many. But some.

It is our first working Variational Hybrid Quantum-Classical Classifier.

# 15. What's Next?

You've reached the end of the preview of **Hands-On Quantum Machine Learning with Python**. I hope you enjoyed reading it thus far. And I hope you stay with me in the journey on learning about quantum machine learning.

We have just scratched the very surface of quantum machine learning. We created a simple **Variational Hybrid Quantum-Classical Classification Algorithm**.

But this algorithm is only the beginning. It is among the simplest classifiers we can imagine. Even though we use a **Parameterized Quantum Circuit**, we didn't do anything classical computers can't do.

In the upcoming chapters, we will explore how to create more sophisticated quantum circuits. And we will learn how to use entanglement and interference to reduce the complexity of a problem at hand.

There is a lot to discover in quantum machine learning. And with **Hands-On Quantum Machine Learning With Python**, you will continue discovering it in a practical and easy to follow manner. You'll get all the knowledge you need to implement quantum-based machine learning algorithms.

In this book, we will go far beyond the basics. We will learn how to create state-of-the-art quantum machine learning algorithms.

**Hands-On Quantum Machine Learning With Python** will equip you with all you need to become a "Quantum Machine Learning Engineer" – the job to be-

come the sexiest job of the 2020s.

**Hands-On Quantum Machine Learning With Python** is currently work in process. While I continue working on the book, I'd appreciate your interest and I'll be happy to provide you with the newest insights I gathered.

Don't miss the regular updates on Substack, Medium, and www.pyqml.com.

If you like, please provide me with feedback at mail@pyqml.com.

You can also mail me if you have any other question regarding quantum machine learning in general. I'll strive to reply. Most likely, others will have the same question, so I'll be happy to include the answers in the book once it is ready.

Thank you for reading.