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Essential Math for Data Science

Take Control of Your Data with Fundamental Linear Algebra, Probability, and Statistics

Early Release

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Thomas Nield

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Preface

In the past 10 years or so, there has been a growing interest in applying math and statistics to our everyday work and lives. Why is that? Does it have to do with the accelerated interest in "data science" which Harvard Business Review called "the Sexiest Job of the 21st Century". Or is it the promise of machine learning and "artificial intelligence" changing our lives? Is it because news headlines are inundated with studies, polls, and research findings, but unsure how to scrutinize such claims? Or is it the promise of "self-driving" cars and robots automating jobs in the near future ?

I will make the argument that the disciplines of math and statistics have captured mainstream interest because of the growing availability of data, and we need math, statistics, and machine learning to make sense of it. Yes, we do have scientific tools, machine learning, and other automations that call to us like sirens. We are to blindly trust these "black boxes," devices and softwares we do not understand but we use them anyway.

While it is easy to believe computers are smarter than us (and this idea is frequently marketed), the reality cannot be more the opposite. This disconnect can be precarious on so many levels. Do you really want an "algorithm" or "AI" performing criminal sentencing or driving a vehicle, but nobody including the developer can explain why it came to a specific decision? Explainability is the next frontier of statistical computing and AI. This can only begin when we open up the "black box" and uncover the math.

You may also ask how can a developer not know how their own algorithm works? We will talk about that in the second half of the book when we discuss machine learning techniques, and emphasize why we need to understand the math behind the black boxes we build.

To another point, the reason data is being collected on a massive scale is largely due to connected devices and their presence in our everyday lives. We no longer solely use the internet on a desktop or laptop computer. We now take it with us in our smart phones, cars, and household devices. This has subtly enabled a transition over the past two decades. Data has now evolved from an operational tool to something that is collected and analyzed for less defined objectives. A smartwatch is constantly collecting data on our heart rate, breathing, walking distance, and other markers. Then it uploads that data to a cloud to be analyzed alongside other users. Our driving habits are being collected by computerized cars, and being used by manufacturers to collect data and enable "self-driving" vehicles. Even "smart toothbrushes" are finding their way into drug stores, which track brushing habits and store that data in a cloud. Whether smart toothbrush data is useful and essential is another discussion!

All of this data collection is permeating every corner of our lives. It can be overwhelming, and a whole book can be written on privacy concerns and ethics. But this availability of data also creates opportunities to leverage math and statistics in new ways, and create more exposure outside academic environments. We can learn more about the human experience, improve product design and application, and optimize commercial strategies. If you understand the ideas presented in this book, you will be able to unlock the value held in our data-hording infrastructure. This does not imply that data and statistical tools are a silver bullet to solve all the world's problems, but it has given us new tools that we can use. Sometimes it is just as valuable to recognize certain data projects as rabbit holes, and realize efforts are better spent elsewhere.

This growing availability of data has made way for "data science" and "machine learning" to become demanded professions. We define essential math as an exposure to probability, linear algebra, statistics, and machine learning. If you are seeking a career in data science, machine learning, or engineering, these topics are necessary. I will throw in just enough college math, calculus, and statistics necessary to better understand what goes in the "black box" libraries you will encounter.

With this book, I aim to give readers an exposure to different mathematical, statistical, and machine learning areas that will be applicable to real-world problems. The first four chapters cover foundational math concepts including practical calculus, probability, linear algebra, and statistics. The last three chapters will segue into machine learning. The ultimate purpose of teaching machine learning is to integrate everything we learn, and demonstrate practical insights in using machine learning and statistical libraries beyond a "black box" understanding.

The only tool that is needed to follow examples is a Windows/Mac/Linux computer and a Python 3 environment of your choice. The primary Python libraries we will need are `numpy`, `scipy`, `sympy`, and `sklearn`. If you are unfamiliar with Python, it is a friendly and easy-to-use programming language with massive learning resources behind it. Here are some I recommend:

- *Data Science from Scratch 2nd Edition (O'Reilly)* by Joel Grus - The second chapter of this book has the best crash course in Python I have encountered. Even if you have never written code before, Joel does a fantastic job getting you up and running with Python effectively in the shortest time possible. It is also a great book to have on your shelf and to apply your mathematical knowledge!
- *Python for the Busy Java Developer (Apress)* by Deepak Sarda - If you are a software engineer coming from a statically-typed, object-oriented programming background, this is the book to grab. As someone who started programming with Java, I have a deep appreciation how Deepak shares Python features and relates them to Java developers. If you have done .NET, C++, or other C-like languages you will probably learn Python effectively from this book as well.

This book will not make you an expert or give you PhD knowledge. I do my best to avoid mathematical expressions full of Greek symbols, and instead strive to use plain English in its place. But, what this book will do is

make you more comfortable talking about math and statistics, giving you *essential* knowledge to navigate these areas successfully. I believe the widest path to success is not having deep, specialized knowledge in one topic, but instead having exposure and practical knowledge across several topics. That is the goal of this book, and you will learn just enough to be dangerous and ask those once elusive critical questions.

So let's get started!

Chapter 1. Basic Math and Calculus Review

A NOTE FOR EARLY RELEASE READERS

With Early Release ebooks, you get books in their earliest form—the author's raw and unedited content as they write—so you can take advantage of these technologies long before the official release of these titles.

This will be the 1st chapter of the final book.

If you have comments about how we might improve the content and/or examples in this book, or if you notice missing material within this chapter, please reach out to the author at *thomasnield@live.com*.

We will kick off the first chapter covering what numbers are and how variables and functions work on a Cartesian system. We will then cover exponents and logarithms. After that we will learn the two basic operations of calculus: derivatives and integrals.

Before we dive into the applied areas of essential math such as probability, linear algebra, statistics, and machine learning, we should probably review a few basic math and calculus concepts. Before you drop this book and run screaming, do not worry! I will present how to calculate slopes and areas for a function in a way you were probably not taught in college. We got Python on our side, not a pencil and paper.

I will make these topics as tight and practical as possible, focusing only on what will help us in later chapters and fall under the "essential math" umbrella.

THIS IS NOT A FULL MATH CRASH COURSE!

This is by no means a comprehensive review of high school and college math. If you want that, a great book to check out is *No Bullshit Guide to Math and Physics* by Ivan Savov. The first few chapters contain the best crash course on high school and college math I have ever seen. The book *Mathematics 1001* by Dr. Richard Elwes has some great content as well, and in bite-sized explanations.

Number Theory

What are numbers? I promise to not be too philosophical in this book, but are numbers not a construct we have defined? Why do we have the digits 0 through 9, and not have more digits than that? Why do we have fractions and decimals and not just whole numbers? This area of math where we muse about numbers and why we designed them a certain way is known as number theory.

Number theory goes all the way back to ancient times, where mathematicians study different number systems and why we have accepted them the way we do today. Here are different number systems that you may recognize:

Natural Numbers

> These are the numbers 1, 2, 3, 4, 5… and so on. Only positive numbers are included here, and are the earliest known system. Natural numbers are so ancient cavemen scratched tally marks on bones and cave walls to keep records.

Whole Numbers

> Adding to natural numbers, the concept of "0" was later accepted and we call these "whole numbers." The Babylonians also developed the useful idea for place-holding notation for empty "columns" on numbers greater than 9, such as "10", "1000", or "1090." Those zeros indicate no value occupying that column.

Integers

Integers include positive and negative whole numbers as well as 0. We may take them for granted, but ancient mathematicians were deeply distrusting of the idea of negative numbers. But when you subtract 5 from 3, you get -2. This is useful especially when it comes to finances where we measure profits and losses. In 628 AD, an Indian mathematician named Brahmagupta showed why negative numbers were necessary for arithmetic to progress, and therefore integers became accepted.

Rational Numbers

Any number that you can express as a fraction, such as $\frac{2}{3}$, is a rational number. This includes all finite decimals and integers since they can be expressed as fractions too, such as $\frac{687}{100} = 6.87$ and $\frac{2}{1} = 2$ respectively. They are called *rational* because they are *ratios*. Rational numbers were quickly deemed necessary bececause because time, resources, and other quantities could not always be measured in discrete units. Milk does not always come in gallons. We may have to measure it as parts of a gallon. If I run for 12 minutes, I cannot be forced to measure in whole miles when in actuality I ran $\frac{9}{10}$ of a mile.

Irrational Numbers

Irrational numbers cannot be expressed as a fraction. This includes the famous Pi π, square roots of certain numbers like $\sqrt{2}$, and Euler's number e which we will learn about later. These numbers have an infinite number of decimal digits, such as
$\pi = 3.141592653589793238462...$

There is an interesting history behind irrational numbers. The Greek mathematician Pythagoras believed all numbers are rational. He believed this so fervently, he made a religion that prayed to the number 10. "*Bless us, divine number, thou who generated gods and men!*" he and his followers would pray (why "10" was so special, I do not know).

There is a legend that one of his followers Hippasusus proved not all numbers are rational simply by demonstrating the square root of 2. This severely messed with Pythagoras' belief system, and he responded by drowning Hippasus out at sea.

Regardless, we now know not all numbers are rational.

Real Numbers

Real numbers include rational as well as irrational numbers. In practicality, when you are doing any data science work you can treat any decimals you work with as real numbers.

Complex and Imaginary Numbers

You encounter this number type when you take the square root of a negative number. While imaginary and complex numbers have relevance in certain types of problems, we will mostly steer clear from them for our purposes

In data science, you will find most (if not all) your work will be using natural numbers, integers, and real numbers. Imaginary numbers may be encountered in more advanced use cases such as matrix decomposition, which we will touch on in Chapter 4.

COMPLEX AND IMAGINARY NUMBERS

If you do want to learn about imaginary numbers, there is a great playlist *Imaginary Numbers are Real* on YouTube here: *https://youtu.be/T647CGsuOVU*.

Order of Operations

Hopefully you are familiar with **order of operations** which is the order you solve each part of a mathematical expression. As a brief refresher, recall you evaluate components in parantheses, followed by exponents, then multiplication, division, addition, and subtraction. You can remember the

order of operations by the mnemonic device **PEMDAS** (Please Excuse My Dear Aunt Sally) which corresponds to the ordering paranthesis, exponents, multiplication, division, addition, and subtraction.

Take for example this expression:

$$2*\frac{(3+2)^2}{5}-4$$

First we evaluate the paranetheses $(3+2)$ which evaluates to 5.

$$2*\frac{(\mathbf{5})^2}{5}-4$$

Next we solve the exponent, which we can see is squaring that 5 we just summed. That is 25.

$$2*\frac{\mathbf{25}}{5}-4$$

Next up we have multiplication and division. The ordering of these two is swappable since division is also multiplication (using fractions). Let's go ahead and multiply the 2 with the $\frac{25}{5}$, yielding $\frac{50}{5}$

$$\frac{50}{5}-4$$

Next we will perform the division, dividing 50 by 5 which will yield 10.

$$\mathbf{10}-4$$

And finally we perform any addition and subtraction. Of course, $10-4$ is going to give us 6.

$$10-4=6$$

Sure enough, if we were to express this in Python we would print a value of 6.0 as shown in Example 1-1.

Example 1-1. Solving an expression in Python

```
my_value = 2 * (3 + 2)**2 / 5 - 4

print(my_value) # prints 6.0
```

This may be elementary to you, but it is still criticial nonetheless. In code, even if you get the correct result without them, it is a good practice to liberally use paranthesis in complex expressions so you establish control of the evaluation order.

Here I group up the fractional part of my expression in paranthesis, helping to set it apart from the rest of the expression in Example 1-2.

Example 1-2. Making use of paranthesis for clarity in Python

```
my_value = 2 * ((3 + 2)**2 / 5) - 4

print(my_value) # prints 6.0
```

While both examples are technically correct, the latter one is more clear to us easily confused humans. If you or someone else makes changes to your code, the paranthesis provide an easy reference of operation order as you make changes. This provides a line of defense against code changes to prevent bugs as well.

Variables

If you have done some scripting with Python or another programming language, you have an idea what a variable is. In mathematics, a **variable** is a named placeholder for an unspecified or unknown number.

You may have a variable *x* representing any real number, and you can multiply that variable without declaring what it is. In Example 1-3 we take a variable input *x* from a user, and multiply it by 3.

Example 1-3. A variable in Python that is then multiplied

```
x = int(input("Please input a number\n"))

product = 3 * x
```

```
print(product)
```

There are some standard variable names for certain variable types. If these variable names and concepts are unfamiliar, no worries! But the rest of you readers might recognize we use theta θ to denote angles and beta β for a parameter in a linear regression. Greek symbols make awkward variable names in Python, so we would likely name these variables `theta` and `beta` in Python as shown in Example 1-4.

Example 1-4. Greek variable names in Python

```
beta = 1.75
theta = 30.0
```

Note also that variable names can be subscripted so that several instances of a variable name can be used. For practical purposes, just treat these as separate variables. If you encounter variables x_1, x_2, and x_3, just treat them as three separate variables as shown in Example 1-5.

Example 1-5. Expressing subscripted variables in Python

```
x1 = 3  # or x_1 = 3
x2 = 10 # or x_2 = 10
x3 = 44 # or x_3 = 44
```

Functions

Functions are expressions that define relationships between two or more variables. More specifically, a function takes **input variables** (also called **domain variables** or **independent variables**), plugs them into an expression, and then results in an **output variable** (also called **dependent variable**).

Take this simple linear function $y = 2x + 1$. For any given x value, we solve the expression with that x to find y. When x = 1, then y = 3. When x = 2, y = 5. When x = 3, y = 7 and so on as shown in Table 1-1.

$$y = 2x + 1$$

Table 1-1. Different values for y = 2x + 1

x	2x + 1	y
0	2(0) + 1	1
1	2(1) + 1	3
2	2(2) + 1	5
3	2(3) + 1	7

Functions are useful because they help predict the relationship between variables, such as how many fires y can we expect at x temperature. We will use linear functions to perform linear regressions in Chapter 5.

Another convention you may see for the dependent variable y is to explicitly label it a function of x, such as $f(x)$. So rather than express a function as $y = 2x + 1$ we can also express it as:

$$f(x) = 2x + 1$$

Example 1-6 shows how we can declare a mathematical function and iterate it in Python.

Example 1-6. Declaring a linear function in Python

```
def f(x):
    return 2 * x + 1


x_values = [0, 1, 2, 3]

for x in x_values:
    y = f(x)
    print(y)
```

When dealing with real numbers, a subtle but important feature of functions is they often have an infinite number of x values and resulting y values. Ask yourself this: how many x values can we put through the function

$y = 2x + 1$? Rather than just 0, 1, 2, 3… why not 0, .5, 1, 1.5, 2, 2.5, 3 as shown in Table 1-2 below?

Table 1-2. Different values for y = 2x + 1

x	2x + 1	y
0.0	2(0) + 1	1
0.5	2(.5) + 1	2
1.0	2(1) + 1	3
1.5	2(1.5) + 1	4
2.0	2(2) + 1	5
2.5	2(2.5) + 1	6
3.0	2(3) + 1	7

Or why not do quarter steps for x? $\frac{1}{10}$ of a step? We can make these steps infinitely small effectively showing $y = 2x + 1$ is a **continuous function**, where for every possible value of x there is a value for y. This segues us nicely to visualize our function as a line as shown in Figure 1-1.

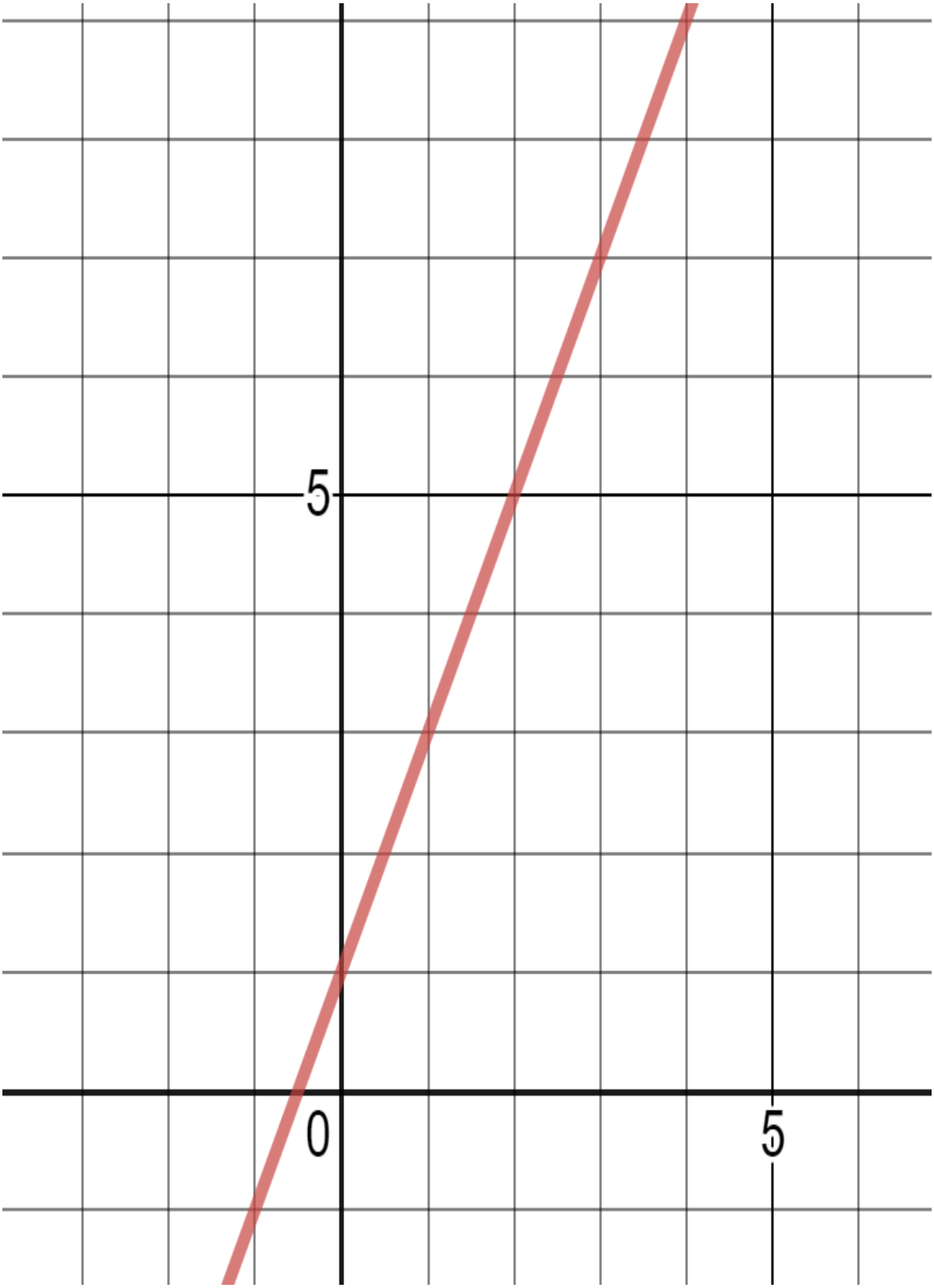


Figure 1-1. Graph for function y = 2x + 1

When we plot on a two-dimensional plane with two number lines (one for each variable) it is known as a **Cartesian plane**, **x-y plane**, or **coordinate plane**. We trace a given *x* value and then look up the corresponding *y* value, and plot the intersections as a line. Notice that due to the nature of real numbers (or decimals, if you prefer), there are an infinite number of *x* values. This is why when we plot the function `f(x)` we get a continuous line with no breaks in it. There are an infinite number of points on that line, or any part of that line.

If you want to plot this using Python, there are a number of charting libraries from Plotly to matplotlib. However, SymPy gives us a quick, clean way to plot a function. It uses matplotlib so make sure you have that package installed, otherwise it will print an ugly text-based graph to your console. After that, just declare the *x* variable to SymPy using `symbols()`, declare your function, and then plot it as shown in Example 1-7 and Figure 1-2.

Example 1-7. Charting a linear function in Python using SymPy

```
from sympy import *

x = symbols('x')
f = 2*x + 1
plot(f)
```

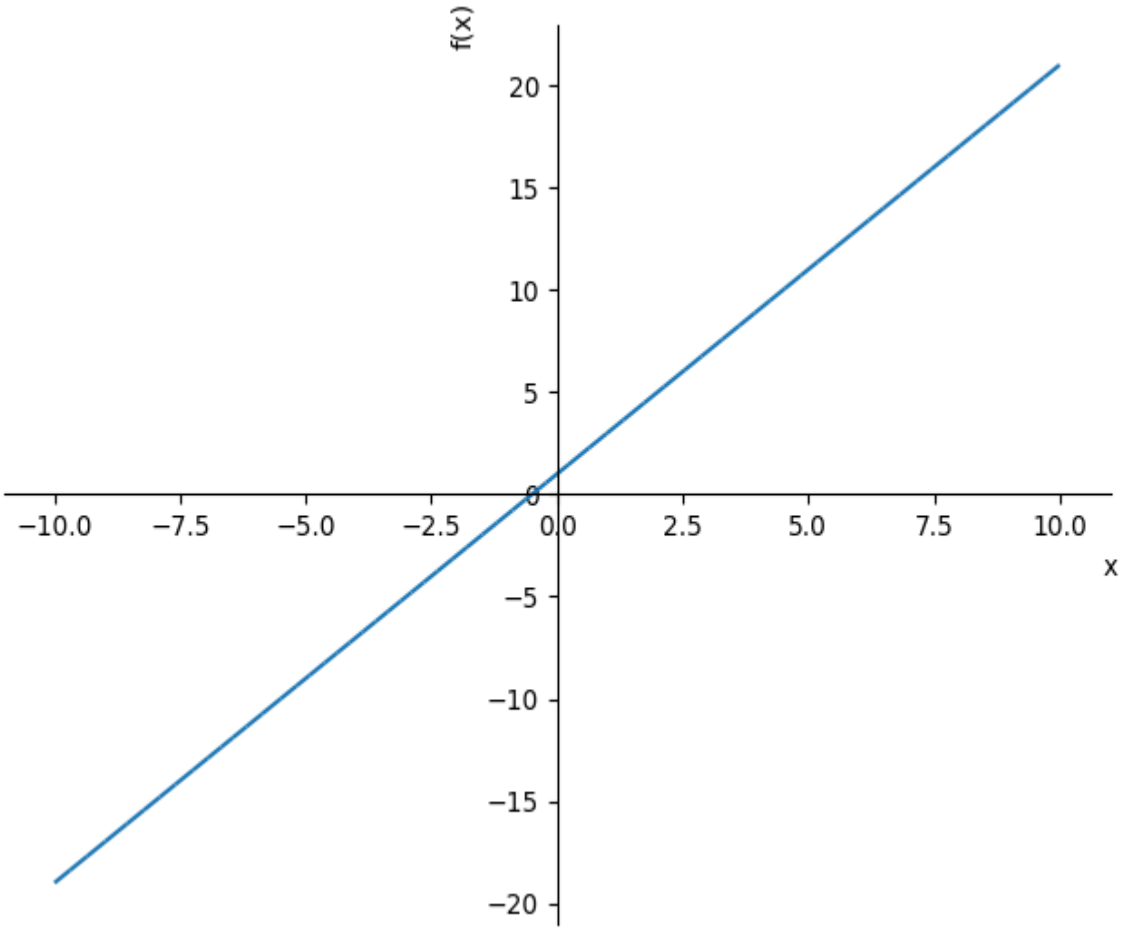


Figure 1-2. Using SymPy to graph a linear function

Example 1-8 and Figure 1-3 are another example showing the function $y = x^2 + 1$.

Example 1-8. Charting a linear function in Python using SymPy

```
from sympy import *

x = symbols('x')
f = x**2 + 1
plot(f)
```

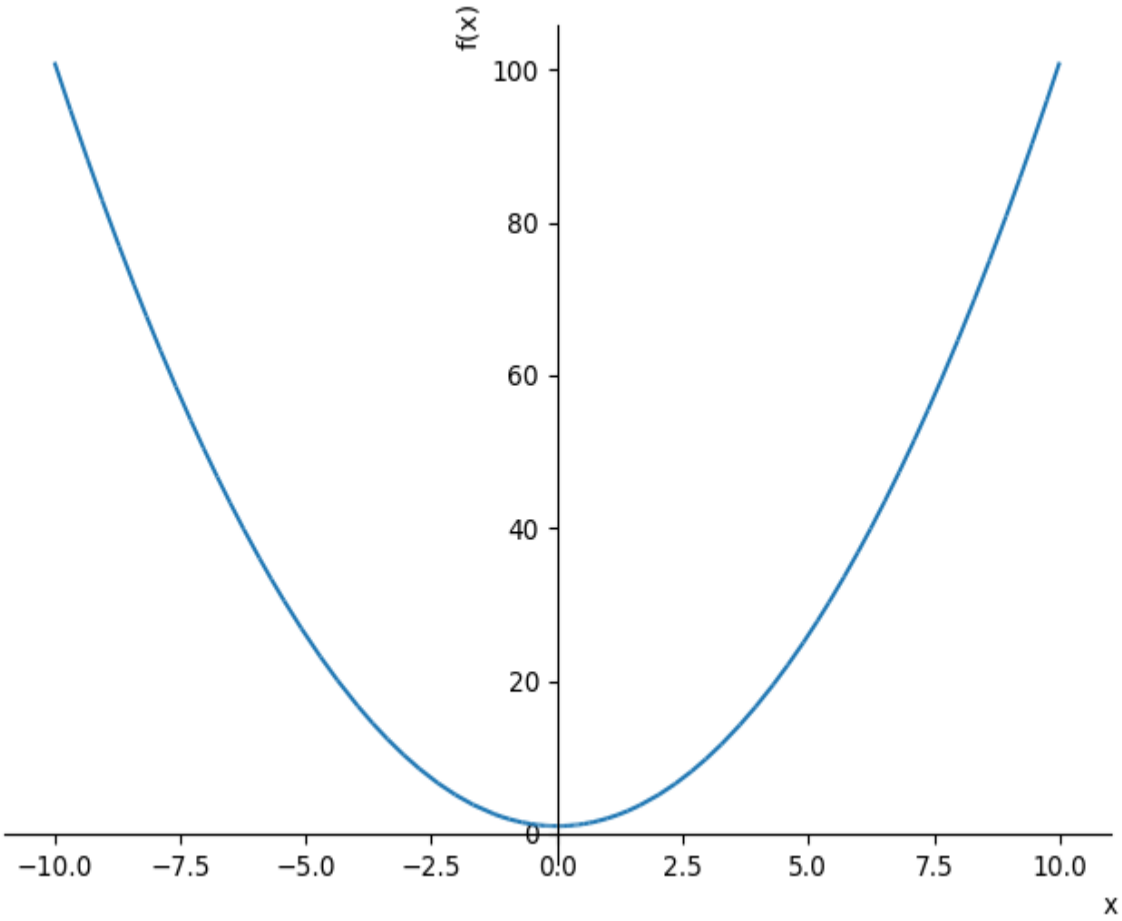


Figure 1-3. Using SymPy to graph an exponential function

Notice in Figure 1-3 we do not get a straight line but rather a smooth, symmetrical curve known as a parabola. It is continuous but not linear, as it does not produce values in a straight line. Curvy functions like this are mathematically harder to work with, but we will learn some tricks to make it not so bad.

CURVILINEAR FUNCTIONS

When a function is continuous but curvy, rather than linear and straight, we call it a *curvilinear function*.

Note that functions can utilize multiple input variables and not just one. For example, we can have a function with independent variables x and y. Note

that y is not dependent like in previous examples.

$$f(x, y) = 2x + 3y$$

Since we have 2 independent variables (x and y) and 1 dependent variable (the output of `f(x,y)`) we need to plot this graph on 3 dimensions to produce a plane of values rather than a line as shown in Example 1-9 and Figure 1-4.

Example 1-9. Declaring a function with 2 independent variables in Python:

```
from sympy import *
from sympy.plotting import plot3d

x, y = symbols('x y')
f = 2*x + 3*y
plot3d(f)
```

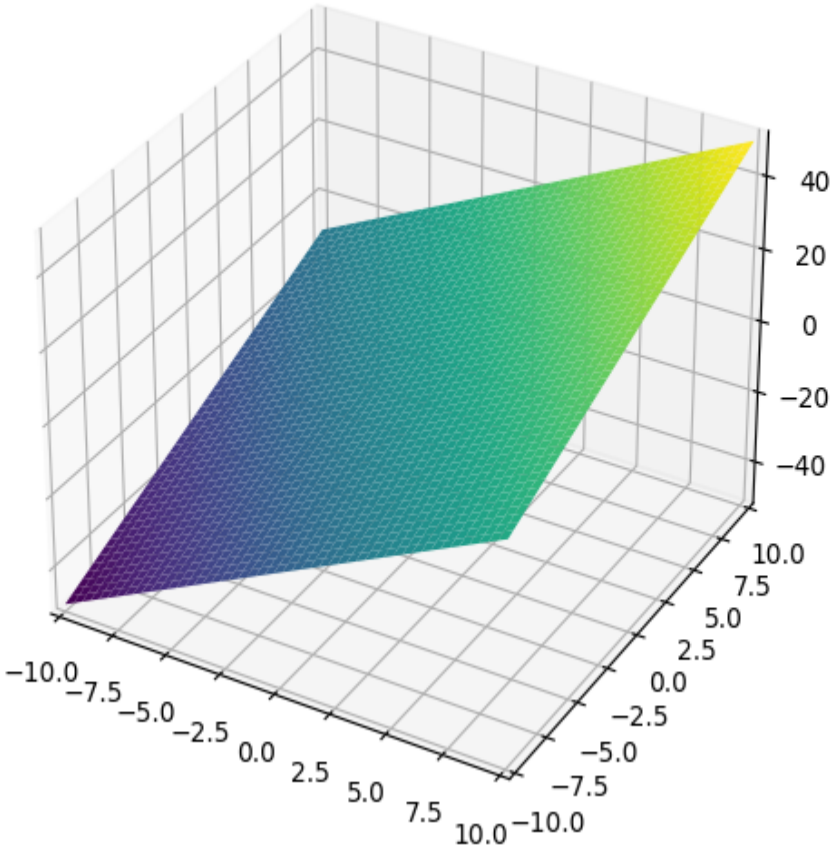


Figure 1-4. Using SymPy to graph a 3-dimensional function

No matter how many independent variables you have, your function will typically only output one dependent variable. When you solve for multiple dependent variables, you will likely be using separate functions for each one.

Summations

I promised not to use equations full of Greek symbols in this book. However, there is one that is so common and useful that it would be remiss to not cover it. A **summation** is expressed as a sigma Σ and adds elements together.

For example, if I wanted to iterate the numbers 1 through 5, multiply each by 2, and sum them here is how I would express that using a summation. Example 1-10 shows how to execute this in Python.

$$\sum_{i=1}^{5} 2i$$

$$= (2)1 + (2)2 + (2)3 + (2)4 + (2)5 = 30$$

Example 1-10. Performing a summation in Python

```
summation = sum(2*i for i in range(1,6))
print(summation)
```

Note that *i* is a placeholder variable representing each consecutive index value we are iterating in the loop, which we multiply by 2 and then sum all together. When you are iterating data, you may see variables like x_i indicating an element in a collection at index *i*.

THE RANGE() FUNCTION

Recall that the `range()` function in Python is end exclusive, meaning if you invoke `range(1,4)` it will iterate the numbers 1, 2, and 3. It excludes the 4 as an upper boundary.

It is also common to see n represent the number of items in a collection, like the number of records in a dataset. Here is one such example where we iterate a collection of numbers of size n, multiply each one by 10, and sum them.

$$\sum_{i=1}^{n} 10x_i$$

In Example 1-11 we use Python we execute this expression on a collection of 4 numbers. Note that in Python (and most programming languages in general) we typically reference items starting at index 0, while in math we start at index 1. Therefore we shift accordingly in our iteration by starting at 0 in our `range()`.

Example 1-11. Summation of elements in Python

```
x = [1, 4, 6, 2]
n = len(x)

summation = sum(10*x[i] for i in range(0,n))
print(summation)
```

That is the gist of summation. In a nutshell, a summation Σ says "add a bunch of things together" and uses an index i and a maximum value n to express each iteration feeding into the sum. We will see them in almost every other chapter in this book.

SUMMATIONS IN SYMPY

Later in this chapter we will earn about SymPy, a symbolic math library. Here's a sidebar for reference. A summation operation in SymPy is performed using the `Sum()` operator. Below in Example 1-12 we iterate *i* from 1 through *n*, multiply each *i*, and sum them. But then we use the `subs()` function to specify *n* as 5, which will then iterate and sum all *i* elements from `1` through *n*.

Example 1-12.

```
from sympy import *

i,n = symbols('i n')

# iterate each element i from 1 to n,
# then multiply and sum
summation = Sum(2*i,(i,1,n))

# specify n as 5,
# iterating the numbers 1 through 5
up_to_5 = summation.subs(n, 5)
print(up_to_5.doit()) # 30
```

Note that summations in SymPy are lazy, meaning they do not automatically calculate or get simplified. So use the `doit()` function to execute the expression.

Exponents

Exponents multiplies a number by itself a specified number of times. When you raise 2 to the 3rd power (expressed as 2^3 using `3` as a superscript), that is multiplying three 2's together:

$$2^3 = 2*2*2 = 8$$

The **base** is the variable or value we are exponentiating, and the **exponent** is the number of times we multiply the base value. For the expression 2^3, 2 is the base and 3 is the exponent.

Exponents have a few interesting properties. Say we multiplied x^2 and x^3 together. Observe what happens below when I expand the exponents with simple multiplication, and then consolidate into a single exponent:

$$x^2x^3 = (x*x)*(x*x*x) = x^{2+3} = x^5$$

When we multiply exponents together with the same base, we simply add the exponents which is known as the **product rule**. Note that the base of all multiplied exponents must be the same for the product rule to apply.

Let's explore division next. What happens when we divide x^2 by x^5 ?

$$\frac{x^2}{x^5}$$

$$\frac{x*x}{x*x*x*x*x}$$

$$\frac{1}{x*x*x}$$

$$\frac{1}{x^3} = x^{-3}$$

As you can see above, when we divide x^2 by x^5 we can cancel out two *x*'s in numerator and denominator, leaving us with $\frac{1}{x^3}$. Without tangenting into algebra rules too much, here is what happens. When a factor exists in both the numerator and denominator, we can cancel out that factor.

This is a good point to introduce negative exponents, which is another way of expressing an exponent operation in the denominator of a fraction. To demonstrate, $\frac{1}{x^3}$ is the same as x^{-3}.

$$\frac{1}{x^3} = x^{-3}$$

Tying back the product rule, we can see it applies to negative exponents too. To get intuition behind this, let's approach this problem a different way. We

can express this division of two exponents by making the "5" exponent of x^5 negative, and then multiplying it with x^2. When you add a negative number, it is effectively performing subtraction. Therefore, the exponent product rule summing the multiplied exponenents still holds up as shown below:

$$\frac{x^2}{x^5}x^2\frac{1}{x^5} = x^2x^{-5} = x^{2+-5} = x^{-3}$$

SIMPLIFY EXPRESSIONS WITH SYMPY

If you get uncomfortable with simplifying algebraic expressions, you can use the SymPy library to do the work for you. Example 1-13 shows how to simplify our previous example.

Example 1-13.

```
from sympy import *

x = symbols('x')
expr = x**2 / x**5
print(expr) # x**(-3)
```

Now what about fractional exponents? They are just an alternative way to represent roots, such as the square root. As a brief refresher, a square root of 4 asks "what number multiplied by itself will give me 4?", which of course is 2. Note here that $4^{1/2}$ is the same as $\sqrt{4}$.

$$4^{1/2} = \sqrt{4} = 2$$

Cubed roots are similar to square roots, but they seek a number multiplied by itself 3 times to give a result. A cubed root of 8 is expressed as $\sqrt[3]{8}$, and asks "what number multiplied by itself 3 times gives me 8"? This number would be 2 because 2*2*2 = 8. In exponents, a cubed root is expressed as a fractional exponent, and $\sqrt[3]{8}$ can be re-expressed as $8^{1/3}$.

$$8^{1/3} = \sqrt[3]{8} = 2$$

To bring it back full circle, what happens when you multiply the cubed root of 8 three times? This will undo the cubed root and yield us 8. Alternatively, if we express the cubed root as fractional exponenents $8^{1/3}$, it becomes clear we add the exponents together to get an exponent of 1. That also undoes the cubed root.

$$\sqrt[3]{8} * \sqrt[3]{8} * \sqrt[3]{8} = 8^{\frac{1}{3}} \times 8^{\frac{1}{3}} * 8^{\frac{1}{3}} = 8^{\frac{1}{3}+\frac{1}{3}+\frac{1}{3}} = 8^1 = 8$$

And one last property: with an exponent of an exponent, that would multiply the exponents together. This is known as the **power rule**. So $\left(8^3\right)^2$ would simplify to 8^6.

$$\left(8^3\right)^2 = 8^{3*2} = 8^6$$

If you are skeptical why this is, try expanding it and you will see the sum rule makes it clear:

$$\left(8^3\right)^2 = 8^3 8^3 = 8^{3+3} = 8^6$$

Lastly, what does it mean when we have a fractional exponent with a numerator other than 1, such as $8^{\frac{2}{3}}$? Well that is taking the cube root of 8 and then squaring it. Take a look below:

$$8^{\frac{2}{3}} = \left(8^{\frac{1}{3}}\right)^2 = 2^2 = 4$$

And yes, irrational numbers can serve as exponents like 8^{π} which is 687.2913. This may feel unintuitive, and understandably so! In the interest of time we will not dive deep into this as it requires some Calculus. But essentially, we can calculate irrational exponents by approximating with a rational number. This is effectively what computers do since they can only compute to so many decimal places anyway.

For example Pi π has an infinite number of decimal places. But if we take the first 11 digits, 3.1415926535, we can approximate Pi as a rational

number `31415926535 / 10000000000`. Sure enough, this gives us approximately 687.2913 which should approximately match any calculator.

$$8^{\pi} \approx 8^{\frac{31415926535}{10000000000}} \approx 687.2913$$

Logarithms

A **logarithm** is a math function that finds a power for a specific number and base. It may not sound interesting at first, but it actually has many applications. From measuring earthquakes to managing volume on your stereo, the logarithm is found everywhere. It also finds its way into machine learning and data science a lot. As a matter of fact, logarithms will be a key part of logistic regressions in Chapter 6.

Start your thinking by asking "2 raised to *what power* gives me 8?" One way to express this mathematically is to use an x for the exponent:

$$2^x = 8$$

We intuitively know the answer, $x = 3$, but we need a more elegant way to express this common math operation. This is what the $log()$ function is for.

$$log_2 8 = x$$

As you can see in the logarithm expression above, we have a base 2 and are finding a power to give us 8. More generally, we can re-express a variable exponent as a logarithm:

$$a^x = b$$

$$log_a b = x$$

Algebraically speaking, this is a way of isolating the x which is important to solve for x.

Example 1-14 shows how we calculate this logarithm in Python.

Example 1-14. Using the log function in Python:

```
from math import log

# 2 raised to what power gives me 8?
x = log(8, 2)

print(x) # prints 3.0
```

When you do not supply a base argument to a `log()` function on a platform like Python, it will typically have a default base. In some fields, like earthquake measurements, the default base for the log is 10, but in data science, the default base for the log is Euler's number *e*. Python uses the latter and we will talk about *e* shortly.

Just like exponents, logarithms have several properties when it comes to multiplication, division, exponentiation, and so on. In the interest of time and focus, I will just present this table below in Table 1-3. The key idea to focus on is a logarithm finds an exponent for a given base to result in a certain number.

If you need need to dive into logarithmic properties, Table 1-3 displays exponent and logarithm behaviors side-by-side you can use for reference.

Table 1-3. Properties for Exponents and

L
o
g
a
r
i
t
h
m
s

Operator	Exponent Property	Logarithm Property
Multiplication	$x^m * x^n = x^{m+n}$	$log(a*b) = log(a) + log(b)$
Division	$\frac{x^m}{x^n} = x^{m-n}$	$log\left(\frac{a}{b}\right) = log\left(a\right) - log\left(b\right)$
Exponentiation	$\left(x^m\right)^n = x^{mn}$	$log\left(a^n\right) = n*log\left(a\right)$
Zero Exponent	$x^0 = 1$	$log(1) = 0$
Inverse	$x^{-1} = \frac{1}{x}$	$log\left(x^{-1}\right) = log(\frac{1}{x} = -log\left(x\right)$

Euler's Number and Natural Logarithms

There is a special number that shows up quite a bit in math called Euler's number *e*. It is a special number much like Pi π, and is approximately 2.71828. *e* is used a lot because it mathematically simplifies a lot of problems.

Back in high school, my Calculus teacher demonstrated Euler's number in several exponential problems. Finally I asked "Mr. Nowe, what is *e* anyway? Where does it come from?" I remember never being fully satisfied with the explanations involving rabbit populations and other natural phenomena. I hope to give a more satisfying explanation here.

WHY EULER'S NUMBER IS USED SO MUCH

Another property of Euler's number is its exponential function is a derivative to itself, which is convenient for exponential and logarithmic functions. We will learn about derivatives later in this chapter. In many applications where the base does not really matter, we pick the one that results in the simplest derivative, and that is Euler's number. That is also why it is the default base in many data science functions.

Here is how I like to discover Euler's number. Let's say you loan $100 to somebody with 20% interest annually. Typically interest will be compounded monthly, so the interest each month would be $.20/12 = .01666$. How much will the loan balance be after two years? To keep it simple, let's assume the loan does not require payments (and no payments are made) until the end of those two years.

Putting together the exponent concepts we learned so far (or perhaps pulling it out a finance textbook), we can come up with a formula to calculate interest. It consists of a balance *A* for a starting investment *P*, interest rate *r*, time span *t* (number of years), and periods *n* (number of months in each year). Here it is as follows:

$$A = P \times \left(1 + \frac{r}{n}\right)^{nt}$$

So if we were to compound interest every month, the loan would grow to $148.69 as calculated below:

$$A = P^{*}\left(1 + \frac{r}{n}\right)^{nt}$$

$$100^{*}\left(1 + \frac{.20}{12}\right)^{12^{*}2} = 148.6914618$$

If you want to do this in Python, try it out with the code in Example 1-15.

Example 1-15. Calculating compound interest in Python

```
from math import exp

p = 100
r = .20
t = 2.0
n = 12

a = p * (1 + (r/n))**(n * t)

print(a) # prints 148.69146179463576
```

But what if we compounded interest daily? What happens then? Change *n* to 365.

$$A = P^*\left(1 + \frac{r}{n}\right)^{nt}$$

$$100^*\left(1 + \frac{.20}{365}\right)^{365^*2} = 149.1661279$$

Huh! If we compound our interest daily instead of monthly, we would earn 47.4666 cents more at the end of two years. If we got greedy why not compound every hour as shown below? Will that give us even more? There are 8760 hours in a year, so set *n* to that value:

$$A = P^*\left(1 + \frac{r}{n}\right)^{nt}$$

$$100^*\left(1 + \frac{.20}{8760}\right)^{8760^*2} = 149.1817886$$

Ah, we squeezed out roughly 2 cents more in interest! But are we experiencing a diminishing return? Let's try to compound every minute! Note that there are 525,600 minutes in a year, so let's set that value to *n*:

$$A = P^*\left(1 + \frac{r}{n}\right)^{nt}$$

$$100*\left(1+\frac{.20}{525600}\right)^{525600*2}=149.1824584$$

Okay we are only gaining smaller and smaller fractions of a cent the more frequently we compound. So if I keep making these periods infinitely smaller to the point of compounding continuously, where does this lead to?

Let me introduce you to Euler's number *e*, which is approximately 2.71828. Here is the formula to compound "continuously," meaning we are compounding nonstop:

$$A=P*e^{rt}$$

Returning to our example, let's calculate the balance of our loan after 2 years if we compounded continuously:

$$A=P*e^{rt}$$

$$A=100*e^{.20*2}=149.1824698$$

Okay this is not too surpising considering compounding every minute got us a balance of 149.1824584. That got us really close to our value of 149.1824698 when compounding continuously.

Typically you use *e* as an exponent base in Python, Excel, and other platforms using the `exp()` function. You will find that *e* is so commonly used, it is the default base for both exponent and logarithm functions.

Example 1-16 calculates continuous interest in Python using the `exp()` function.

Example 1-16. Calculating continuous interest in Python

```
from math import exp

p = 100 # principal, starting amount
r = .20 # interest rate, by year
t = 2.0 # time, number of years

a = p * exp(r*t)
```

```
print(a) # prints 149.18246976412703
```

So where do we derive this constant *e*? Compare the compounding interest formula and the continuous interest formula. They structurally look similar, but with some differences:

$$A = P^*\left(1 + \frac{r}{n}\right)^{nt}$$

$$A = P^*e^{rt}$$

More technically speaking, *e* is the resulting value of the expression $\left(1 + \frac{1}{n}\right)^n$ as *n* forever gets bigger and bigger, thus approaching infinity. Try experimenting with increasingly large values for *n*. By making it larger and larger you will notice something:

$$\left(1 + \frac{1}{n}\right)^n$$

$$\left(1 + \frac{1}{100}\right)^{100} = 2.70481382942$$

$$\left(1 + \frac{1}{1000}\right)^{1000} = 2.71692393224$$

$$\left(1 + \frac{1}{10000}\right)^{10000} = 2.71814592682$$

$$\left(1 + \frac{1}{10000000}\right)^{10000000} = 2.71828169413$$

As you make *n* larger, there is a diminishing return and it converges approximately on the value 2.71828, which is our value *e*. You will find this number *e* used not just in studying populations and their growth. It plays a key role in many areas of mathematics.

Later in the book, we will use it to build normal distributions in Chapter 3 and logistic regressions in Chapter 6.

Natural Logarithms

When we use e as our base for a logarithm, we call it a **natural logarithm**. Depending on the platform, we may use `ln()` instead of `log()` to specify a natural logarithm. So rather than express a natural logarithm expressed as $log_e 10$ to find the power raised on e to get 10, we would shorthand it as $ln(10)$.

$$log_e 10 = ln\,(10)$$

However in Python, a natural logarithm is specified by the `log()` function. As said earlier, the default base for the `log()` function is e. Just leave the second argument for the base empty and it will default to using e as the base shown in Example 1-17.

Example 1-17. Calculating natural logarithm of 10 in Python

```
from math import log

# e raised to what power gives us 10?
x = log(10)

print(x) # prints 2.302585092994046
```

We will use e in a number of places throughout this book. Feel free to experiment with exponents and logarithms for awhile using Excel, Python, Desmos.com, or any other calculation platform of your choice. Make graphs and get comfortable with functions!

Limits

As we have seen with Euler's number, some interesting ideas emerge when we forever increase or decrease an input variable and the output variable keeps approaching a value but never reaching it. Let's formally explore this idea.

Take this function which is plotted in Figure 1-5:

$$f(x) = \frac{1}{x}$$

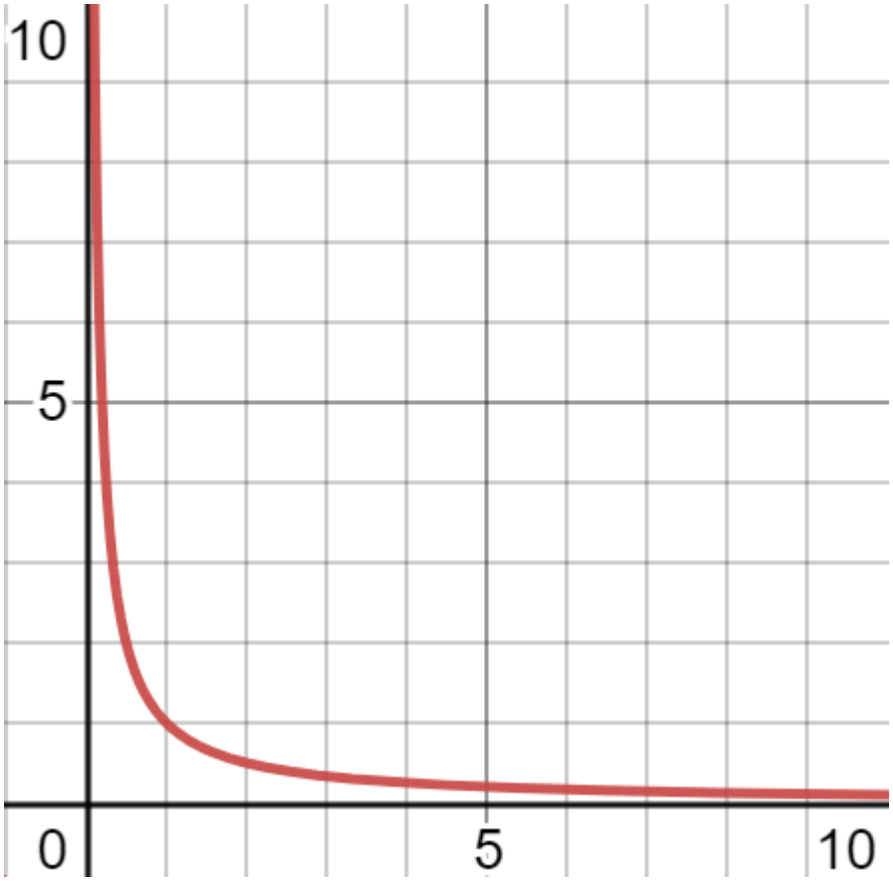


Figure 1-5. A function that forever approaches 0 in either direction but never reaches 0

We are only looking at positive *x* values. Notice that as *x* forever increases *f(x)* gets closer to 0. Fascinatingly, *f(x)* never actually reaches 0. It just forever keeps getting closer.

Therefore, the fate of this function is as x forever extends into infinity, it will keep getting closer to 0 but never reach 0. The way we express a value that is forever being approached, but never reached, is through a limit.

$$\lim_{x \to \infty} \frac{1}{x} = 0$$

The way we read this is “as x approaches infinity, the function 1/x approaches 0 (but never reaches 0).” You will see this kind of “approach but never touch” behavior a lot especially when we dive into derivatives and integrals.

Using SymPy, we can calculate what value we approach for $f(x) = \frac{1}{x}$ as x approaches infinity ∞.

Example 1-18. Using SymPy to calculate limits

```
from sympy import *

x = symbols('x')
f = 1 / x
result = limit(f, x, oo)

print(result) # 0
```

As you have seen, we discovered Euler’s number *e* this way too. It is the result of forever extending *n* into infinity for this function.

$$\lim_{n \to \infty} \left(1 + \frac{1}{n}\right)^n = e = 2.71828169413\ldots$$

Funny enough, when we calculate Euler’s number with limits in SymPy (shown in Example 1-19), SymPy immediately recognizes it as Euler’s Number. We can call `evalf()` so we can actually display it as a number.

Example 1-19.

```
from sympy import *

n = symbols('n')
f = (1 + (1/n))**n
result = limit(f, n, oo)

print(result) # E
print(result.evalf()) # 2.71828182845905
```

THE POWER OF SYMPY

SymPy is a powerful and fantastic computer algebra system (CAS) for Python that uses exact symbolic computation rather than approximate computation using decimals. It's helpful for those situations you would use "pencil and paper" to solve math and Calculus problems, with the benefit of using familiar Python syntax. Rather than represent the square root of 2 by approximating `1.4142135623730951`, it will preserve it as exactly $sqrt(2)$.

So why not use SymPy for everything math-related? While we will use it throughout this book, it is important to still be comfortable doing Python math with plain decimals, as SciKit-Learn and other data science libraries take this approach. It is much faster for computers to use decimals rather than symbols. But keep SymPy in your back pocket as your advantage, and do not tell your high school and college-age kids about it. They can literally use it to do their math homework.

https://docs.sympy.org/latest/tutorial/intro.html

Derivatives

Let's go back to talking about functions and look at them from a Calculus perspective, starting with derivatives. A **derivative** tells the slope of a function, and it is useful to measure the rate of change at any point in a function.

Why do we care about derivatives? They are often used in machine learning and other mathematical algorithms, especially with gradient descent. When the slope is 0, that means we are at the minimum or maximum of an output variable. This concept will be useful later when we do linear regression, logistic regression, and neural networks.

But let's start with a simple example. A derivative provides the slope at that given x value. Let's take a look at the function $f(x) = x^2$ in Figure 1-6.

How “steep” is the curve at $x = 2$?

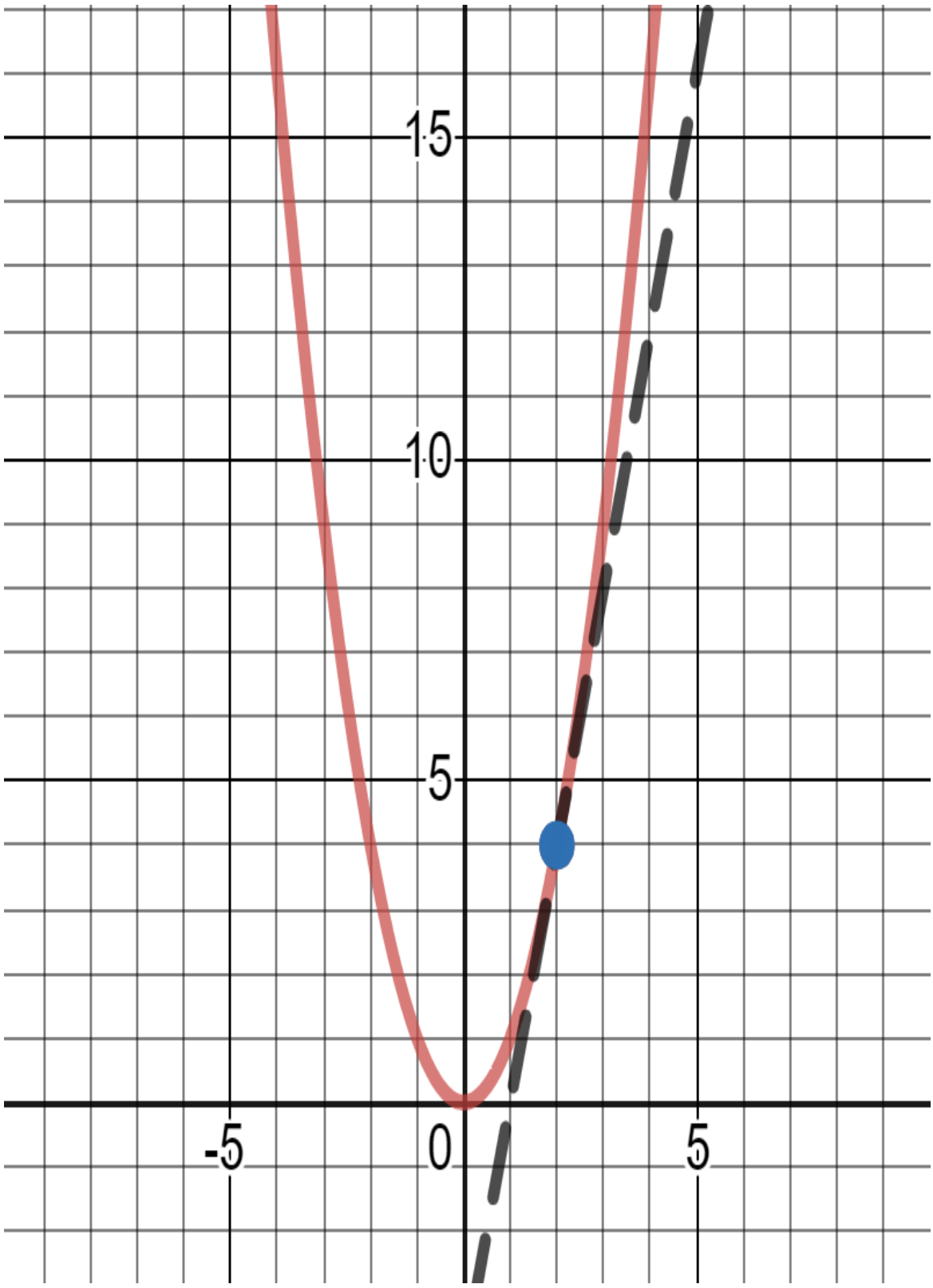


Figure 1-6. Observing steepness at a given part of the function

Notice above we can measure "steepness" at any point in the curve, and we can visualize this with a tangent line. Think of a **tangent line** as a straight line that "just touches" the curve at a given point. It also provides the slope at a given point. You can crudely estimate a tangent line at a given *x* value by creating a line intersecting that *x* value and a *really close* neighboring *x* value on the function.

Take $x = 2$ and a nearby value $x = 2.1$, which when passed to the function $f(x) = x^2$ will yield $f(2) = 4$ and $f(2.1) = 4.41$ as shown in Figure 1-7. The resulting line that passes through these two points has a slope of 4.41.

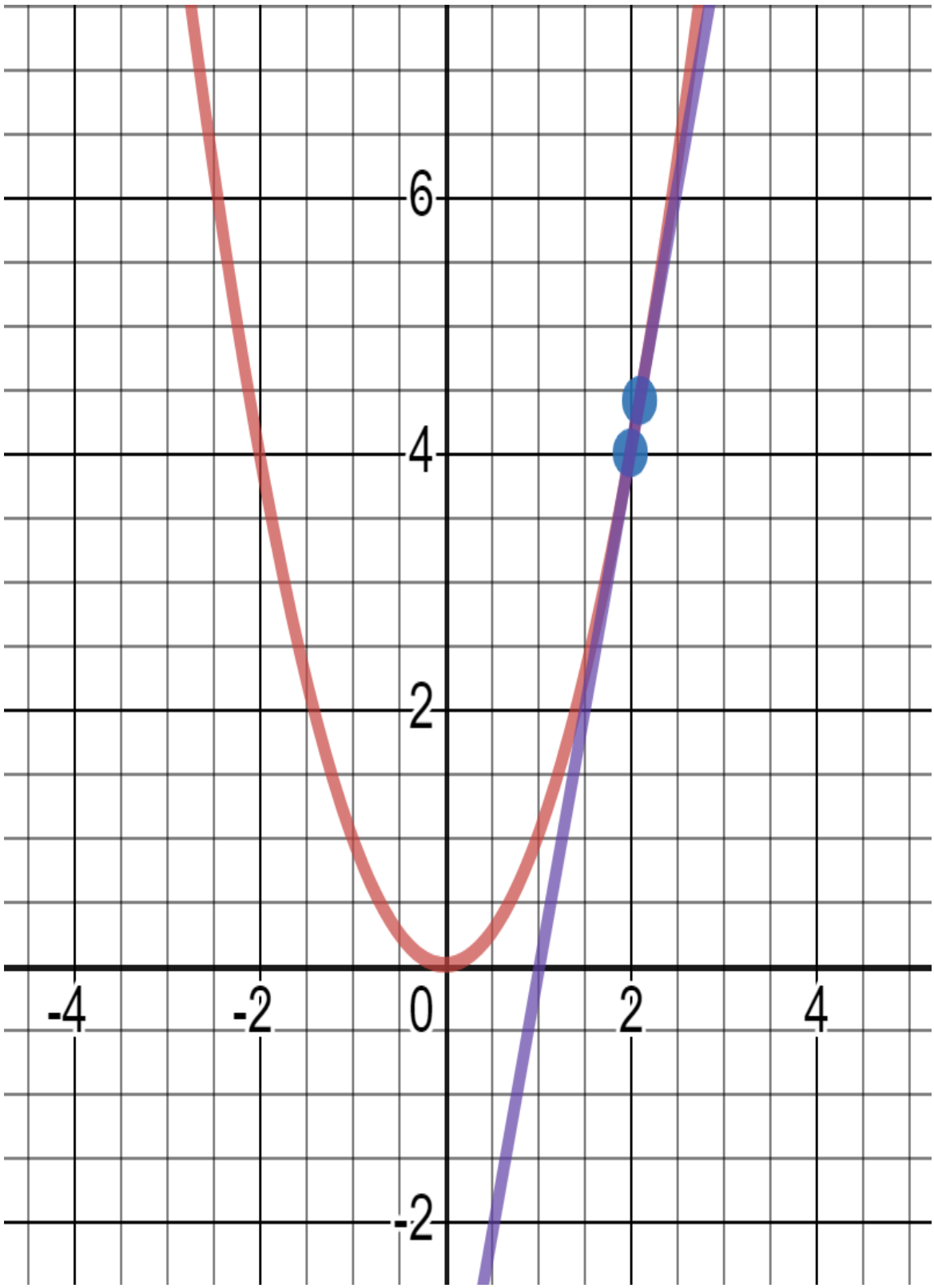


Figure 1-7. A crude way of calculating slope

You can quickly calculate the slope m between two points using the simple rise-over-run formula:

$$m = \frac{y_2 - y_1}{x_2 - x_1}$$

$$m = \frac{4.41 - 4.0}{2.1 - 2.0}$$

$$m = 4.41$$

If I made the *x* step between the two points even smaller, like *x = 2* and *x = 2.00001* which would result in *f(2) = 4* and *f(2.00001) = 4.00004*, that would get *really* close to the actual slope of 4. So the smaller our step is to the neighboring value, the closer we get to the slope value at a given point in the curve. Like so many important concepts in math, we find something meaningful as we approach infinitely large or infinitely small values.

Example 1-20 shows a derivative calculator implemented in Python.

Example 1-20. A derivative calculator in Python

```
def derivative_x(f, x, step_size):
    m = (f(x + step_size) - f(x)) / ((x + step_size) - x)
    return m


def my_function(x):
    return x**2

slope_at_2 = derivative_x(my_function, 2, .00001)

print(slope_at_2) # prints 4.000010000000827
```

Now the good news is there is a cleaner way to calculate the slope anywhere on a function. We have already been using SymPy to plot graphs, but I will show you how it can also do tasks like derivatives for you using the magic of symbolic computation.

When you encounter an exponential function like $f(x) = x^2$ the derivative function will make the exponent a multiplier and then decrement the exponent by 1, leaving us with the derivative $\frac{d}{dx}x^2 = 2x$. The $\frac{d}{dx}$ indicates

a *derivative with respect to x*, which says we are building a derivative targeting the *x* value to get its slope. So if we want to find the slope at `x = 2`, and we have the derivative function, we just plug in that *x* value to get the slope.

$$f(x) = x^2$$

$$\frac{d}{dx} f(x) = \frac{d}{dx} x^2 = 2x$$

$$\frac{d}{dx} f(2) = 2(2) = 4$$

If you intend on learning these rules to hand-calculate derivatives, there are plenty of Calculus books for that. But there are some nice tools to calculate derivatives symbolically for you. The Python library SymPy is free and open-source, and it nicely adapts to using the Python syntax. Example 1-21 shows how we calculate the derivative for $f(x) = x^2$ on SymPy.

Example 1-21. Calculating a derivative in SymPy

```
from sympy import *

# Declare 'x' to SymPy
x = symbols('x')

# Now just use Python syntax to declare function
f = x**2

# Calculate the derivative of the function
dx_f = diff(f)
print(dx_f) # prints 2*x
```

Wow! So by declaring variables using the `symbols()` function in SymPy, I can then proceed to use normal Python syntax to declare my function. After that I can use `diff()` to calculate the derivative function for me. In Example 1-22 can then take our derivative function back to plain Python and simply declare it as another function.

Example 1-22. A derivative calculator in Python

```
def f(x):
    return x**2

def dx_f(x):
    return 2*x

slope_at_2 = dx_f(2.0)

print(slope_at_2) # prints 4.0
```

If you wanted to keep using SymPy, you can call the `subs()` function to swap the *x* variable with the value `2` as shown in Example 1-23.

Example 1-23. Using the substitution feature in SymPy

```
# Calculate the slope at x = 2
print(dx_f.subs(x,2)) # prints 4
```

Another concept we will encounter in this book is **partial derivatives** in Chapter 5, Chapter 6, and Chapter 7, which are derivatives on functions that have multiple input variables. Think of it this way. Rather than finding the slope on a 1-dimensional function, we have slopes with respect to multiple variables in several directions. For each given variable derivative, we assume the other variables are held constant. Take a look at the 3D graph of $f(x,y) = 2x^3 + 3y^3$ in Figure 1-8 and you will see we have slopes in two directions for two variables.

Let's take the function $f(x,y) = 2x^3 + 3y^3$. The *x* and *y* variable each get their own derivatives $\frac{d}{dx}$ and $\frac{d}{dy}$. These represent the slope values with respect to each variable on a multidimensional surface. These are the derivatives for *x* and *y*, followed by the SymPy code to calculate those derivatives:

$$f(x,y) = 2x^3 + 3y^3$$

$$\frac{d}{dx} 2x^3 + 3y^3 = 4x$$

$$\frac{d}{dy} 2x^3 + 3y^3 = 9y^2$$

Example 1-24 and Figure 1-8 shows how we calculate the partial derivatives for *x* and *y* respectively with SymPy.

Example 1-24. Calculating partial derivatives with SymPy

```
from sympy import *
from sympy.plotting import plot3d

# Declare x and y to SymPy
x,y = symbols('x y')

# Now just use Python syntax to declare function
f = 2*x**3 + 3*y**3

# Calculate the partial derivatives for x and y
dx_f = diff(f, x)
dy_f = diff(f, y)

print(dx_f) # prints 6*x**2
print(dy_f) # prints 9*y**2

# plot the function
plot3d(f)
```

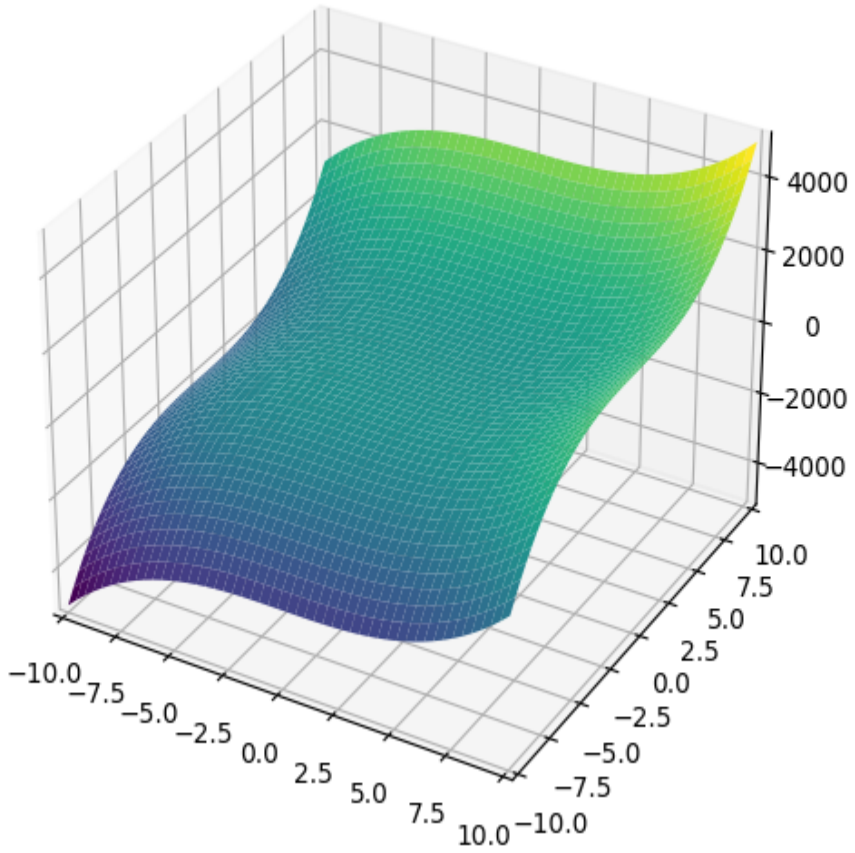


Figure 1-8. Plotting a 3-dimensional exponential function

So for (x,y) values (1,2), the slope with respect to x is $6(1) = 4$ and the slope with respect to y is $9(2)^2 = 36$.

USING LIMITS TO CALCULATE DERIVATIVES

Want to see where limits come into play calculating derivatives? If you are feeling good about what we learned so far, proceed! If you are still digesting, maybe consider coming back to this sidebar later.

SymPy allows us to do some interesting explorations about math. Take our function $f(x) = x^2$ and we approximated a slope for $x = 2$ by drawing a line through a close neighboring point $x = 2.0001$ by adding a step $.0001$. Why not use a limit to forever decrease that step s and see what slope it approaches?

$$\lim_{s \to 0} \frac{(x+s)^2 - x^2}{(x+s) - x}$$

In our example, we are interested in the slope where $x = 2$ so let's substitute that.

$$\lim_{s \to 0} \frac{(2+s)^2 - 2^2}{(2+s) - 2} = 4$$

By forever approaching a step size s to 0 but never reaching it (remember the neighboring point cannot touch the point at $x = 2$ else we have no line!), we can use a limit to see we converge on a slope of 4 as shown in Example 1-25.

Example 1-25. Using limits to calculate a slope

```
from sympy import *

# "x" and step size "s"
x, s = symbols('x s')

# declare function
f = x**2

# slope between two points with gap "s"
# substitute into rise-over-run formula
slope_f = (f.subs(x, x + s) - f) / ((x+s) - x)
```

```
# substitute 2 for x
slope_2 = slope_f.subs(x, 2)

# calculate slope at x = 2
# infinitely approach step size _s_ to 0
result = limit(slope_2, s, 0)

print(result) # 4
```

Now what if we do not assign a specific value to *x* and leave it alone? What happens if we decrease our step size *s* infinitely towards 0 then? Let's look in Example 1-26.

Example 1-26. Using limits to calculate a derivative

```
from sympy import *

# "x" and step size "s"
x, s = symbols('x s')

# declare function
f = x**2

# slope between two points with gap "s"
# substitute into rise-over-run formula
slope_f = (f.subs(x, x + s) - f) / ((x+s) - x)

# calculate derivative function
# infinitely approach step size +s+ to 0
result = limit(slope_f, s, 0)

print(result) # 2x
```

Wow! That gave us our derivative function `2x`. SymPy was smart enough to figure out to never let our step size reach 0 but forever approach 0. This converges $f(x) = x^2$ to reach its derivative counterpart $2x$.

Integrals

The opposite of a derivative is an **integral**, which finds the area under the curve for a given range. We will find ourselves using integrals quite a bit in

this book to find areas under probability distributions.

I want to take an intuitive approach for learning integrals called the Reimann Sums, one that flexibly adapts to any continuous function.

First, let's point out that finding the area for a range under a straight line is easy. Let's say I have a function $f(x) = 2x$ and I want to find the area under the line between 0 and 1, as shaded in Figure 1-9.

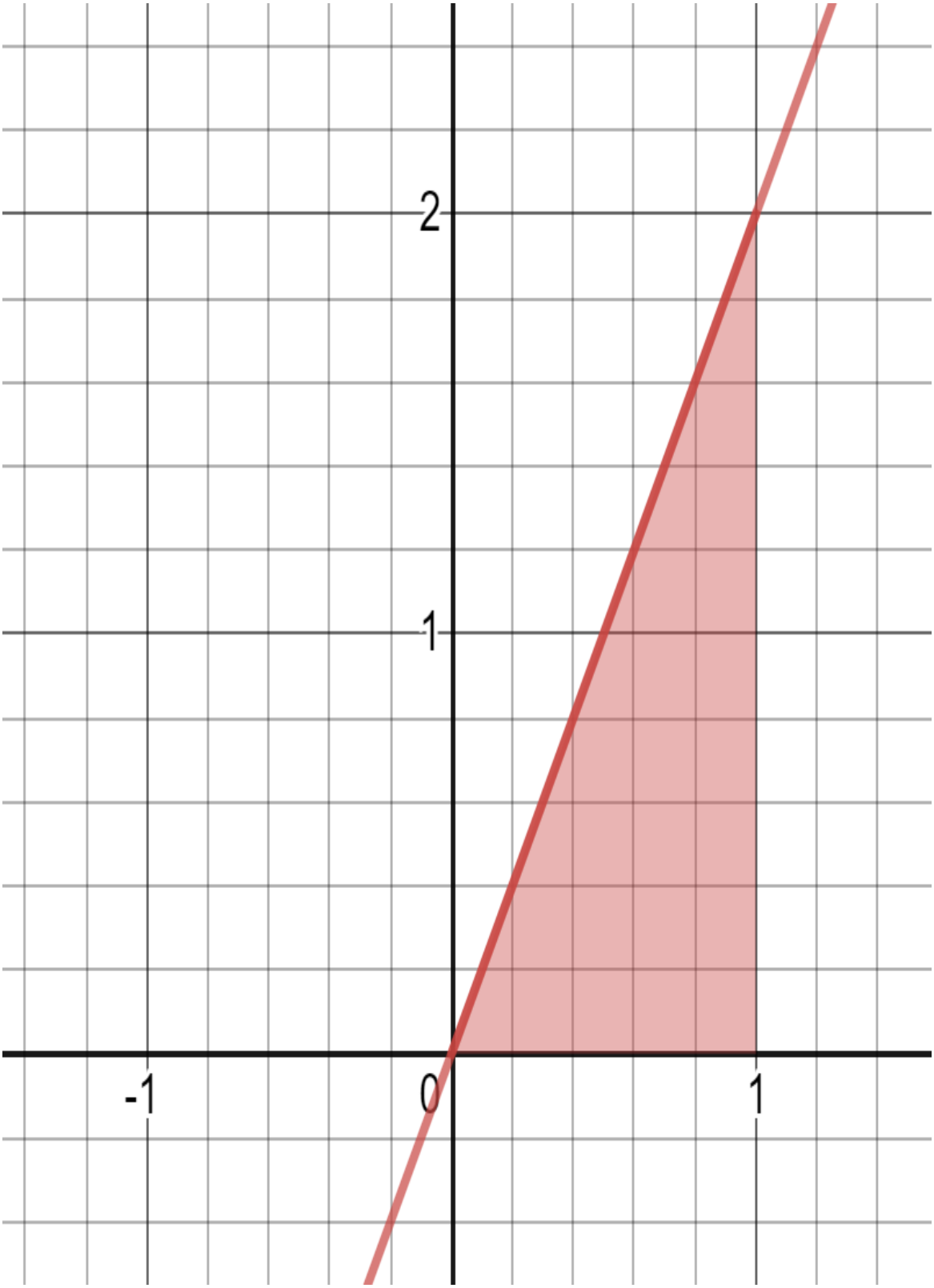


Figure 1-9. Calculating an area under a linear function

Notice that I am finding the area bounded between the line and the x-axis, and in the *x* range 0 to 1.0. If you recall basic geometry formulas, the area *A* for a triangle is $A = \frac{1}{2}b*h$ where *b* is the length of the base and *h* is the height. We can visually spot above that $b = 1$ and $h = 2$. So plugging into the formula we get for our area 1.0 as calculated below:

$$A = \frac{1}{2}bh$$

$$A = \frac{1}{2}*1.0*2.0$$

$$A = 1.0$$

That was not bad, right? But let's look at a function that is difficult to find the area under: $f(x) = x^2 + 1$. What is the area between 0 and 1 as shaded in Figure 1-10?

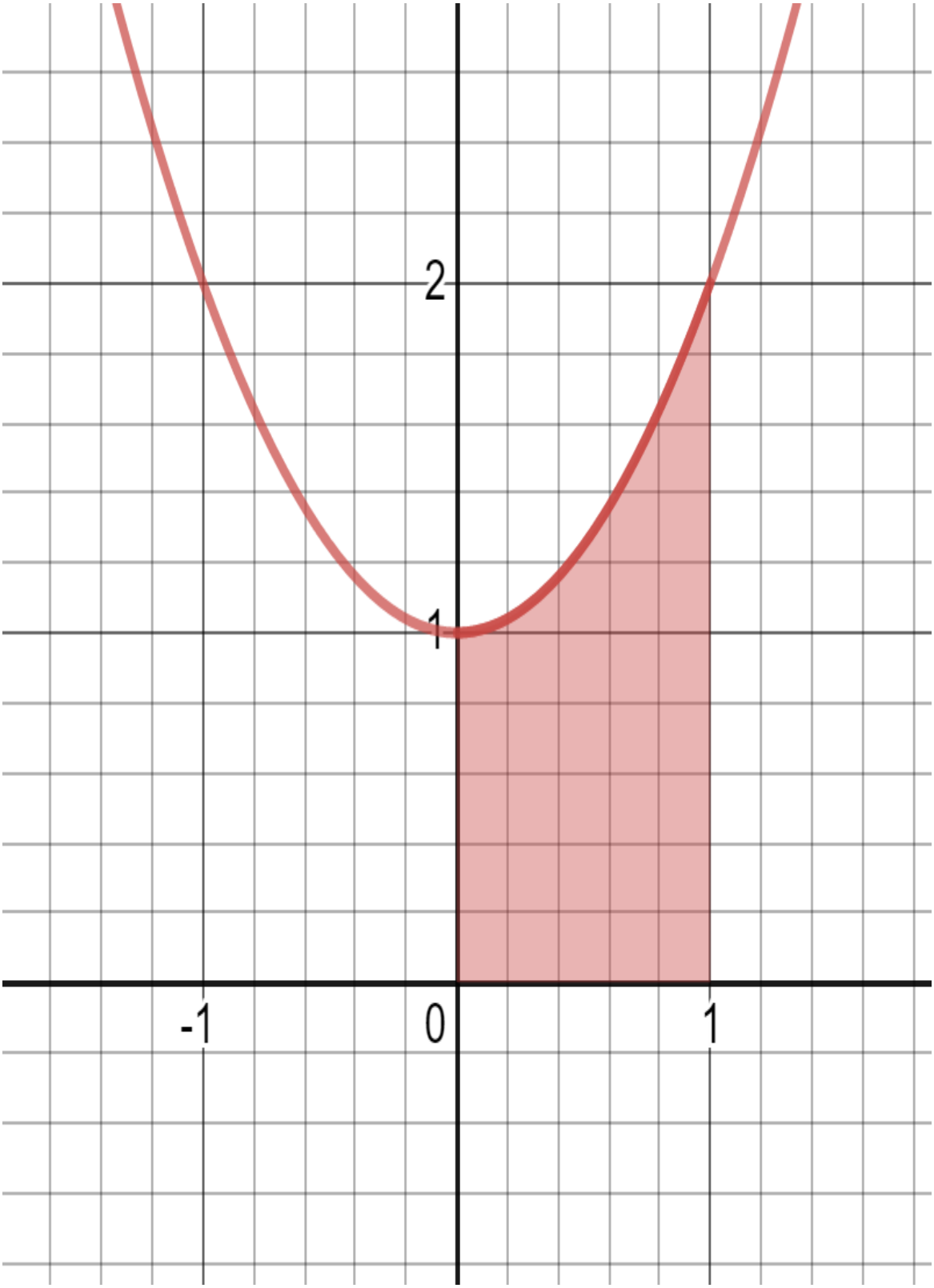


Figure 1-10. Calculating area under nonlinear functions is less straightforward

Again we are only interested in the area below the curve and above the x-axis, only within the *x* range between 0 and 1. The curviness here does not give us a clean geometric formula to find the area, but here is a clever little hack you can do.

What if we packed 5 rectangles of equal length under the curve as shown in Figure 1-11, where the height of each one extends from the x-axis to where the midpoint touches the curve?

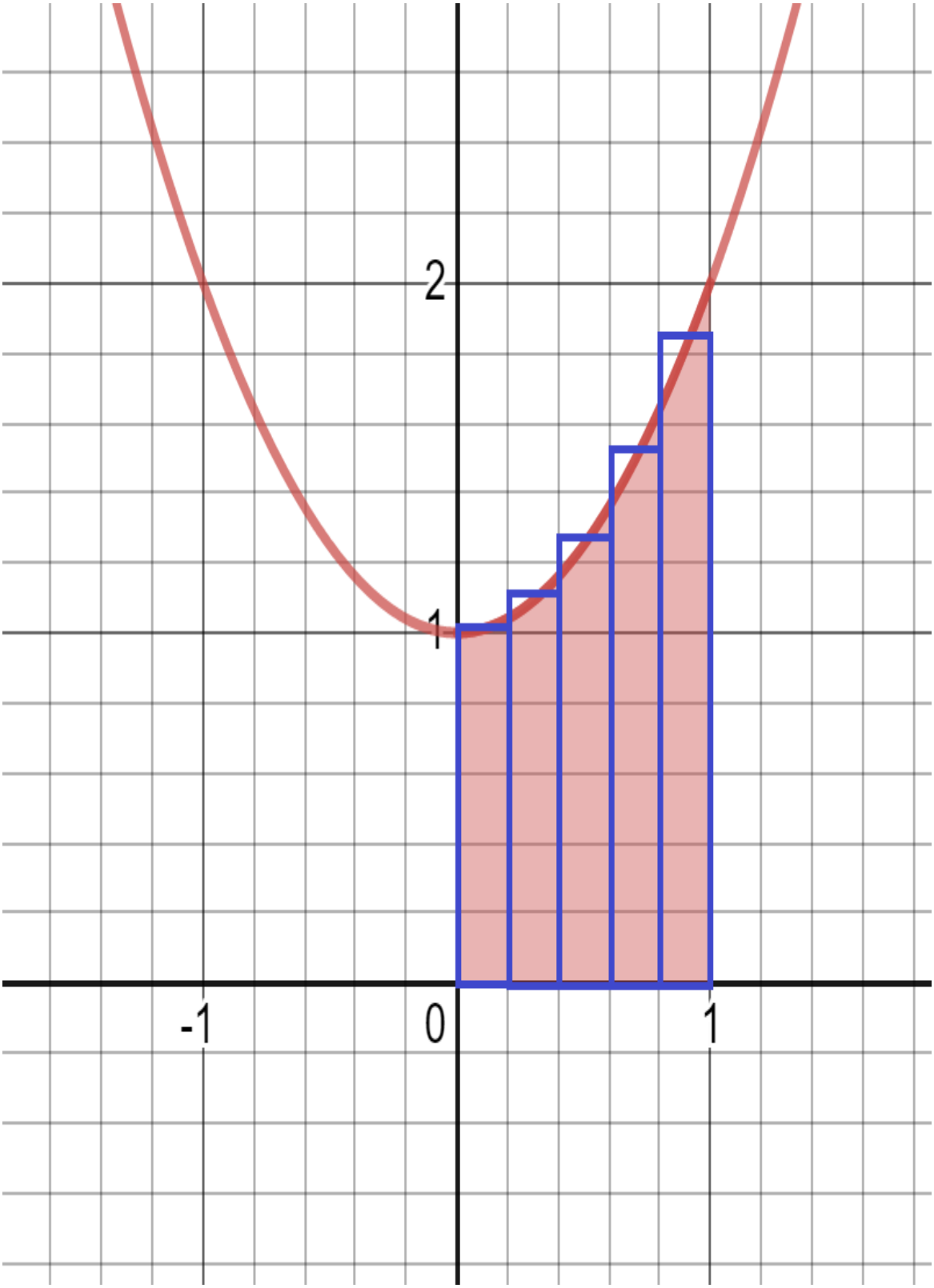


Figure 1-11. Packing rectangles under a curve to approximate area

The area of a rectangle is *A = length * width*, so we could easily sum the areas of the rectangles. Would that give us a good approximation of the area under the curve? What if we packed 100 rectangles? 1000? 100,000? As we increase the number of rectangles while decreasing their width, would we not get closer to the area under the curve? Yes we would, and it is yet another case where we increase/decrease something towards infinity to approach an actual value.

Let's try it out in Python! First we need a function that approximates an integral which we will call `approximate_integral()`. The arguments *a* and *b* will specify the min and max of the *x* range respectively. *n* will be the number of rectangles to pack, and *f* will be the function we are integrating. We implement the function in Example 1-27, and then use it to integrate our function $f(x) = x^2 + 1$ with 5 rectangles, between 0.0 and 1.0.

Example 1-27. An integral approximation in Python

```
def approximate_integral(a, b, n, f):
    delta_x = (b - a) / n
    total_sum = 0

    for i in range(1, n + 1):
        midpoint = 0.5 * (2 * a + delta_x * (2 * i - 1))
        total_sum += f(midpoint)

    return total_sum * delta_x

def my_function(x):
    return x**2 + 1

area = approximate_integral(a=0, b=1, n=5, f=my_function)

print(area) # prints 1.33
```

So we get an area of 1.33. What happens if we use 1000 rectangles? Let's try it out in Example 1-28.

Example 1-28. An integral approximation in Python

```
area = approximate_integral(a=0, b=1, n=1000, f=my_function)

print(area) # prints 1.333333250000001
```

Okay we are getting some more precision here, and getting some more decimal places. What about 1 million rectangles as shown in Example 1-29?

Example 1-29. An integral approximation in Python

```
area = approximate_integral(a=0, b=1, n=1_000_000, f=my_function)

print(area) # prints 1.3333333333332733
```

Okay I think we are getting a diminishing return here, and are converging on the value 1.333 where the ".333" part is forever recurring. If this were a rational number, it is likely $\frac{4}{3} = 1.333$. As we increase the number of rectangles, the approximation starts to reach its limit at smaller and smaller decimals.

Now that we got some intuition on what we are trying to achieve and why, let's do a more exact approach with SymPy which happens to support rational numbers in Example 1-30.

Example 1-30. Using SymPy to perform integration

```
from sympy import *

# Declare 'x' to SymPy
x = symbols('x')

# Now just use Python syntax to declare function
f = x**2 + 1

# Calculate the integral of the function with respect to x
# for the area between x = 0 and 1
area = integrate(f, (x, 0, 1))

print(area) # prints 4/3
```

Cool! So the area actually is `4/3`, which is what our previous method converged on. Unfortunately plain Python (and many programming languages) only support decimals but computer algebra systems like SymPy give us exact rational numbers. We will be using integrals to find areas under curves in Chapter 2 and Chapter 3, although we will have Scikit-Learn do the work for us when available.

CALCULATING INTEGRALS WITH LIMITS

For the super curious, here is how we calculate definite integrals using limits in SymPy. Please! Skip or come back to this sidebar later if you have enough to digest. But if you are feeling good and want to deep dive how integrals are derived using limits, proceed!

The main idea follows much what we did earlier: pack rectangles under a curve and make them infinitely smaller until we approach the exact area. But of course, the rectangles cannot have a width of 0… they just have to keep getting closer to 0 without ever reaching 0. It is another case of using limits.

Khan Academy has a great article explaining how to use limits for Reimann Sums but here is how we do it in SymPy as shown in Example 1-31.

Example 1-31. Using Limits to Calculate Integrals

```
from sympy import *

# Declare variables to SymPy
x, i, n = symbols('x i n')

# Declare function and range
f = x**2 + 1
lower, upper = 0, 1

# Calculate width and each rectangle height at index "i"
delta_x = ((upper - lower) / n)
x_i = (lower + delta_x * i)
fx_i = f.subs(x, x_i)

# Iterate all "n" rectangles and sum their areas
n_rectangles = Sum(delta_x * fx_i, (i, 1, n)).doit()

# Calculate the area by approaching the number
# of rectangles "n" to infinity
area = limit(n_rectangles, n, oo)

print(area) # prints 4/3
```

Above we determine the length of each rectangle `delta_x_` and the start of each rectangle `+x_i_` where *i* is the index of each rectangle. `+fx_i_` is the height of each rectangle at index *i*. We declare *n* number of rectangles and sum their areas `+delta_x * fx_i_`, but we have no area value yet because we have not committed a number for *n*. Instead we approach *n* towards infinity to see what area we converge on, and you should get +4/3!

Conclusion

In this chapter we covered some foundations we will use for the rest of this book. From number theory to logarithms and calculus integrals, we cherrypicked some important mathematical concepts that have relevance in data science, machine learning, and analytics. You may have questions about why these concepts are useful. That will come next!

Before we move on to discuss probability, take a little bit of time to skim these concepts one more time and then do the following exercise. You can always revisit this chapter as you progress through this book, and refresh as necessary when you start applying these mathematical ideas.

Exercises

1. Is the value 62.6738 rational or irrational? Why or why not?
2. Evaluate the expression: $10^7 10^{-5}$
3. Evaluate the expression: $81^{\frac{1}{2}}$
4. Evaluate the expression: $25^{\frac{3}{2}}$
5. Assuming no payments are made, how much would a $1000 loan be worth at 5% interest compounded monthly after 3 years?

6. Assuming no payments are made, how much would a $1000 loan be worth at 5% interest compounded continuously after 3 years?
7. For the function $f(x) = 3x^2 + 1$ what is the slope at $x = 3$?
8. For the function $f(x) = 3x^2 + 1$ what is the area under the curve for x between 0 and 2?

Chapter 2. Probability

> **A NOTE FOR EARLY RELEASE READERS**
>
> With Early Release ebooks, you get books in their earliest form—the author's raw and unedited content as they write—so you can take advantage of these technologies long before the official release of these titles.
>
> This will be the 2nd chapter of the final book.
>
> If you have comments about how we might improve the content and/or examples in this book, or if you notice missing material within this chapter, please reach out to the author at *thomasnield@live.com*.

When you think of probability, what images come to mind? Perhaps you think of gambling-related examples, like the probability of winning the lottery or getting a pair with two dice. Maybe it is predicting stock performance, the outcome of a political election, or whether your flight will arrive on time. Our world is full of uncertainties we want to measure.

Maybe that is the word we should focus on: uncertainty. How do we measure something that we are uncertain about?

In the end, probability is the theoretical study of measuring certainty that an event will happen. It is a foundational discipline for statistics, hypothesis testing, machine learning, and other topics in this book. A lot of folks take probability for granted and assume they understand it. However, it is more nuanced and complicated than most people think. While the theorems and ideas of probability are mathematically sound, it gets more complex when we introduce data and venture into statistics. We will cover that in Chapter 4 and hypothesis testing.

In this chapter, we will discuss what probability is. Then we will cover probability math concepts, Bayes Theorem, the Binomial Distribution, and the Beta Distribution.

Understanding Probability

Probability is how strongly we believe an event will happen, often expressed as a percentage. Here are some questions that might warrant a probability for an answer:

- How likely will I get 7 heads in 10 fair coin flips?
- What are my chances in winning an election?
- Will my flight be late?
- How certain am I a product is defective?

The most popular way to express probability is as a percentage, as in “There is a 70% chance my flight will be late.” We will call this probability $P(X)$, where X is the event of interest. As you work with probabilities though, you will more likely see it expressed as a decimal (in this case .70) which must be between 0.0 and 1.0.

$P(X) = .70$

Likelihood is similar to probability, and it is easy to confuse the two (many dictionaries do as well). You can get away with using “probability” and “likelihood” interchangeably in everyday conversation. However, we should pin down these differences. Probability is about quantifying predictions of events yet to happen, whereas likelihood is measuring the frequency of events that already occurred. In statistics and machine learning, we often use likelihood (the past) in the form of data to predict probability (the future).

It is important to note that a probability of an event happening must be strictly between 0% and 100%, or 0.0 and 1.0. Logically, this means the probability of an event *NOT* happening is calculated by subtracting the probability of the event from 1.0.

$$P(X) = .70$$

$$P(\text{not X}) = 1.0 - .70 = .30$$

Alternatively, probability can be expressed as an **odds** $O(X)$ expressed as 7:3, $\frac{7}{3}$, or 2.333.

ODDS ARE USEFUL!

While many people feel more comfortable expressing probabilities as percentages or proportions, odds can be a helpful tool. If I have an odds of 2.0, that means I feel an event is 2 times more likely to happen than not to happen. That can be more intuitive to describe a belief than a percentage of 66.666%. For this reason, odds are helpful quantifying subjective beliefs especially in a gambling/betting context. It plays a role in Bayesian statistics (including the Bayes Factor) as well as logistic regressions with the log-odds which we will cover in Chapter 6.

To turn an odds $O(X)$ into a proportional probability $P(X)$, use the formula below:

$$P\left(X\right) = \frac{O(X)}{1.0 + O(X)}$$

So if have an odds $\frac{7}{3}$, I can convert it into a proportional probability like this:

$$P\left(X\right) = \frac{O(X)}{1.0 + O(X)}$$

$$P\left(X\right) = \frac{\frac{7}{3}}{1.0 + \frac{7}{3}}$$

$$P(X) = .7$$

Conversely, you can turn an odds into a probability simply by dividing the probability of the event occuring by the probability it will not occur:

$$O\left(X\right) = \frac{P(X)}{1.0 - P(X)}$$

$$O\left(X\right) = \frac{.70}{1.0 - .70}$$

$$O\left(X\right) = \frac{7}{3}$$

Probability versus Statistics

Sometimes people use the terms *probability* and *statistics* interchangeably, and while this is understandable to conflate the two disciplines they do have distinctions. **Probability** is purely theoretical of how likely an event is to happen, and does not require data. **Statistics** on the other hand cannot exist without data, and uses it to discover probability and provides tools to decribe data.

Think of predicting the outcome of rolling a "4" on a die (that's the singular of "dice"). Approaching the problem with a pure probability mindset, one simply says there are 6 sides on a die. We assume each side is equally likely, so the probability of getting a "4" is $\frac{1}{6}$, or 16.666%.

However, a zealous statistician might say "No! We need to roll the die to get data. If we can get 30 rolls or more, and the more rolls we do the better, only then will we have data to determine the probability of getting a *4*." This approach may seem silly if we assume the die is fair, but what if it's not? If that's the case, collecting data is the only way to discover the probability of rolling a "4". We will talk about hypothesis testing in Chapter 3.

> **BAYESIAN AND FREQUENTIST STATISTICS**
>
> If you are curious to learn the differences between Bayesian and Frequentist thinking, turn to Appendix A.

Probability Math

When we work with a single probability of an event $P(X)$, known as a **marginal probability**, the idea is fairly straightforward as discussed previously. But when we start combining probabilities of different events together, it gets a little less intuitive.

Joint Probabilities

Let's say you have a fair coin and a fair 6-sided die. You want to find the probability of flipping a "Heads" and rolling a "6" on the coin and die respectively. These are two separate probabilities of two separate events, but we want to find the probability that both events will occur together. This is known as a **joint probability**.

Think of a joint probability as an AND operator. I want to find the probability of flipping a *heads* AND rolling a *six.* We want both events to happen together, so how do we calculate this probability?

There are 2 sides on a coin and 6 sides on the die, so the probability of heads is $\frac{1}{2}$ and probability of six is $\frac{1}{6}$. The probability of both events occurring (assuming they are independent, more on this later!) is simply multiplying the two together:

$$P(\text{A AND B}) = P(A)*P(B)$$

$$P\left(\text{Heads}\right) = \frac{1}{2}$$

$$P\left(6\right) = \frac{1}{6}$$

$$P\left(\text{Heads AND 6}\right) = \frac{1}{2}*\frac{1}{6} = \frac{1}{12} = .08333$$

Easy enough, but why is this the case? A lot of probability rules can be discovered by generating all possible combinations of events, which comes from an area of math known as permutations and combinations. For this case, generate every possible outcome between the coin and die, pairing heads (H) and tails (T) with the numbers 1 through 6. Note I put asterisks "*" around the outcome of interest where we got heads and a six.

```
H1  H2  H3  H4  H5  *H6*  T1  T2  T3  T4  T5  T6
```

Notice there are 12 possible outcomes when flipping our coin and rolling our die. The only one that is of interest to us is "H6," getting a heads and a six. So because there is only 1 outcome that satisfies our condition, and there are 12 possible outcomes, the probability of getting a heads and a six is $\frac{1}{12}$.

Rather than generate all possible combinations and counting the ones of interest to us, we can again use the multiplication as a shortcut to find the joint probability. This is known as the **product rule**.

$$P(\text{A AND B}) = P(A)*P(B)$$

$$P\left(\text{Heads AND 6}\right) = \frac{1}{2}*\frac{1}{6} = \frac{1}{12} = .08333$$

Union Probabilities

We discussed joint probabilities, which is the probability of two or more events occurring simultaneously. But what about the probability of getting event A or B?

When we deal with “OR” operations with probabilities, this is known as a **union probability**.

Let’s start with **mutually exclusive** events, which are events that cannot occur simultaneously. For example, if I roll a die I cannot simultaneously get a “4” and a “6”. I can only get one outcome. Getting the union probability for these cases are easy. I just simply add them together. If I want to find the probability of getting a “4” or “6” on a die roll, it is going to be $\frac{2}{6} = \frac{1}{3}$.

$$P(4) = \frac{1}{6}$$

$$P(6) = \frac{1}{6}$$

$$P(4 \text{ OR } 6) = \frac{1}{6} + \frac{1}{6} = \frac{1}{3}$$

But what about **non-mutally exclusive** events, which are events that can occur simulataneously? Let’s go back to the coin flip and die roll example. What is the probability of getting a heads OR a “six”? Before you are tempted to add those probabilities, let’s generate all possible outcomes again and highlight the ones we are interested in:

```
*H1*  *H2*  *H3*  *H4*  *H5*  *H6*  T1  T2  T3  T4  T5  *T6*
```

Above we are interested in all the “heads” outcome as well as the “6” outcomes. If we proportion the 7 out of 12 outcomes we are interested in, $\frac{7}{12}$, we get a correct probability of $.58333$.

But what happens if we add the probabilities of heads and “6” together? We get a different (and wrong!) answer of $.666$.

$$P(HEADS) = \frac{1}{2}$$

$$P(6) = \frac{1}{6}$$

$$P(\text{HEADS OR } 6) = \frac{1}{2} + \frac{1}{6} = \frac{4}{6} = .666$$

Why is that? Study the combinations of coin flip and die outcomes again and see if you can find something fishy. Notice when we add the probabilities, we double-count the probability of getting a “6” in both “H6” and “T6”! If this is not clear, try finding the probability of getting “Heads” and a die roll of 1 through 5.

$$P\left(HEADS\right) = \frac{1}{2}$$

$$P\left(1 \text{ through } 5\right) = \frac{5}{6}$$

$$P\left(\text{HEADS OR 1 through 5}\right) = \frac{1}{2} + \frac{5}{6} = \frac{8}{6} = 1.333$$

We get a probability of 133.333% which is definitely not correct, as a probability must be no more than 100% or 1.0. The problem again is we are double-counting outcomes.

If you ponder long enough, you may realize the logical way to remove double-counting in a union probability is to subract the joint probability. This is known as the **sum rule of probability** and ensures every joint event is only counted once.

$$P(\text{A OR B}) = P(A) + P(B) - P(\text{A AND B})$$

$$P(\text{A OR B}) = P(A) + P(B) - P(\text{A})*P(\text{B})$$

So going back to our example of calculating the probability of a Heads or a “six”, we need to subtact the joint probability of getting a Heads or a “six” from the union probability:

$$P\left(HEADS\right) = \frac{1}{2}$$

$$P\left(6\right) = \frac{1}{6}$$

$$P(\text{A OR B}) = P(A) + P(B) - P(A)*P(B)$$

$$P\left(\text{HEADS OR 6}\right) = \frac{1}{2} + \frac{1}{6} - \left(\frac{1}{2}*\frac{1}{6}\right) = .58333$$

Note that this formula also applies to mutually exclusive events. If the events are mutually exclusive where only one outcome A or B is allowed but not both, then the

joint probability $P(\text{A AND B})$ is going to be 0, and therefore remove itself from the formula. You are then left with simply summing the events as we did earlier.

In summary, when you have a union probability between two or more events that are not mutually exclusive, be sure to subtract the joint probability so no probabilities are double-counted.

Conditional Probability and Bayes Theorem

A probability topic that people easily get confused by is the concept of **conditional probability**, which is the probability of an event A occuring given event B has occurred. It is typically expressed as $P(\text{A GIVEN B})$ or $P(\text{A}|\text{B})$.

Let's say some study makes a claim that 85% of cancer patients drank coffee. How do you react to this claim? Does this alarm you and make you want to abandon your favorite morning drink? Let's first define this as a conditonal probability $P(\text{Coffee given Cancer})$ or $P(\text{Coffee}|\text{Cancer})$. This represents a probability of people who drink coffee given they have cancer.

Within the United States, let's compare this to the percentage of people diagnosed with cancer (0.5% according to cancer.gov) and the percentage of people who drink coffee (65% according to statista.com):

$$P(\text{Coffee}) = .65$$

$$P(\text{Cancer}) = .005$$

$$P(\text{Coffee}|\text{Cancer}) = .85$$

Hmmmm… study these numbers for a moment and ask whether coffee is really contributing to cancer here. Notice again that only 0.5% of the population has cancer at any given time. However 65% of the population drinks coffee regularly. If coffee contributes to cancer, should we not have much higher cancer numbers than 0.5%? Would it not be closer to 65%?

This is the sneaky thing about proportional numbers. They may seem significant without any given context, and media headlines can certainly exploit this for clicks: "New Study Reveals 85% of Cancer Patients Drink Coffee" it might read. Of course, this is silly because we have taken a common attribute (drinking coffee) and associated it with an uncommon one (having cancer).

The reason people can be so easily confused by conditional probabilities is because the direction of the condition matters, and the two conditions are conflated as

somehow being equal. The "probability of having cancer given you are a coffee drinker" is different than the "probability of being a coffee drinker given you have cancer." To put it simply: few coffee drinkers have cancer, but many cancer patients drink coffee.

If we are interested in studying whether coffee contributes to cancer, we really are interested in the first conditional probability: the probability of somone having cancer given they are a coffee drinker.

$$P(\text{Coffee}|\text{Cancer}) = .85$$

$$P(\text{Cancer}|\text{Coffee}) = ?$$

How do we flip the condition? There's a powerful little formula called **Bayes Theorem** and we can use it to flip conditional probabilities.

$$P(\text{A}|\text{B}) = \frac{P(\text{B}|\text{A})*P(B)}{P(A)}$$

If we plug the information we already have into this formula, we can solve for the probability someone has cancer given they drink coffee:

$$P(\text{A}|\text{B}) = \frac{P(\text{B}|\text{A})*P(B)}{P(A)}$$

$$P(\text{Cancer}|\text{Coffee}) = \frac{P(\text{Coffee}|\text{Cancer})*P(\text{Coffee})}{P(\text{Cancer})}$$

$$P(\text{Cancer}|\text{Coffee}) = \frac{P(.85)*P(.005)}{P(.65)} = .0065$$

If you want to calculate this in Python, check out Example 2-1.

Example 2-1. Using Bayes Theorem in Python

```
p_coffee_drinker = .65
p_cancer = .005
p_coffee_drinker_given_cancer = .85

p_cancer_given_coffee_drinker = p_coffee_drinker_given_cancer *
    p_cancer / p_coffee_drinker

# prints 0.006538461538461539
print(p_cancer_given_coffee_drinker)
```

Wow! So the probability someone has cancer given they are a coffee drinker is only 0.65%! This number is very different than the probability someone is a coffee drinker given they have cancer, which is 85%. Now do you see why the direction of the condition matters? Bayes Theorem is helpful for this reason, and it can be used to chain several conditional probabilities together to keep updating our beliefs based on new information.

WHAT DEFINES A "COFFEE DRINKER"?

Note that I could have accounted for other variables here, in particular what qualifies someone as a "coffee drinker." If someone drinks coffee once a month, as opposed to somone who drinks coffee every day, should I equally qualify both as "coffee drinkers"? What about the person who started drinking coffee a month ago as opposed to someone who drank coffee for 20 years? How often and how long do people have to drink coffee before they meet the threshhold of being a "coffee drinker" in this cancer study?

These are important questions to consider, and shows why data rarely tells a whole story. If someone gives you a spreadsheet of patients with a simple "YES/NO" flag on whether they are a coffee drinker, that threshhold needs to be defined! Or we need a more weightful metric like "number of coffee drinks consumed in the last 3 years." I kept this thought experiment simple and didn't define how someone qualifies as a "coffee drinker", but be aware that out in the field, always ask for context about the data.

If you want to explore the intuition behind Bayes Theorem more deeply, turn to Appendix A. For now just know it helps us flip a conditional probability. Let's talk about how conditional probabilities interact with joint and union operations next.

NAIVE BAYES

Bayes Theorem plays a central role to a common machine learning algorithm called Naive Bayes. Joel Grus covers it in his book Data Science from Scratch[*https://www.oreilly.com/library/view/data-science-from/9781492041122/*].

Joint and Union Conditional Probabilities

Let's revist joint probabilities and how they interact with conditional probabilities. I want to find the probability somebody is a coffee drinker AND they have cancer.

Should I multiply $P(\text{Coffee})$ and $P(\text{Cancer})$? Or should I use $P(\text{Coffee}|\text{Cancer})$ in place of $P(\text{Coffee})$ if it is available? Which one do I use?

$$\text{OPTION 1:}$$

$$P(\text{Coffee}) \times P(\text{Cancer}) = .65 \times .005 = .00325$$

$$\text{OPTION 2:}$$

$$P(\text{Coffee}|\text{Cancer}) \times P(\text{Cancer}) = .85 \times .005 = .00425$$

If we already have established our probability only applies to people with Cancer, does it not make sense to use $P(\text{Coffee}|\text{Cancer})$ instead of $P(\text{Coffee})$? One is more specific and applies to a condition that's already been established. So we should use $P(\text{Coffee}|\text{Cancer})$ as $P(Cancer)$ is already part of our joint probability. This means the probability of somone having cancer and being a coffee drinker is 0.425%.

$$P(\text{Coffee and Cancer}) = P(\text{Coffee}|\text{Cancer}) \times P(Cancer) = .85 \times .005 = .00425$$

This joint probability also applies in the other direction. I can find the probability of someone being a coffee drinker and having cancer by multiplying $P(\text{Cancer}|\text{Coffee})$ and $P(\text{Coffee})$. As you can observe, I arrive at the same answer:

$$P(\text{Cancer}|\text{Coffee}) \times P(\text{Coffee}) = .0065 \times .65 = .00425$$

If we did not have any conditional probabilities available, then the best we can do is multiply P(Coffee Drinker) and P(Cancer) as shown here:

$$P(\text{Coffee Drinker}) \times P(Cancer) = .65 \times .005 = .00325$$

Now think about this: if event A has no impact on event B, then what does that mean for conditional probability $P(\text{B}|\text{A})$? That means $P(\text{B}|\text{A}) = P(B)$, meaning event A occuring makes no difference to how likely event B is to occur. Therefore we can update our joint probability formula to be, regardless if the two events are dependent, to be:

$$P(\text{A AND B}) = P(\text{B}) \times P(\text{A}|\text{B})$$

And finally let's talk about unions and conditional probability. If I wanted to calculate the probability of A or B occuring, but A may affect the probability of B, we update our sum rule like this:

$$P(\text{A OR B}) = P(A) + P(B) - P(\text{A}|\text{B}) \times P(\text{B})$$

As a reminder, this applies to mutually exclusive events as well. The sum rule $P(\mathrm{A}|\mathrm{B})*P(\mathrm{B})$ would yield 0 if the events A and B cannot happen simultaneously.

Binomial Distribution

Let's say you are working on a new turbine jet engine and ran 10 tests. The outcomes yielded 8 successes and 2 failures:

✓ ✓ ✓ ✓ ✓ ✗ ✓ ✗ ✓ ✓

You were hoping to get a 90% success rate, but based on the data above you conclude that your tests have failed with only 80% success. Each test is time-consuming and expensive, so you decide it is time to go back to the drawing board to re-engineer the design.

However one of your engineers insists there should be more tests. "The only way we will know for sure is to run more tests," she argues. "What if more tests yield 90% or greater success? After all, if you flip a coin 10 times and get 8 heads, it does not mean the coin is fixed at 80%."

You briefly consider the engineer's argument and realize she has a point. Even a fair coin flip will not always have an equally split outcome, especially with only 10 flips. You are most likely to get 5 heads but you can also get 3, 4, 6, or 7 heads. You could even get 10 heads, although this is unlikely. So how do you determine the likelihood of 80% success assuming the underlying probability is 90%?

One tool that might be relevant here is the **binomial distribution**, which measures how likely *k* successes can happen out of *n* trials given *p* probability.

Visually, a binomial distribution looks like Figure 2-1.

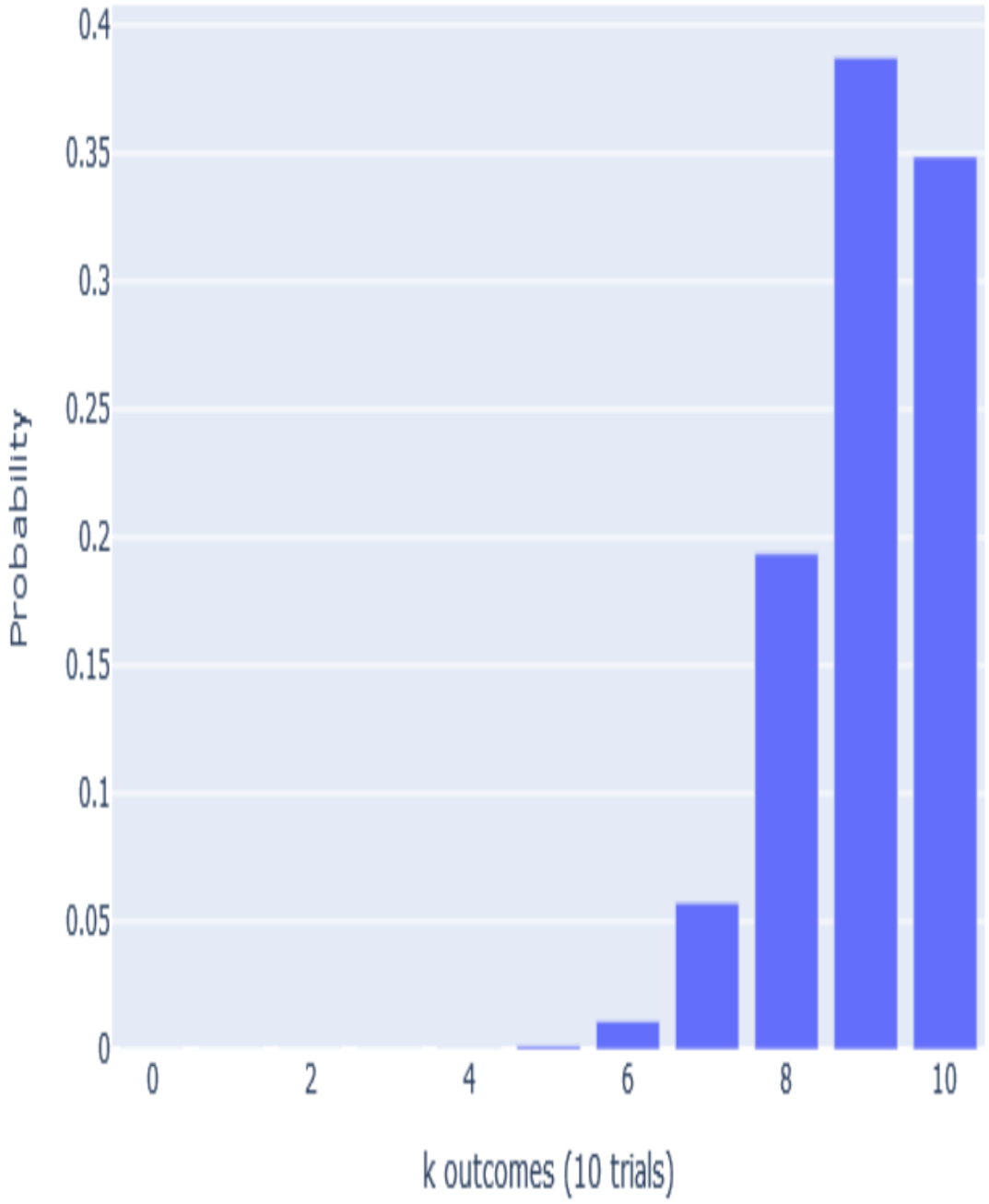


Figure 2-1. A binomial distribution

As you see above, we see the probability of *k* successes for each bar out of 10 trials. This binomial distribution assumes a probability *p* of 90%, meaning there is a .90 (or

90%) chance for a success to occur. If this is true, that means there is a .1937 probability we would get 8 successes out of 10 trials. The probability of getting 1 success out of 10 trials is extremely unlikely, .000000008999, hence why the bar is not even visible.

We can also calculate the probability of 8 or less successes by adding up bars for 8 or less successes. This would give us .2639 probabilty of 8 or less successes.

So how do we implement the binomial distribution? We can do it from scratch relatively easily (as shared in Appendix A, or we can use libraries like SciPy. Example 2-2 shows how we use SciPy's `binom.pmf()` function (PMF stands for "probability mass function") to print all 11 probabilities for our binomial distribution from 0 to 10 successes.

Example 2-2. Using SciPy for the binomial distribution

```
from scipy.stats import binom

n = 10
p = 0.9

for k in range(n + 1):
    probability = binom.pmf(k, n, p)
    print("{0} - {1}".format(k, probability))


# OUTPUT:

# 0 - 9.99999999999996e-11
# 1 - 8.999999999999996e-09
# 2 - 3.644999999999996e-07
# 3 - 8.748000000000003e-06
# 4 - 0.0001377809999999999
# 5 - 0.0014880347999999988
# 6 - 0.011160260999999996
# 7 - 0.05739562800000001
# 8 - 0.19371024449999993
# 9 - 0.38742048900000037
# 10 - 0.34867844010000004
```

As you can see, we provide *n* as the number of trials, *p* as the probability of success for each trial, and *k* is the number of successes we want to look up the likelihood for. We iterate each number of successes *x* with the corresponding probability we would see that many successes. As we can see above in the output, the most likely number of successes is 9.

But if you add up the probability of 8 or less succcesses, we would get .2639. This means there is a 26.39% chance we would see 8 or less successes even if the

underlying succcess rate is 90%. So maybe the engineer is right. 26.39% chance is not nothing and certainly possible.

However we did make an assumption here in our model which we will discuss with the Beta Distribution.

> **BINOMIAL DISTRIBUTION FROM SCRATCH**
>
> Turn to Appendix A to learn how to build the Binomial Distribution from scratch rather than using Scikit-Learn.

Beta Distribution

What did I assume with my engine test model using the binomial distribution? Is there a parameter I assumed to be true and then built my entire model around it? Think carefully and read on.

What might be problematic about my binomial distribution above is I *ASSUMED* the underlying success rate is 90%. That's not to say my model is worthless. I just showed if the underlying success rate is 90%, there is a 26.39% chance I would see 8 or less successes with 10 trials. So the engineer is certainly not wrong that there could be an underlying success rate of 90%.

But let's flip the question and consider this: what if there are other underlying rates of success that would yield 8/10 successes besides 90%? Could we see 8/10 successes with an underlying 80% success rate? 70%? 30%? When we fix the 8/10 successes, can we explore the probabilities of probabilities?

Rather than create countless binomial distributions to answer this question, there is one tool that we can use. The **beta distribution** allows us to see the likelihood of different underlying probabilities for an event to occur given *alpha* successes and *beta* failures.

Here is a chart of the beta distribution given 8 successes and 2 failures in Figure 2-2.

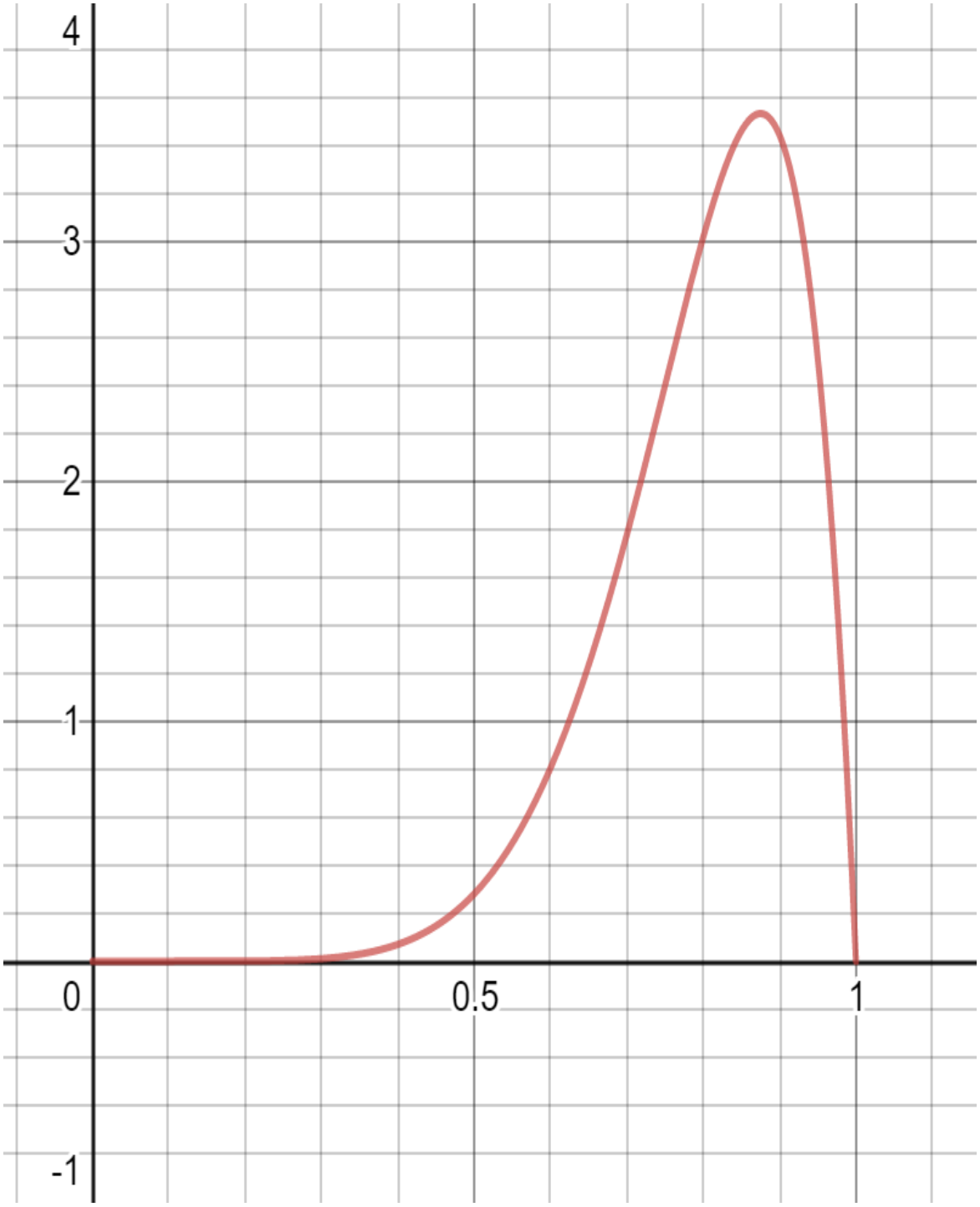


Figure 2-2. Beta distribution

BETA DISTRIBUTION ON DESMOS

If you want to interact with the Beta Distribution, a Desmos graph is provided here:
https://www.desmos.com/calculator/xylhmcwo71

Notice that the x-axis represents all underlying rates of success from 0.0 to 1.0 (0% to 100%), and the y-axis represents the likelihood of that probability given 8 successes and 2 failures. In other words, the beta distribution allows us to see the probabilities of probabilities given 8/10 successes. Think of it as a meta-probability so take your time grasping this idea!

Notice also that the beta distribution is a continuous function, meaning it forms a continuous curve of decimal values (as opposed to the tidy and discrete integers in the binomial distribution). This is going to make the math with the beta distribution a bit harder, as a given density value on the y-axis is not a probability. We instead find probabilities using areas under the curve.

The beta distribution is a type of **probability distribution**, which means the area under the entire curve is 1.0, or 100%. To find a probability, we need to find the area within a range. For example, if we want to evaluate the probability 8/10 successes would yield 90% or higher success rate, we need to find the area between 90% and 100%, which is 22.5%, as shaded in Figure 2-3.

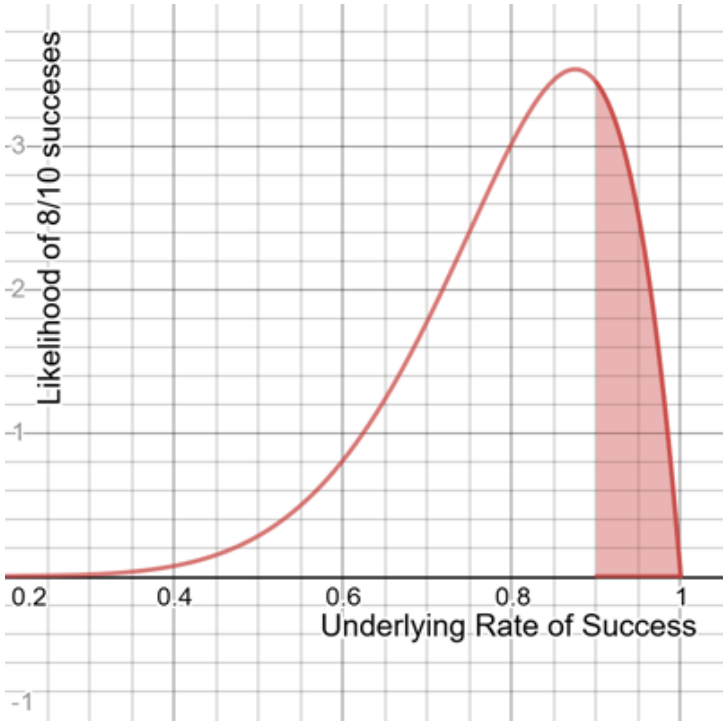


Figure 2-3. The area between 90% and 100%, which is 22.5%

As we did with the binomial distribution, we can use SciPy to implement the beta distribution. Every continuous probability distribution has a **cumulative density function (CDF)** which calculates the area up to a given *x* value. Let's say I wanted to calculate the area up to 90% (0.0 to .90) as shaded in Figure 2-4.

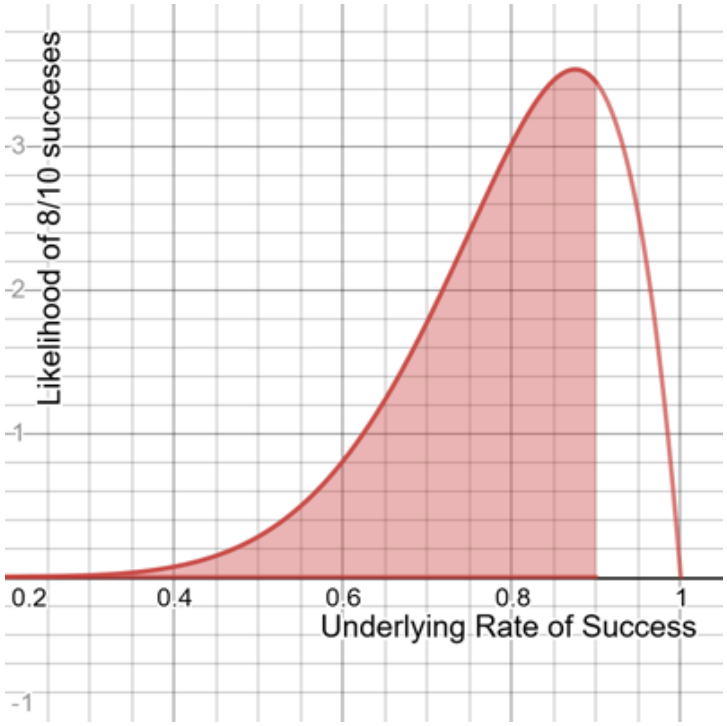


Figure 2-4. Calculating the area up to 90% (0.0 to .90)

It is easy enough to use SciPy with its `beta.cdf()` function, and the only parameters I need to provide are the *x* value, the number of successes *a*, and the number of failures *b* as shown in Example 2-3.

Example 2-3. Beta distribution using SciPy

```
from scipy.stats import beta

a = 8
b = 2

p = beta.cdf(.90, a, b)

# 0.7748409780000001
print(p)
```

So according to our calculation above, there is a 77.48% chance the underlying probability of success is 90% or less.

How do we calculate the probability of success being 90% or more as shaded below in Figure 2-5?

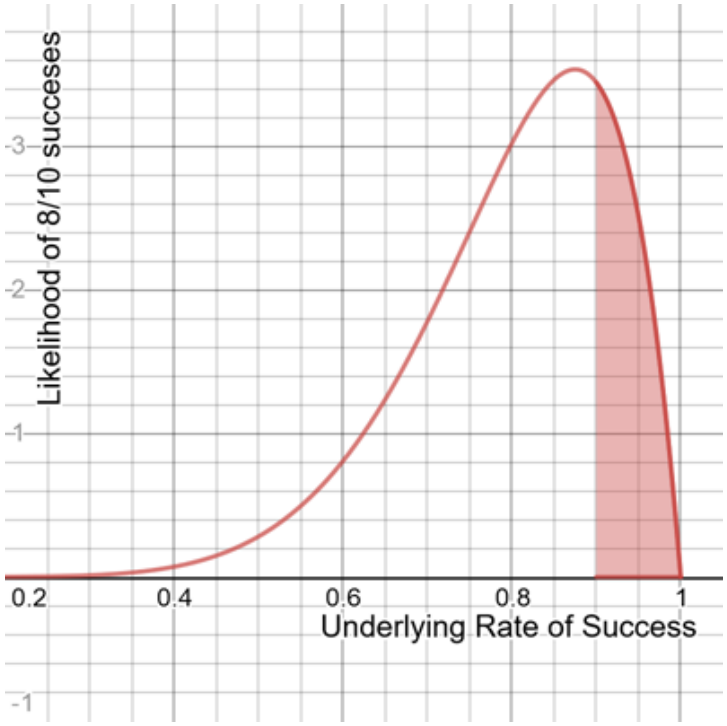


Figure 2-5. The probability of success being 90% or more

Our CDF only calculates area to the left of our boundary, not the right. Think about our rules of probability, and with a probability distribution the total area under the curve is 1.0. If we want to find the opposite probability of an event (greater than .90 as opposed to less than .90), just subtract the probability of being less than .90 from 1.0, and the remaining probability will capture being greater than .90. Here's a visual demonstrating how we do this subtraction in Figure 2-6.

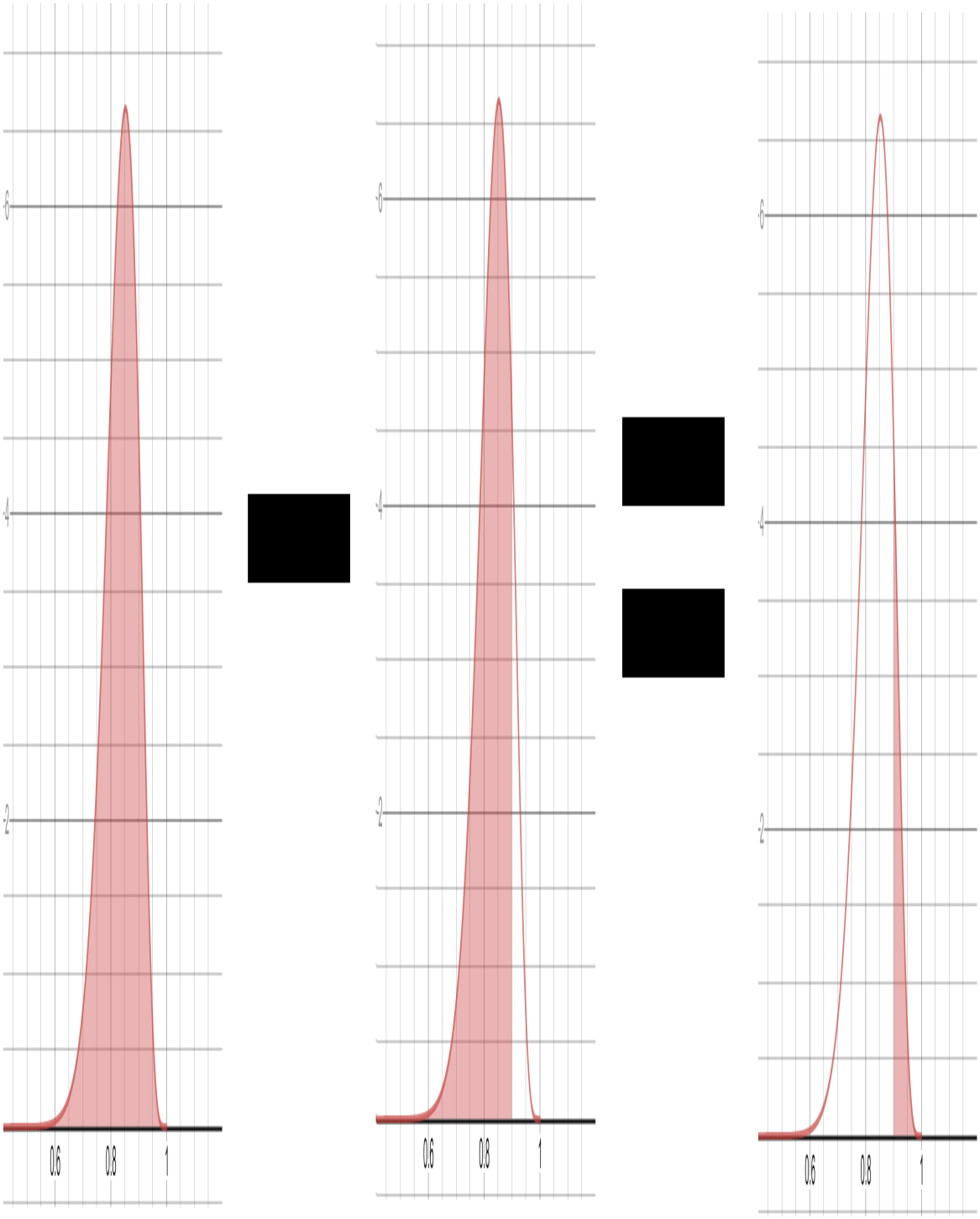


Figure 2-6. Finding the probability of success being greater than 90%

Example 2-4 shows how we calculate this subtraction operation in Python.

Example 2-4. Beta distribution using SciPy

```
from scipy.stats import beta

a = 8
b = 2

p = 1.0 - beta.cdf(.90, a, b)

# 0.22515902199999993
print(p)
```

So this means out of 8/10 successful engine tests, there is only a 22.5% chance the underlying success rate is 90% or greater. But there is about a 77.5% chance it is less than 90%. The odds are not in our favor here that our tests were successful, but we could gamble on that 22.5% chance with more tests if we are feeling lucky. If our CFO granted funding for 26 more tests resulting in 30 successes and 6 failures, here is what our Beta distribution would look now in Figure 2-7.

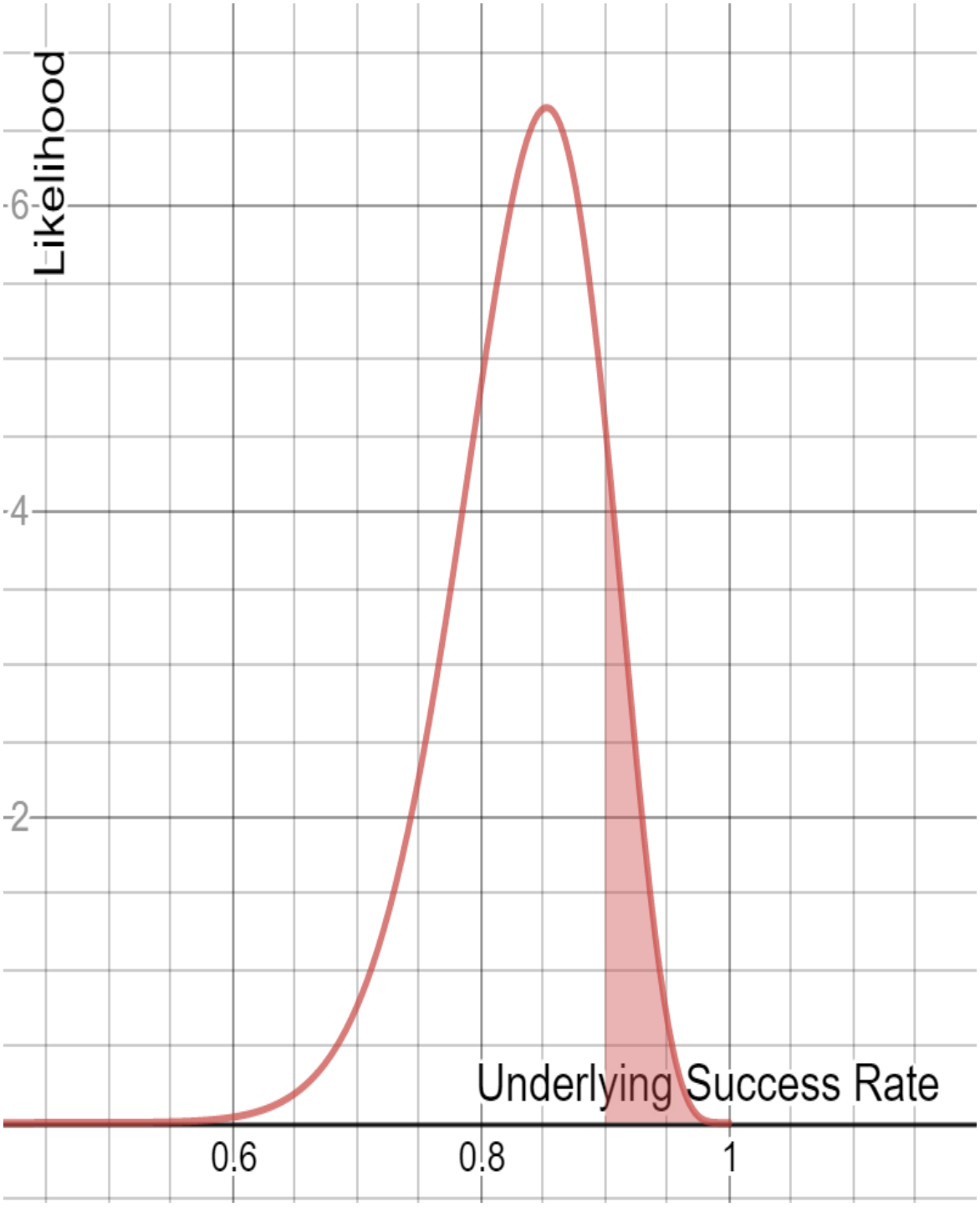


Figure 2-7. Beta distribution after 30 successes and 6 failures

Notice our distribution became narrower, thus becoming more confident that the underlying rate of success is in a smaller range. Unfortunately our probability of meeting our 90% success rate minimum has only decreased, going from 22.5% to 13.16% as shown in Example 2-5.

Example 2-5. Beta distribution using SciPy

```
from scipy.stats import beta

a = 30
b = 6

p = 1.0 - beta.cdf(.90, a, b)

# 0.13163577484183708
print(p)
```

At this point, it might be a good idea to walk away and stop doing tests, unless you want to keep gambling against that 13.16% chance and hope the peak moves to the right.

Last but not least, how would we calculate an area in the middle? What if I want to find the probability my underlying rate of success is between 80% and 90% as shown in Figure 2-8?

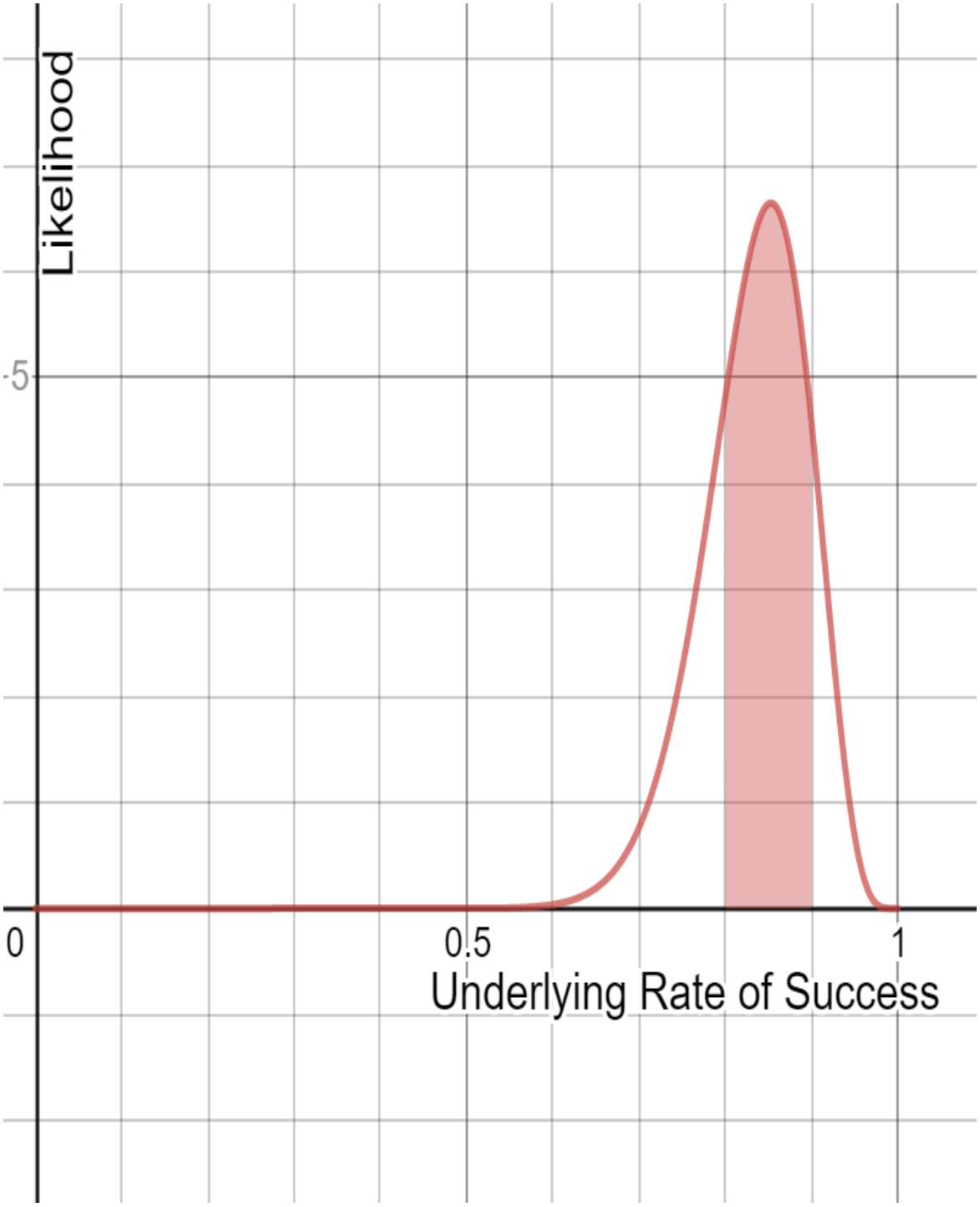


Figure 2-8. Probability the underlying rate of success is between 80% and 90%

Think carefully how you might approach this. What if we were to subtract the area behind .80 from the area behind .90 like in Figure 2-9?

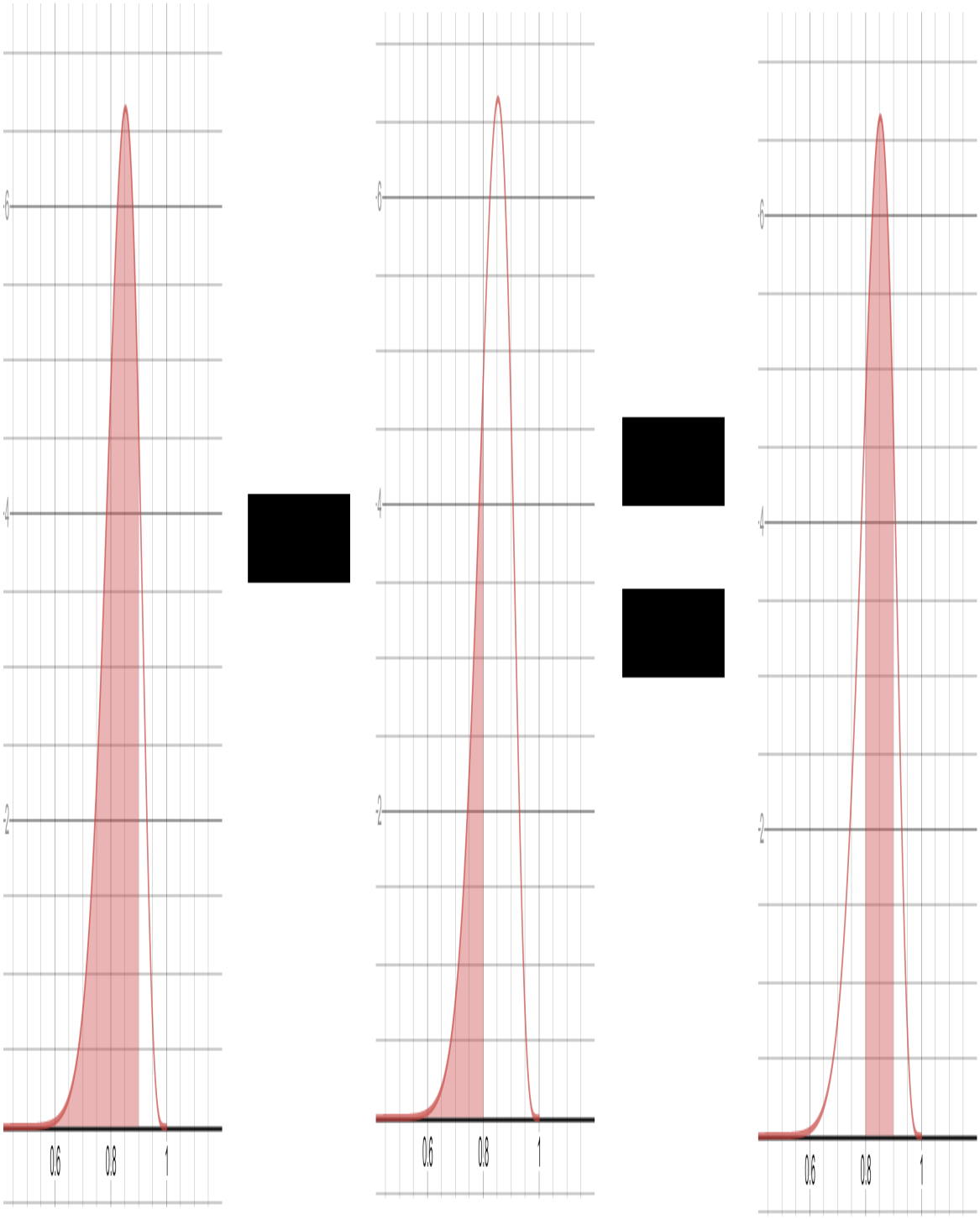


Figure 2-9. Obtaining the area between .80 and .90

Would that not give us the area between .80 and .90? Yes it would, and it would yield an area of .3386 or 33.86% probability. Here is how we would calculate it in Python in Example 2-6.

Example 2-6. Beta distribution middle area using SciPy

```
from scipy.stats import beta

a = 8
b = 2

p = beta.cdf(.90, a, b) - beta.cdf(.80, a, b)

# 0.33863336200000016
print(p)
```

The beta distribution is a fascinating tool to measure the probability of an event occuring versus not occurring, based on a limited set of observations. It allows us to reason about probabilities of probabilities, and we can update it as we get new data. We can also use it for hypothesis testing, but we will put more emphasis on using the normal distribution and t-distribution for that purpose in Chapter 3.

> **BETA DISTRIBUTION FROM SCRATCH**
>
> To learn how to implement the beta distribution from scratch, refer to Appendix A.

Conclusion

We covered a lot in this section! We not only covered the fundamentals of probability, its logical operators, and Bayes Theorem but we introduced probability distributions including the binomial and beta distributions. In the next chapter we will cover one of the more famous distributions, the normal distribution, and how it relates to hypothesis testing.

If you want to learn more about Bayesian probability and statistics, a great book is *Bayesian Statistics the Fun Way* by Will Kurt. There are also interactive Katacoda scenarios available on the O'Reilly platform. (NOTE TO EDITOR AND SELF: put links here?).

Exercises

1. There is a 30% chance of rain today, and a 40% chance your umbrella order will arrive on time. You are eager to walk in the rain today and cannot do so without either!

   What is the probability it will rain AND your umbrella will arrive?

2. There is a 30% chance of rain today, and a 40% chance your umbrella order will arrive on time.

   You will only be able to run errands if it does not rain or your umbrella arrives.

   What is the probability it will not rain OR your umbrella arrives?

3. There is a 30% chance of rain today, and a 40% chance your umbrella order will arrive on time.

   However, you found out if it rains there is only 20% chance your umbrella will arrive on time.

   What is the probability it will rain and your umbrella will arrive on time?

4. You have 137 passengers booked on a flight from Las Vegas to Dallas. However it is Las Vegas on a Sunday morning and you estimate each passenger is 40% likely to not show up.

   You are trying to figure out how many seats to overbook so the plane does not fly empty.

   How likely is it at least 50 passengers will not show up?

5. You flipped a coin 19 times and got heads 15 times and tails 4 times.

   Do you think this coin has any good probability of being fair? Why or why not?

Chapter 3. Descriptive and Inferential Statistics

A NOTE FOR EARLY RELEASE READERS

With Early Release ebooks, you get books in their earliest form—the author's raw and unedited content as they write—so you can take advantage of these technologies long before the official release of these titles.

This will be the 3rd chapter of the final book.

If you have comments about how we might improve the content and/or examples in this book, or if you notice missing material within this chapter, please reach out to the author at *thomasnield@live.com*.

Statistics is the practice of collecting and analyzing data to discover findings that are useful, or predict what causes those findings to happen. Probability often plays a large role in statistics, as we use data to estimate how likely an event is to happen.

It may not always get credit, but statistics is the heart of so many data-driven innovations. Machine learning in itself is a statistical tool, searching for possible hypotheses to correlate relationships between different variables in data. However there are a lot of blind sides in statistics, even for professional statisticians. We can so easily get caught up in the data that we forget to ask what is not captured in the data. These concerns become all the more important as "big data", "data mining", and "machine learning" all accelerate the automation of statistical algorithms. Therefore it is important to have a solid foundation in statistics and hypothesis testing, so you do not treat these automations as black boxes as so many do.

In this section we will cover the fundamentals of statistics and hypothesis testing. Starting with descriptive statistics, we will learn common ways to summarize data. After that we will venture into inferential statistics where we try to uncover attributes of a population based on a sample.

What is Data?

It may seem odd I have to define data, something we all use and take for granted. But I think it needs to be done. Chances are if you asked any person what is data, they might answer to the effect of "you know… data! It's… you know… information!" and not venture further than that. Nowadays it seems to be marketed as the be all and end all. The source of not just truth… but intelligence! It's the fuel for "artificial intelligence" and it is believed that the more data you have, the more truth you have. Therefore you can never have enough data. It will unlock the secrets needed to redefine your business strategy and maybe even create artificial general intelligence. But let me offer a pragmatic perspective on what data is. Data is not important in itself. It's the analysis of data (and how it is produced) that is the driver of all these innovations and solutions.

Imagine you were provided a photo of a family. Can you glean this family's story based on this one photo? What if you had 20 photos? 200 photos? 2000 photos? How many photos do you need to know their story? Do you need photos of them in different situations? Alone and together? With relatives and friends? At home and at work?

Data is just like photographs; it provides snapshots of a story. The continuous reality and contexts are not fully captured, as well as the infinite number of variables that are driving that story. As we will discuss, data may be biased. It can have gaps and be missing relevant variables. Ideally we would love to have an infinite amount of data capturing an infinite number of variables, with so much detail we could virtually recreate reality and construct alternate ones! But is this possible? Currently, no. Not even the greatest supercomputers in the world combined can come close to capturing the entirety of the world as data.

Therefore we have to narrow our scope to make our objectives feasible. A few strategic photos of the father playing golf can easily tell us whether he is good at golf. But trying to decipher his entire life story just through photos? That might be impossible. There is so much that cannot be captured in snapshots. These practical concerns should also be applied when working with data projects, because data is actually just snapshots of a given time capturing only what it is aimed at (much like a camera). We need to keep our objectives focused, as this hones in on gathering data that is relevant and complete. If we make our

objectives broad and open-ended, we can get into trouble with spurrious findings and incomplete datasets. This practice, known as **data mining**, has a time and place but it must be done carefully. We will revisit this at the end of the chapter.

Even with narrowly defined objectives, we can still run into problems with our data. Let's return to the question of determining whether a few strategic photos can tell whether the father is good at golf. Perhaps if you had a photo of him mid-swing you would be able to tell if he had good form. Or perhaps if you saw him cheering and fist-pumping at a hole, you can infer he got a good score. Maybe you can just take a photo of his scorecard! But it's important to note all these instances can be faked or taken out of context. Maybe he was cheering for someone else, or maybe the scorecard was not his or even forged. Just like these photographs, data does not capture context or truth. This is an incredibly important point because data provides clues, not truth. These clues can lead us to the truth or mislead us into erroneous conclusions.

This is why being curious about where data comes from is such an important skill. Ask questions on how the data was created, who it was created by, and what the data is not capturing. Nowadays it is too easy to get caught up in what the data says, and forgetting to ask where it came from. Even worse there are widespread sentiments that one can shovel data into machine learning algorithms and expect the computer to work it all out. But as the old adage goes, "garbage in, garbage out." No wonder only 13% of machine learning projects succeed according to VentureBeat [1]. Successful machine learning projects put thought and analysis into the data, as well as what produced the data.

[1] *https://venturebeat.com/2019/07/19/why-do-87-of-data-science-projects-never-make-it-into-production/*

Descriptive versus Inferential Statistics

What comes to mind when you hear the word "statistics"? Is it calculating mean, median, mode, charts, bell curves, and other tools to describe data? This is the most commonly understood part of statistics called **descriptive statistics** and we use it to summarize data. After all, is it more meaningful to scroll through a million records of data or have it summarized? We will cover this area of statistics first.

Inferential statistics tries to uncover attributes about a larger population, often based on a sample. It is often misunderstood and less intuitive than descriptive statistics. Oftentimes we are interested in studying a group that is too large to observe (e.g. average height of adolescents in North America) and we have to resort to using only a few members of that group to infer conclusions about them. As you can guess, this is not easy to get right. After all, we are trying to represent a population with a sample which may not be representative. We will explore these caveats along the way.

Populations, Samples, and Bias

Before we dive deeper into descriptive and inferential statistics, it might be a good idea to lay out some definitions and relate them with tangible examples.

A **population** is a particular group of interest we want to study, such as "all seniors over the age of 65 in the North America", "all golden retrievers in Scotland," or "current high school sophomores at Los Altos High School." Notice how we have boundaries on defining our population. Some of these boundaries are broad and capture a large group over a vast geography or age group. Others are highly specific and small such as the sophomores at Los Altos High School. How you hone in on defining a population depends on what you are interested in studying.

A **sample** is a subset of the population that is ideally random and unbiased, which we use to infer attributes about the population. We often have to study samples because polling the entire population is not always possible. Of course, some populations are easier to get a hold of if they are small and accessible. But measuring all seniors over 65 in North America? That is unlikely to be practical!

POPULATIONS CAN BE ABSTRACT!

It is important to note that populations can be theoretical and not physically tangible. In these cases our "population" acts more like a sample from something abstract. Here's my favorite example: we are interested in flights that depart between 2PM and 3PM at an airport, but we lack enough flights at that time to reliably predict how often these flights are late. Therefore we may treat this "population" as a sample instead… from an underlying population of all theoretical flights taking off between 2PM and 3PM.

Problems like this are why many researchers resort to simulations to generate data. Simulations can be useful but rarely are accurate, as simulations only capture so many variables and have assumptions built in.

If we are going to infer attributes about a population based on a sample, it's important the sample be as random as possible so we do not skew our conclusions. Here's an example. Let's say I'm a college student at Arizona State University. I want to find the average number of hours college students watch television per week in the United States. I walk right outside my dorm and start polling random students walking by, finishing my data gathering in a few hours. What's the problem here?

The problem is our student sample is going to have **bias**, meaning it skews our findings by overrepresenting a certain group at the expense of other groups. My study defined the population to be "college students in the United States," not "college students at Arizona State University." I am only polling students at one specific university to represent all college students in the entire United States! Is that really fair?

It is unlikely all colleges across the country homogeneously have the same student attributes. What if Arizona State students watch far more TV than other students at other universities? Would that not distort the results using them to represent the entire country? Maybe this is possible because it is usually too hot to go outside in Tempe, Arizona. Therefore TV is a common pastime (anecdotally I would know, I lived in Phoenix for many years). Other college students in milder climates may do more outdoor activities and watch less TV.

This is just one possible variable showing why it's a bad idea to represent college students across the entire United States with just a sample of students from one university. Ideally, I should be randomly polling college students all

over the country at different universities. That way I have a more representative sample.

However, bias is not always geographic. Let's say I put a sincere effort to poll students across the United States. I arrange a social media campaign to have a poll shared by various universities on Twitter and Facebook. This way their students see it and hopefully fill it out. I get hundreds of responses on students' TV habits across the country and feel I've conquered the bias beast… or have I?

What if students who are on social media enough to see the poll are also likely to watch more TV? If they are on social media a lot, they probably do not mind recreational screen time. It's easy to imagine they have Netflix and Hulu ready to stream on that other tab! This particular type of bias where a specific group is more likely to include themselves in a sample is known as **self-selection bias**.

SAMPLES AND BIAS IN MACHINE LEARNING

These problems with sampling and bias extends to machine learning as well. Whether it is linear regression, logistic regression, or neural networks, a sample of data is used to infer predictions. If that data is biased then it will steer the machine learning algorithm to make biased conclusions.

There are many documented cases of this. Criminal justice has been a precarious application of machine learning because it has repeatedly shown to be biased in every sense of the word, discriminating against minorities due to minority-heavy datasets. In 2017, Volvo tested "self-driving cars" that were trained on datasets capturing deer, elk, and caribou. However it had no driving data in Australia and therefore could not recognize kangaroos, much less make sense of their jumping movements! Both of these are examples of biased data.

Darn it! You just can't win, can you?! If you think about it long enough, data bias just feels inevitable! And oftentimes it is. So many **confounding variables**, or factors we did not account for, can influence our study. This problem of data bias is expensive and difficult to overcome, and machine learning is especially vulnerable to it.

The way to overcome this problem is to truly at random select students from the entire population, and they cannot elect themselves into or out of the sample voluntarily. This is the most effective way to mitigate bias, but as you can imagine it takes a lot of coordinated resources to do.

A WHIRLWIND TOUR OF BIAS TYPES

As humans, we are strangely wired to be biased. We look for patterns even if they do not exist. Perhaps this was a necessity for survial in our early history, as finding patterns make hunting, gathering, and farming more productive.

There are many types of bias, but they all have the same effect of distorting findings. **Confirmation bias** is only gathering data that supports your belief, which can even be done unknowningly. An example of this is only following social media accounts you politically agree with, reinforcing your beliefs rather than challenging them.

We just discussed **self-selection bias**, which is when certain types of subjects are more likely to include themselves in the experiment. Walking onto a flight and polling the customers if they like the airline over other airlines, and using that to rank customer satisfaction amongst all airlines, is silly. Why? Many of those customers are likely repeat customers, and they have created self-selection bias. We do not know how many are first-time fliers or repeat fliers, and of course the latter is going to prefer that airline over other airlines. Even first-time fliers may be biased and self-selected, because they chose to fly that airline and we are not sampling all airlines.

Survival bias only captures living and survived subjects, while the deceased ones are never accounted for. It is the most fascinating type of bias in my opinion, because the examples are so diverse and unobvious.

Probably the most famous example of survival bias is this: The Royal Air Force in WWII was having trouble with German enemy fire causing casualties on its bombers. Their initial solution was to armor bombers where bullet holes were found, reasoning this would improve their likelihood of survival. However a mathemetican named Abraham Wald pointed to them this was fatally wrong. He proposed armoring areas on the aircraft that *did not* have bullet holes. Was he insane? Far from. The bombers that returned obviously did not have fatal damage where bullet holes were found. How do we know this? Because they returned from their mission! But what of the aircraft that did not return? Where were they hit? Wald's theory was likely in the areas untouched in the aircraft *that survived* and returned to base, and

this proved right. Those areas without bullet holes were armored and the survivability of aircraft and pilots increased. This unorthodox observation is credited with turning the tide of war in favor of the Allies.

There are other fascinating examples of survivor bias that are less obvious. Many management consulting companies and book publishers like to identify traits of successful companies/individuals and use them as predictors for future successes. These works are pure survival bias (and XKCD has a funny cartoon about this. These works do not account for companies/individuals that failed in obscurity, and these "success" qualities may be commonplace with failed ones as well. We just have not heard about them because they never had a spotlight.

An anecdotal example that comes to my mind is Steve Jobs. On many accounts, he was said to be passionate and hot-tempered… but he also created one of the most valuable companies of all time. Therefore some people believed being passionate and even temperamental might correlate with success. Again, this is survivor bias. I am willing to bet there are many companies run by passionate leaders that failed in obscurity, but we fixate and latch onto outlier success stories like Apple.

Lastly, in 1987 there was a veterinary study showing that cats who fell from 6 stories or less had greater injuries than those that fell more than 6 stories. Prevailing scientific theories postulated that cats righted themselves at about 5 stories, giving them enough time to brace for impact and inflict less injury. But then a publication *The Straight Dope* posed an important question: what happened to the dead cats? People are not likely to bring a dead cat to the vet and therefore it is unreported how many cats died from higher falls. In the words of Homer Simpson, "*D'oh!*".

Alright, enough talk about populations, samples, and bias. Let's move onto some math and descriptive statistics. Just remember that math and computers do not recognize bias in your data. That is on you to detect as a good data science professional! Always ask questions about how the data was obtained, and then scrutinize how that process could have biased the data.

Descriptive Statistics

Descriptive statistics is the area most people are familiar with. We will touch on the basics like mean, median, and mode followed by variance, standard deviation, and the normal distribution.

Mean and Weighted Mean

The **mean** is the average of a set of values. The operation is simple to do: sum the values and divide by the number of values. The mean is useful because it shows where the "center of gravity" exists for an observed set of values.

The mean is calculated the same way for both populations and samples. Example 3-1 shows a sample of 8 values and how to calculate their mean in Python.

Example 3-1. Calculating mean in Python

```
# Number of pets each person owns
sample = [1, 3, 2, 5, 7, 0, 2, 3]

mean = sum(sample) / len(sample)

print(mean) # prints 2.875
```

As you can see, we polled 8 people and the number of pets they own. The sum of the sample is 23 and the number of items in the sample is 8, so this gives us a mean of 2.875 as $23/8 = 2.875$.

There are two versions of the mean you will see: the sample mean $\overline{x}$ and the population mean μ as expressed below:

$$\overline{x} = \frac{x_1 + x_2 + x_3 + \ldots + x_n}{n} = \sum \frac{x_i}{n}$$

$$\mu = \frac{x_1 + x_2 + x_3 + \ldots + x_n}{N} = \sum \frac{x_i}{N}$$

Recall the summation symbol $\sum$ means add all the items together. The *n* and the *N* represent the sample and population size respectively, but mathematically they represent the same thing: the number of items. The same goes for calling the sample mean $\overline{x}$ ("x-bar") and the population mean μ ("mu"). Both $\overline{x}$ and μ are the same calculation, just different names depending on whether it's a sample or population we are working with.

The mean is likely familar to you, but here's something less known about the mean: the mean is actually a weighted average called the **weighted mean**. The mean we commonly use gives equal importance to each value. But we can manipulate the mean and give each item a different weight.

$$\text{weighted mean} = \frac{(x_1 \cdot w_1) + (x_2 \cdot w_2) + (x_3 \cdot w_3) + \ldots (x_n \cdot w_n)}{w_1 + w_2 + w_3 + \ldots + w_n}$$

This can be helpful when we want some values to contribute to the mean more than others. A common example of this is weighting academic exams to give a final grade. If you have 3 exams and a final exam, and we give each of the 3 exams 20% weight and the final exam 40% weight of the final grade, here is how we express it in Example 3-2.

Example 3-2. Calculating a weighted mean in Python

```
# Three exams of .20 weight each and final exam of .40 weight
sample = [90, 80, 63, 87]
weights = [.20, .20, .20, .40]

weighted_mean = sum(s * w for s,w in zip(sample, weights)) /
sum(weights)

print(weighted_mean) # prints 81.4
```

We weight each exam score through multiplication accordingly and instead of dividing by the value count, we divide by the sum of weights. Weightings don't have to be percentages, as any numbers used for weights will end up being proportionalized. In Example 3-3, we weight each exam with "1" but weight the final exam with "2", giving it twice the weight of the exams. We will still get the same answer of `81.4` as these values will still be proportionalized.

Example 3-3. Calculating a weighted mean in Python

```
# Three exams of .20 weight each and final exam of .40 weight
sample = [90, 80, 63, 87]
weights = [1.0, 1.0, 1.0, 2.0]

weighted_mean = sum(s * w for s,w in zip(sample, weights)) /
sum(weights)

print(weighted_mean) # prints 81.4
```

Median

The **median** is the middle-most value in a set of ordered values. You sequentially order the values, and the median will be the center-most value. If you have an even number of values, you average the two center-most values. We can see in Example 3-4 the median number of pets owned in our sample is 7.

```
  0, 1, 5, *7*, 9, 10, 14
```

Example 3-4. Calculating the median in Python

```
# Number of pets each person owns
sample = [0, 1, 5, 7, 9, 10, 14]

def median(values):
    ordered = sorted(values)
    print(ordered)
    n = len(ordered)
    mid = int(n / 2) - 1 if n % 2 == 0 else int(n/2)

    if n % 2 == 0:
        return (ordered[mid] + ordered[mid+1]) / 2.0
    else:
        return ordered[mid]

print(median(sample)) # prints 5
```

The median can be a helpful alternative to the mean when data is skewed by **outliers**, or values that are extremely large and small compared to the rest of the values. Here's an interesting anecdote to understand why. In 1986, the mean annual starting salary of geography graduates in the University of North Carolina was $250,000. Other universities averaged $22,000. Wow, UNC must have an amazing geography program!

But in reality, what was so lucrative about UNC's geography program? Well… they had Michael Jordan as one of their graduates. One of the most famous NBA players of all time indeed graduated with a geography degree from University of North Carolina. However he started his career playing basketball, not studying maps. Obviously this is a confounding variable which has created a huge outlier, and it majorly skewed the income average.

This is why the median can be preferable in outlier-heavy situations (such as income-related data) over the mean. It is less senstive to outliers and cuts data strictly down the middle based on their relative order, rather than where they fall

exactly on a number line. When your median is very different from mean, that means you have a skewed dataset with outliers.

THE MEDIAN IS A QUANTILE

There is a concept of **quantiles** in descriptive statistics. The concept of quantiles is essentially the same as a median, just cutting the data in other places besides the middle. The median is actually the 50% quantile, or the value where 50% of ordered values are behind it. Then there is the 25%, 50%, 75% quantiles which are known as **quartiles** as they cut data in 25% increments.

Mode

The **mode** is the most frequently occurring set of values. It primarily becomes useful when your data is repetitive and you want to find which values occur the most frequently.

When no value occurs more than once, there is no mode. When two values occur with an equal amount of frequency, then the dataset is considered **bimodal**. In Example 3-5 we calculate the mode for our pet dataset, and sure enough we see this is bimodal as both 2 and 3 occur the most (and equally) as often.

Example 3-5. Calculating the mode in Python

```
# Number of pets each person owns
from collections import defaultdict

sample = [1, 3, 2, 5, 7, 0, 2, 3]

def mode(values):
    counts = defaultdict(lambda: 0)

    for s in values:
        counts[s] += 1

    max_count = max(counts.values())
    modes = [v for v in set(values) if counts[v] == max_count]
    return modes

print(mode(sample)) # [2, 3]
```

In practicality, the mode is often not used a lot unless your data is repetitive. This is commonly encountered with integers, categories, and other discrete variables.

Variance and Standard Deviation

When we start talking about variance and standard deviation, this is where it gets interesting. One thing that confuses people with variance and standard deviation is there are some calculation differences for the sample versus the population. We will do our best to cover these differences clearly.

Population Variance and Standard Deviation

In describing data, we are often interested in measuring the differences between the mean and every data point. This gives us a sense of how "spread out" the data is.

Let's say I'm interested in studying the number of pets owned by members of my work staff (note that I'm defining this as my population, not a sample). I have 7 people on my staff.

I take the mean of all the numbers of pets they own, and I get 6.571. Let's subtract this mean from each value. This will show us how far each value is from the mean as shown in Table 3-1.

Table 3-1. Number of pets my staff owns

Value	Mean	Difference

0	6.571	-6.571
1	6.571	-5.571
5	6.571	-1.571
7	6.571	0.429
9	6.571	2.429
10	6.571	3.429
14	6.571	7.429

Let's visualize this on a number line with "X" showing the mean in Figure 3-1.

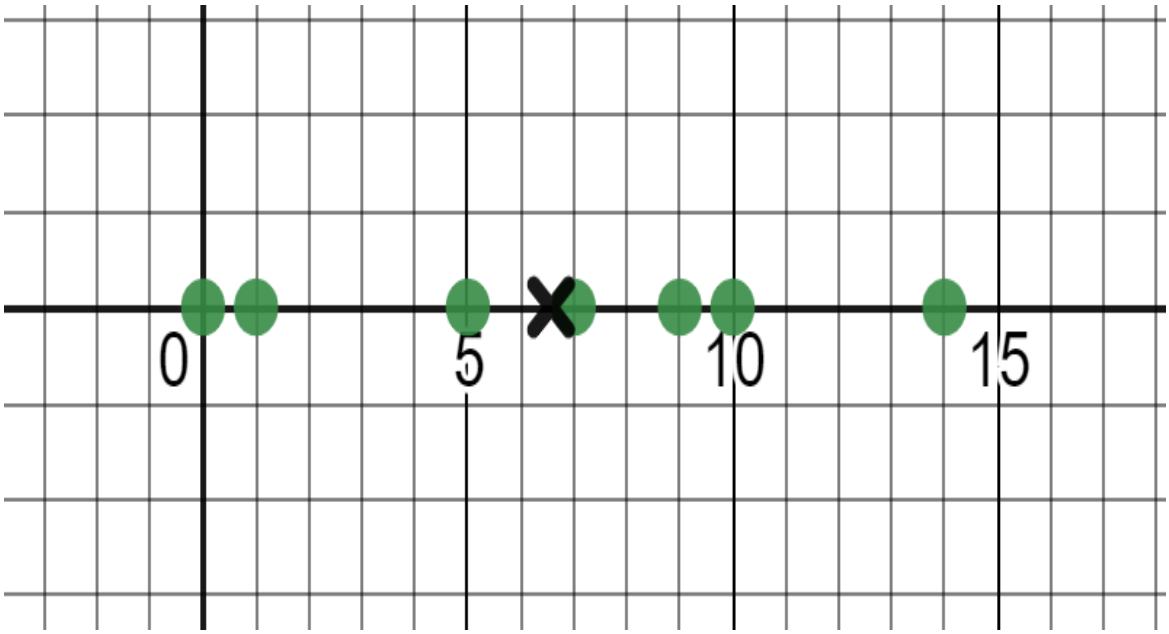


Figure 3-1. Visualizing the spread of our data, where "X" is the mean

Hmmm… now consider why the information above can be useful. The differences give us a sense of how "spread out" the data is, and how far values are from the mean. Is there a way we can consolidate these differences into a single number to quickly describe how spread out the data is?

You may be tempted to take the average of the differences, but the negatives and positives will cancel each other out when they are summed. We could sum the

absolute values (rid the negative signs and make all values positive). An even better approach would be to square these differences before summing them. This not only rids the negative values (because squaring a negative number makes it positive), but it amplifies larger differences. After that, average the squared differences. This will give us the **variance**, a measure of how spread out our data is.

Here is a math formula showing how to calculate variance:

$$\text{population variance} = \frac{(x_1 - mean)^2 + (x_2 - mean)^2 + \ldots + (x_n - mean)^2}{N}$$

More formally, here is the variance for a population.

$$\sigma^2 = \frac{\sum (x_i - \mu)^2}{N}$$

Calculating the population variance of our pet example in Python is shown in Example 3-6.

Example 3-6. Calculating variance in Python

```
# Number of pets each person owns
data = [0, 1, 5, 7, 9, 10, 14]

def variance(values):
    mean = sum(values) / len(values)
    _variance = sum((v - mean) ** 2 for v in values) / len(values)
    return _variance

print(variance(data))  # prints 21.387755102040813
```

So the variance for number of pets owned by my office staff is 21.387755. Okay, but what does it exactly mean? It's reasonable to conclude that a higher variance means more spread, but how do we relate this back to our data? This number is larger than any of our observations because we did a lot squaring and summing, putting it on an entirely different metric. So how do we squeeze it back down so it's back on the scale we started with?

The opposite of a square is a square root, so let's take the square root of the variance which gives us the **standard deviation**. This is the variance scaled into a number expressed in terms of "number of pets" which makes it a bit more meaningful.

$$\sigma = \sqrt{\frac{\sum (x_i - \mu)^2}{N}}$$

To implement in Python, we can reuse the `variance()` function and `sqrt()` its result. We now have a `std_dev()` function shown in Example 3-7.

Example 3-7. Calculating standard deviation in Python

```
from math import sqrt

# Number of pets each person owns
data = [0, 1, 5, 7, 9, 10, 14]

def variance(values):
    mean = sum(values) / len(values)
    _variance = sum((v - mean) ** 2 for v in values) / len(values)
    return _variance

def std_dev(values):
    return sqrt(variance(values))

print(std_dev(data))  # prints 4.624689730353898
```

Running the code in Example 3-7, you will see our standard deviation is approximately 4.62 pets. So we can express our spread on a scale we started with, and this makes our variance a bit easier to interpret. We will see some important applications of the standard deviation in this chapter as well as future chapters, including Chapter 5.

> **WHY THE SQUARE?**
>
> If the exponent in σ^2 bothers you, it's because it is prompting you to take the square root of it to get the standard deviation. It's like a little reminder you are dealing with squared values that need to be square-rooted.

Sample Variance and Standard Deviation

In the previous section we talked about variance and standard deviation for a population. However there is an important tweak we need to apply to these two formulas when we calculate for a sample:

$$s^2 = \frac{\sum (x_i - \overline{x})^2}{n - 1}$$

$$s = \sqrt{\frac{\sum (x_i - \overline{x})^2}{n - 1}}$$

Did you catch the difference? When we average the squared differences, we divide by `n-1` rather than the total number of items *n*. Why would we do this? We do this to decrease any bias in a sample, and not underestimate the variance of the population based on our sample. By counting values short of 1 item in our divisor, we increase the variance and therefore capture greater uncertainty in our sample.

WHY DO WE SUBTRACT 1 FOR SAMPLE SIZE?

On YouTube, Josh Starmer has an excellent video series called StatQuest. In one, he gives an excellent breakdown why we treat samples differently in calculating variance and subtract one element from the number of items.

https://www.youtube.com/watch?v=sHRBg6BhKjI

If our pets data were a sample, not a population, we should make that adjustment accordingly. In Example 3-8, I modify my previous `variance()` and `std_dev()` Python code to optionally provide a parameter `is_sample`, which if *True* will subtract 1 from the divisor in the variance.

Example 3-8. Calculating standard deviation in Python

```
from math import sqrt

# Number of pets each person owns
data = [0, 1, 5, 7, 9, 10, 14]


def variance(values, is_sample: bool = False):
    mean = sum(values) / len(values)
    _variance = sum((v - mean) ** 2 for v in values) /
      (len(values) - (1 if is_sample else 0))

    return _variance
```

```
def std_dev(values, is_sample: bool = False):
    return sqrt(variance(values, is_sample))

print("VARIANCE = {}".format(variance(data, is_sample=True))) #
24.95238095238095
print("STD DEV = {}".format(std_dev(data, is_sample=True))) #
4.99523582550223
```

Notice in Example 3-8 my variance and standard deviation have increased compared to previous examples that treated them as a population, not a sample. Recall in Example 3-7 that the standard deviation was about 4.62 treating as a population. But here treating as a sample (by subtracting 1 from the variance denominator) we get approximately 4.99. This is correct as a sample could be biased and imperfect representing the population. Therefore we increase the variance (and thus the standard deviation) to increase our estimate how spread out the values are. A larger variance/standard deviation shows less confidence with a larger range.

To recap, just like the mean ($\overline{x}$ for sample and μ for population), you will often see certain symbols for variance and standard deviation. The standard deviation for a sample and mean are specified by s and sigma σ respectively. Here again are the sample and population standard deviation formulas:

$$s = \sqrt{\frac{\sum (x_i - \overline{x})^2}{n - 1}}$$

$$\sigma = \sqrt{\frac{\sum (x_i - \mu)^2}{N}}$$

The variance will be the square of these two formulas, undoing the square root. Therefore the variance for sample and population are s^2 and σ^2 respectively.

$$s^2 = \frac{\sum (x_i - \overline{x})^2}{n - 1}$$

$$\sigma^2 = \frac{\sum (x_i - \mu)^2}{N}$$

The square helps imply that a square root should be taken to get the standard deviation.

The Normal Distribution

We touched on probability distributions in the last chapter, particularly the binomial distribution and beta distribution. However the most famous distribution of all is the normal distribution. The **normal distribution**, also known as the **Gaussian distribution**, is a symmetrical bell-shaped distribution that has most mass around the mean, and its spread is defined as a standard deviation. The "tails" on either side become thinner as you move away from the mean.

Here is a normal distribution for golden retriever weights. Notice how most of the mass is around the mean of 64.43 pounds. Let's explore how we encounter the normal distribution in Figure 3-2.

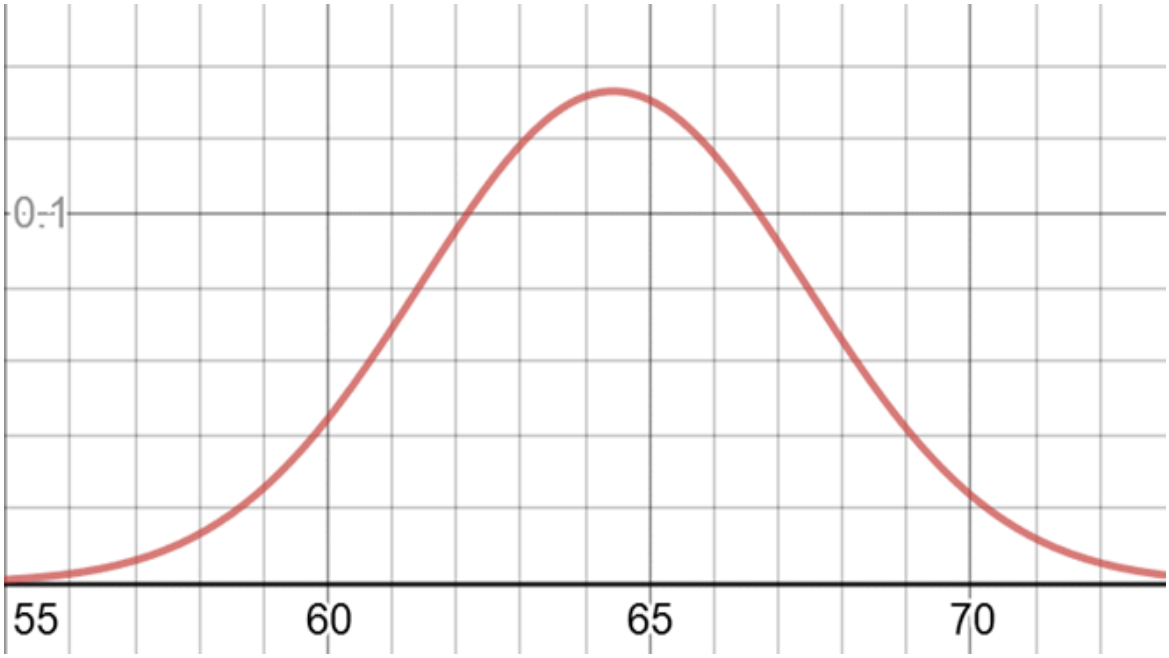


Figure 3-2. A normal distribution

Discovering the Normal Distribution

The normal distribution is seen a lot in nature, engineering, science, and other domains. How do we discover it? Let's say we sample the weight of 50 adult golden retrievers and plot them on a number line as shown in Figure 3-3.

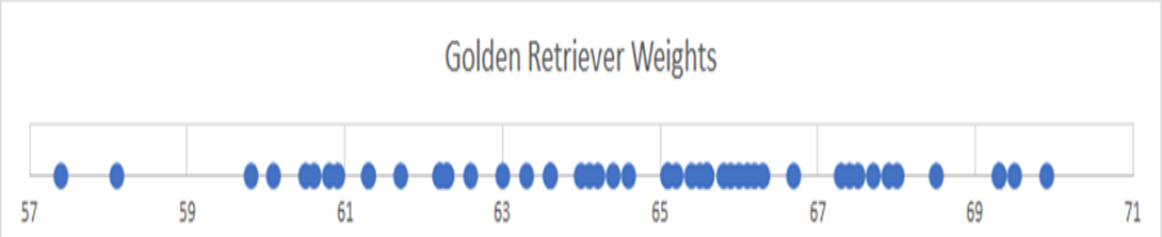


Figure 3-3. A sample of 50 golden retriever weights

Notice how we have more values towards a center, but as we move further left or right we see less values. Based on our sample, it seems highly unlikely we would see a golden retriever with a weight of 57 or 71. But having a weight of 64 or 65? Yeah that certainly seems likely.

Is there a better way to visualize this likelihood to see which golden retriever weights we are more likely to see sampled from the population? We can try to create a **histogram**, which buckets (or "bins") up values based on numeric ranges of equal length, and then uses a bar chart showing the number of values within each range. In Figure 3-4 we create a histogram that bins up values in ranges of .5 pounds.

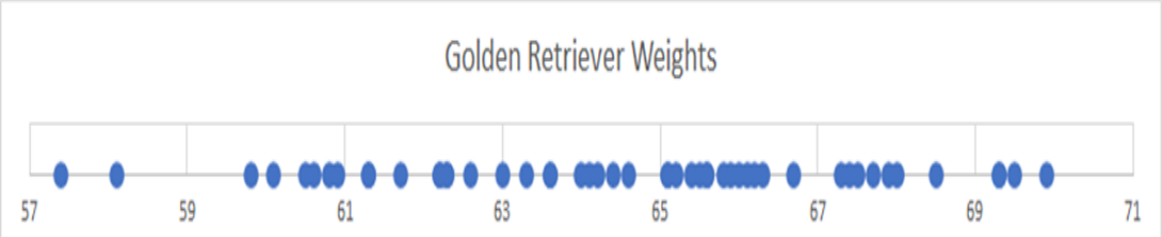


Figure 3-4. A histogram of golden retriever weights

This histogram above does reveal any meaningful shape to our data. The reason is because our bins are too small. We do not have an extremely large or infinite amount of data to meaningfully have enough points in each bin. Therefore we will have to make our bins larger. Let's make the bins each have a length of 3 pounds in Figure 3-5.

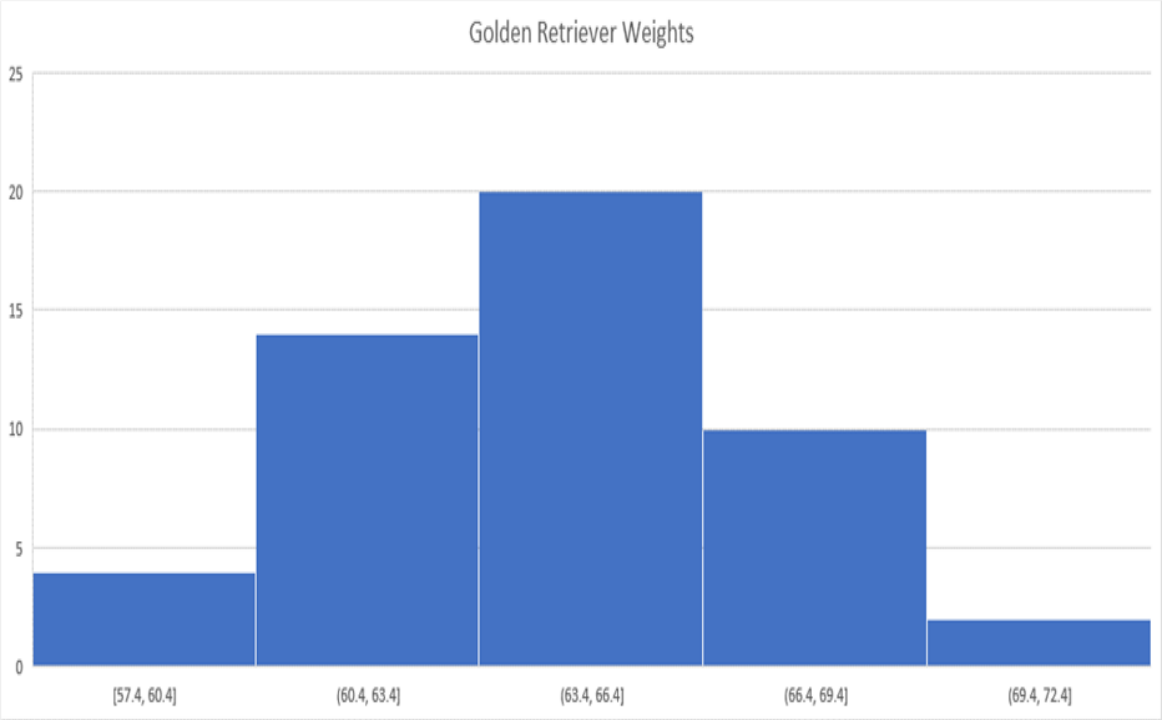


Figure 3-5. A more productive histogram

Alright now we are getting somewhere! As you can see above, if we get the bin sizes just right (in this case each has a range of 3 lbs), we start to get a meaningful bell shape to our data. It's not a perfect bell shape because our samples are never going to be perfectly representative of the population, but this is likely evidence our sample follows a normal distribution. If we fit a histogram with adequate bin sizes, scale it so it has an area of 1.0 (which a probability distribution requires), we roughly see a bell curve representing our sample. Let's show it alongside our original data points in Figure 3-6.

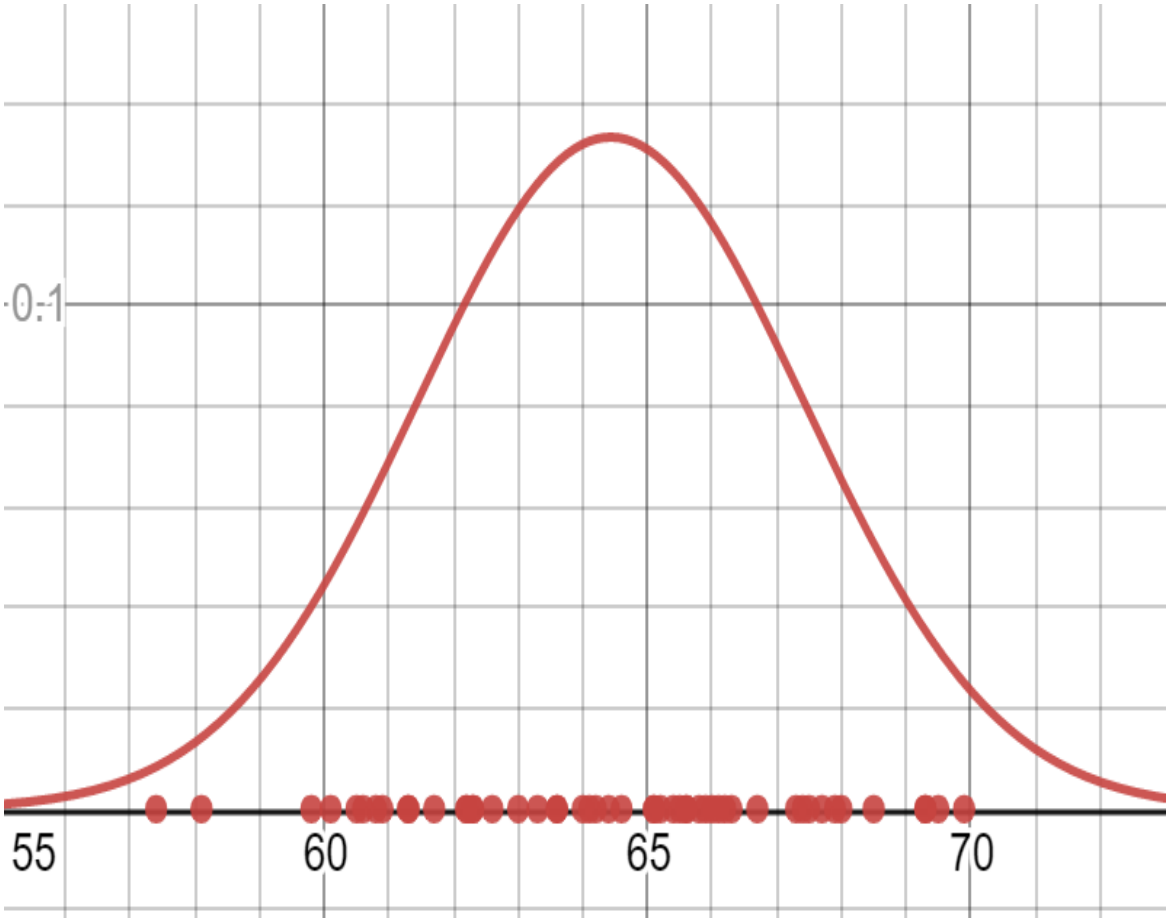


Figure 3-6. A normal distribution fitted to data points

Looking at the bell curve above, we can reasonably expect a golden retriever to have a weight most likely around 64.43 (the mean), but is unlikely at 55 or 73. Anything more extreme than that becomes virtually unlikely.

Properties of a Normal Distribution

The normal distribution has several important properties that make it useful:

- It's symmetrical, both sides are identically mirrored at the mean which is the center
- Most mass is at the center around the mean
- It has a spread (being narrow or wide) that is specified by standard deviation.
- The "tails" are the least likely outcomes, and approach zero infinitely but never touch zero.

- It resembles a lot of phenomena in nature and daily life, and even generalizes non-normal problems because of the central limit theorem which we will talk about shortly.

The Probability Density Function (PDF)

The standard deviation plays an important role in the normal distribution, because it defines how "spread out" it is. It is actually one of the parameters alongside the mean. The **probability density function (PDF)** that creates the normal distribution is as follows:

$$f(x) = \frac{1}{(\text{std dev}) * \sqrt{2\pi}} * e^{-\frac{1}{2}\left(\frac{x-mean}{(\text{std dev})}\right)^2}$$

Wow that's a mouthful, isn't it? We even see our friend Euler's Number *e* from Chapter 1 and some crazy exponents. Here is how we can express it in Python in Example 3-9.

Example 3-9. The normal distribution function in Python

```
# normal distribution, returns likelihood
def normal_pdf(x: float, mean: float, std_dev: float) -> float:
    return (1.0 / (2.0 * math.pi * std_dev ** 2) ** 0.5) *
        math.exp(-1.0 * ((x - mean) ** 2 / (2.0 * std_dev ** 2)))
```

There's a lot to take apart here in this formula, but what's important is that it accepts a mean and standard deviation as parameters, as well as an *x* value so you can look up the likelihood at that given value.

Just like the beta distribution in Chapter 2, the normal distribution is continuous. This means to retrieve a probability we need to integrate a range of x values to find an area.

In practice though, we will use SciPy to do these calculations for us.

Integrating the Normal Distribution

With the normal distribution, the vertical axis is not the probability but rather the likelihood for the data. To find the probability we need to look at a given range, and then find the area under the curve for that range. Let's say I want to find the probability of a golden retriever weighing between 62 and 66 pounds. Here is a visual in Figure 3-7 of the range we want to find the area for.

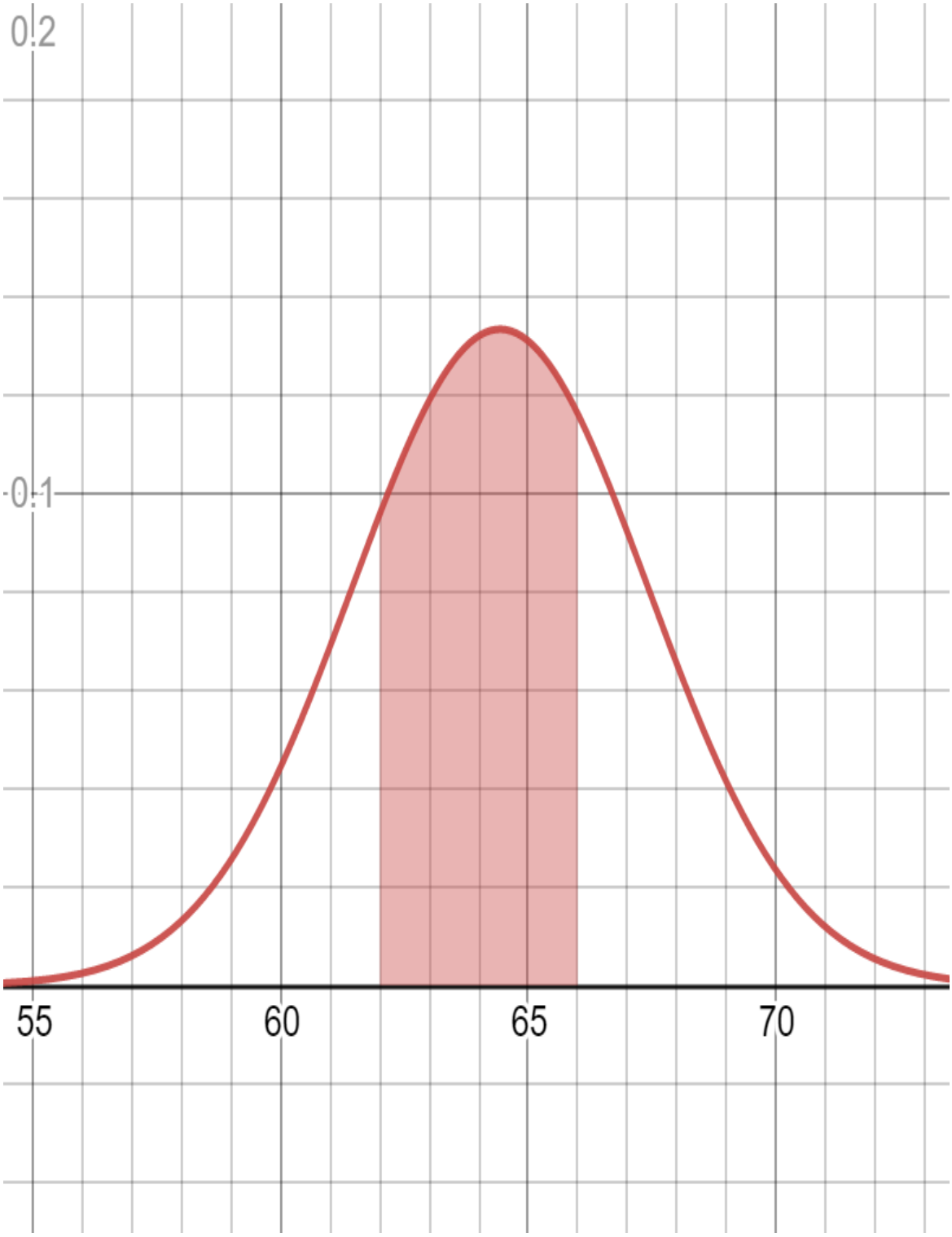


Figure 3-7. A cumulative density function (CDF) measuring probability between 62 and 66 pounds

We already did this task in Chapter 2 with the Beta distribution, and just like the Beta distribution there is a cumulative density function (CDF). Let's follow this

approach.

Integrating using the Cumulative Density Function (CDF)

As we learned in the last chapter, the cumulative density function (CDF) provides the area *up to* a given x-value for a given distribution. Let's see what the CDF looks like for our golden retriever normal distribution, and put it alongside the PDF for reference in Figure 3-8.

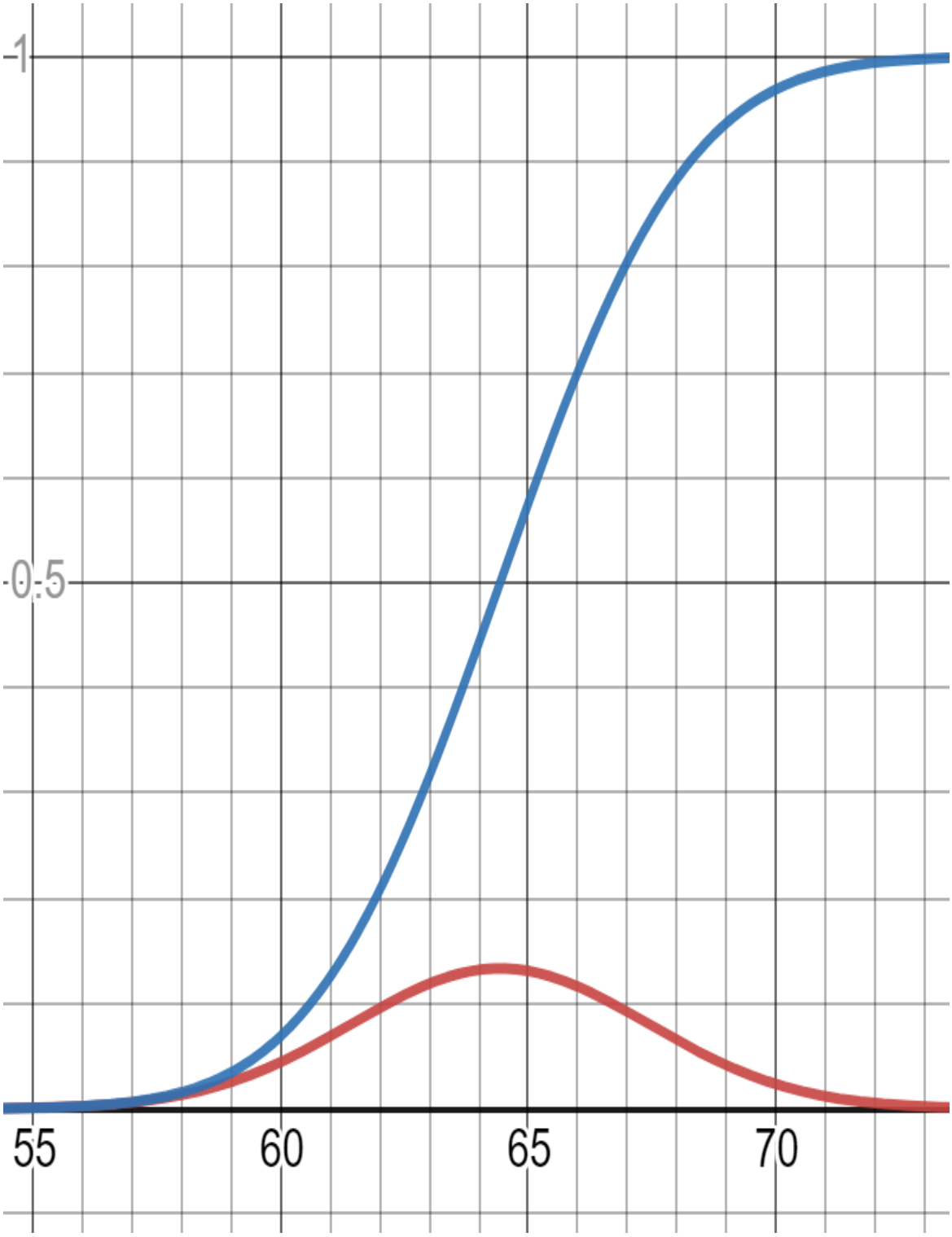


Figure 3-8. A probability density function (PDF) alongside its cumulative density function (CDF)

Notice there's a relationship between the two graphs. The CDF, which is an S-shaped curve (called a sigmoid curve), projects the area up to that range in the

PDF. Observe in Figure 3-9 that when we capture the area from negative infinity up to 64.43 (the mean), our CDF shows a value of exactly .5 or 50%!

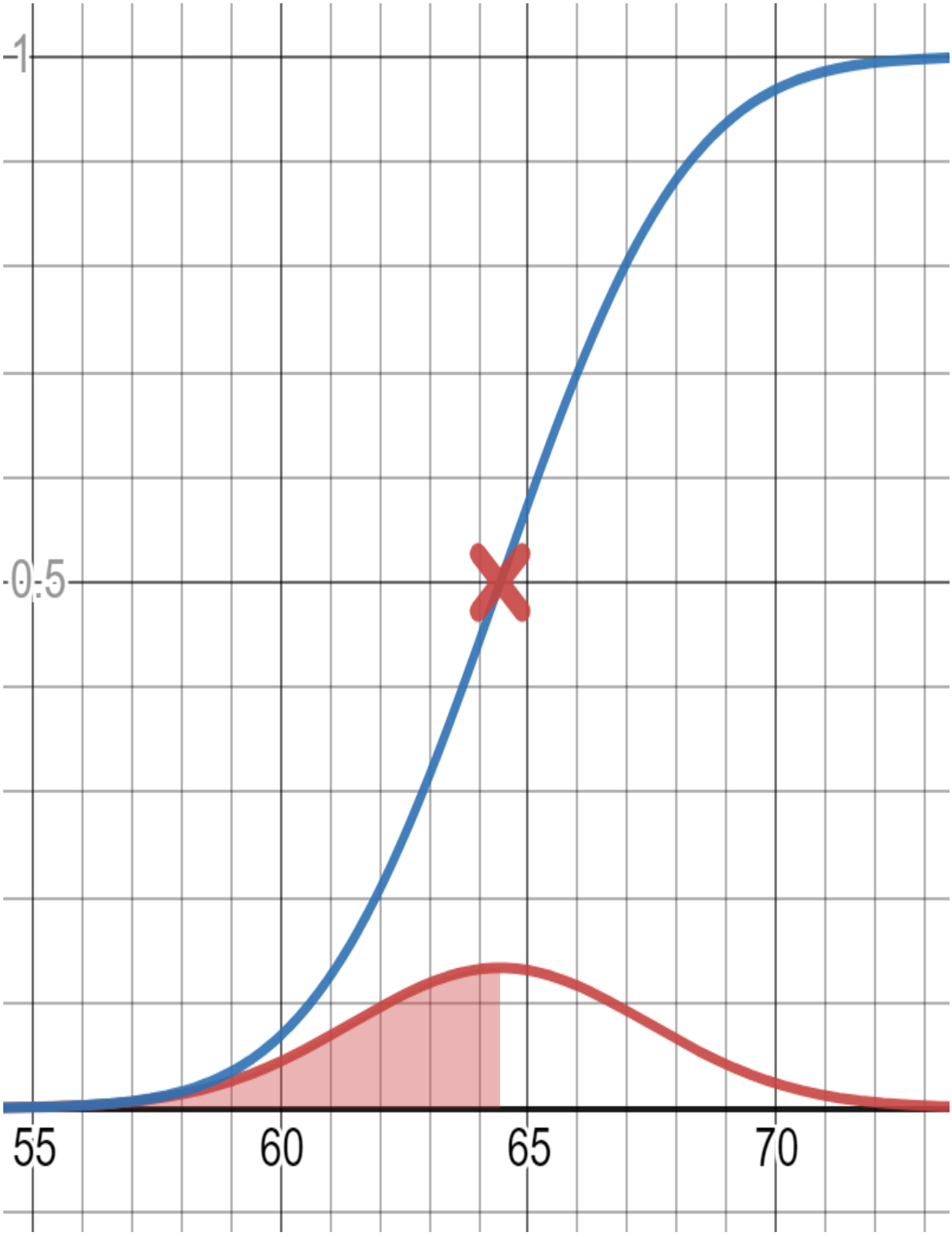


Figure 3-9. A PDF and CDF for golden retriever weights measuring probability up to the mean

This area of .50 or 50% up to the mean is known because of the symmetry of our normal distribution, and we can expect the other side of the bell curve to also have 50% of the area.

To calculate this area up to 64.43 in Python using SciPy, use the `norm.cdf()` function as shown in Example 3-10.

Example 3-10. The normal distribution CDF in Python

```
from scipy.stats import norm

mean = 64.43
std_dev = 2.99

x = norm.cdf(64.43, mean, std_dev)

print(x) # prints 0.5
```

Just like we did in Chapter 2, we can deductively find the area for a given range by subtracting areas. If we wanted to find the probability of observing a golden retriever between 62 and 66 pounds, we would calculate the area up to 66 and subtract the area up to 62 as visualized in Figure 3-10.

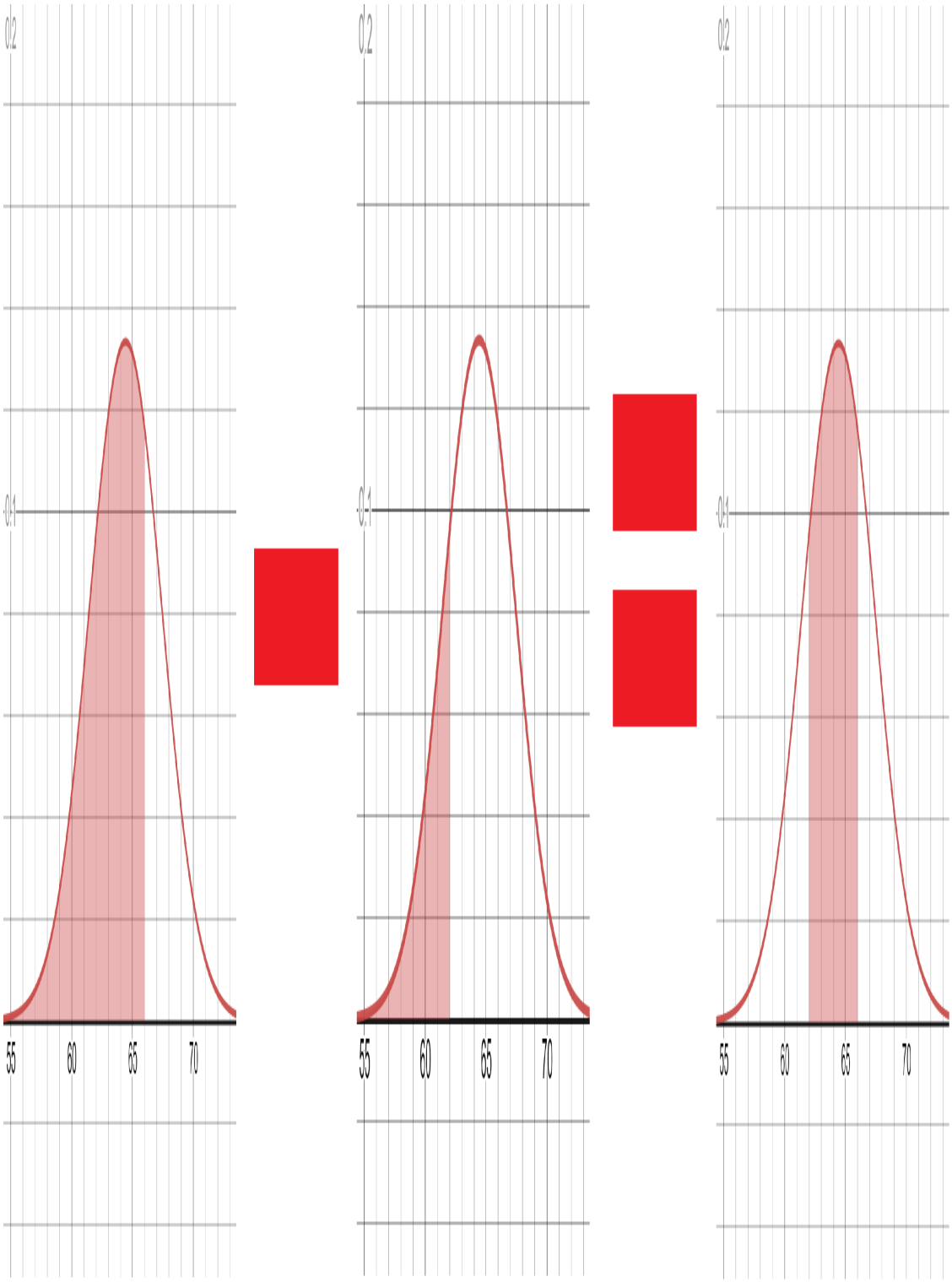


Figure 3-10. Finding a middle range of probability

Doing this in Python using SciPy is as simple as subtracting the two CDF operations shown in Example 3-11.

Example 3-11. Getting a middle range probability using the CDF

```
from scipy.stats import norm

mean = 64.43
std_dev = 2.99

x = norm.cdf(66, mean, std_dev) - norm.cdf(62, mean, std_dev)

print(x) # prints 0.4920450147062894
```

You should find the probability of observing a golden retriever between 62 and 66 pounds to be 0.4920450147062894, or approximately 49.2%

The Inverse Cumulative Density Function (CDF)

When we start doing hypothesis testing later in this chapter, you will encounter situations where you need to look up an area on the CDF and then return the corresponding x-value. Of course this is a backwards usage of the CDF, so we will need to use the inverse CDF which flips the axes as shown in Figure 3-11.

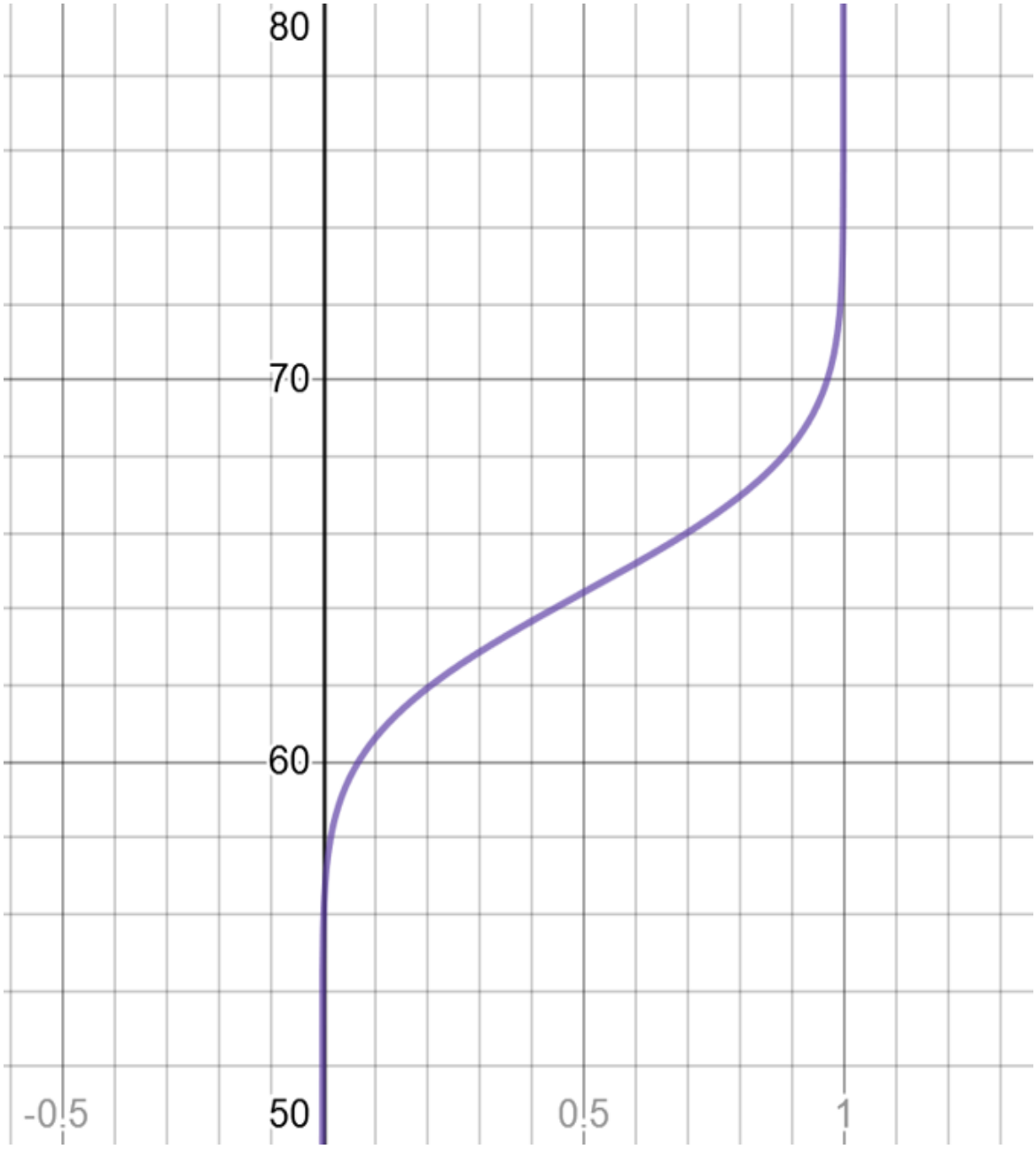


Figure 3-11. The inverse CDF, also called the PPF or quantile function

This way we can now look up a probability and then return the corresponding x-value, and in SciPy we would use the `norm.ppf()` function. For example, I want to find the weight that 95% of golden retrievers fall under. This is easy to do when I use the inverse CDF in Example 3-12.

Example 3-12. Using the inverse CDF (called ppf()) in Python

```
from scipy.stats import norm
```

```
x = norm.ppf(.95, loc=64.43, scale=2.99)
print(x) # 69.3481123445849
```

I find that 95% of golden retrievers are 69.348 pounds or less.

You can also use the inverse CDF to generate random numbers that follow the normal distribution. If I want to create a simulation that generates 1,000 realistic golden retriever weights, I just generate a random value between 0.0 and 1.0, pass it to the inverse CDF, and return the weight value as shown in Example 3-13.

Example 3-13. Generating random numbers from a normal distribution

```
import random
from scipy.stats import norm

for i in range(0,1000):
    random_p = random.uniform(0.0, 1.0)
    random_weight = norm.ppf(random_p,  loc=64.43, scale=2.99)
    print(random_weight)
```

Of course NumPy and other libraries can generate random values off a distribution for you, but this highlights one use case where the inverse CDF is handy.

> **CDF AND INVERSE CDF FROM SCRATCH**
>
> To learn how to implement the CDF and inverse CDF from scratch in Python, refer to Appendix A.

Z-Scores

It is common to re-scale a normal distribution so that the mean is 0 and the standard deviation is 1, which is known as the **standard normal distribution**. This allows us to make it easy to compare the spread of one normal distribution to another normal distribution, even if they have different means and variances.

Something that is of particular importance with the standard normal distribution is it expresses all x-values in terms of standard deviations, known as **Z-scores**. Turning an x-value into a Z-score uses a basic scaling formula.

$$z = \frac{x - \text{mean}}{\text{standard deviation}}$$

Here is an example. We have two homes from two different neighborhoods. Neighborhoood A has a mean home value of $140,000 and standard deviation of $3,000. Neighborhoood B has a mean home value of $800,000 and standard deviation of $10,000.

$$\mu_A = 140,000$$

$$\mu_B = 800,000$$

$$\sigma_A = 3,000$$

$$\sigma_B = 10,000$$

Now we have two homes from each respective neighborhood. House A from neighborhood A is worth $150,000 and House B from neighborhood B is worth $815,000. Which home is more expensive relative to the average home in its neighborhood?

$$x_A = 150,000$$

$$x_B = 815,000$$

If we express these two values in terms of standard deviations, we can compare them relative to each neighborhood mean. Use the Z-score formula:

$$z = \frac{x - \text{mean}}{\text{standard deviation}}$$

$$z_A = \frac{150000 - 140000}{3000} = 3.\overline{333}$$

$$z_B = \frac{815000 - 800000}{10000} = 1.5$$

So the house in neighborhood A is actually much more expensive relative to its neighrbood than the house in neighborhood B, as they have values $3.\overline{333}$ and 1.5 respectively.

Here is how we can convert an x-value coming from a given distribution with a mean and standard deviation into a z-score, and vice versa, as shown in Example 3-14.

Example 3-14. Turn Z-scores in x values and vice versa

```
def z_score(x, mean, std):
    return (x - mean) / std


def z_to_x(z, mean, std):
    return (z * std) + mean


mean = 140000
std_dev = 3000
x = 150000

# Convert to Z-score and then back to X
z = z_score(x, mean, std_dev)
back_to_x = z_to_x(z, mean, std_dev)

print("Z-Score: {}".format(z))  # Z-Score: 3.333
print("Back to X: {}".format(back_to_x))  # Back to X: 150000.0
```

Above the `z_score()` function will take an x-value and scale it in terms of standard deviations, given a mean and standard deviation. The `z_to_x()` function takes a Z-score and converts it back to an x-value. Studying the two functions you can see their algebraic relationship, one solving for the Z-score and the other for the x-value. We then turn an x-value of 8.0 into a Z-score and then turn that Z-score back into an x-value.

COEFFICIENT OF VARIATION

A helpful tool related to measuring spread is the coefficient of variation. It compares two distributions and quantifies how spread out each of them are. It is simple to calculate: divide the standard deviation by the mean. Here is the formula alongside the example comparing two neighborhoods.

$$\text{cv} = \frac{\sigma}{\mu}$$

$$\text{cv}_A = \frac{3000}{140000} = 0.0214$$

$$\text{cv}_B = \frac{10000}{800000} = 0.0125$$

As seen above neighborhood A, while cheaper than than neighborhood B, has more spread and therefore more price diversity than neighborhood B.

Inferential Statistics

Descriptive statistics, which we covered so far, is commonly understood. However when we get into inferential statistics the abstract relationships between sample and population comes into full play. These abstract nuances are not something you want to rush through, but rather take your time and absorb thoughtfully. As stated earlier, we are wired as humans to be biased and quickly come to conclusions. Being a good data science professional requires you to suppress that primal desire and consider the possibility that other explanations can exist. It is acceptable (perhaps even enlightened) to theorize there is no explanation at all and a finding is just coincidental and random.

First let's start with the theorem that lays the foundation for all inferential statistics.

The Central Limit Theorem

One of the reasons the normal distribution is useful is because it appears a lot in nature, such as adult golden retriever weights. However it shows up in a more

fascinating context outside of natural populations. When we start measuring large enough samples from a population, even if that population does not follow a normal distribution, the normal distribution still makes an appearance.

Let's pretend I am measuring a population that is truly and uniformly random. Any value between 0.0 and 1.0 is equally likely, and no value has any preference. But something fascinating happens when we take increasingly large samples from this population, take the average of each, and then plot them into a histogram. Run this Python code in Example 3-15 and observe the plot in Figure 3-12.

Example 3-15. Exploring the central limit theorem in Python

```
# Samples of the uniform distribution will average out to a normal
distribution.
import random
import plotly.express as px

sample_size = 31
sample_count = 1000

# Central limit theorem, 1000 samples each with 31 random numbers
between 0.0 and 1.0
x_values = [(sum([random.uniform(0.0, 1.0) for i in range(sample_size)])
/ sample_size)
            for _ in range(sample_count)]

y_values = [1 for _ in range(sample_count)]

px.histogram(x=x_values, y = y_values, nbins=20).show()
```

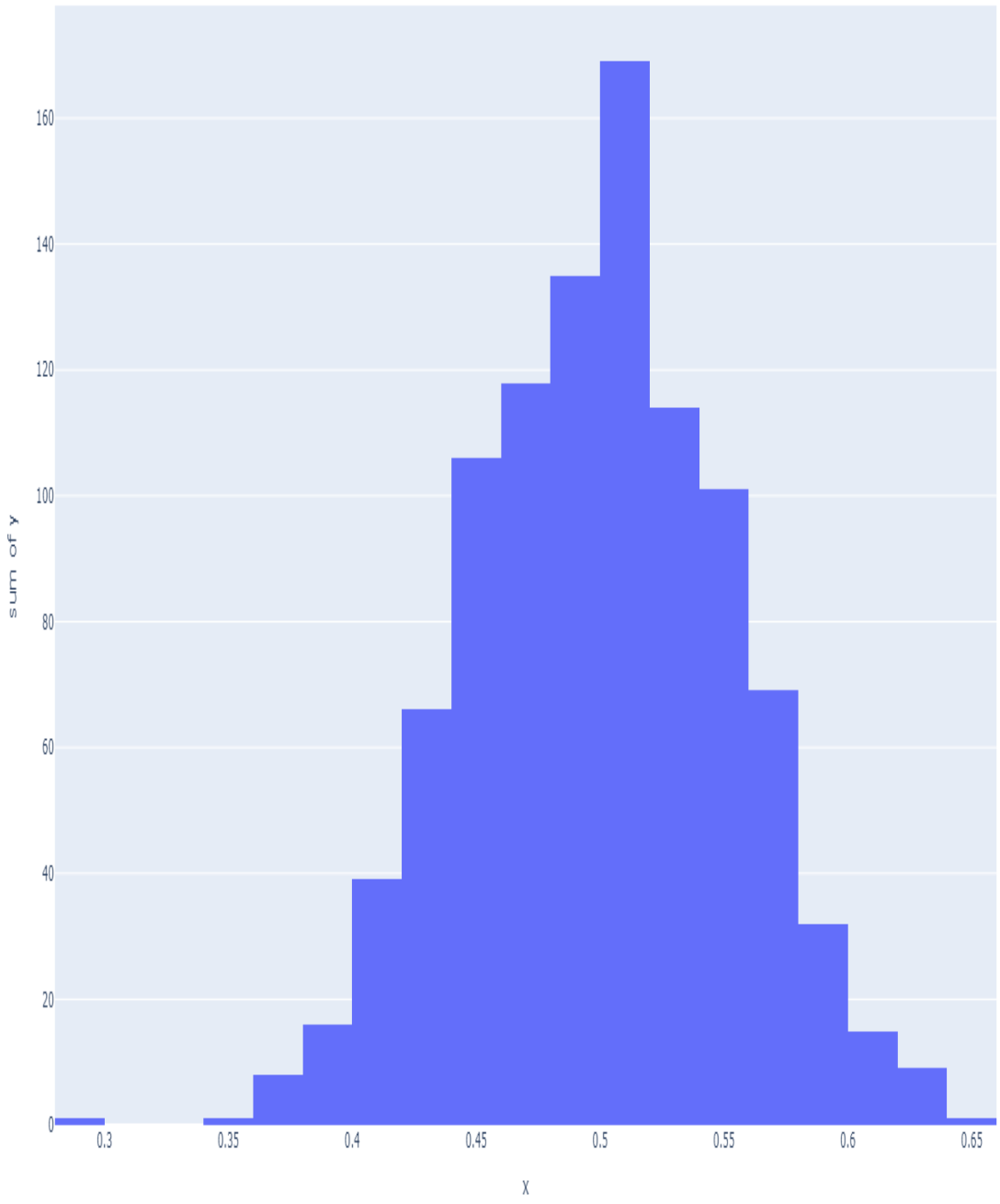


Figure 3-12. Taking the means of samples (each of size 31) and plotting them.

Wait how did uniformly random numbers, when sampled as groups of 31 and then averaged, roughly form a normal distribution? Any number is equally likely, right? Shouldn't the distribution be flat rather than bell-curved?

Here's what happening. The individual numbers in the samples alone will not create a normal distribution. The distribution will be flat where any number is equally likely (known as a **uniform distribution**). But when we group them as samples and average them they form a normal distribution.

This is because of the **central limit theorem**, which states interesting things happen when we take large enough samples of a population, calculate the mean of each, and plot them as a distribution:

1. The mean of the sample means is equal to the population mean.
2. If the population is normal, then the sample means will be normal.
3. If the population is not normal, but the sample size is greater than 30, roughly the sample means will still form a normal distribution.
4. The standard deviation of the sample means equals the population standard deviation divided by the square root of *n*.

$$\text{sample standard deviation} = \frac{\text{population standard deviation}}{\sqrt{\text{sample size}}}$$

Why is all the above important? These behaviors allows us to infer useful things about populations based on samples, even for non-normal populations. If you modify the code above and try smaller sample sizes of 1 or 2, you will not really see a normal distribution emerge. But as you approach 31 or more, you will see that we converge onto a normal distribution as shown in Figure 3-13.

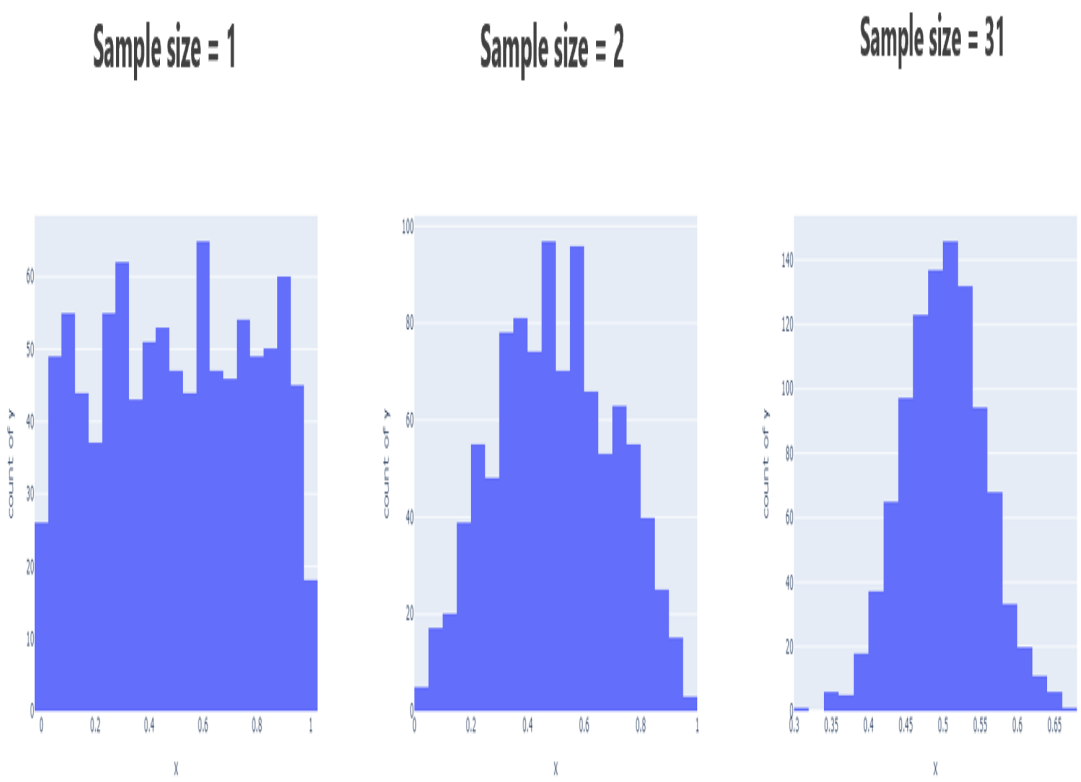


Figure 3-13. Larger sample sizes approach the normal distribution

31 is the textbook number in statistics because that is when our sample distribution often converges onto the population distribution, particularly when we measure sample means or other parameters. When you have less than 31 items in your sample, that is when you have to rely on the T-Distribution rather than the normal distribution, which has increasingly fatter tails the smaller your sample size is. We will briefly talk about this later, but first let's assume we have at least 31 items in our samples when we talk about confidence intervals and testing.

HOW MUCH SAMPLE IS ENOUGH?

While 31 is the textbook number of items you need in a sample to satisfy the central limit theorem and see a normal distribution, this sometimes is not the case. There are cases you will need an even larger sample, such as when the underlying distribution is asymmetrical or multimodal (meaning it has several peaks rather than one at the mean).

In summary, having larger samples are better when you are uncertain of the underlying probability distribution. You can read more in this article.

Confidence Intervals

You may have heard the term confidence interval, which often confuses statistics newcomers and students. A **confidence interval** is a range calculation showing how confidently we believe a sample mean (or other parameter) falls in a range for the population mean.

Base on a sample of 31 golden retrievers with a sample mean of 64.408 and a sample standard deviation of 2.05, I am 95% confident that the population mean lies between 63.686 and 65.1296. How do I know this? Let me show you and if you get confused, circle back to this paragraph and remember what we are trying to achieve. I highlighted that in bold for a reason!

I first start out by choosing a **level of confidence (LOC)**, which will contain the desired probability for the population mean range. I want to be 95% confident that my sample mean falls in the population mean range I will calculate. That's my LOC. We can leverage the central limit theorem and infer what this range for the population mean is. First, I need the **critical Z value** which is the symmetrical range in a standard normal distribution that gives me 95% probability in the center as highlighted in Figure 3-14.

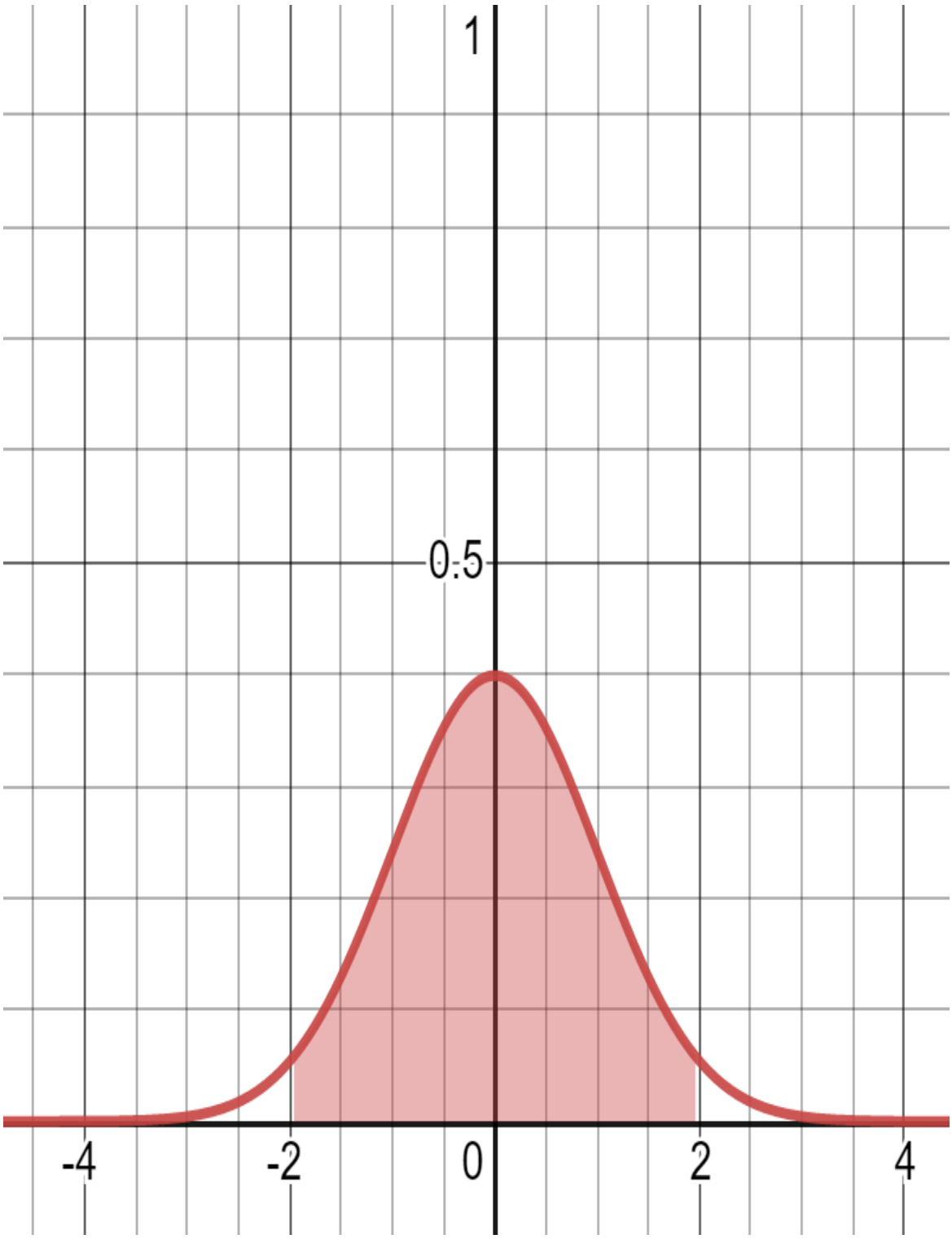


Figure 3-14. 95% symmetrical probability in the center of a standard normal distribution

How do we calculate this symmetral range containing .95 of the area? It's easier to grasp as a concept than as a calculation. You may instinctively want to use the

CDF, but then you may realize there's a few more moving parts here.

First you need to leverage the inverse CDF. Logically to get 95% of the symmetrical area in the center, we would chop off the tails which have the remaining 5% of area. Splitting that remaining 5% area in half would give us 2.5% area in each tail. Therefore, the areas we want to look up the x-values for are .025 and .975 as shown in Figure 3-15.

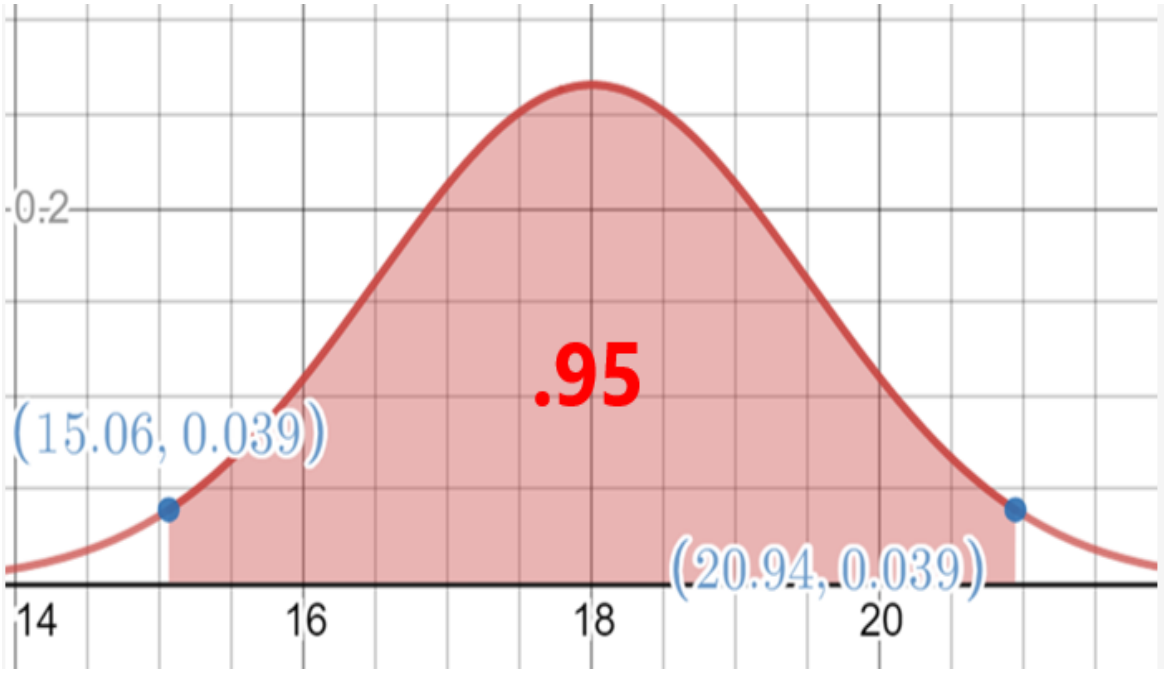


Figure 3-15. We want the x-values that give us areas .025 and .975

We can look up the x-value for area .025, and the x-value for area .975, and that will give us our center range containing 95% of the area. We will then return the corresponding lower and upper z-values containing this area (remember, we are using standard normal distribution here!). Let's calculate this in Python as shown in Example 3-16.

Example 3-16. Retrieving a critical Z-value

```
from scipy.stats import norm

def critical_z_value(p):
    norm_dist = norm(loc=0.0, scale=1.0)
    left_tail_area = (1.0 - p) / 2.0
    upper_area = 1.0 - ((1.0 - p) / 2.0)
    return norm_dist.ppf(left_tail_area), norm_dist.ppf(upper_area)

print(critical_z_value(p=.95))
# (-1.959963984540054, 1.959963984540054)
```

Okay so we get ± 1.95996 which is our critical Z-value capturing 95% of probability at the center of the standard normal distribution. Next I'm going to leverage the central limit theorem to produce the **margin of error (E)**, which is the range around the sample mean that contains the population mean at that level of confidence. Recall that our sample of 31 golden retrievers has a mean of 64.408 and standard deviation of 2.05. The formula to get this margin of error is as shown:

$$E = \pm z_c \frac{s}{\sqrt{n}}$$

$$E = \pm 1.95996 * \frac{2.05}{\sqrt{31}}$$

$$E = \pm 0.72164$$

If we apply that margin of error against the sample mean, we finally get the confidence interval!

$$95\% \text{confidence interval} = 64.408 \pm 0.72164$$

Here is how we calculate this confidence interval in Python from beginning to end in Example 3-17.

Example 3-17. Calculating a confidence interval in Python

```
from math import sqrt
from scipy.stats import norm


def critical_z_value(p):
    norm_dist = norm(loc=0.0, scale=1.0)
    left_tail_area = (1.0 - p) / 2.0
    upper_area = 1.0 - ((1.0 - p) / 2.0)
    return norm_dist.ppf(left_tail_area), norm_dist.ppf(upper_area)


def confidence_interval(p, sample_mean, sample_std, n):
    # Sample size must be greater than 30

    lower, upper = critical_z_value(p)
    lower_ci = lower * (sample_std / sqrt(n))
    upper_ci = upper * (sample_std / sqrt(n))

    return sample_mean + lower_ci, sample_mean + upper_ci
```

```
print(confidence_interval(p=.95, sample_mean=64.408, sample_std=2.05,
n=31))
# (63.68635915701992, 65.12964084298008)
```

So the way to interpret this is "based on my sample of 31 golden retriever weights with sample mean 64.408 and sample standard deviation of 2.05, I am 95% confident the population mean lies between 63.686 and 65.1296". That is how we describe our confidence interval.

One interesting thing to note here too is that in our margin of error formula, the larger *n* becomes the narrower our confidence interval becomes! This makes sense because if we have a larger sample, we are more confident in the population mean falling in a smaller range, hence why it's called a confidence interval.

One caveat to put here is that for this to work, our sample size must be at least 31 items. This goes back to the central limit theorem and if we want to apply a confidence interval to a smaller sample, we need to use a distribution with higher variance (fatter tails reflecting more uncertainty). This is what the T-distribution is for and we will visit that at the end of this chapter.

In Chapter 5 we will continue to use confidence intervals for linear regressions.

Understanding P-Values

When we say something is *statistically significant*, what do we mean by that? We hear it used loosely and frequently but what does it mathematically mean? Technically, it has to do with something called the p-value which is a hard concept for many folks to grasp. But I think the concept of p-values makes more sense when you trace it back to its invention. While this is an imperfect example, it gets across some big ideas.

In 1925, a mathematician named Ronald Fisher was at a party. One of his colleagues Muriel Bristol claimed she could detect when tea was poured before milk simply by tasting it. Intrigued by the claim, Ronald set up an experiment on the spot.

He prepared 8 cups of tea. 4 had milk poured first, the other 4 had tea poured first. He then presented them to his connoisseur colleague and asked her to

identify the pour order for each. Remarkably she identified them all correctly, and the probability of this happening by chance is 1 in 70, or 0.01428571.

This 1.4% probability is what we call the **p-value**, the probability something occuring by chance rather than because of a hypothesized explanation. Without going down a rabbit hole of combinatorial math, the probability that Muriel completely guessed the cups correctly is 1.4%. What exactly does that tell you?

When we frame an experiment, whether it is determining if organic donuts cause weight gain or living near power lines causes cancer, we always have to entertain the possiblity that random luck played a role. Just like there is a 1.4% chance Muriel identified the cups of tea correctly simply by guessing, there's always a chance randomness just gave us a good hand like a slot machine. This helps us frame our **null hypothesis (H0)**, saying that the variable in question had no impact on the experiment and any positive results is just random luck. The **alternative hypothesis (H1)** poses that a variable in question (called the **controlled variable**) is causing a positive result.

Traditionally the threshold for statistical significance is a p-value of 5% or less, or .05. Since .014 is less than .05, this would mean we can reject our null hypothesis that Muriel was randomly guessing. We can then promote the alternative hypothesis that Muriel has as special ability to detect whether tea or milk was poured first.

Now one thing this tea party example did not capture is that when we calculate a p-value, we capture all probability of that event or rarer. We will address this as we dive into the next example using the normal distribution.

Hypothesis Testing

Past studies has shown that the mean recovery time for a cold is 18 days, with a standard deviation of 1.5 days, and follows a normal distribution.

This means there is approximately 95% chance of of recovery taking between 15 and 21 days as shown in Figure 3-16 and Example 3-18.

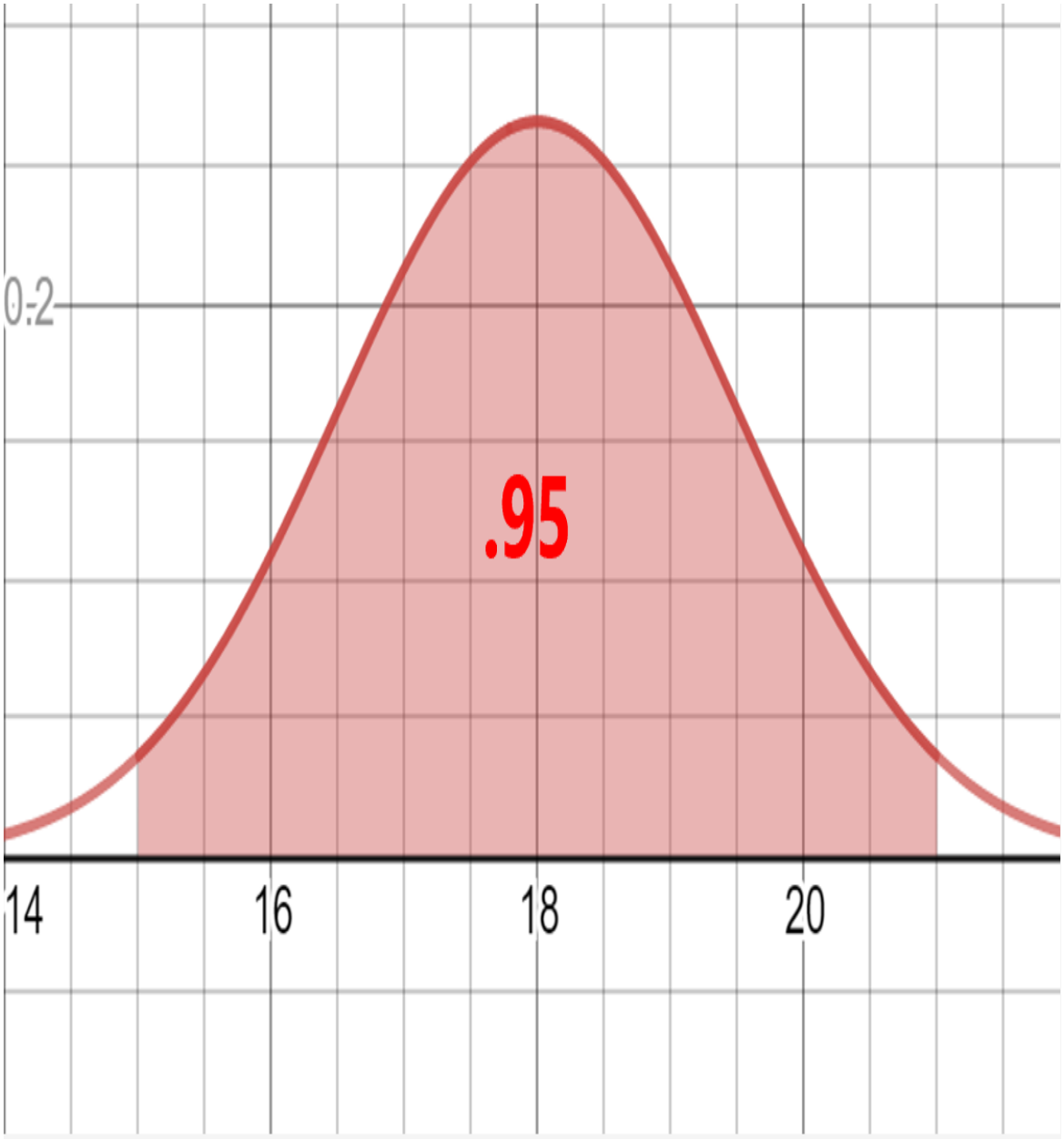


Figure 3-16. There is 95% chance of recovery between 15 and 21 days

Example 3-18. Calculating the probability of recovery between 15 and 21 days

```
from scipy.stats import norm

# Cold has 18 day mean recovery, 1.5 std dev
mean = 18
std_dev = 1.5

# 95% probability recovery time takes between 15 and 21 days.
x = norm.cdf(21, mean, std_dev) - norm.cdf(15, mean, std_dev)

print(x) # 0.9544997361036416
```

We can infer then from the remaining 5% probability that there's a 2.5% chance of recovery taking longer than 21 days and a 2.5% chance of less than 15 days. Hold onto that bit of information because it will be critical later! That drives our p-value.

Now let's say an experimental new drug was given to a test group of 40 people and it took an average of 16 days for them to recover from the cold as shown in Figure 3-17.

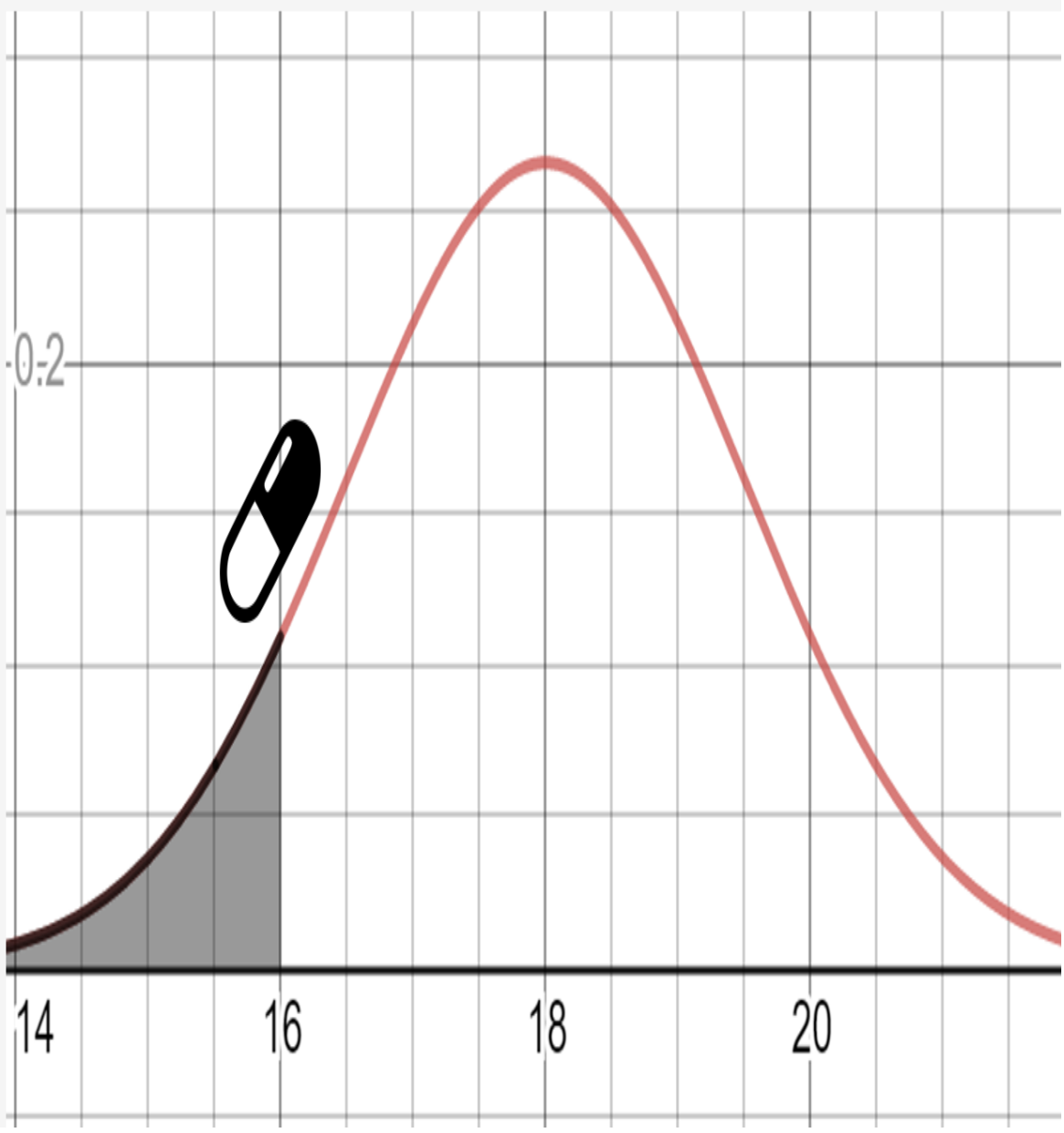


Figure 3-17. A group taking a drug took 16 days to recover

Did the drug have an impact? If you reason long enough, you may realize what we are asking is this: does the drug show a statistically signficant result? Or did the drug not work and the 16-day recovery was a coincidence with the test group? That first question frames our alternative hypothesis, while the second question frames our null hypothesis.

There are two ways we can calculate this: the One-tailed and two-tailed test. We will start with the one-tailed.

One-Tailed Test

When we approach the **one-tailed test**, we typically frame our null and alternative hypotheses using inequalities. We hypothesize around the population mean and say that it either is greater than/equal to 18 (the null hypothesis H_0) or less than 18 (the alternative hypothesis H_1).

$$H_0 : \text{population mean} \geq 18$$

$$H_1 : \text{population mean} < 18$$

To reject our null hypothesis, we need to show that our sample mean (of the patients who took the drug) is not likely to have been coincidental. Since a P-value of .05 or less is traditionally considered statistically signficant, we will use that as our threshold (Figure 3-17). When we calculate this in Python using the inverse CDF as shown in Figure 3-18 and Example 3-19, we find that approximately 15.51 is the number of recovery days that gives us .05 area on the left tail.

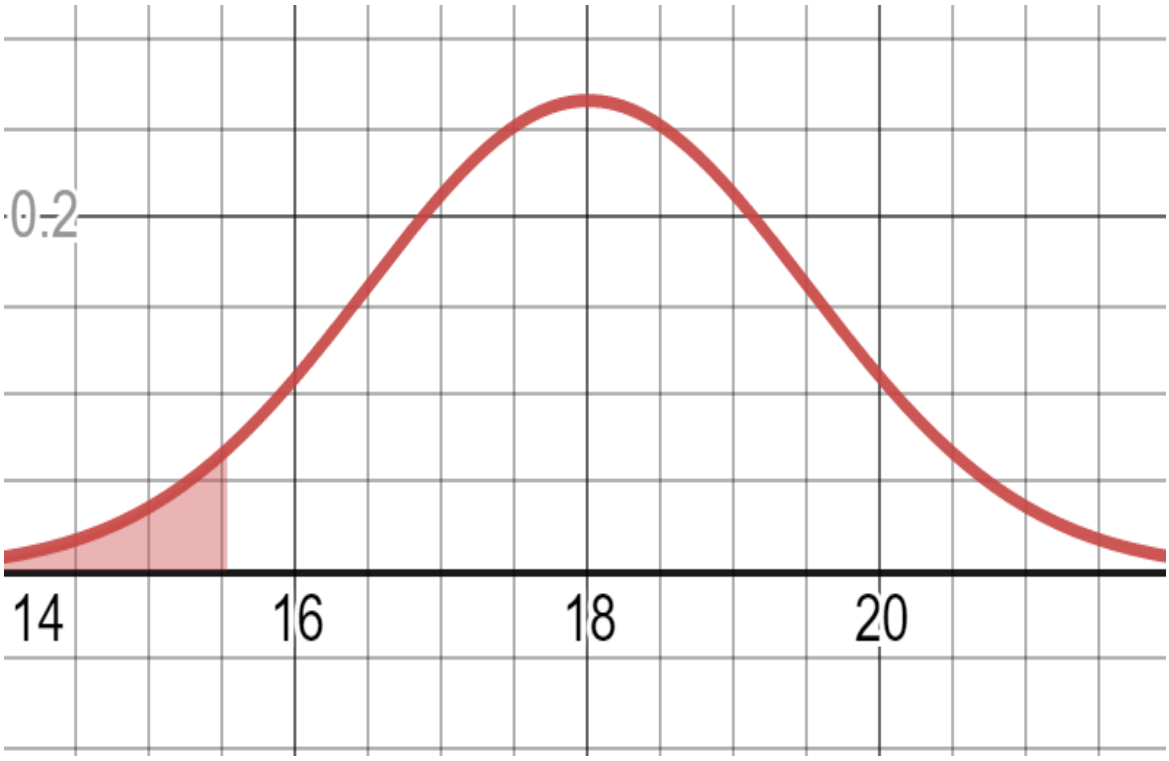


Figure 3-18. Getting the x-value with 5% of area behind it

Example 3-19. Python code for getting x-value with 5% of area behind it

```
from scipy.stats import norm

# Cold has 18 day mean recovery, 1.5 std dev
mean = 18
std_dev = 1.5

# What x-value has 5% of area behind it?
x = norm.ppf(.05, mean, std_dev)

print(x) # 15.53271955957279
```

Therefore if we achieve an average 15.53 or less days of recovery time in our sample group, our drug is considered statistically significant enough to have shown an impact. However, our sample mean of recovery time is actually 16 days and does not fall into this null hypothesis rejection zone. Therefore the statistical significance test has failed as shown in Figure 3-19.

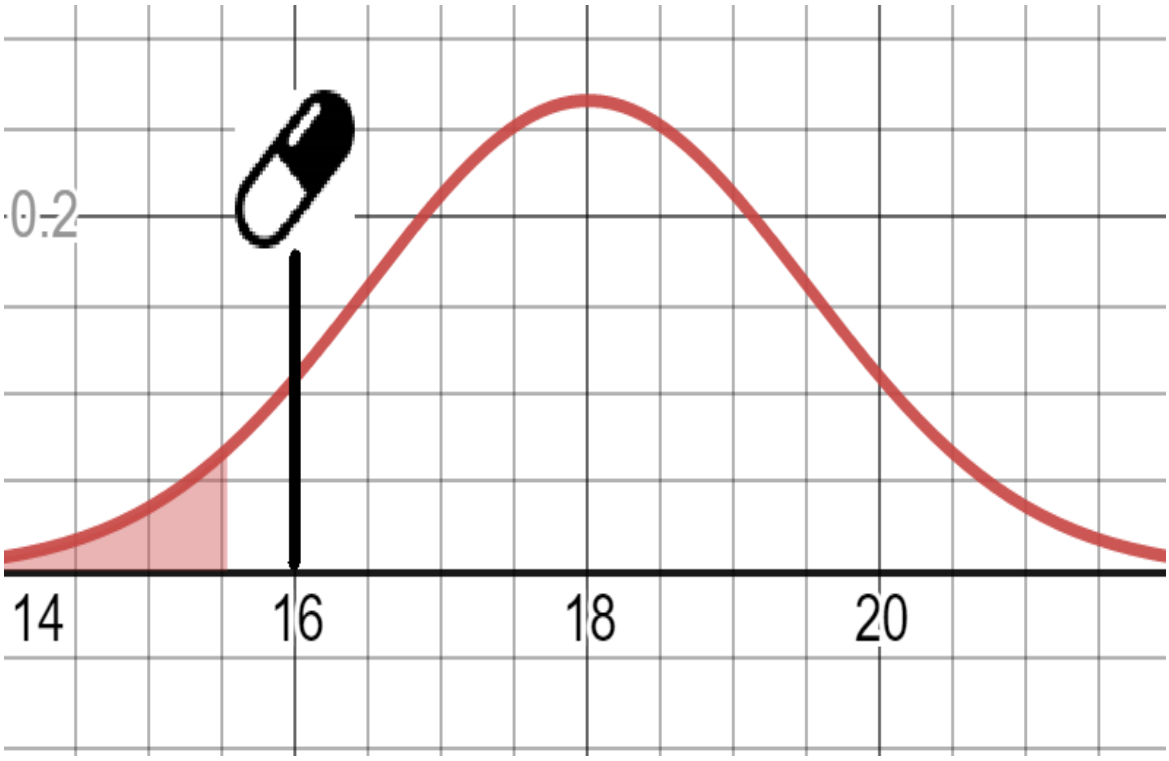


Figure 3-19. We have failed to prove our drug test result is statistically significant

The area up to that 16-day mark is our p-value, which is .0912 and we calculate it in Python as shown in Example 3-20.

Example 3-20. Calculating the 1-tailed p-value

```
from scipy.stats import norm

# Cold has 18 day mean recovery, 1.5 std dev
mean = 18
std_dev = 1.5

# Probability of 16 or less days
p_value = norm.cdf(16, mean, std_dev)

print(p_value) # 0.09121121972586788
```

Since the p-value of .0912 is greater than our statistical significance threshold of .05, we do not consider the drug trial a success and fail to reject our null hypothesis.

Two-Tailed Test

The previous test we performed is called the one-tailed test because it only looks for statistical significance on one tail. However it is often safer and better

practice to use a two-tailed test. We will elaborate why later.

To do a **two-tailed test**, we frame our null and alternative hypothesis in an "equal" and "not equal" structure. In our drug test, we will say the null hypothesis has a mean recovery time of 18 days. But our alternative hypothesis is the mean recovery time is not 18 days thanks to the new drug.

$$H_0 : \text{population mean} = 18$$

$$H_1 : \text{population mean} \neq 18$$

This has an important implication. We are structuring our alternative hypothesis to not test whether the drug improves cold recovery time, but if it had *any* impact. This includes testing if it increased the duration of the cold. Is this helpful? Hold that thought.

Naturally this means we spread our p-value statistical significance threshhold to both tails, not just one. If we are testing for a statistical significance of 5% then we split it and give each 2.5% half to each tail. If our drug mean recovery time falls in either region our test is successful and we reject the null hypothesis (Figure 3-20).

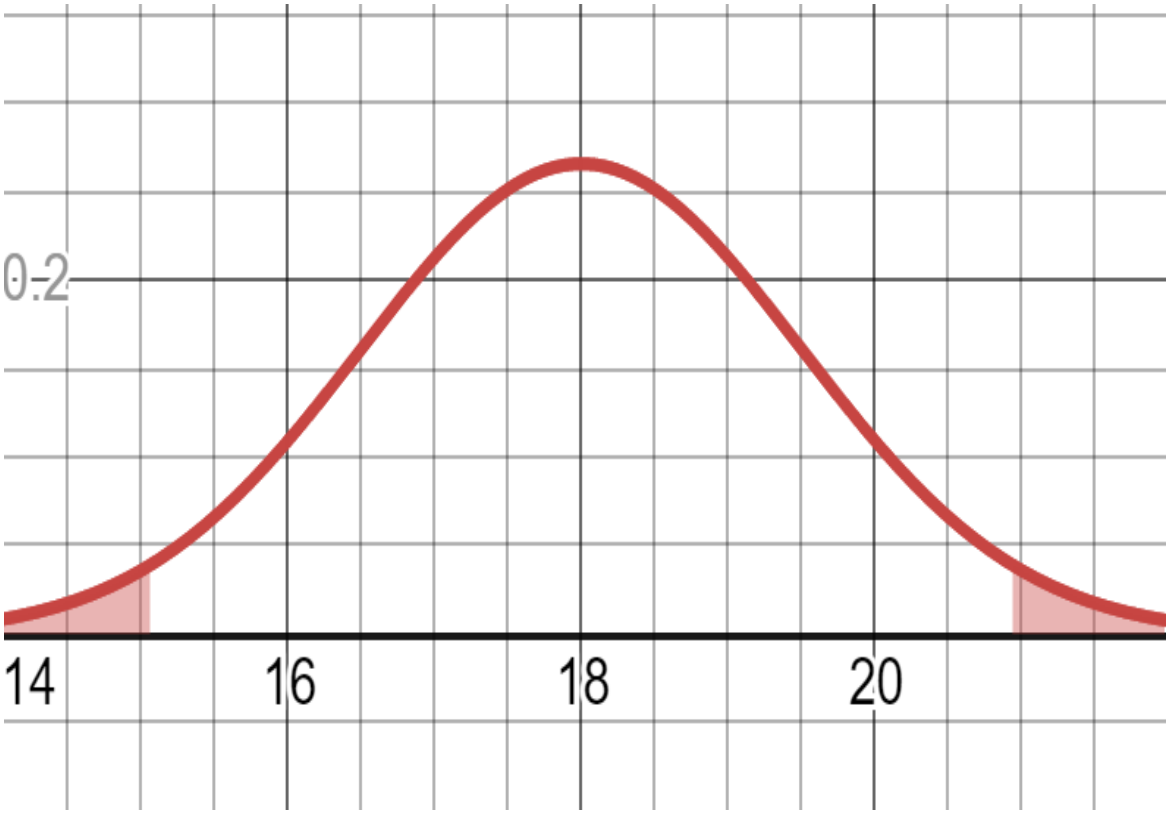


Figure 3-20. A 2-tailed test

The x-values for the lower tail and upper tail are 15.06 and 20.93, meaning if we are under or over respectively we reject the null hypothesis. Here are those two values calculated using the inverse CDF below in Figure 3-21 and Example 3-21. Remember, to get the upper tail we take .95 and then add the .025 piece of significance threshhold to it, giving us .975.

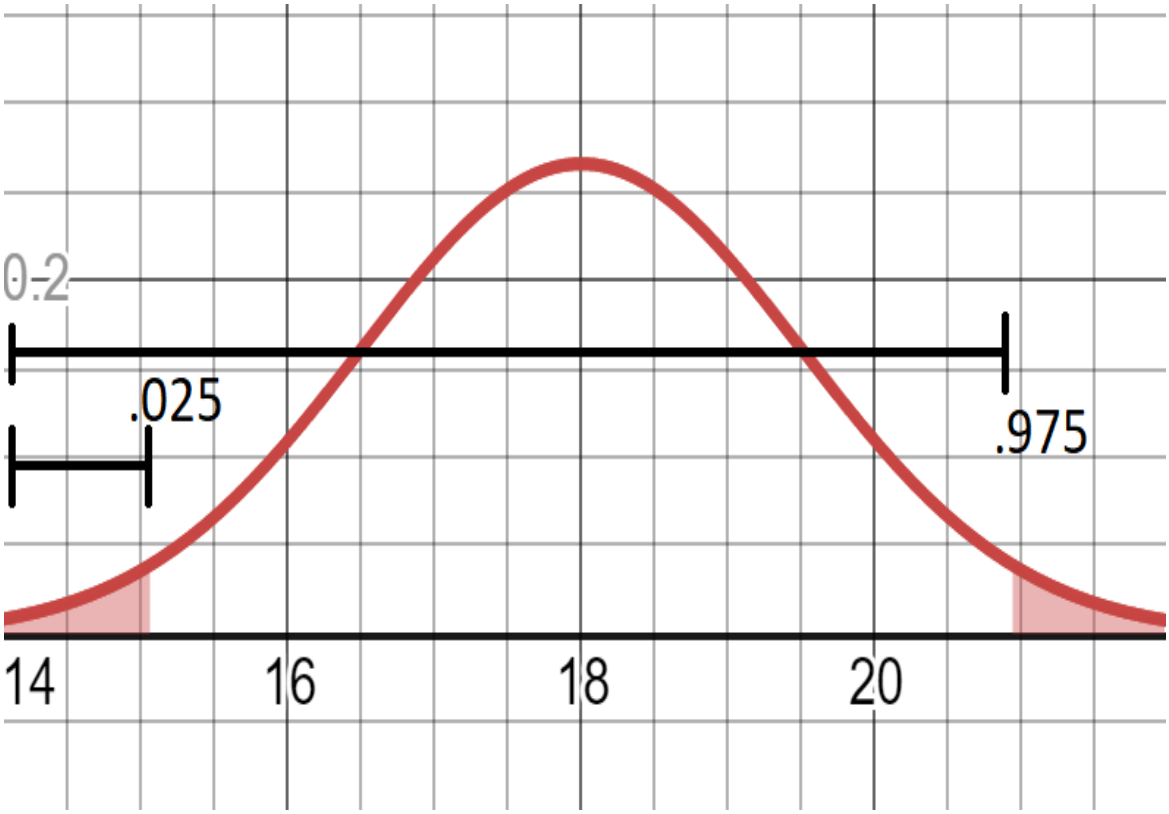


Figure 3-21. Calculating the central 95% of normal distribution area

Example 3-21.

```
from scipy.stats import norm

# Cold has 18 day mean recovery, 1.5 std dev
mean = 18
std_dev = 1.5

# What x-value has 2.5% of area behind it?
x1 = norm.ppf(.025, mean, std_dev)

# What x-value has 97.5% of area behind it
x2 = norm.ppf(.975, mean, std_dev)

print(x1) # 15.060054023189918
print(x2) # 20.93994597681008
```

The sample mean value for the drug test group is 16, and 16 is not less than 15.06 nor greater than 20.9399. So like the 1-tailed test we still fail to reject the null hypothesis. Our drug still has not shown any statistical significance to have any impact as shown in Figure 3-22.

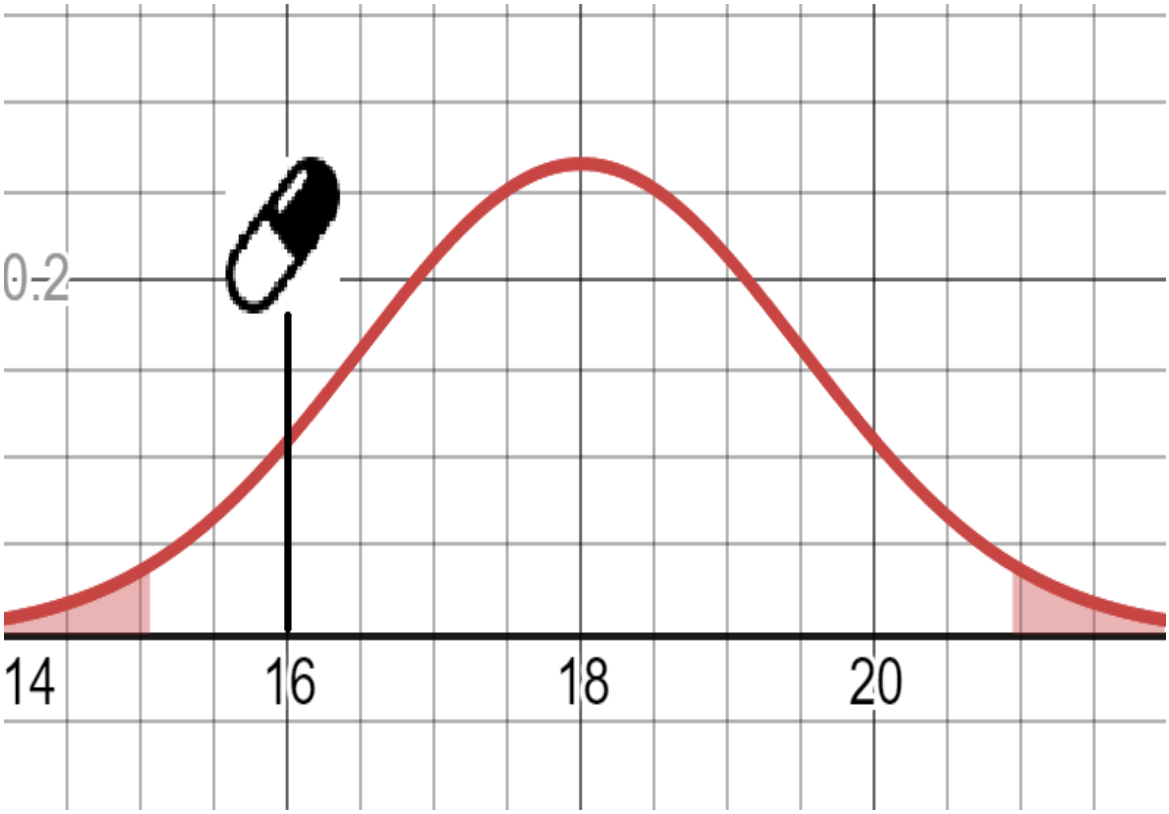


Figure 3-22. The 2-tailed test has failed to prove statistical significance

But what is the p-value? This is where it gets interesting with 2-tailed tests. Our p-value is going to not just capture the area to the left of 16, but also the symmetrical equivalent area on the right tail as well. Since 16 is 4 days below the mean, we will also capture the area above 20 which is 4 days above the mean (Figure 3-23). This is capturing the probability of an event or rarer, on both sides of the bell curve.

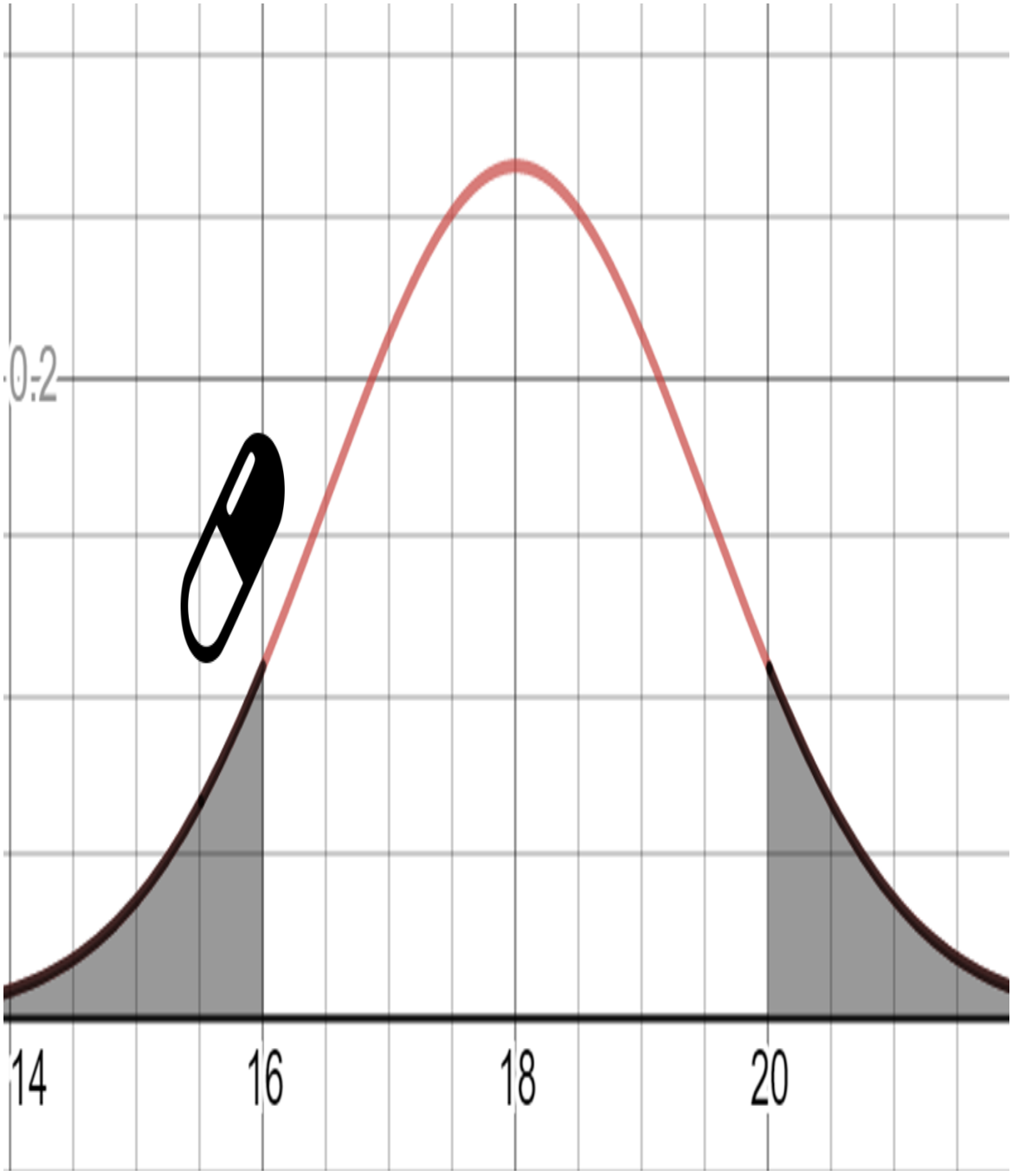


Figure 3-23. The p-value adds symmetrical sides for statistical significance

When we sum both those areas, we get a p-value of .1824. This is a lot greater than .05, so it definitely does not pass our p-value threshold of .05 (Example 3-22).

Example 3-22. Calculating the 2-tailed p-value

```
from scipy.stats import norm
```

```
# Cold has 18 day mean recovery, 1.5 std dev
mean = 18
std_dev = 1.5

# Probability of 16 or less days
p1 = norm.cdf(16, mean, std_dev)

# Probability of 20 or more days
p2 = 1.0 -  norm.cdf(20, mean, std_dev)

# P-value of both tails
p_value = p1 + p2

print(p_value) # 0.18242243945173575
```

So why do we also add the symmetrical area on the opposite side in a 2-tailed test? This may not be the most intuitive concept, but first remember how we structured our hypotheses:

$$H_0 : \text{population mean} = 18$$

$$H_1 : \text{population mean} \neq 18$$

If we are testing in an “equals 18” versus “not equals 18” capacity, we have to capture any probability that is of equal or less value on both sides. After all we are trying to prove significance, and that includes anything that is equally or less likely to happen. We did not have this special consideration with the 1-tailed test that used only “greater/less than” logic. But when we are dealing with “equals/not equals” our interest area goes in both directions..

So what are the practical implications of the 2-tailed test? How does it affect whether we reject the null hypothesis? Ask yourself this: which one sets a higher threshhold? You will notice that even when our objective is to show we may have lessened something (the cold recovery time using a drug), reframing our hypothesis to show any impact (greater or lesser) creates a higher significance threshhold. If our significance threshhold is a p-value of .05 or less, our 1-tailed test was closer to acceptance at p-value .0912 as opposed to the 2-tailed test which was about double that at p-value .182.

This means the 2-tailed test makes it harder to reject the null hypothesis and demands stronger evidence to pass a test. Also think of this: what if our drug could worsen colds and make them last longer? It may be helpful to capture that probability too and account for variation in that direction. This is why 2-tailed

tests are preferrable in most cases. They tend to be more reliable and not bias the hypothesis in just one direction.

We will use hypothesis testing and P-values again in Chapter 5 and Chapter 6.

BEWARE OF P-HACKING!

There is a growing problem in the scientific research community called p-hacking, where researchers shop for statistically significant p-values of .05 or less. This is not hard to do with "big data", machine learning, and data mining where we can traverse hundreds or thousands of variables and then find statistically significant (but coincidental) relationships between them.

Why do so many researchers p-hack? Many are probably not aware they are doing it. It's easy to keep tuning and tuning a model, omitting "noisy" data and changing parameters, until it gives the "right" result. Others are simply under pressure by academia and industry to produce lucrative, not objective, results.

If you are hired by the Calvin Cereal Company to study whether Frosted Chocolate Sugar Bombs causes diabetes, do you expect to give an honest analysis and get hired again? What if a manager asks you to produce a forecast showing $15 million in sales next quarter for a new product launch? You have no control over what sales will be, but you're asked for a model that produces a pre-determined result. In the worst case, you may even be held accountable when it proves wrong. Unfair, but it happens!

This is why soft skills like diplomacy can make a difference in a data science professional's career. If you can share difficult and inconvenient stories in a way that productively gets an audience, that is a tremendous feat. Just be mindful of the organization's managerial climate and always propose alternate solutions. If you end up in a no-win situation where you are asked to p-hack, and could be held accountable for when it backfires, then definitely change work environments!

The T-Distribution: Dealing with Small Samples

Let's briefly address how to deal with smaller samples of 30 or less, and we will need this when we do linear regression in Chapter 5. Whether we are calculating confidence intervals or doing hypothesis testing, if we have 30 or less items in a sample we would opt to use a T-Distribution instead of a normal distribution. The **T-distribution** is like a normal distribution but has fatter tails to reflect more variance and uncertainty. Figure 3-24 shows a normal distribution (dashed) alongside a T-distribution with 1 degree of freedom (solid):

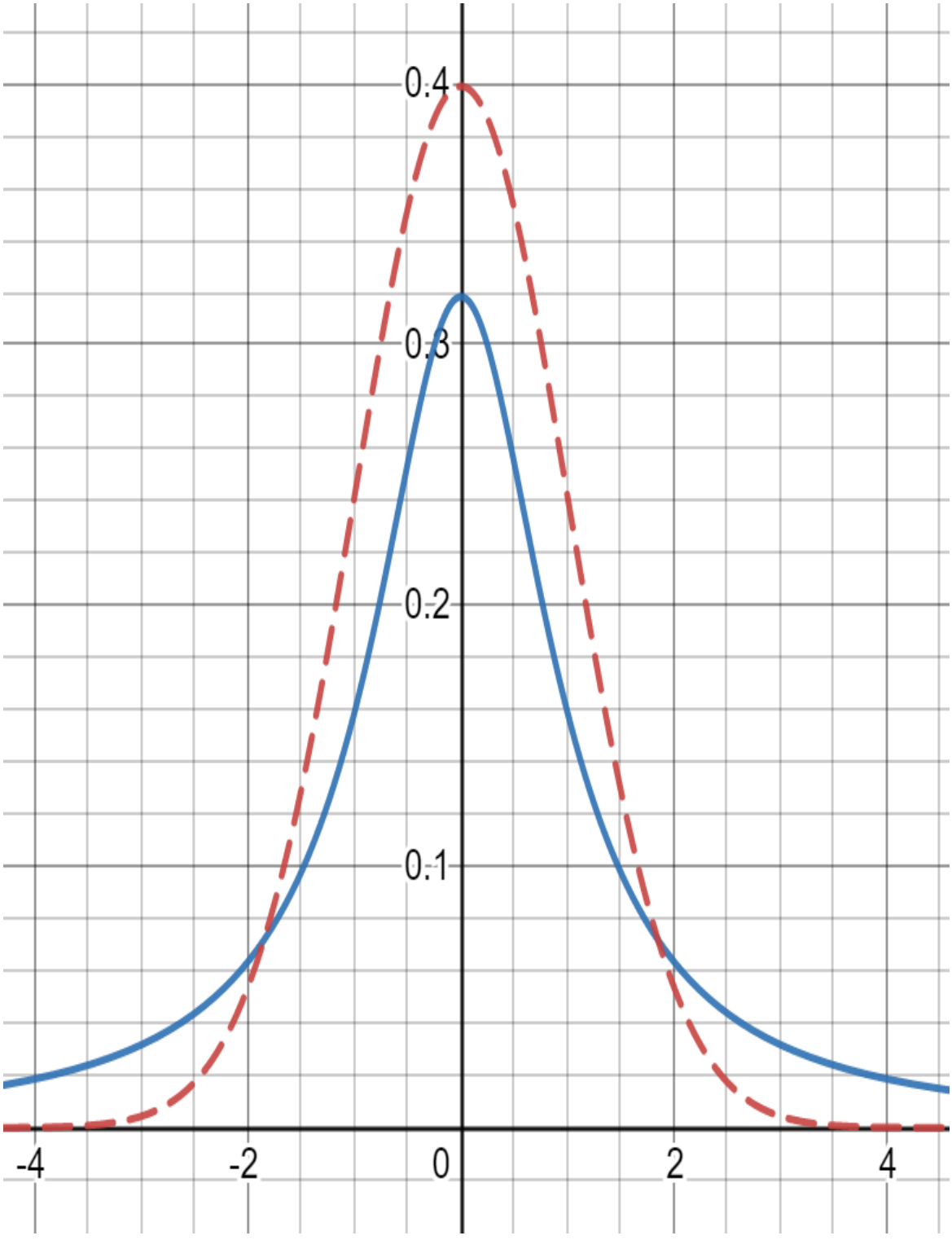


Figure 3-24. The T-Distribution alongside a normal distribution. Note the fatter tails.

The smaller the sample size is, the fatter the tails get in a T-distribution. But what's interesting is after you approach 31 items the T-distribution is nearly

indistinguishable from the normal distribution, which neatly reflects the ideas behind the central limit theorem.

Example 3-23 below shows how to find the **critical t-value** for 95% confdicence. You can use this for confidence intervals and hypothesis testing when you have a sample size of 30 or less. It's conceptually the same as the critical z-value, but we are usign a T-distribution instead of a normal distribution to reflect greater uncertainty. The smaller the sample size, the larger the range reflecting greater uncertainty.

Example 3-23.

```
from scipy.stats import t

# get critical value range for 95% confidence
# with a sample size of 25

n = 25
lower = t.ppf(.025, df=n-1)
upper = t.ppf(.975, df=n-1)

print(lower, upper)
-2.063898561628021 2.0638985616280205
```

Note that `df` is the "degrees of freedom" parameter, and as outlined earlier it should be 1 less of the sample size.

BEYOND THE MEAN

We can use confidence intervals and hypothesis testing to measure other parameters besides the mean, including variance/standard deviation as well as proportions (e.g. 60% of people report improved happiness after walking 1 hour a day). These require other distributions such as the Chi-Square distribution instead of the normal distribution. As stated, these are all beyond the scope of this book but hopefully you have a strong conceptual foundation to extend into these areas if needed.

We will however use confidence intervals and hypothesis testing throughout Chapter 5 and Chapter 6.

Big Data Considerations and Texas Sharpshooter Fallacy

One final thought before we close this chapter. As we have discussed, randomness plays such a role in validating our findings and we always have to account for its possibility. Unfortunately with "big data", machine learning, and other data-mining tools the scientific method has suddenly become a practice done backwards. This can be precarious and allow me to demonstrate why, adapting an example from Gary Smith in his book *Standard Deviations*.

Let's pretend I draw 4 playing cards from a fair deck. There's no game or objective here other than to draw 4 cards and observe them. I get 2 tens, a three, and a two. "This is interesting" I say. "I got 2 tens, a three, and a two. Is this meaningful? Are the next four cards I draw also going to be two consecutive numbers and a pair? What's the underlying model here?"

See what I did there? I took something that was completely random and I not only looked for patterns, but I tried to make a predictive model out of them. What has subtly happened here is I never made it my objective to get these four cards with these particular patterns. I observed them *after* they occurred.

This is exactly what data mining falls victim to every day: finding coincidental patterns in random events. With huge amounts of data and fast algorithms looking for patterns, it's not hard to find things that look meaningful but actually are just random coincidences.

This is analogous to me firing a gun at a wall. I then draw a target around the hole and I then bring my friends over to show off my amazing marksmanship. Silly, right? Well many people in data science figuratively do this everyday and it is known as the **Texas Sharpshooter Fallacy**. They set out to act without an objective, stumble on something rare, and then point out what they found somehow creates predictive value.

The problem is the law of truly large numbers says rare events are likely to be found, we just do not know which ones. When we encounter rare events, we highlight and even speculate what might have caused them. The probability of a specific person winning the lottery is highly unlikely, but yet someone *is* going to win the lottery. Why should we be surprised when there is a winner? Unless

somebody predicted the winner, nothing meaningful happened other than a random person got lucky.

This also applies to correlations which we will study in Chapter 5. With an enormous dataset with thousands of variables, is it hard to find statistically significant findings with a .05 p-value? You betcha! I'll find thousands of those. I'll even show evidence *http://www.tylervigen.com/spurious-correlations* [the number of Nicholas Cage movies correlates with the number of pool drownings in a year].

So to prevent the Texas Sharpshooter Fallacy and falling victim to big data fallacies, try to use structured hypothesis testing and gather data for that objective. If you utilize data mining, try to obtain fresh data to see if your findings still hold up. Finally, always consider the possibility that things can be coincidental and if there is not a common sense explanation then it probably was coincidental.

We learned how to hypothesize before gathering data, but data mining gathers data then hypothesizes. Ironically, we are often more objective starting with a hypothesis, because we then seek out data to deliberately prove and disprove our hypothesis.

Conclusions

We learned a lot in this chapter, and you should feel good about getting this far. This was probably one of the harder topics in this book! We learned not only descriptive statistics from the mean to the normal distribution, but we also tackled confidence intervals and hypothesis testing.

Hopefully you see data a little differently. It is snapshots of something rather than a complete capturing of its context. Data on its own is not very useful, and we need context, curiosity, and analysis of where it came from before we can make meaningful insights with it. We covered how to describe data as well as infer attributes about a larger population based on a sample. Finally we addressed some of the data mining fallacies we can stumble into if we are not careful, and how to remedy that with fresh data and common sense.

Do not feel bad if you need to go back and review some of the content in this chapter, because there's a lot to digest. It is also important to get in the

hypothesis testing mindset if you want to be successful at a data science and machine learning career. Few practitioners take time to link statistics and hypothesis testing concepts to machine learning, and it unfortunately has slowed progress in the field substantially. Understandability and explainability is the next frontier of machine learning, so continue to learn and integrate these ideas as you progress throughout the rest of this book and the rest of your career.

Exercises

1. You bought a spool of 1.75mm filament for your 3D printer. You want to measure how close the filament diameter really is to 1.75 mm. You use a caliper tool and sample the diameter five times on the spool:

   1.78, 1.75, 1.72, 1.74, 1.77

   Calculate the mean and standard deviation for this set of values.

2. A manufacturer says the Z-Phone smart phone has a mean consumer life of 42 months with a standard deviation of 8 months. Assuming a normal distribution, what is the probability a given random Z-Phone will last between 20 and 30 months?

3. I am skeptical that my 3D printer filament is not 1.75mm in average diameter as advertised. I sampled 34 measurements with my tool. The sample mean is 1.715588 and the sample standard deviation is 0.029252.

   What is the 99% confidence interval for the mean of my entire spool of filament?

4. Your marketing department has started a new advertising campaign and wants to know if it affected sales, which in the past averaged $10,345 a day with a standard deviation of $552. The new advertising campaign ran for 45 days and averaged $11,641 in sales.

   Did the campaign affect sales? Why or why not? (Use a 2-tailed test for more reliable significance)

Chapter 4. Linear Algebra

> **A NOTE FOR EARLY RELEASE READERS**
>
> With Early Release ebooks, you get books in their earliest form—the author's raw and unedited content as they write—so you can take advantage of these technologies long before the official release of these titles.
>
> This will be the 4th chapter of the final book.
>
> If you have comments about how we might improve the content and/or examples in this book, or if you notice missing material within this chapter, please reach out to the author at *thomasnield@live.com*.

Changing gears a little bit, let's venture away from probability and statistics and into linear algebra. Sometimes people confuse linear algebra with basic algebra, thinking maybe it has to do with plotting lines using the algebraic function `y = mx + b`. This is why linear algebra should probably have been called "vector algebra" or "matrix algebra" because it is much more abstract. Linear systems play a role, but in a much more metaphysical way.

So, what exactly is linear algebra? Well, **linear algebra** concerns itself with linear systems, but represents them through vector spaces and matrices. If you do not know what a vector or a matrix is, do not worry! We will define and explore them in depth. Linear algebra is hugely fundamantal to many applied areas of math, statistics, operations research, data science, and machine learning. When we work with data in any of these areas, we are using linear algebra and perhaps you may not even know it.

You can get away with not learning linear algebra for awhile, using machine learning and statistics libraries that do it all for you. But if we are going to get intuition behind these black boxes and be more effective at working with data, understanding the fundamentals of linear algebra is an

inevitability. Linear algebra is an enormous topic that can fill thick textbooks, so of course we cannot gain total mastery in just one chapter of this book. However, we can learn enough to be more comfortable with it and navigate the data science domain effectively. There will also be opportunities to apply it in later chapters of this book.

What is a Vector?

Simply put a **vector** is an arrow in space with a specific direction and length, often representing a piece of data. It is the central building block to linear algebra, including matrices and linear transformations. In its fundamental form, it has no concept of location so always imagine its tail starts at the origin of a Cartesian plane (0,0).

Figure 4-1 shows a vector $\vec{v}$ that moves 3 steps in the horizontal direction and 2 steps in the vertical direction.

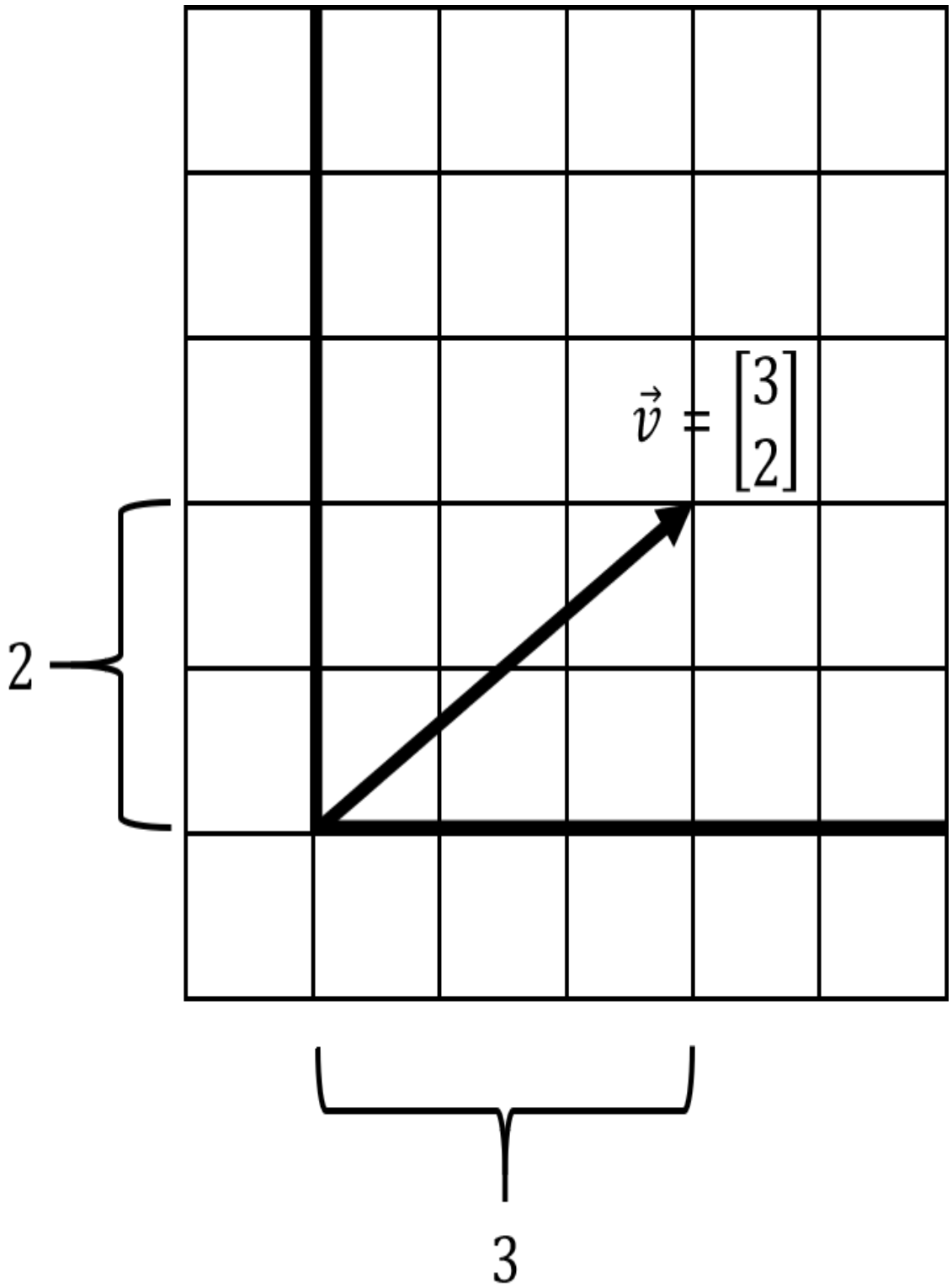


Figure 4-1. A simple vector

To emphasize again, the purpose of the vector is to visually represent a piece of data. If you have a data record for the square footage of a house 18,000 square feet and its valuation $260,000, we could express that as a vector `[18000 2600000]`, stepping 18,000 steps in the horizontal direction and 260,000 steps in the vertical direction.

We declare a vector mathematically like this:

$$\overrightarrow{v} = \begin{bmatrix} x \\ y \end{bmatrix}$$

$$\overrightarrow{v} = \begin{bmatrix} 3 \\ 2 \end{bmatrix}$$

We can declare a vector using a simple Python collection, like a Python list as shown in Example 4-1.

Example 4-1. Declaring a vector in Python using a list

```
v = [3, 2]
print(v)
```

However when we start doing mathematical computations with vectors, especially when doing tasks like machine learning, we should probably use the NumPy library as it is more efficient than plain Python. You can also use SymPy to perform linear algebra operations, and we will use it occasionally in this chapter when decimals become inconvenient. However, NumPy is what you will likely use in practice so that is what we will mainly stick to.

To declare a vector, you can use NumPy's `array()` function and then can pass a collection of numbers to it as shown in Example 4-2.

Example 4-2. Declaring a vector in Python using NumPy

```
import numpy as np
v = np.array([3, 2])
print(v)
```

PYTHON LIBRARIES ARE MORE EFFICIENT

Python is slow but its numeric and scientific libraries are not. Libraries like NumPy are typically written in low-level languages like C and C++, hence why they are computationally efficient. Python really acts as "glue code" integrating these libraries for your task.

A vector has countless practical applications. In physics, a vector is often thought of as a direction and magnitude. In math it is a direction and scale on an XY plane, kind of like a movement. In computer science, it is an array of numbers storing data. The computer science context is the one we will become the most familiar with as data science professionals. However it is important we never forget the visual aspect so we do not think of vectors as esoteric grids of numbers. Without a visual understanding it is almost impossible to grasp many fundamental linear algebra concepts like linear dependence and determinants.

Here are some more examples of vectors. In Figure 4-2 note that some of these vectors have negative directions on the X and Y scales. Vectors with negative directions will have an impact when we combine them later, essentially subtracting rather than adding them together.

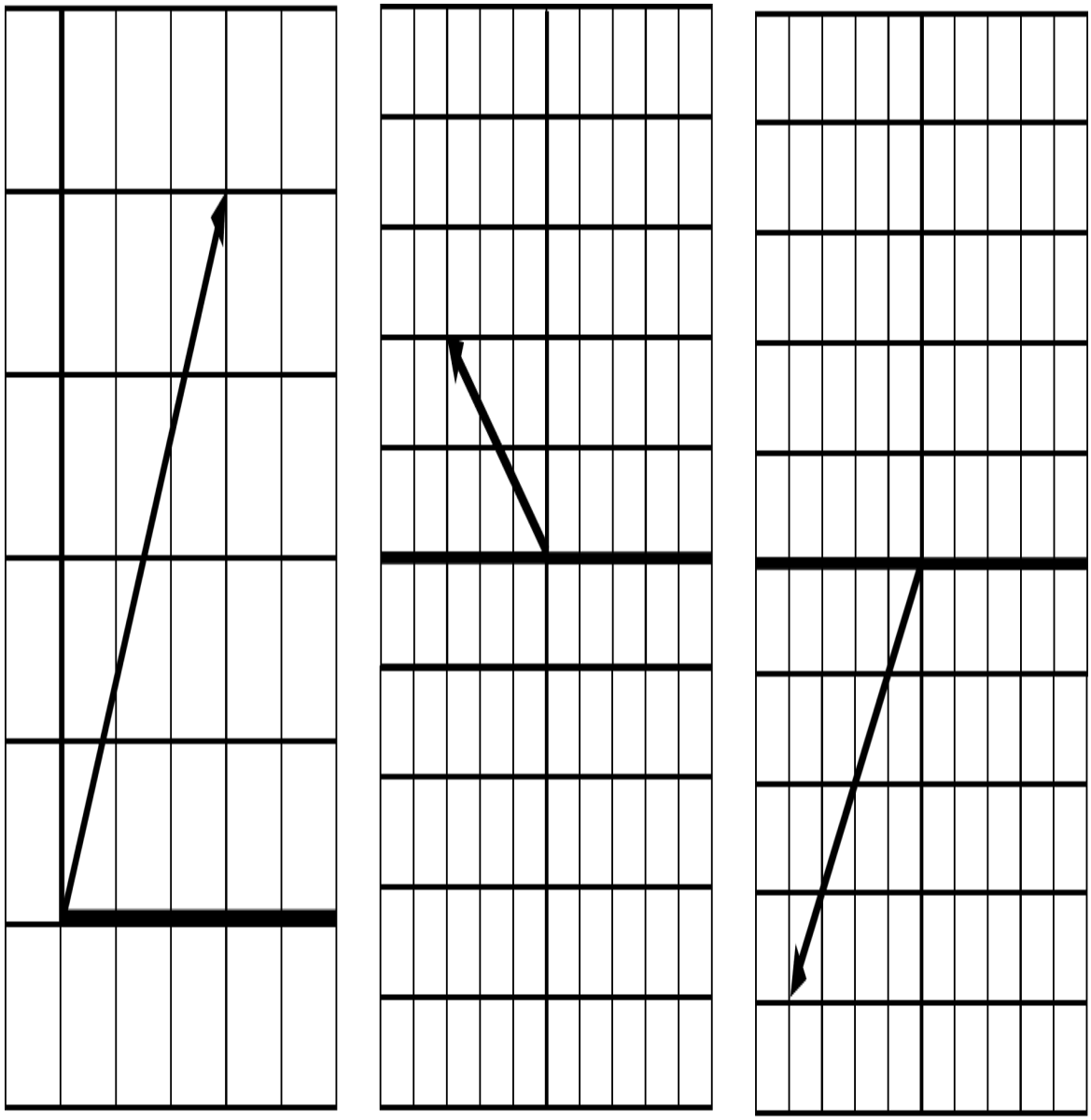


Figure 4-2. A sampling of different vectors

WHY ARE VECTORS USEFUL?

A struggle many people have with vectors (and linear algebra in general) is understanding why it is useful. It's a highly abstract concept but it has many tangible applications. Computer graphics are easier to work with when you have a grasp of vectors and linear transformations. When doing statistics and machine learning work, data is often imported and turned into numerical vectors so we can work with it. Solvers like the one in Excel or Python PuLP use linear programming, which uses vectors to maximize a solution while meeting those constraints. Even video games and flight simulators use vectors and linear algebra not just to model graphics but also physics. I think what makes vectors so hard to grasp is not that their application is unobvious, but rather these applications are so diverse it is hard to see the generalization.

Note also vectors can exist on more than two dimensions. Below we declare a 3-dimensional vector along axes x, y, and z:

$$\vec{v} = \begin{bmatrix} x \\ y \\ z \end{bmatrix} = \begin{bmatrix} 4 \\ 1 \\ 2 \end{bmatrix}$$

Note to create the vector above we are stepping 4 steps in the x direction, 1 in the y direction, and 2 in the z direction. Here it is visualized in Figure 4-3. Note that we no longer are showing a vector on a 2-dimensional grid but rather a 3-dimensional space with 3 axes: *x*, *y*, and *z*.

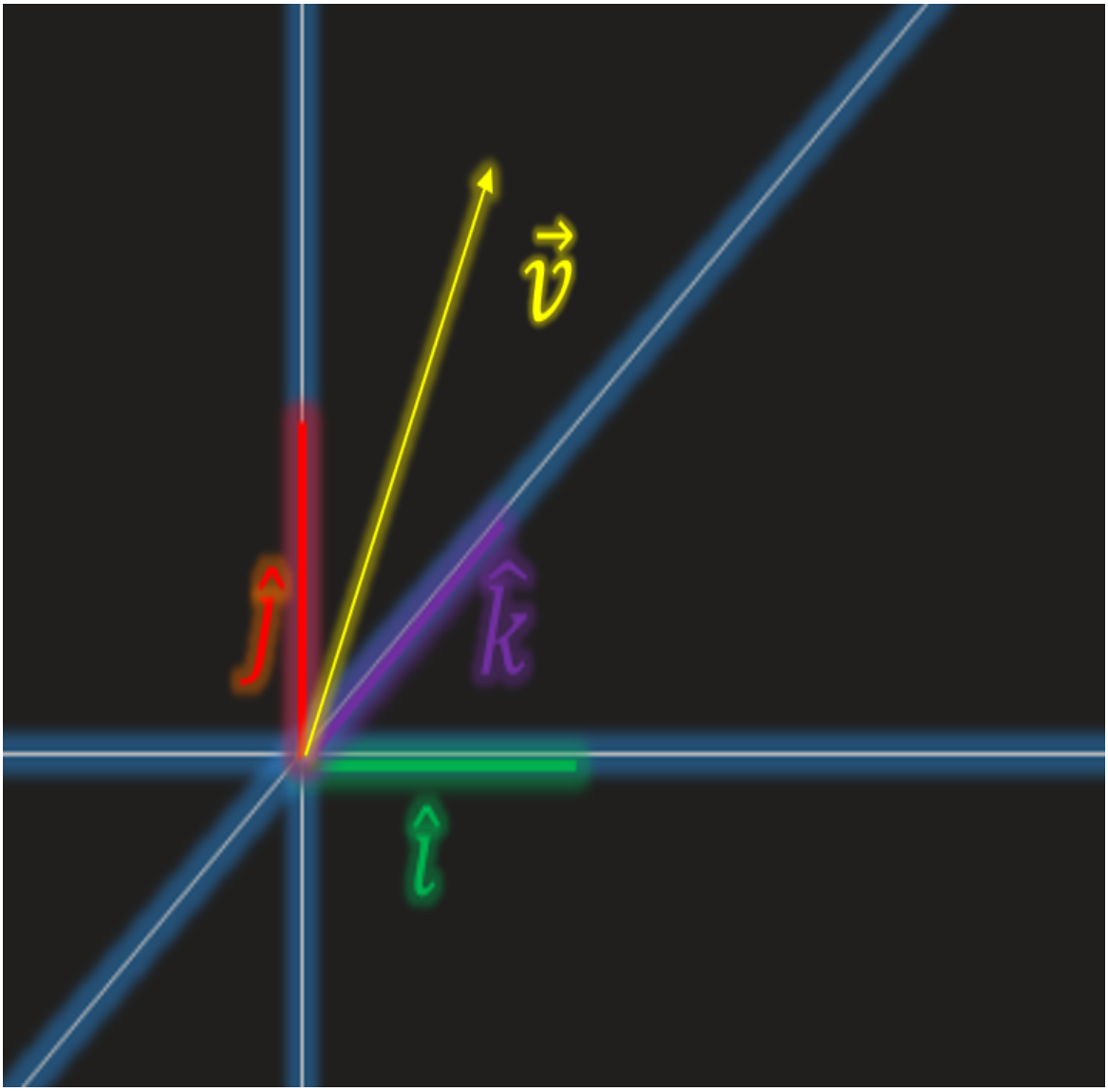


Figure 4-3. A 3-dimensional vector

Naturally we can express this 3-dimensional vector in Python using 3 numeric values, as declared in Example 4-3.

Example 4-3. Declaring a 3-dimensional vector in Python using NumPy

```
import numpy as np
v = np.array([4, 1, 2])
print(v)
```

Like many mathematical models, visualizing more than 3 dimensions is challenging and something we will not expense energy doing so in this

book. But numerically it is still straightforward. Example 4-4 shows how we declare a 5-dimensional vector mathematically in Python.

$$\overrightarrow{v} = \begin{bmatrix} 6 \\ 1 \\ 5 \\ 8 \\ 3 \end{bmatrix}$$

Example 4-4. Declaring a 5-dimensional vector in Python using NumPy

```
import numpy as np
v = np.array([6, 1, 5, 8, 3])
print(v)
```

Adding and Combining Vectors

On their own, vectors are not terribly interesting. You express a direction and size, kind of like a movement of space. But when you start combining vectors, known as **vector addition**, it starts to get interesting. We effectively combine the movements of two vectors into a single vector.

Say we have two vectors $\overrightarrow{v}$ and $\overrightarrow{w}$ as shown in Figure 4-4. How do we add these two vectors together?

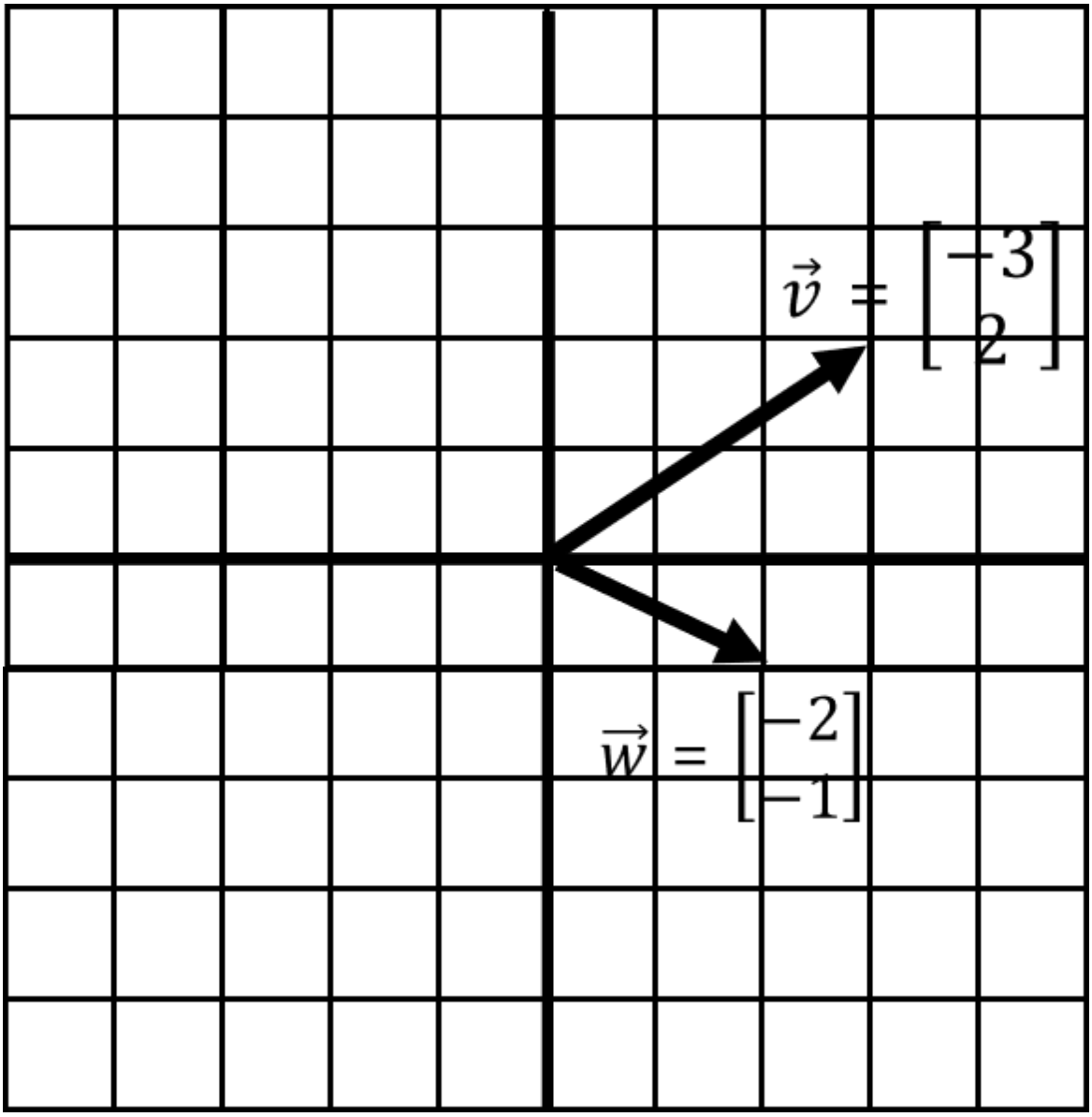


Figure 4-4. Adding two vectors together

We will get to why adding vectors is useful in a moment. But if we wanted to combine these two vectors, including their direction and scale, what would that look like? Numerically this is straightforward. You simply add the respective *x* values and then the *y* values into a new vector as shown in Example 4-5.

$$\vec{v} = \begin{bmatrix} 3 \\ 2 \end{bmatrix}$$

$$\vec{w} = \begin{bmatrix} 2 \\ -1 \end{bmatrix}$$

$$\vec{v} + \vec{w} = \begin{bmatrix} 3+2 \\ 2+-1 \end{bmatrix} = \begin{bmatrix} 5 \\ 1 \end{bmatrix}$$

Example 4-5. Adding two vectors in Python using NumPy

```
from numpy import array

v = array([3,2])
w = array([2,-1])

# sum the vectors
v_plus_w = v + w

# display summed vector
print(v_plus_w) # [5, 1]
```

But what does this mean visually? To visually add these two vectors together, connect one vector after the other and walk to the tip of the last vector (Figure 4-5). The point you end at is a new vector, the result of summing the two vectors.

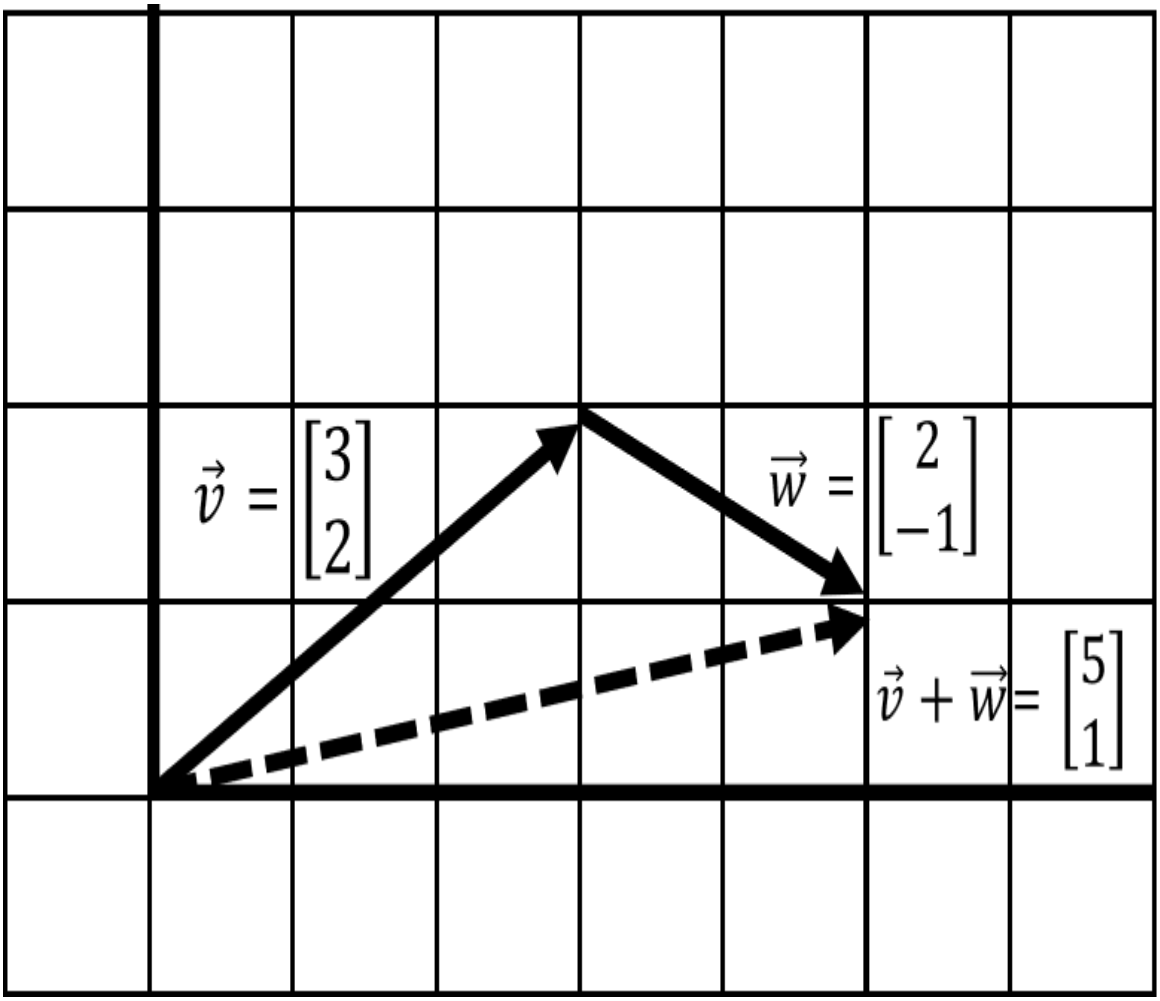


Figure 4-5. Adding two vectors into a new vector

As seen above in Figure 4-5, when we walk to the end of the last vector $\vec{w}$ we end up with a new vector `[5, 1]`. This new vector is the result of summing $\vec{v}$ and $\vec{w}$. In practice, this can be simply adding data together. If we were totaling housing values and their square footage in an area, we would be adding several vectors into a single vector in this manner.

Note that it does not matter whether we add $\vec{v}$ before $\vec{w}$ or vice versa, which means it is **commutative** and order of operation does not matter. If we walk $\vec{w}$ before $\vec{v}$ we end up with the same resulting vector `[5, 1]` as visualized in Figure 4-6.

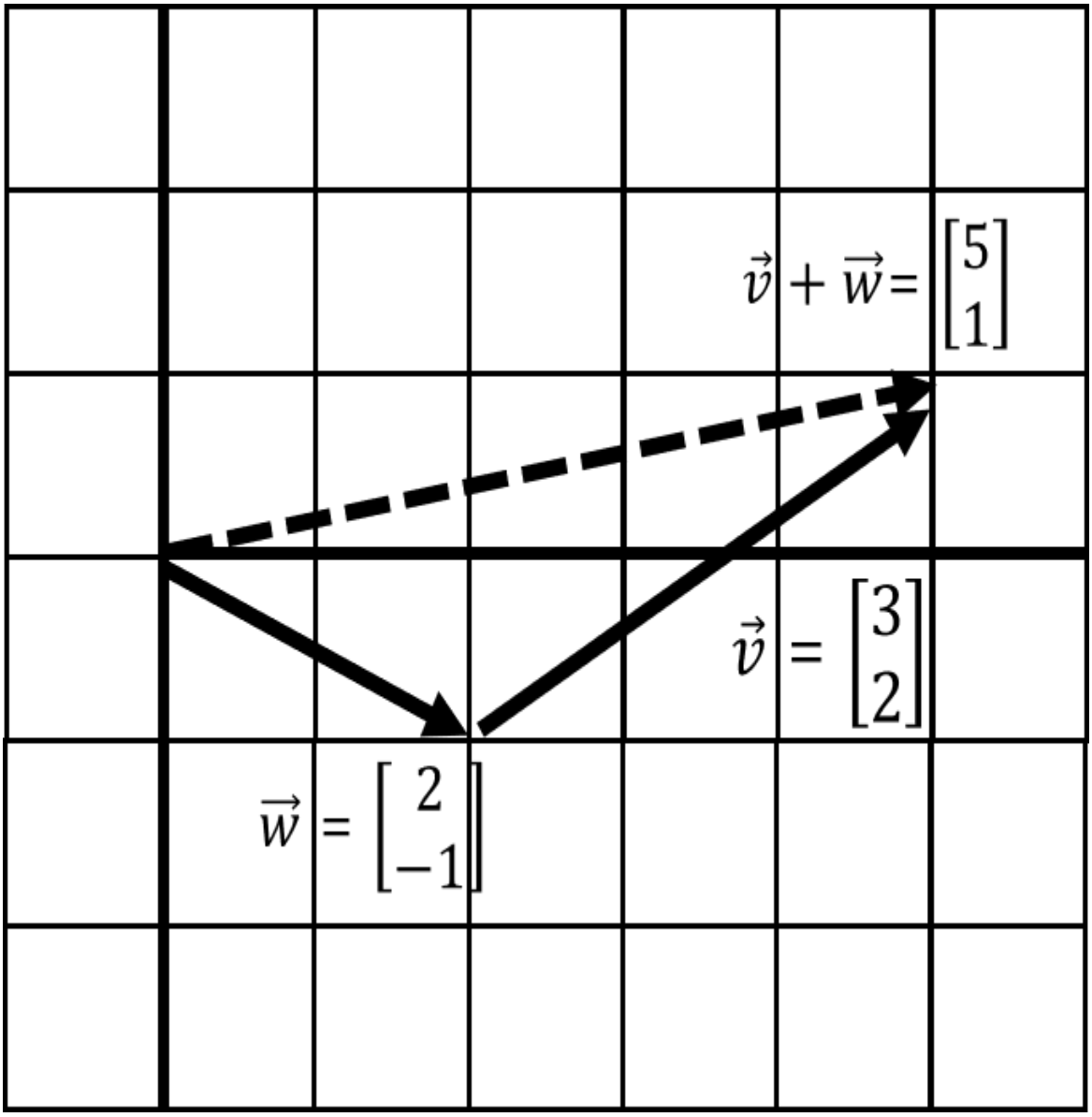


Figure 4-6. Adding vectors is commutatitive

Scaling Vectors

Scaling is growing or shrinking a vector's length. You can grow/shrink a vector by multiplying or scaling it with a single value, known as a **scalar**. Figure 4-7 is vector $\vec{v}$ being scaled by a factor of 2, which doubles it.

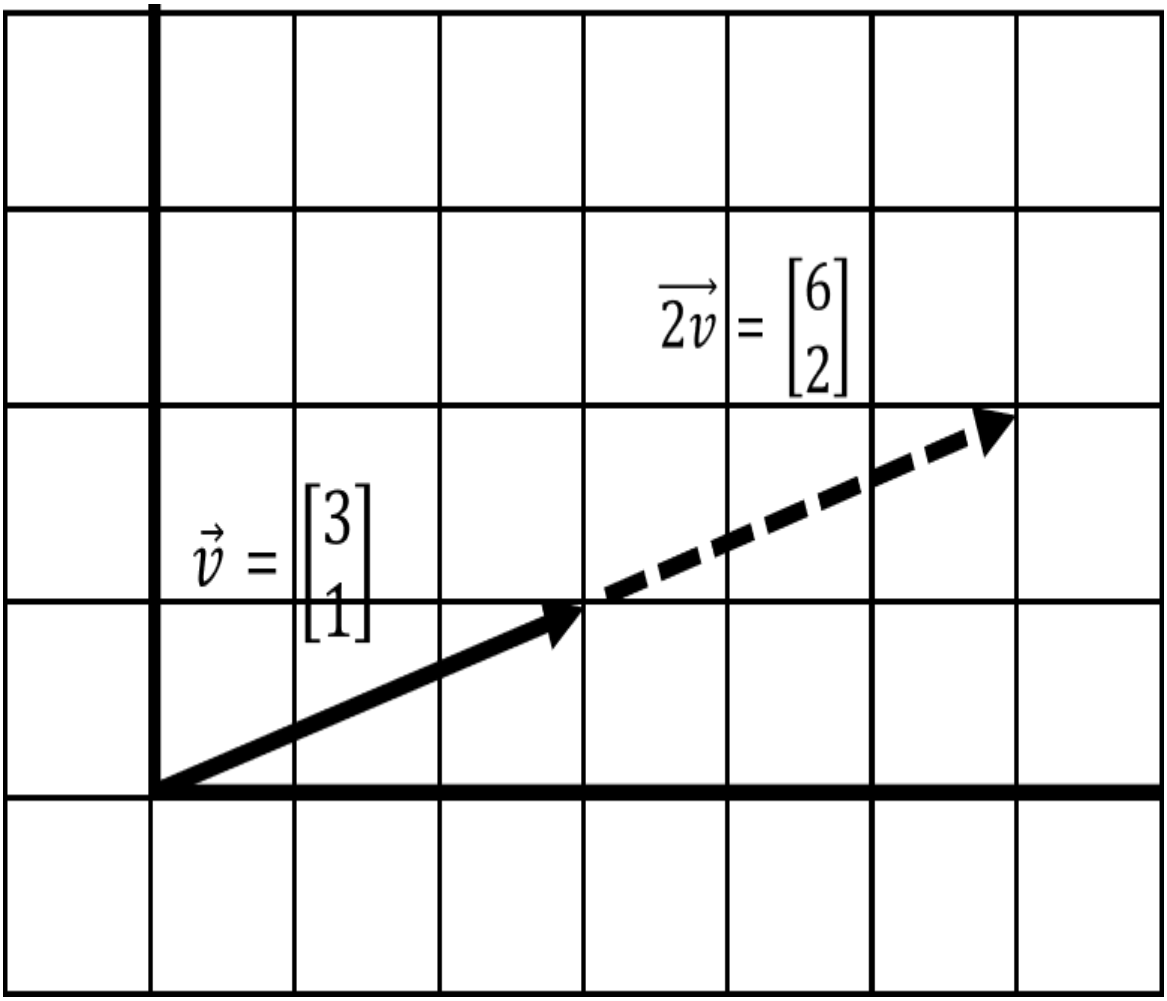


Figure 4-7. Scaling a vector

Mathematically you multiply each element of the vector by the scalar value.

$$\overrightarrow{v} = \begin{bmatrix} 3 \\ 2 \end{bmatrix}$$

$$2\overrightarrow{v} = 2\begin{bmatrix} 3 \\ 2 \end{bmatrix} = \begin{bmatrix} 3 \times 2 \\ 2 \times 2 \end{bmatrix} = \begin{bmatrix} 6 \\ 4 \end{bmatrix}$$

Performing this scaling operation in Python is as easy as multiplying a vector by the scaler, as coded in Example 4-6.

Example 4-6. Scaling a number in Python using NumPy

```
from numpy import array
```

```
v = array([3,1])

# scale the vector
scaled_v = 2.0 * v

# display scaled vector
print(scaled_v) # [6 2]
```

Here in Figure 4-8 is $\overrightarrow{v}$ being scaled down by factor of .5, which halves it.

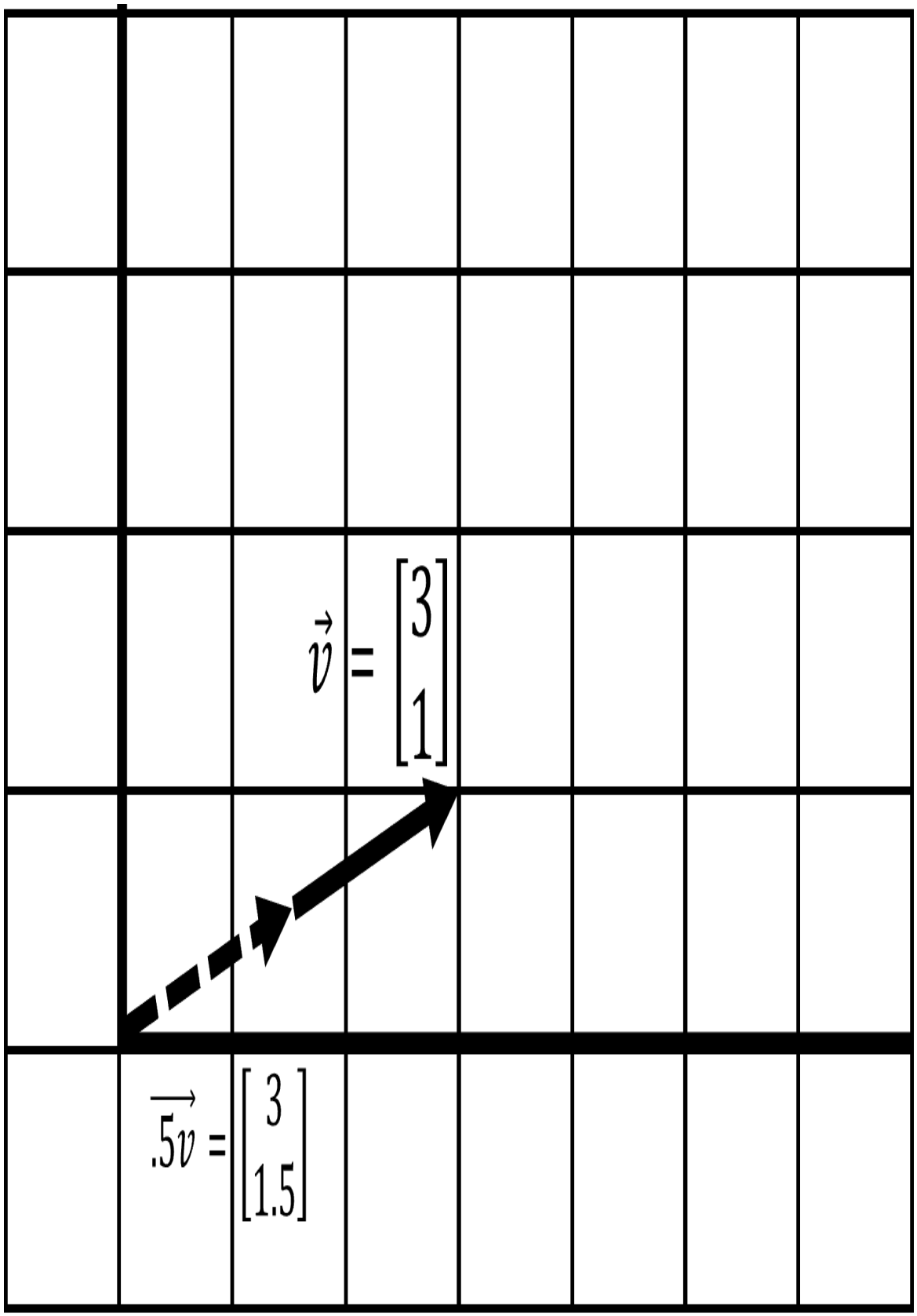

$\vec{v} = \begin{bmatrix} 3 \\ 1 \end{bmatrix}$
$.5\vec{v} = \begin{bmatrix} 3 \\ 1.5 \end{bmatrix}$

Figure 4-8. Scaling down a vector by half

MANIPULATING DATA IS MANIPULATING VECTORS

Every data operation can be thought of in terms of vectors, even simple averages.

Take scaling for example. Let's say we were trying to get the average house value and average square footage for an entire neighborhood. We would add the vectors together to combine their value and square footage respectively, giving us one giant vector containing both total value and total square footage. We then scale down the vector by dividing by the number of houses N, which really is multiplying by $\frac{1}{N}$. We now have a vector containing the average house value and average square footage.

An important detail to note here is that scaling a vector does not change its direction, only its magnitude. But there is one slight exception to this rule as visualized in Figure 4-9. When you multiply a vector by a negative number, it flips the direction of the vector as shown below:

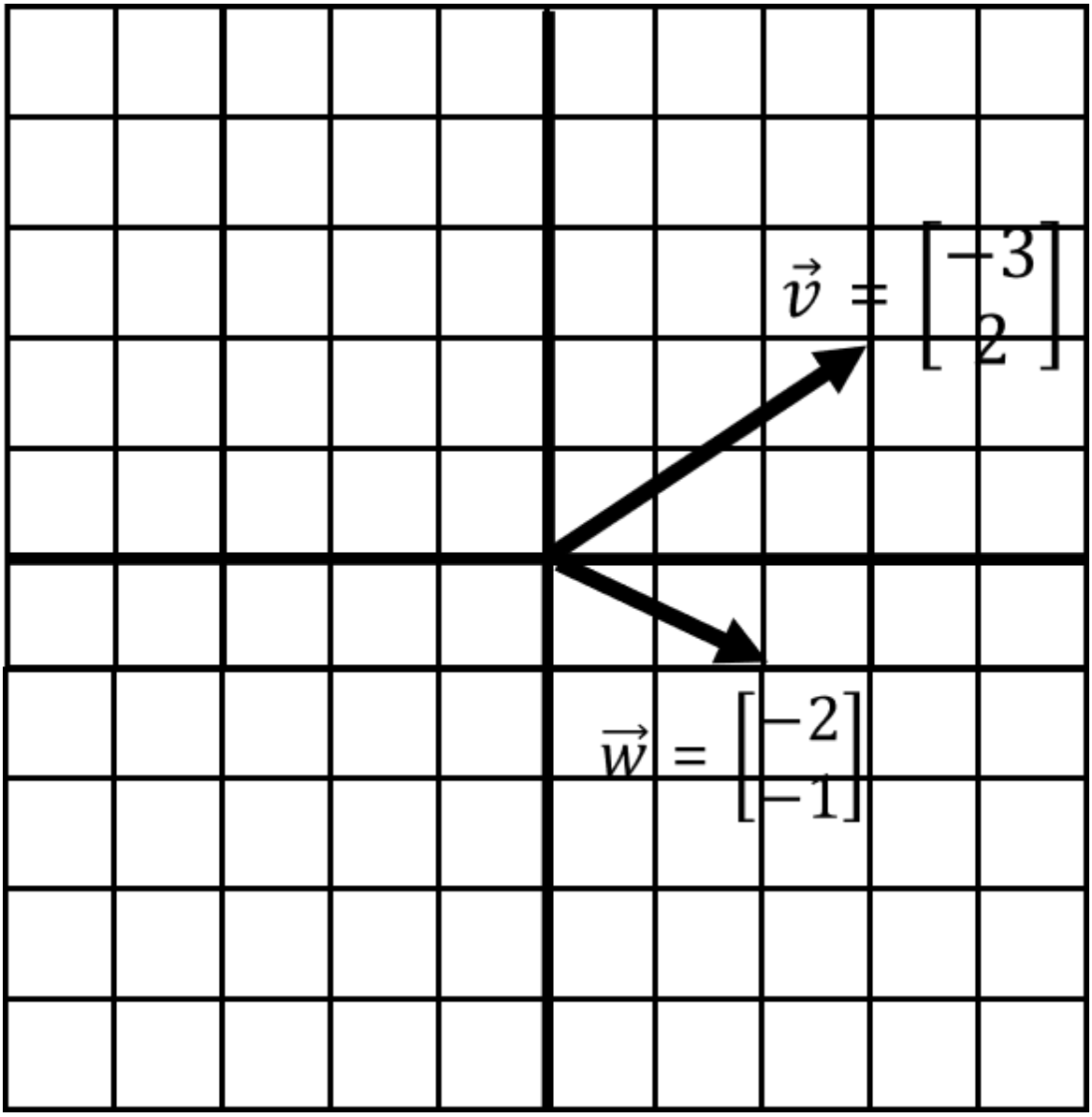


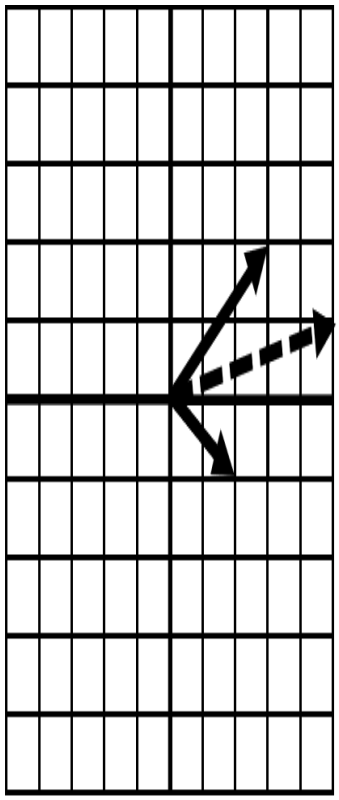
Figure 4-9. A negative scalar flips the vector direction

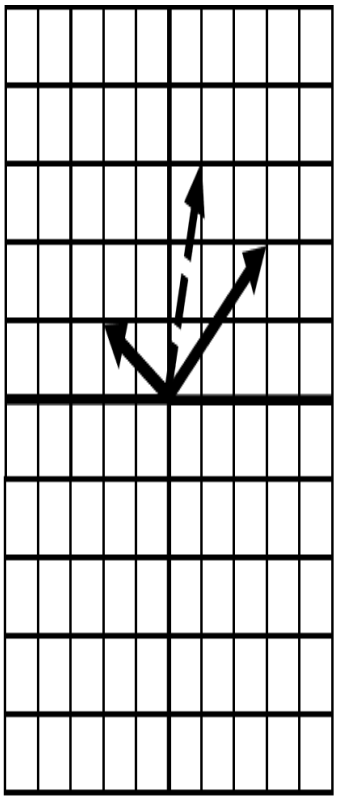
When you think about it though, scaling by a negative number has not really changed direction in that it still exists on the same line. This segues us into a key concept called linear dependence.

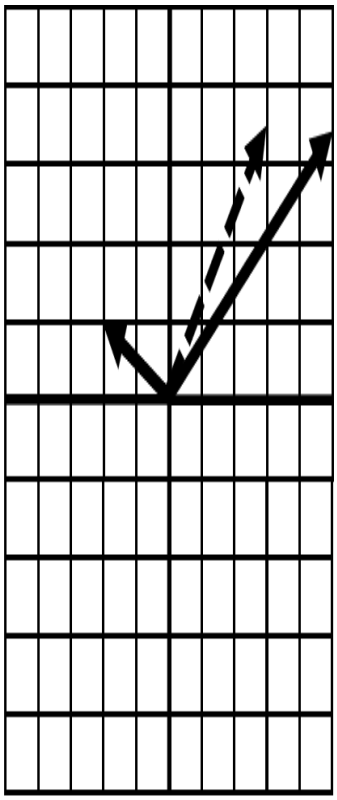
Span and Linear Dependence

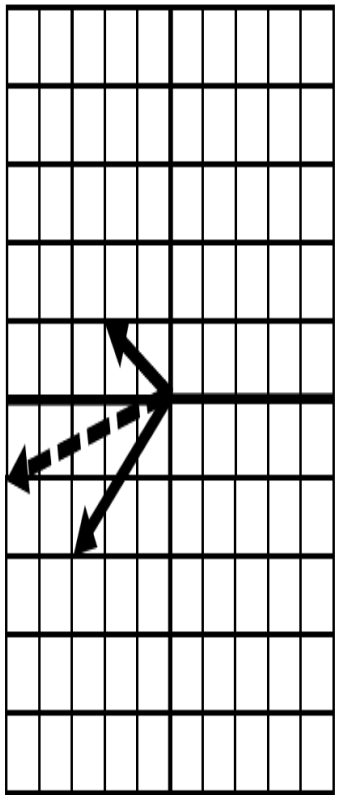
These two operations, adding two vectors and scaling them, brings about a simple but powerful idea. With these two operations, we can combine two vectors and scale them to create any resulting vector we want. Figure 4-10

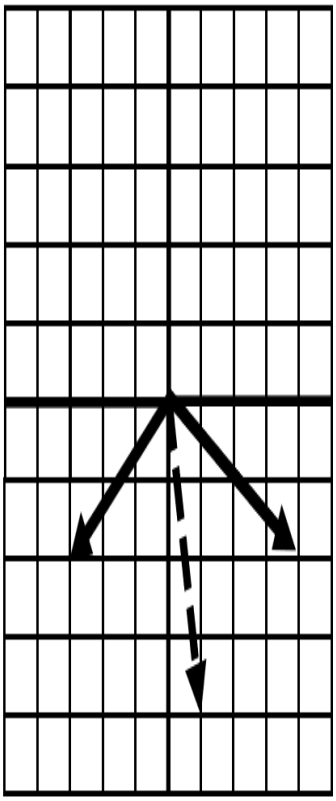
shows six examples of taking two vectors $\overrightarrow{v}$ and $\overrightarrow{w}$, and scaling and combining. These vectors $\overrightarrow{v}$ and $\overrightarrow{w}$, fixed in two different directions, can be scaled and added to create ANY new vector $\overrightarrow{v+w}$.











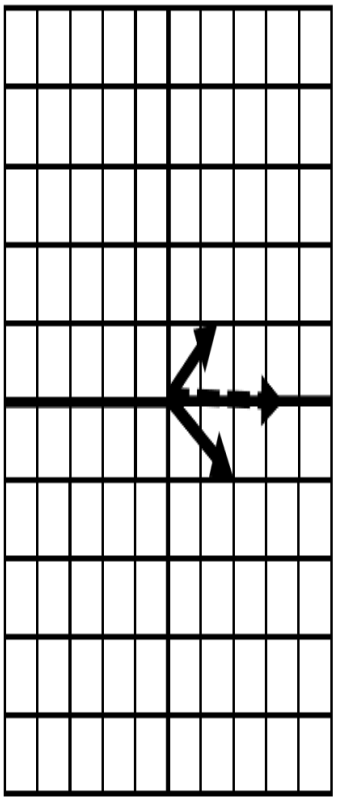


Figure 4-10. Scaling two added vectors allows us to create any new vector

AGAIN, $\overrightarrow{v}$ and $\overrightarrow{w}$ are fixed in direction, except for flipping with negative scalars, but we can use scaling to freely create any vector composed of $\overrightarrow{v + w}$.

This whole space of possible vectors is called **span**, and in most cases our span can create unlimited vectors off those two vectors, simply by scaling and summing them. When we have two vectors in two different directions, they are **linearly independent** and have this unlimited span.

But in what case are we limited in the vectors we can create? Think about it and read on.

What happens when two vectors exist in the same direction, or exist on the same line? The combination of those vectors is also stuck on the same line, limiting our span to just that line. No matterhow you scale it, the resulting sum vector is also stuck on that same line. This makes them **linearly dependent** as shown in Figure 4-11.

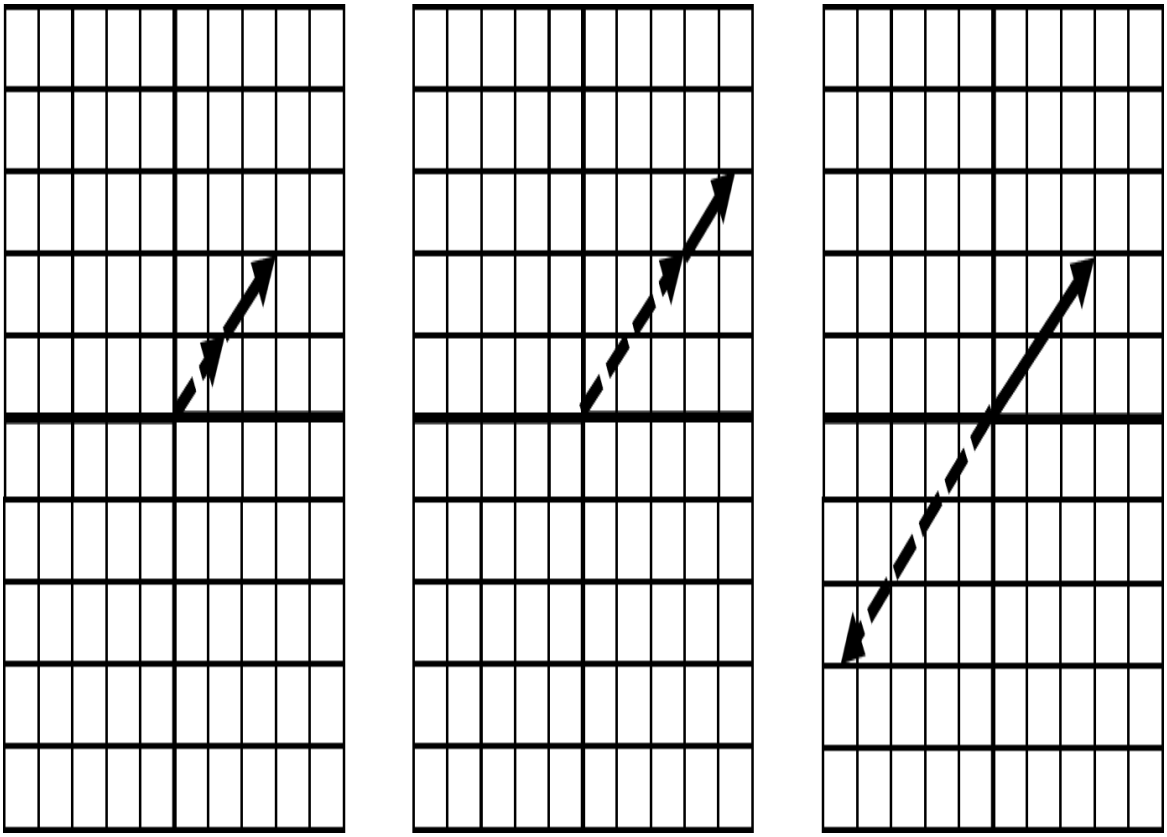


Figure 4-11. Linearly dependent vectors

The span here is stuck on the same line as the two vectors it is made out of. Because the two vectors exist in the same direction (or share the same line), we cannot flexibly create any new vector through scaling. Any resulting vector is stuck on that line.

In 3 or more dimensions, when we have a linearly dependent set of vectors we often get stuck on a plane in a smaller number of dimensions. Here is an example of being stuck on a 2-dimensional plane even though we have 3-dimensional vectors as declared in Figure 4-12.

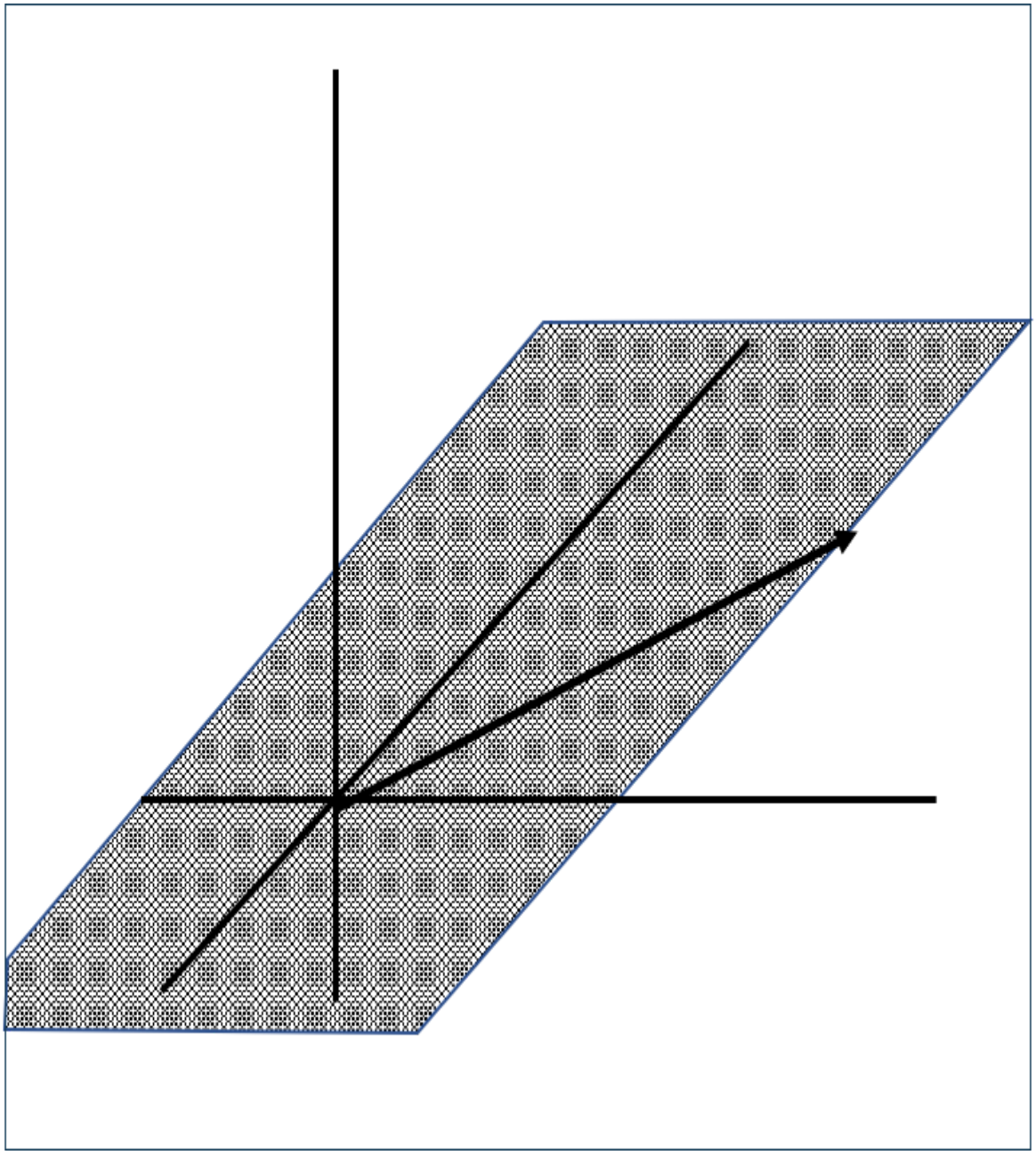


Figure 4-12. Linear dependence in 3 dimensions, note our span is limited to a flat plane

Later we will learn a simple tool called the determinant to check for linear dependence, but why do we care whether two vectors are linear depenendent or independent? A lot of problems become difficult or unsolvable when they are linearly dependent. For example, when we learn about systems of equations later in this chapter, a linearly dependent set of equations can cause variables to disappear and make the problem unsolvable. But if you have linear independence, that flexibility to create

any vector you need from two or more vectors becomes invaluable to solve for a solution!

Linear Transformations

This concept of adding two vectors with fixed direction, but scaling them to get different combined vectors, is hugely important. This combined vector, except in cases of linear dependence, can point in any direction and have any length we choose. This sets up an intuition for linear transformations where we use a vector to transform another vector in a functional-like manner.

Basis Vectors

Imagine we have two simple vectors $\hat{i}$ and $\hat{j}$ ("i-hat" and "j-hat"). These are known as **basis vectors**, which are used to describe transformations on other vectors. They typically have a length of 1 and point in perpendicular positive directions as visualized in Figure 4-13.

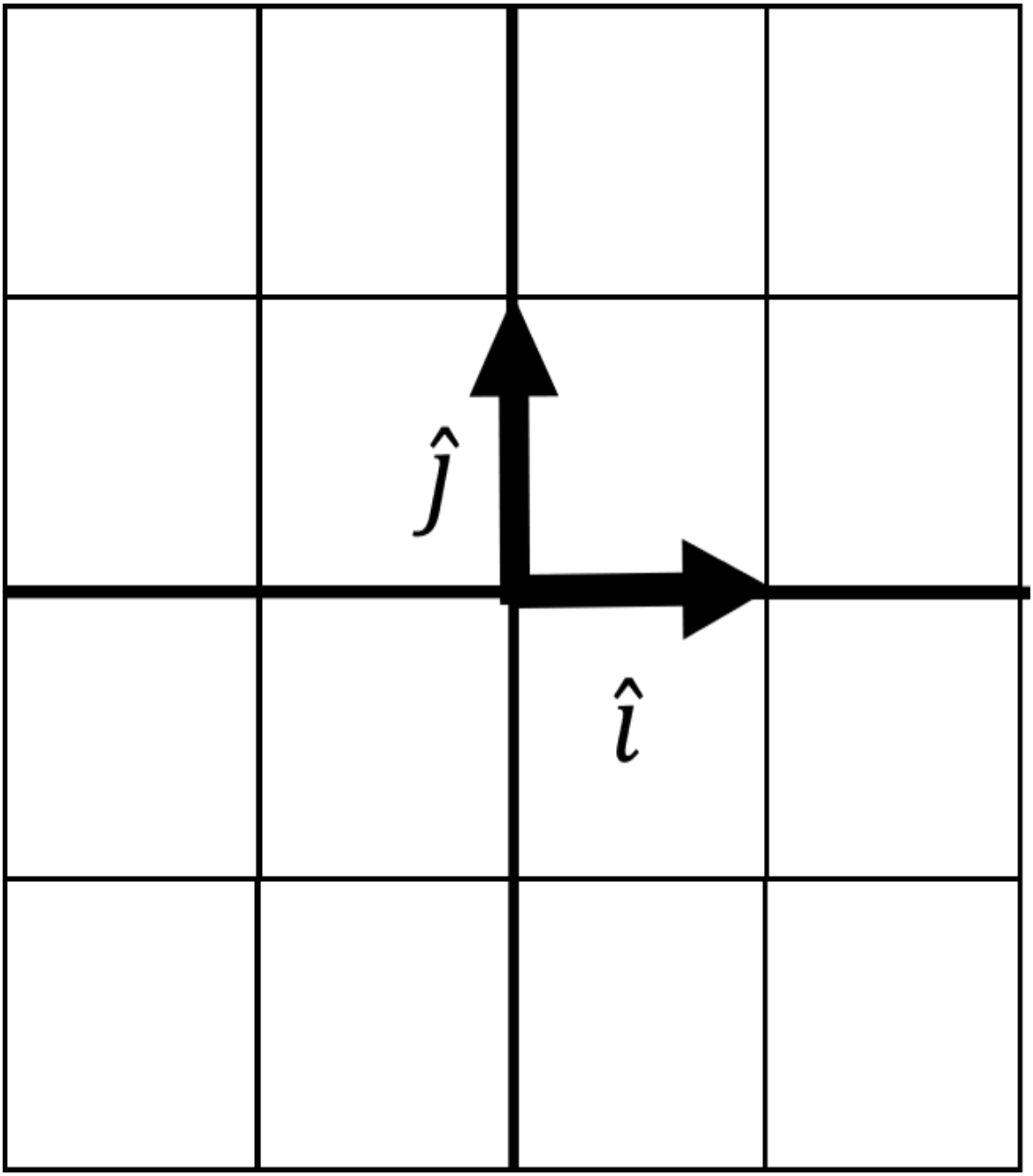


Figure 4-13. Basis vectors $\hat{i}$ and $\hat{j}$

Think of the basis vectors as building blocks to build or transform any vector. Our basis vector is expressed in a 2 x 2 matrix, where the first column is $\hat{i}$ and the second column is $\hat{j}$.

$$\hat{i} = \begin{bmatrix} 1 \\ 0 \end{bmatrix}$$

$$\hat{j} = \begin{bmatrix} 0 \\ 1 \end{bmatrix}$$

$$\text{basis} = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$$

A **matrix** is a collection of vectors (such as $\hat{i}$, $\hat{j}$), can have multiple rows and columns, and is a convenient way to package data. We can use $\hat{i}$ and $\hat{j}$ to create any vector we want by scaling and adding them. Let's start with each having a length of 1 and showing the resulting vector $\overrightarrow{v}$ in Figure 4-14.

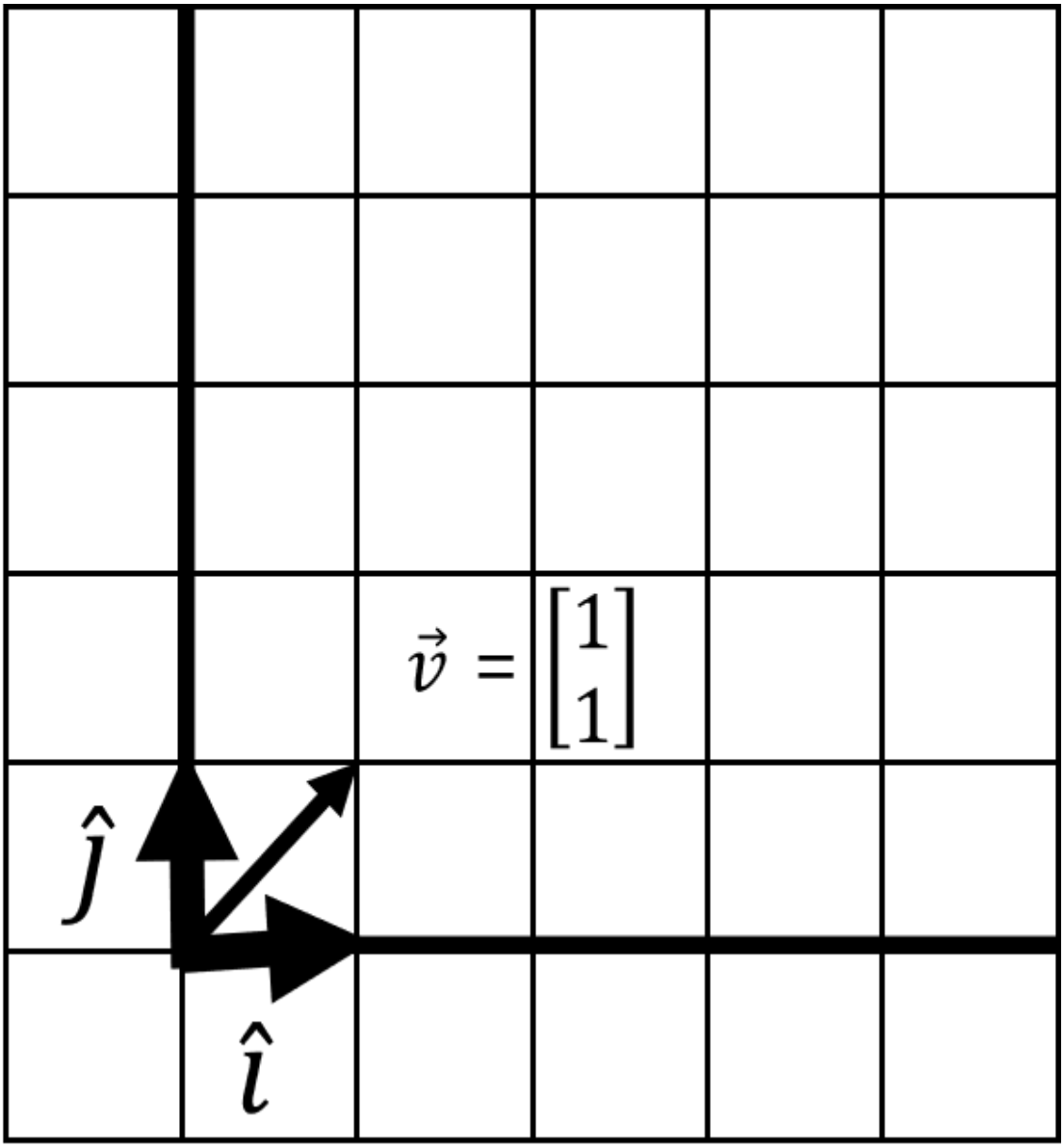


Figure 4-14. Creating a vector off of basis vectors

I want vector $\vec{v}$ to land at `[3, 2]`. What happens to $\vec{v}$ if we stretch $\hat{i}$ by a factor of 3 and $\hat{j}$ by a factor of 2? First we scale them individually as shown here:

$$3\hat{i} = 3\begin{bmatrix} 1 \\ 0 \end{bmatrix} = \begin{bmatrix} 3 \\ 0 \end{bmatrix}$$

$$2\hat{j} = 2\begin{bmatrix}0\\1\end{bmatrix} = \begin{bmatrix}0\\2\end{bmatrix}$$

If we stretched space in these two directions, what does this do to $\overrightarrow{v}$? Well it is going to stretch with $\hat{i}$ and $\hat{j}$. This is known as a **linear transformation**, where we transform a vector with stretching, squishing, sheering, or rotating by tracking basis vector movements. In this case of Figure 4-15, scaling $\hat{i}$ and $\hat{j}$ has stretched space along with our vector $\overrightarrow{v}$.

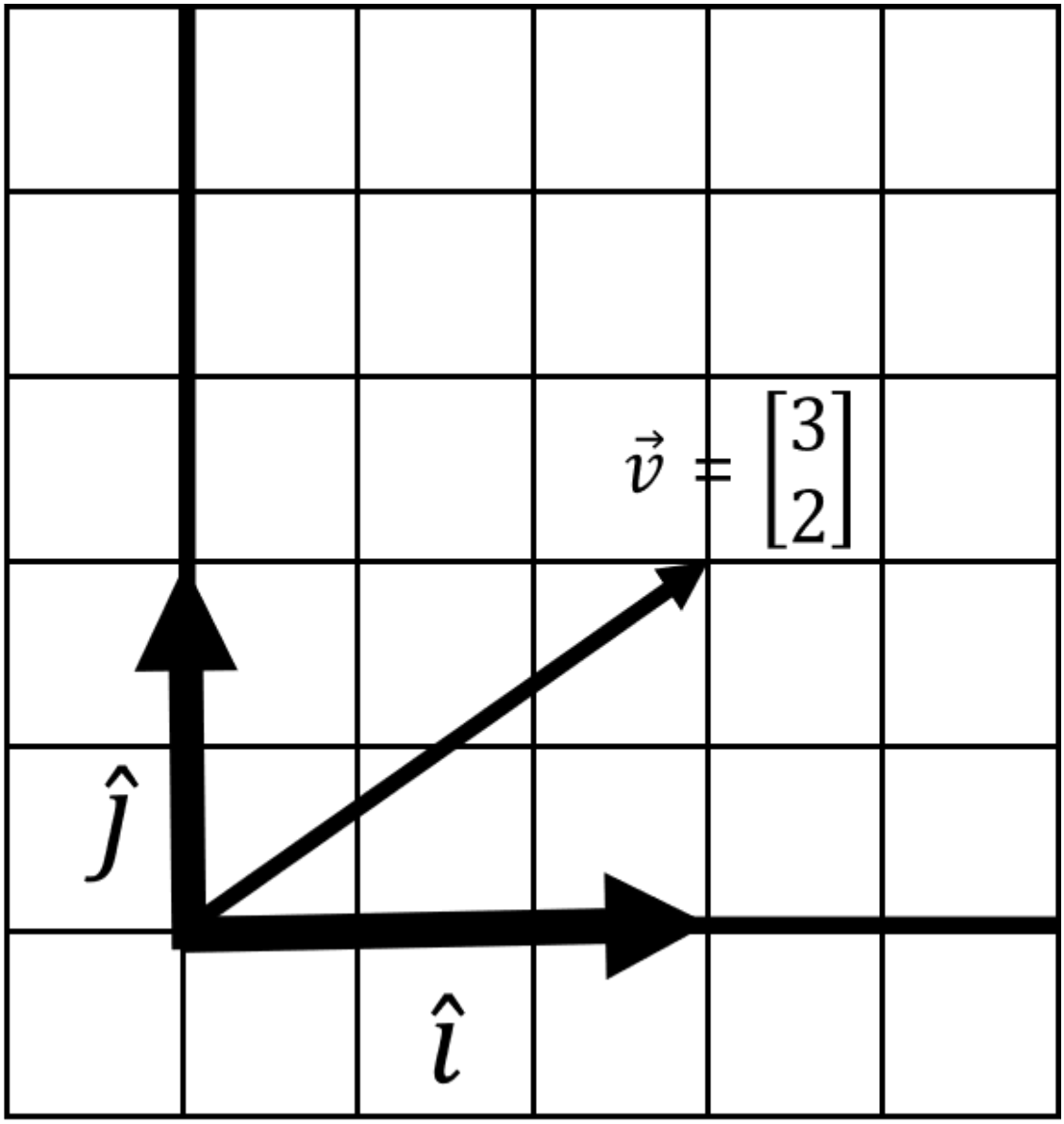
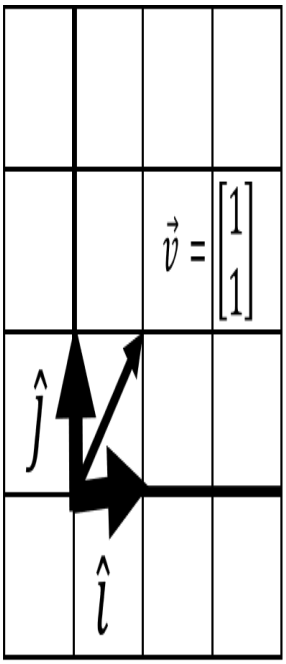


Figure 4-15. A linear transformation

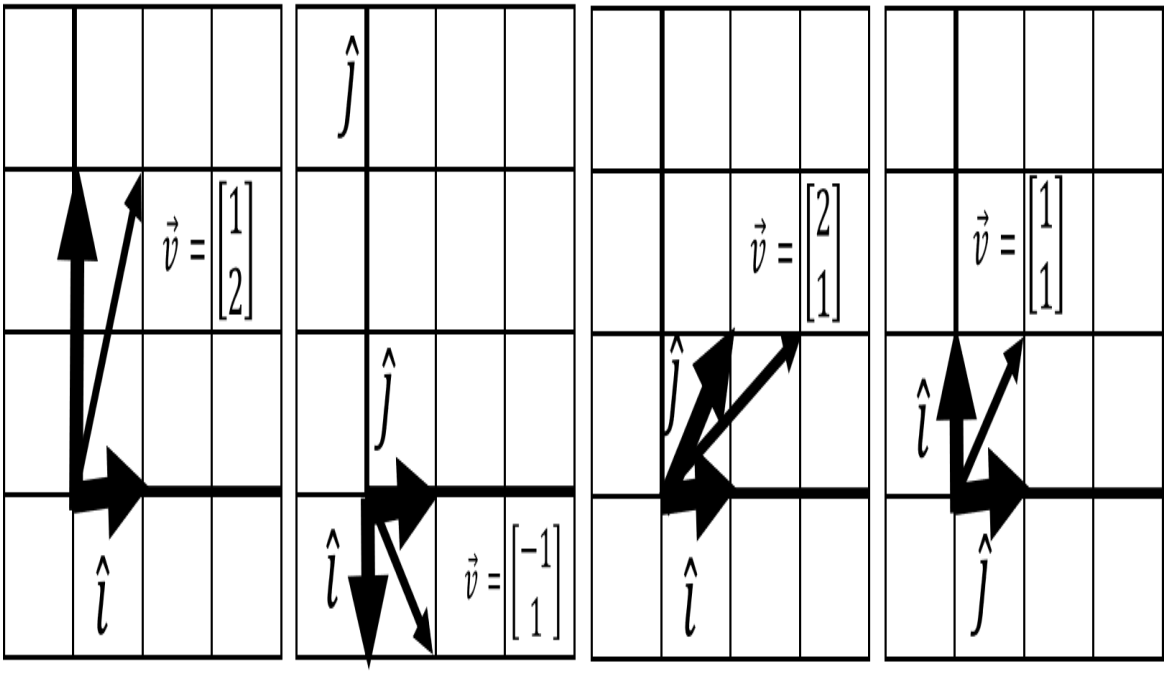
But where does $\overrightarrow{v}$ land? It is easy to visually see where it lands here, which is `[3, 2]`. Recall that vector $\overrightarrow{v}$ is composed off of adding $\hat{i}$ and $\hat{j}$. So we simply take the stretched $\hat{i}$ and $\hat{j}$ and add them together to see where vector $\overrightarrow{v}$ has landed.

$$\overrightarrow{v}_{new} = \begin{bmatrix} 3 \\ 0 \end{bmatrix} + \begin{bmatrix} 0 \\ 2 \end{bmatrix} = \begin{bmatrix} 3 \\ 2 \end{bmatrix}$$

Generally with linear transformations, there are four movements you can achieve shown in Figure 4-16.



BASIS



SCALE ROTATE SHEAR INVERSION

Figure 4-16. Four movements can be achieved with linear transformations

These four linear transformations are a central part of linear algebra. Scaling a vector will stretch or squeeze it. Rotations will turn the vector space, and inversions will flip the vector space so that $\hat{i}$ and $\hat{j}$ swap respective places.

It is important to note that you cannot have transformations that are nonlinear, resulting in curvy or squiggly transformations that no longer respect a straight line. This is why we call it linear algebra, not nonlinear algebra!

Matrix Vector Multiplication

This brings us to our next big idea in linear algebra. This concept of tracking where $\hat{i}$ and $\hat{j}$ land after a transformation is important because it allows us not just to create vectors but also transform existing vectors. If you want true linear algebra enlightenment, think why creating vectors and transforming vectors are actually the same thing. It's all a matter of relativity given your basis vectors being a starting point before and after a transformation.

The formula to transform a vector $\overrightarrow{v}$ given basis vectors $\hat{i}$ and $\hat{j}$ packaged as a matrix is as follows:

$$\begin{bmatrix} x_{new} \\ y_{new} \end{bmatrix} = \begin{bmatrix} a & b \\ c & d \end{bmatrix} \begin{bmatrix} x \\ y \end{bmatrix}$$

$$\begin{bmatrix} x_{new} \\ y_{new} \end{bmatrix} = \begin{bmatrix} ax + by \\ cx + dy \end{bmatrix}$$

$\hat{i}$ is the first column `[a c]` and $\hat{j}$ is the column `[b d]`. We package both of these basis vectors as a matrix, which again is a collection of vectors expressed as a grid of numbers in two or more dimensions. This transformation of a vector by applying basis vectors is known as **matrix vector multiplication**. This may seem contrived at first, but this formula is

a shortcut for scaling and adding $\hat{i}$ and $\hat{j}$ just like we did earlier adding two vectors, and applying the transformation to any vector $\vec{v}$. $\hat{i}$ is the first column `[a c]` and $\hat{j}$ is the column `[b d]`. We package both of these basis vectors as a matrix, which again is a collection of vectors expressed as a grid of numbers in two or more dimensions. This transformation of a vector by applying basis vectors is known as **matrix vector multiplication**. This may seem contrived at first, but this formula is a shortcut for scaling and adding $\hat{i}$ and $\hat{j}$ just like we did earlier adding two vectors, and applying the transformation to any vector $\vec{v}$. So in effect, a matrix really is a transformation expressed as basis vectors.

To execute this transformation in Python using NumPy, we will need to declare our basis vectors as a matrix and then apply it to vector $\vec{v}$ using the `dot()` operator (Example 4-7). The dot operator will perform this scaling and addition between our matrix and vector as we just described above. This is known as the **dot product** and we will explore it throughout this chapter.

Example 4-7. Matrix vector multiplication in NumPy

```
from numpy import array

# compose basis matrix with i-hat and j-hat
basis = array(
    [[3, 0],
     [0, 2]]
 )

# declare vector v
v = array([1,1])

# create new vector
# by transforming v with dot product
new_v = basis.dot(v)

print(new_v) # [3, 2]
```

When thinking in terms of basis vectors, I prefer to break out the basis vectors and then compose them together into a matrix. Just note you will need to **transpose**, or swap the columns and rows. This is because NumPy's

`array()` function will do the opposite orientation we want, populating each vector as a row rather than a column. Transposition in NumPy is demonstrated in Example 4-8.

Example 4-8.

```
from numpy import array

# Declare i-hat and j-hat
i_hat = array([2, 0])
j_hat = array([0, 3])

# compose basis matrix using i-hat and j-hat
# also need to transpose rows into columns
basis = array([i_hat, j_hat]).transpose()

# declare vector v
v = array([1,1])

# create new vector
# by transforming v with dot product
new_v = basis.dot(v)

print(new_v) # [2, 3]
```

Here's another example. Let's start with vector $\vec{v}$ being `[2 1]` and $\hat{i}$ and $\hat{j}$ start at `[1 0]` and `[0 1]` respectively. We then transform $\hat{i}$ and $\hat{j}$ to `[2 0]` and `[0 3]`. What happens to vector $\vec{v}$? Working this out mathematically by hand using our formula, we get this.

$$\begin{bmatrix} x_{new} \\ y_{new} \end{bmatrix} = \begin{bmatrix} a & b \\ c & d \end{bmatrix} \begin{bmatrix} x \\ y \end{bmatrix} = \begin{bmatrix} ax + by \\ cx + dy \end{bmatrix}$$

$$\begin{bmatrix} x_{new} \\ y_{new} \end{bmatrix} = \begin{bmatrix} 2 & 0 \\ 0 & 3 \end{bmatrix} \begin{bmatrix} 2 \\ 1 \end{bmatrix} = \begin{bmatrix} (2)(2) + (0)(1) \\ (2)(0) + (3)(1) \end{bmatrix} = \begin{bmatrix} 4 \\ 3 \end{bmatrix}$$

Example 4-9 shows this solution in Python.

Example 4-9. Transforming a vector using NumPy

```
from numpy import array

# Declare i-hat and j-hat
```

```
i_hat = array([2, 0])
j_hat = array([0, 3])

# compose basis matrix using i-hat and j-hat
# also need to transpose rows into columns
basis = array([i_hat, j_hat]).transpose()

# declare vector v 0
v = array([2,1])

# create new vector
# by transforming v with dot product
new_v = basis.dot(v)

print(new_v) # [4 3]
```

The vector $\overrightarrow{v}$ now lands at `[4 3]`. Figure 4-17 shows a visual of what this transformation looks like.

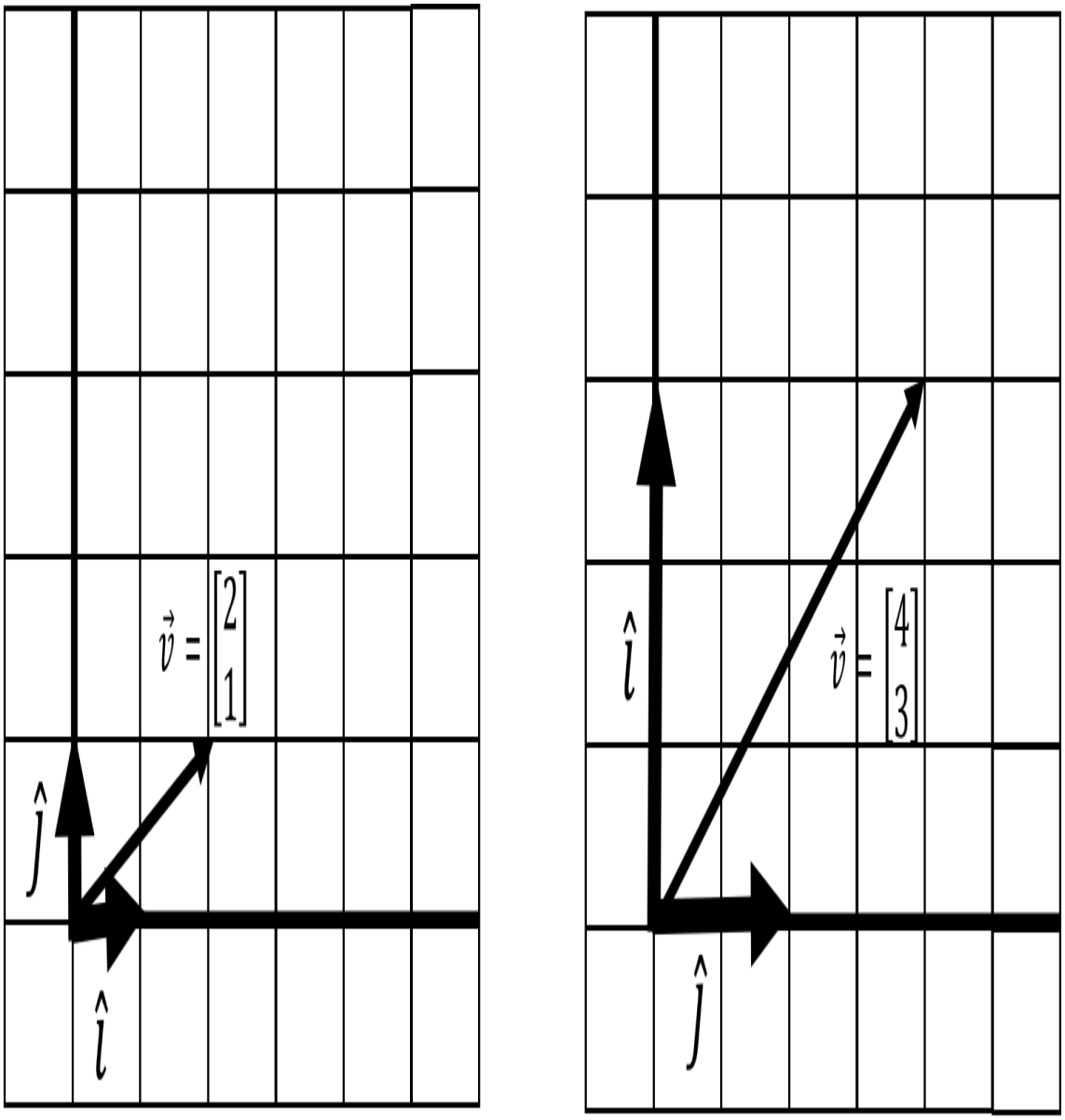


Figure 4-17. A stretching linear transformation

Here is an example that jumps things up a notch. Let's take vector $\vec{v}$ of value `[2 1]`. $\hat{i}$ and $\hat{j}$ start at `[1 0]` and `[0 1]`, but then are transformed and land at `[2 3]` and `[2 -1]`. What happens to $\vec{v}$? Let's look in Figure 4-18 and Example 4-10.

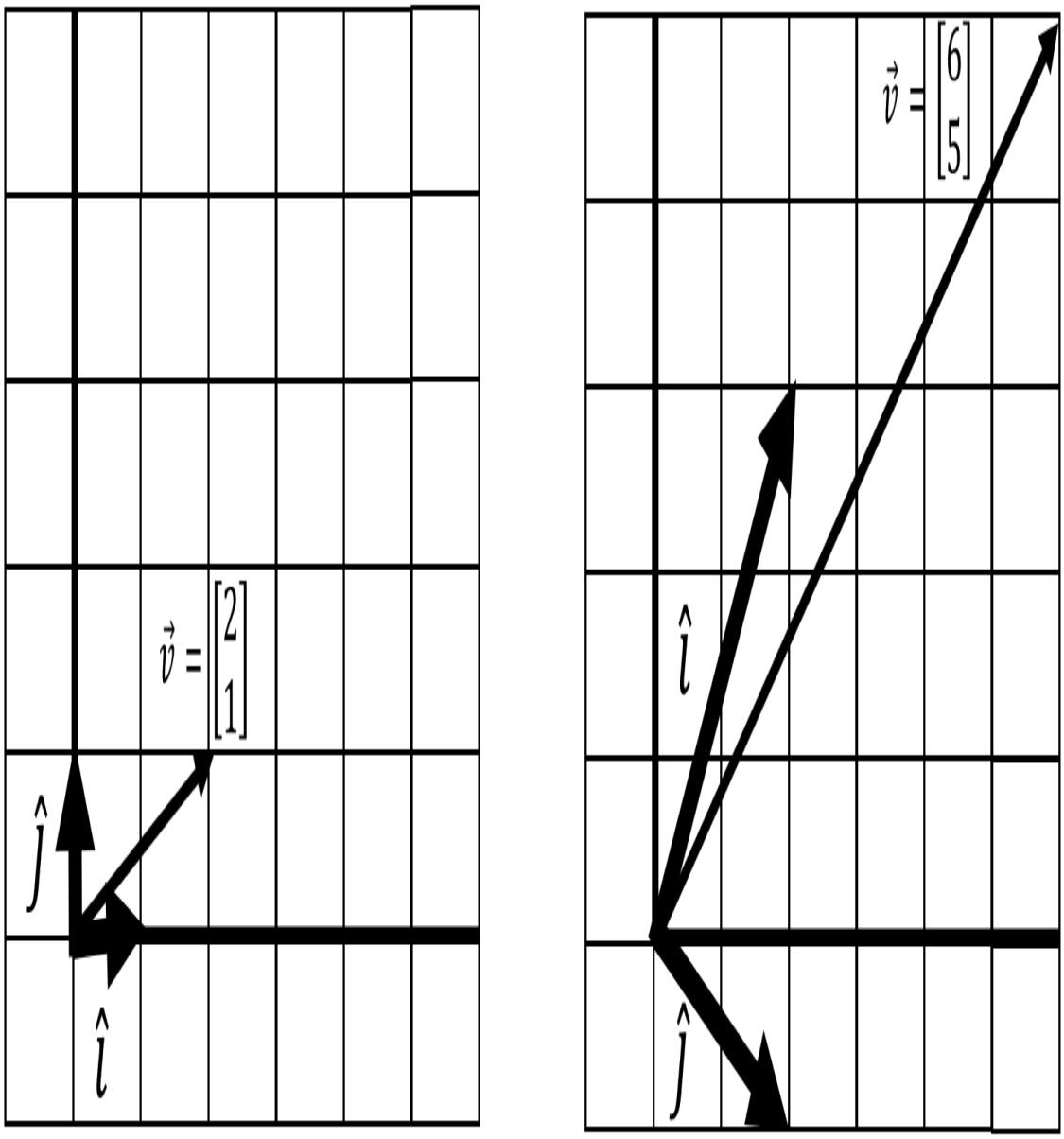


Figure 4-18. A linear transformation that does a rotation, sheer, and flipping of space

Example 4-10.

```
from numpy import array

# Declare i-hat and j-hat
i_hat = array([2, 3])
j_hat = array([2, -1])
```

```
# compose basis matrix using i-hat and j-hat
# also need to transpose rows into columns
basis = array([i_hat, j_hat]).transpose()

# declare vector v 0
v = array([2,1])

# create new vector
# by transforming v with dot product
new_v = basis.dot(v)

print(new_v) # [6, 5]
```

A lot has happened here. Not only did we scale $\hat{i}$ and $\hat{j}$ and elongate vector $\overrightarrow{v}$. We actually sheered, rotated, and flipped space too. You know space was flipped space when $\hat{i}$ and $\hat{j}$ change places in their clockwise orientation, and we will learn how to detect this with determinants later in this chapter.

BASIS VECTORS IN 3D AND BEYOND

You might be wondering how we think of vector transformations in 3 dimensions or more. The concept of basis vectors extends quite nicely. If I have a 3-dimensional vector space, then I have basis vectors $\hat{i}$, $\hat{j}$, and $\hat{k}$. I just keep adding more letters from the alphabet for each new dimension (Figure 4-19).

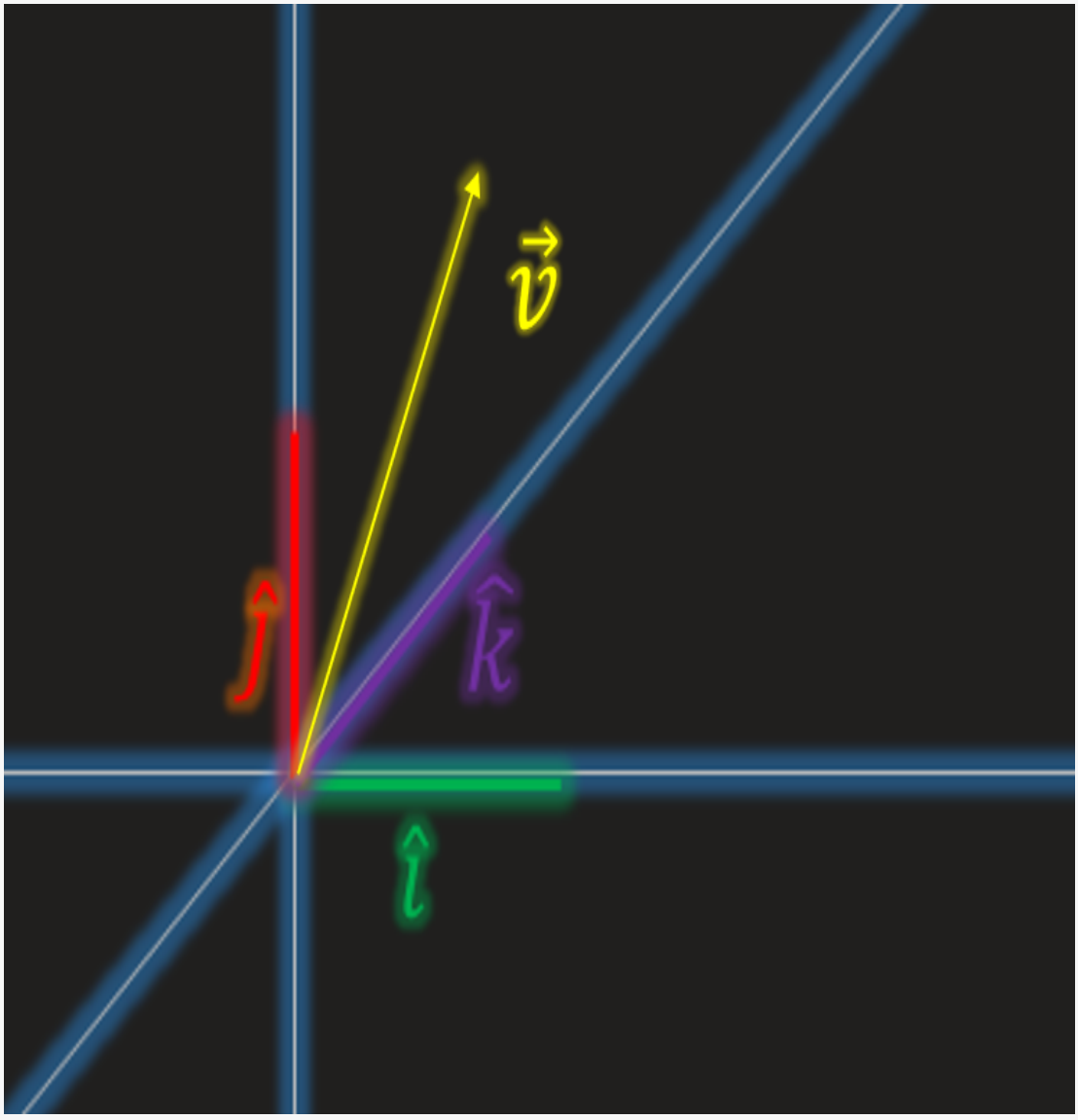


Figure 4-19. 3D basis vector

Something else that is worth pointing out is some linear transformations can shift a vector space into fewer or more dimensions, and that is

exactly what nonsquare matrices will do (where number of rows and columns are not equal). In the interest of time we cannot explore this. But 3Blue1Brown explains and animates this concept beautifully.

Matrix Multiplication

We learned how to multiply a vector and a matrix, but what exactly does multiplying two matrices accomplish? Think of **matrix multiplication** as applying multiple transformations to a vector space. Each transformation is like a function, where we apply the inner-most first and then apply each subsequent transformation outwards.

Here is how we apply a rotation and then a shear to any vector $\overrightarrow{v}$ with value `[x y]`.

$$\begin{bmatrix} 1 & 1 \\ 0 & 1 \end{bmatrix} \begin{bmatrix} 0 & -1 \\ 1 & 0 \end{bmatrix} \begin{bmatrix} x \\ y \end{bmatrix}$$

We can actually consolidate these two transformations by using this formula, applying one tranformation onto the last. You multiply and add each row from the first matrix to each respective column of the second matrix, in an "over-and-down! over-and-down!" pattern.

$$\begin{bmatrix} a & b \\ c & d \end{bmatrix} \begin{bmatrix} e & f \\ g & h \end{bmatrix} = \begin{bmatrix} ae + bg & af + bh \\ ce + dy & cf + dh \end{bmatrix}$$

So we can actually consolidate these two separate transformations (rotation and shear) into a single transformation.

$$\begin{bmatrix} 1 & 1 \\ 0 & 1 \end{bmatrix} \begin{bmatrix} 0 & -1 \\ 1 & 0 \end{bmatrix} \begin{bmatrix} x \\ y \end{bmatrix}$$

$$= \begin{bmatrix} (1)(0) + (1)(1) & (-1)(1) + (1)(0) \\ (0)(0) + (1)(1) & (0)(-1) + (1)(0) \end{bmatrix} \begin{bmatrix} x \\ y \end{bmatrix}$$

$$= \begin{bmatrix} 1 & -1 \\ 1 & 0 \end{bmatrix} \begin{bmatrix} x \\ y \end{bmatrix}$$

To execute this in Python using NumPy, you can combine the two matrices simply using the `matmul()` or `@` operator (Example 4-11). We will then turn around and use this consolidated tranformation and apply it to a vector `[1 2]`.

> **USING `DOT()` VS `MATMULT()` AND `@`**
>
> In general, you want to prefer `matmul()` and its shorthand `@` to combine matrices rather than the `dot()` operator in NumPy. The former generally has a preferable policy for higher-dimensional matrices and how the elements are broadcasted.
>
> To learn more, this StackOverflow question is a good place to start.

Example 4-11.

```
from numpy import array

# Transformation 1
i_hat1 = array([0, 1])
j_hat1 = array([-1, 0])
transform1 = array([i_hat1, j_hat1]).transpose()

# Transformation 2
i_hat2 = array([1, 0])
j_hat2 = array([1, 1])
transform2 = array([i_hat2, j_hat2]).transpose()

# Combine Transformations
combined = transform2 @ transform1

# Test
print("COMBINED MATRIX:\n {}".format(combined))

v = array([1, 2])
print(combined.dot(v))   # [-1 1]
```

Note that we could have also applied each tranformation individually to vector $\vec{v}$ and still have gotten the same result. If you replace the last line

with these three lines applying each transformation (Example 4-12), you will still get `[-1 1]` on that new vector.

Example 4-12.

```
rotated = transform1.dot(v)
sheered = transform2.dot(rotated)
print(sheered) # [-1 1]
```

Note that the order you apply each transformation matters! If we were to apply `transformation1` on `transformation2`, we are going to get a different result of `[-2 3]` as calculed in Example 4-13. So matrix dot products are not commutative, meaning you cannot flip the order and expect the same result!

Example 4-13.

```
from numpy import array

# Transformation 1
i_hat1 = array([0, 1])
j_hat1 = array([-1, 0])
transform1 = array([i_hat1, j_hat1]).transpose()

# Transformation 2
i_hat2 = array([1, 0])
j_hat2 = array([1, 1])
transform2 = array([i_hat2, j_hat2]).transpose()

# Combine Transformations, apply sheer first and then rotation
combined = transform1 @ transform2

# Test
print("COMBINED MATRIX:\n {}".format(combined))

v = array([1, 2])
print(combined.dot(v)) # [-2 3]
```

Think of each transformation as a function, and we apply them from the inner-most to outer-most just like nested function calls.

LINEAR TRANSFORMATIONS IN PRACTICE

You might be wondering what do all these linear transformations and matrices have to do with data science and machine learning. The answer is everything! From importing data to numerical operations with linear regression, logistic regression, and neural networks, linear transformations are the heart of mathematically manipulated data.

In practice however, you will rarely take the time to geometrically visualize your data as vector spaces and linear transformations. You will be dealing with too many dimensions to do this productively. But it is good to be mindful of of the geometric interpretation just to understand what these contrived-looking numerical operations do! Otherwise you just memorizing numerical operation patterns without any context. It also makes new linear algebra concepts like determinants more obvious.

Determinants

When we perform linear transformations, we sometimes "expand" or "squish" space and the degree this happens can be helpful. Take a sampled area from the vector space in Figure 4-20: what happens to it after we scale $\hat{i}$ and $\hat{j}$?

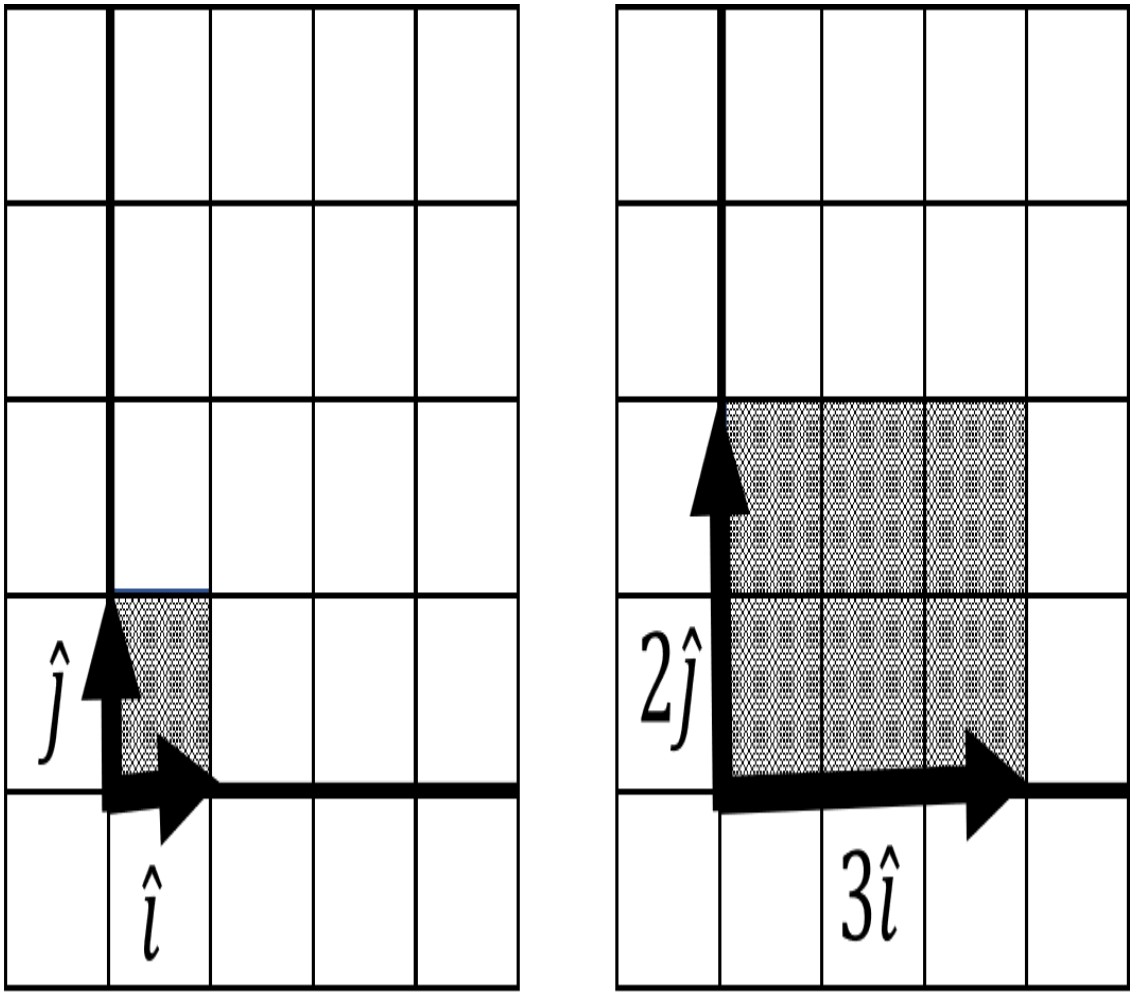


Figure 4-20. A determinant measures how a linear transformation scales an area

Note it increases in area by a factor of 6.0, and this factor is known as a **determinant**. Determinants describe how much a sampled area in a vector space changes in scale with linear transformations, and this can provide helpful information about the transformation.

Example 4-14 shows how to calculate this determinant in Python.

Example 4-14.

```
from numpy.linalg import det
from numpy import array

i_hat = array([3, 0])
j_hat = array([0, 2])

basis = array([i_hat, j_hat]).transpose()
```

```
determinant = det(basis)

print(determinant) # prints 6.0
```

Simple shears and rotations should not affect the determinant as the area will not change. Figure 4-21 and Example 4-15 shows a simple shear and the determinant remains a factor 1.0, showing it is unchanged.

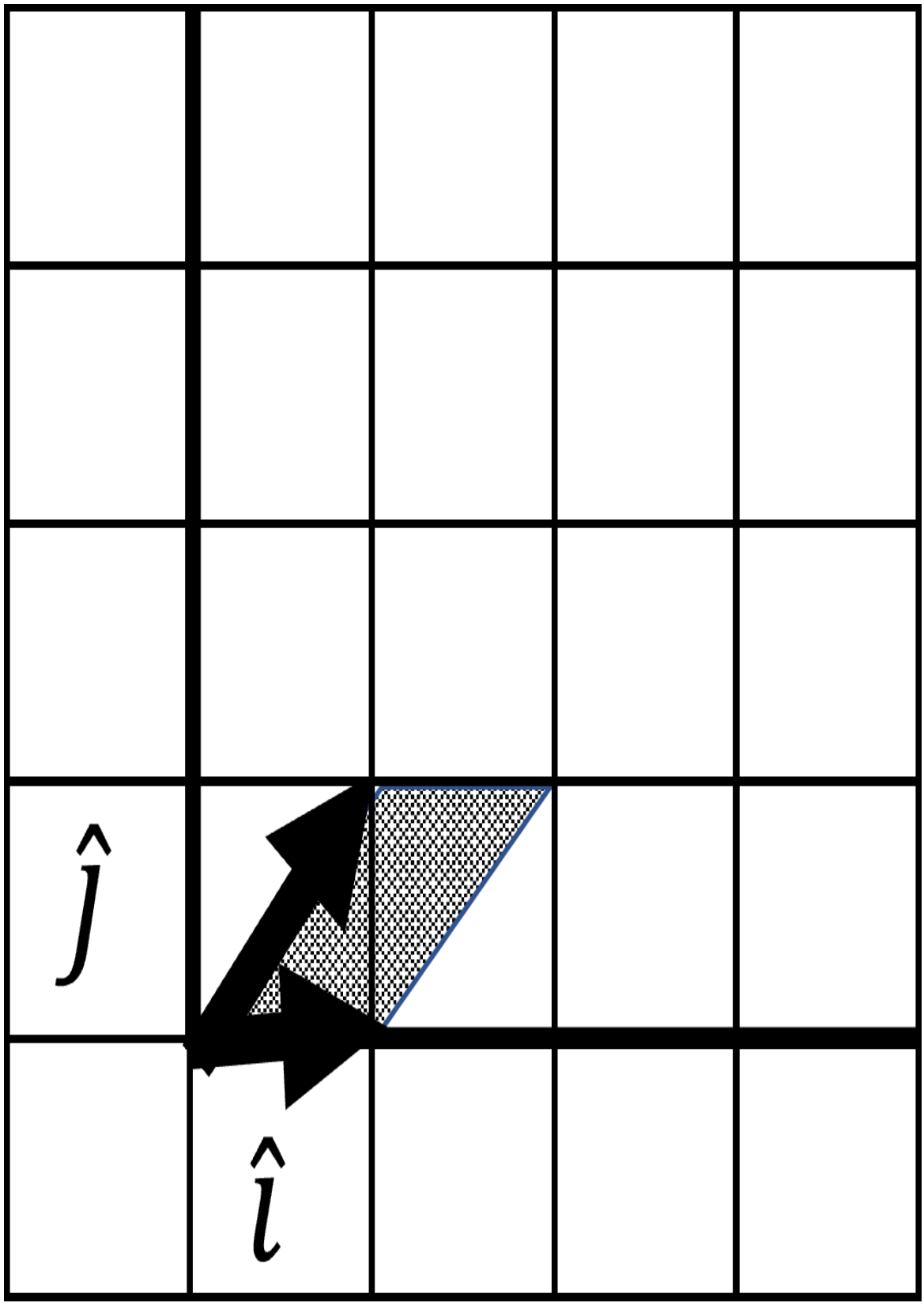

$\hat{j}$
$\hat{i}$

Figure 4-21. A simple shear does not change the determinant

Example 4-15.

```
from numpy.linalg import det
from numpy import array

i_hat = array([1, 0])
j_hat = array([1, 1])

basis = array([i_hat, j_hat]).transpose()

determinant = det(basis)

print(determinant) # prints 1.0
```

But scaling will increase or decrease the determinant, as that will increase/decrease the sampled area. When the orientation flips ($\hat{i}$, $\hat{j}$ swap clockwise positions) then the determinant will be negative. Figure 4-22 and Example 4-16 is a determinant showing a transformation that not only scaled but also flipped the orientation of the vector space.

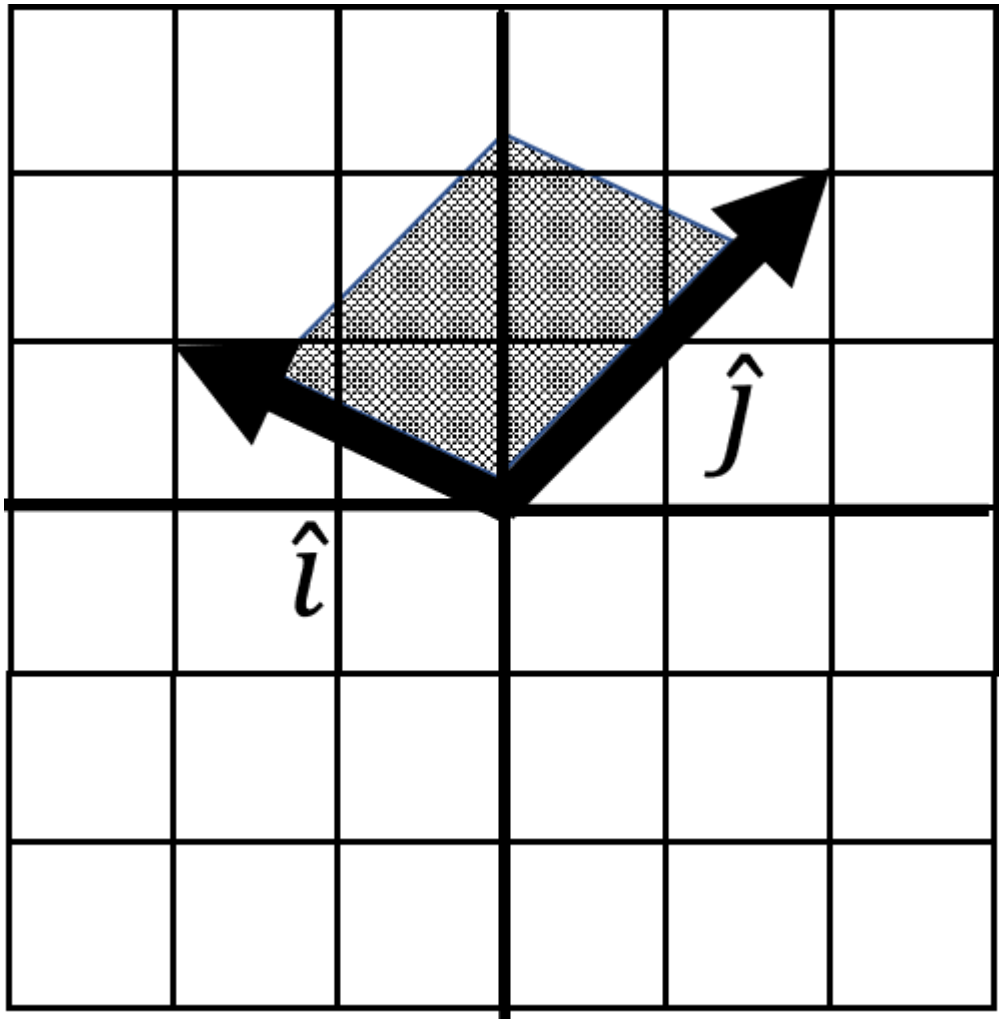


Figure 4-22. A determinant on a flipped space is negative

Example 4-16.

```
from numpy.linalg import det
from numpy import array

i_hat = array([-2, 1])
j_hat = array([1, 2])

basis = array([i_hat, j_hat]).transpose()

determinant = det(basis)

print(determinant) # prints -5.0
```

Because this determinant is negative, we quickly see that the orientation has flipped.

THE RIGHT HAND RULE

The determinant can extend to 3 or more dimensions. It becomes a matter of visualizing a sampled *volume* scaling, rotating, shearing, and flipping as visualized in Figure 4-23.

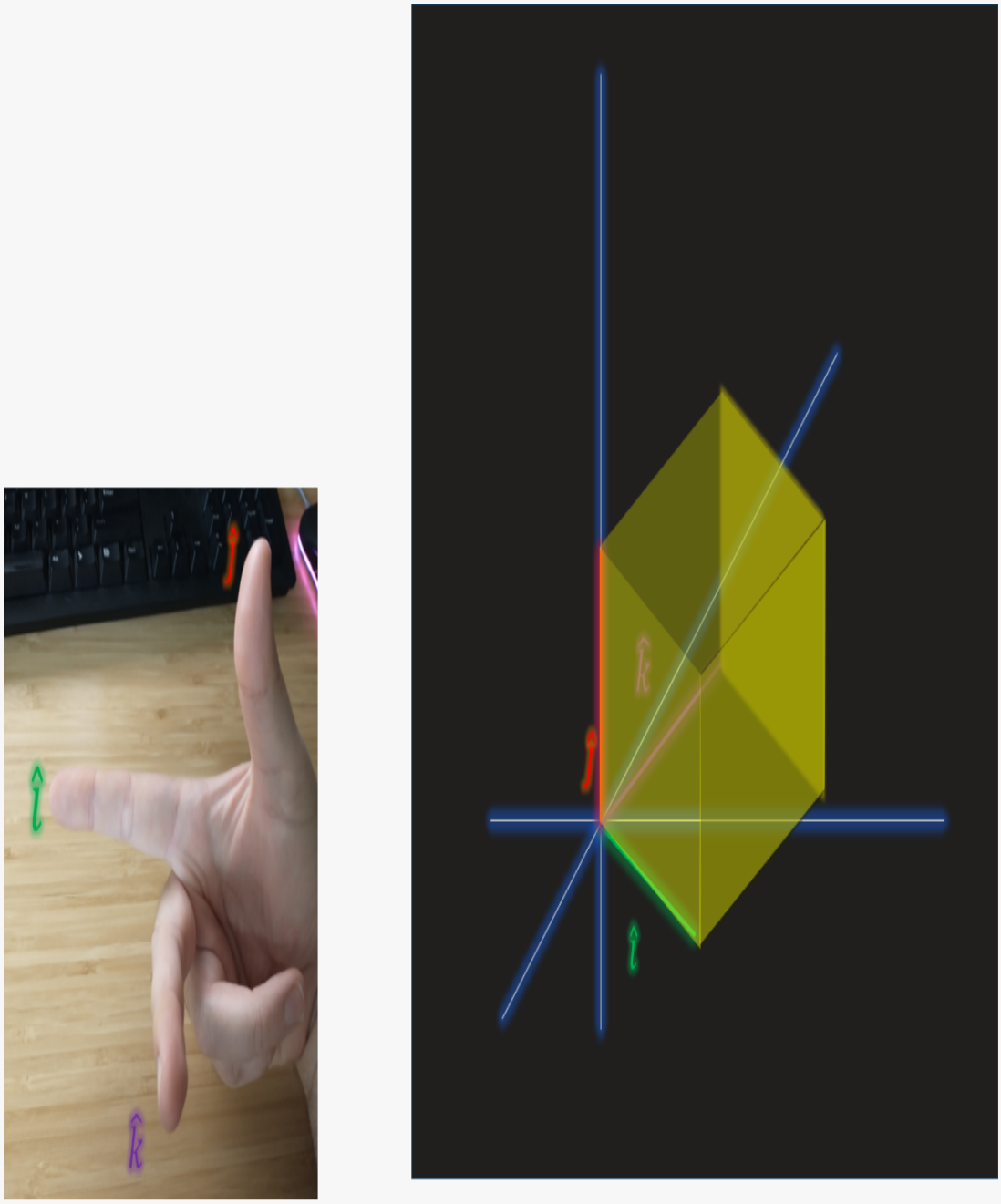


Figure 4-23. The right hand rule

To figure out if a 3D space has flipped, use the **right hand rule**. If you cannot relatively orient $\hat{i}$, $\hat{j}$, and $\hat{k}$ like my hand above the orientation has flipped, and you should have a negative determinant.

But by far, the most critical piece of information the determinant tells you is whether the transformation is linearly dependent. If you have a determinant of 0 that means all of space has been squished into a lesser dimension.

In Figure 4-24 we see two linearly dependent transformations, where a 2D space is compressed into 1 dimension and a 3D space is compressed into 2 dimensions. The area and volume respectively in both cases are 0!

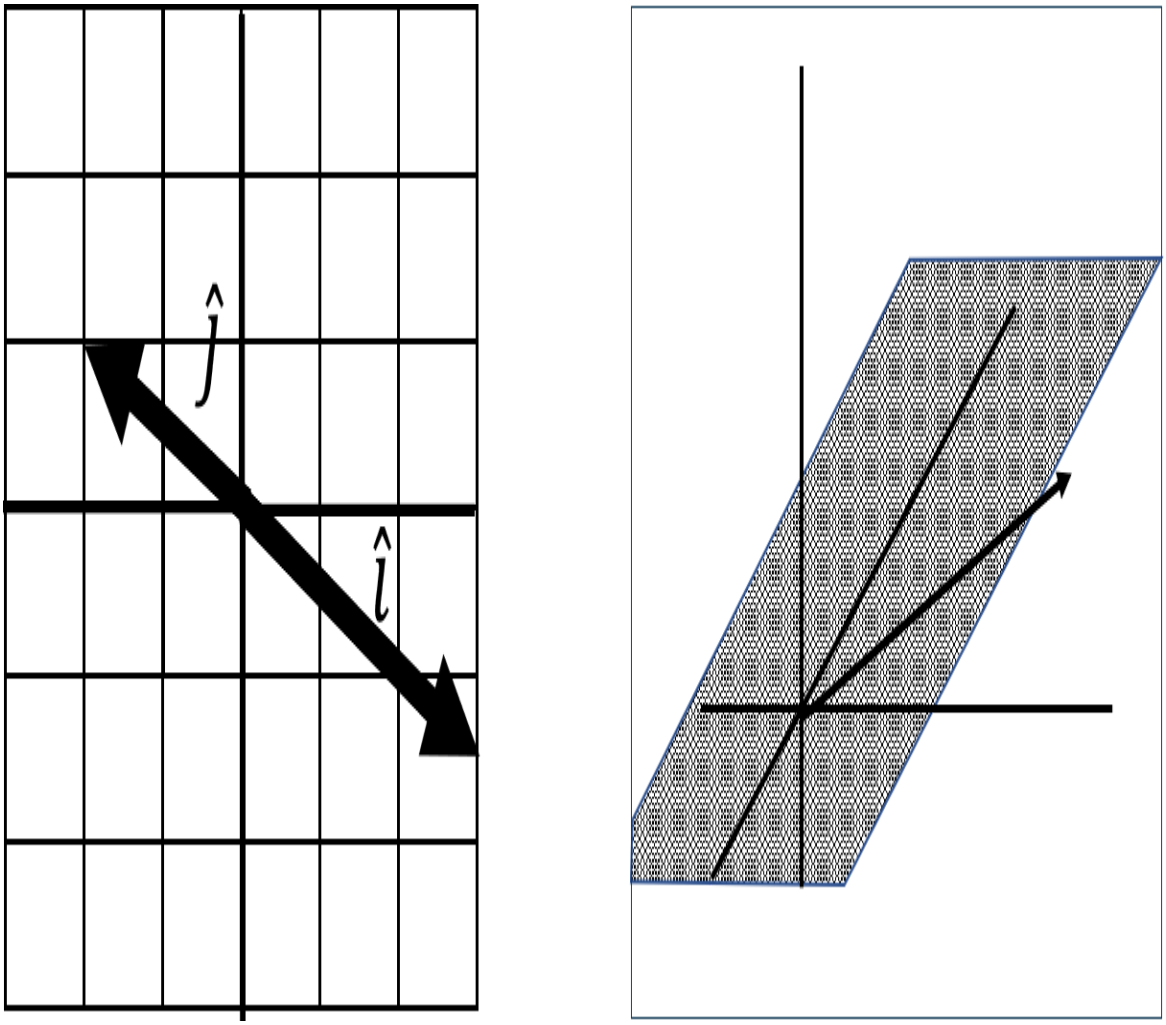


Figure 4-24. Linear dependence in 2D and 3D

Example 4-17 shows the code for the 2D example above squishing an entire 2D space into a single 1-dimensional number line.

Example 4-17.

```
from numpy.linalg import det
from numpy import array

i_hat = array([-2, 1])
j_hat = array([3, -1.5])

basis = array([i_hat, j_hat]).transpose()

determinant = det(basis)

print(determinant) # prints 0.0
```

So testing for a 0 determinant is highly helpful to determine if a transformation has linear dependence. When you encounter this you will likely find a difficult or unsolvable problem on your hands.

Systems of Equations and Inverse Matrices

One of the basic use cases for linear algebra is solving systems of equations. It is also a good application to learn about inverse matrices. Let's say you are provided with the following equations and you need to solve for x, y, and z.

$$4x + 2y + 4z == 44$$

$$5x + 3y + 7z = 56$$

$$9x + 3y + 6z = 72$$

You can try manually experimenting with different algebraic operations to isolate the three variables, but if you want a computer to solve it you will need to express this problem in terms of matrices as shown below. Extract the coefficients into matrix A, the values on the right-side of the equation into matrix B, and the unknown variables into matrix X.

$$A = \begin{bmatrix} 4 & 2 & 4 \\ 5 & 3 & 7 \\ 9 & 3 & 6 \end{bmatrix}$$

$$B = \begin{bmatrix} 44 \\ 56 \\ 72 \end{bmatrix}$$

$$X = \begin{bmatrix} x \\ y \\ z \end{bmatrix}$$

The function for a linear system of equations is `AX = B`, we need to transform matrix A with some other matrix X that will result in matrix B.

$$AX = B$$

$$\begin{bmatrix} 4 & 2 & 4 \\ 5 & 3 & 7 \\ 9 & 3 & 6 \end{bmatrix} \cdot \begin{bmatrix} x \\ y \\ z \end{bmatrix} = \begin{bmatrix} 44 \\ 56 \\ 72 \end{bmatrix}$$

We need to "undo" A so we can isolate X and get the values for x, y, and z. The way you undo A is to take the inverse of A denoted by A^{-1} and apply it to A via matrix multiplication. We can express this algebraically below:

$$AX = B$$

$$A^{-1}AX = A^{-1}B$$

$$X = A^{-1}B$$

To calculate the inverse of matrix A, we should probably use a computer rather than searching for solutions by hand using Gaussian elimination, which we will not venture into in this book (PatrickJMT has some great videos on YouTube). Here is the inverse of matrix A.

$$A^{-1} = \begin{bmatrix} -\frac{1}{2} & 0 & \frac{1}{3} \\ 5.5 & -2 & \frac{4}{3} \\ -2 & 1 & \frac{1}{3} \end{bmatrix}$$

Note when we matrix multiply A^{-1} against A it will create an **identity matrix**, creating a matrix of all zeroes except for 1's in the diagonal. The identity matrix is the linear algebra equivalent of multiplying by "1", meaning it essentially has no effect and will effectively isolate values for x, y, and z.

$$A^{-1} = \begin{bmatrix} -\frac{1}{2} & 0 & \frac{1}{3} \\ 5.5 & -2 & \frac{4}{3} \\ -2 & 1 & \frac{1}{3} \end{bmatrix}$$

$$A = \begin{bmatrix} 4 & 2 & 4 \\ 5 & 3 & 7 \\ 9 & 3 & 6 \end{bmatrix}$$

$$A^{-1}A = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

To see this identity matrix in action in Python, you will probably want to use SymPy here instead of NumPy. The floating point decimals in NumPy will not make the identity matrix so obvious, but doing it symbolically in Example 4-18 we will see a clean, symbolic output. Note that to do matrix multiplication in SymPy we use the asterisk * rather than @.

Example 4-18. Using SymPy to study the inverse and identity matrix

```
from sympy import *

# 4x + 2y + 4z = 44
# 5x + 3y + 7z = 56
# 9x + 3y + 6z = 72

A = Matrix([
```

```
    [4, 2, 4],
    [5, 3, 7],
    [9, 3, 6]
])

# dot product between A and its inverse
# will produce identity function
inverse = A.inv()
identity = inverse * A

# prints Matrix([[-1/2, 0, 1/3], [11/2, -2, -4/3], [-2, 1, 1/3]])
print("INVERSE: {}".format(inverse))

# prints Matrix([[1, 0, 0], [0, 1, 0], [0, 0, 1]])
print("IDENTITY: {}".format(identity))
```

In practice though, the lack of floating point precision will not affect our answers too badly, so using NumPy should be fine to solve for *X*. Example 4-19 shows a solution with NumPy.

Example 4-19. Using NumPy to solve a system of equations

```
from numpy import array
from numpy.linalg import inv

# 4x + 2y + 4z = 44
# 5x + 3y + 7z = 56
# 9x + 3y + 6z = 72

A = array([
    [4, 2, 4],
    [5, 3, 7],
    [9, 3, 6]
])

B = array([
    44,
    56,
    72
])

X = inv(A).dot(B)

print(X) # [ 2. 34. -8.]
```

So `x = 2`, `y = 34`, and `z = 8`. Since I did use SymPy in this problem, Example 4-20 shows the full solution in SymPy as an alternative to NumPy.

Example 4-20. Using SymPy to solve a system of equations

```
from sympy import *

# 4x + 2y + 4z = 44
# 5x + 3y + 7z = 56
# 9x + 3y + 6z = 72

A = Matrix([
    [4, 2, 4],
    [5, 3, 7],
    [9, 3, 6]
])

B = Matrix([
    44,
    56,
    72
])

X = A.inv() * B

print(X) # Matrix([[2], [34], [-8]])
```

Here is the solution in mathematical notation:

$$A^{-1}B = X$$

$$\begin{bmatrix} -\frac{1}{2} & 0 & \frac{1}{3} \\ 5.5 & -2 & \frac{4}{3} \\ -2 & 1 & \frac{1}{3} \end{bmatrix} \begin{bmatrix} 44 \\ 56 \\ 72 \end{bmatrix} = \begin{bmatrix} x \\ y \\ z \end{bmatrix}$$

$$\begin{bmatrix} 2 \\ 34 \\ -8 \end{bmatrix} = \begin{bmatrix} x \\ y \\ z \end{bmatrix}$$

Hopefully this gave you an intuition for inverse matrices and how they can be used to solve a system of equations.

SYSTEMS OF EQUATIONS IN LINEAR PROGRAMMING

This method of solving systems of equations is used for linear programming as well, where inequalities define constraints and an objective is minimized/maximized.

PatrickJMT has a lot of good videos on Linear Programming

In practicality you should rarely find it necessary to calculate inverse matrices by hand and can have a computer do it for you. But if you have a need or are curious, you will want to learn about Gaussian elimination. PatrickJMT on YouTube has a number of videos demonstrating Gaussian elimination.

Eigenvectors and Eigenvalues

Matrix decomposition is breaking up a matrix into its basic components, much like factoring numbers (e.g. 10 can be factored to 2 x 5).

Matrix decomposition is helpful for tasks like finding inverse matrices, calculating determinants, as well as linear regression. There are many ways to decompose a matrix depending on your task. In Chapter 5 we will use a matrix decomposition technique, QR decomposition, to perform a linear regression. But in this chapter let's focus on a common method called eigendecomposition, which is often used for machine learning and Principal Component Analysis (PCA). At this level we do not have the bandwidth to dive into each of these applications. For now, just know eigendecomposition is helpful for breaking up a matrix into components that are easier to work with in different machine learning tasks.

In eigendecomposition, there are two components: the eigenvalues denoted by lambda λ and eigenvector by v shown in Figure 4-25.

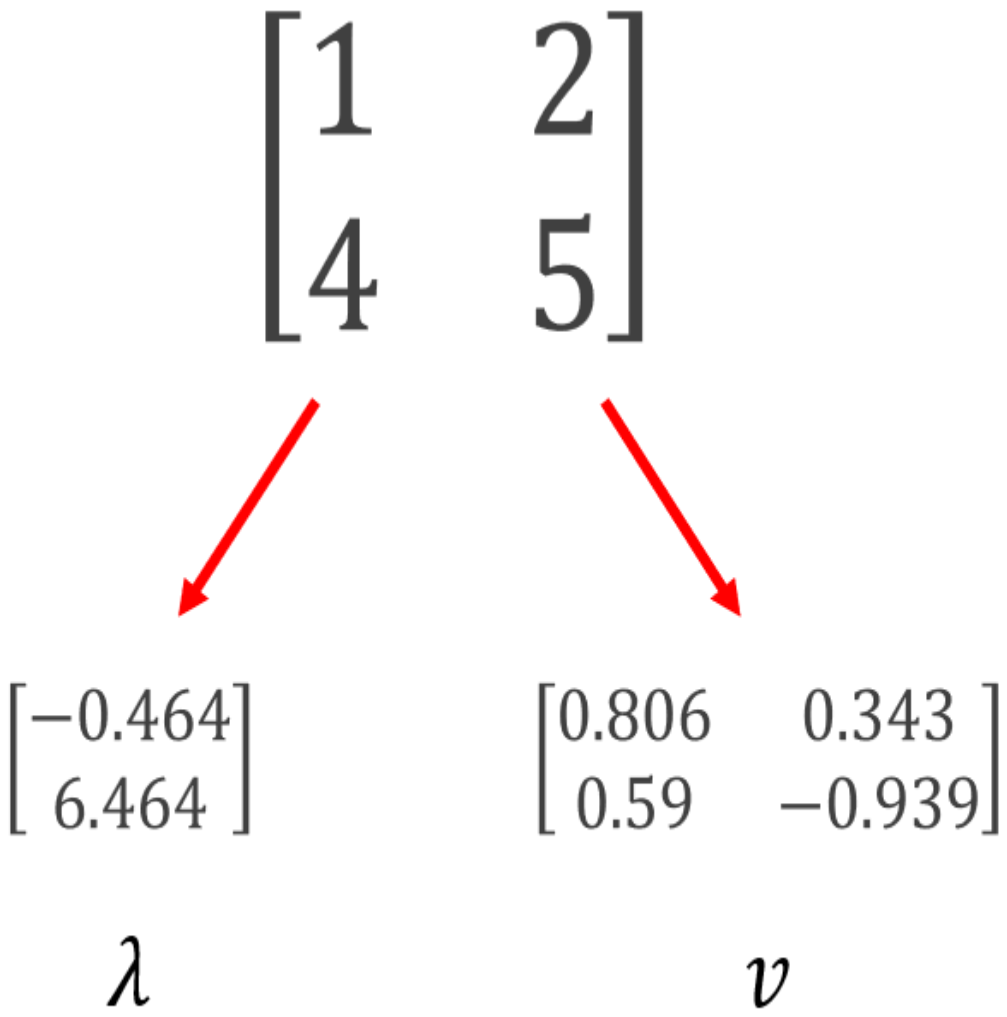


Figure 4-25. The eigenvector and eigenvalues

If we have a square matrix A, it has the following eigenvalue equation:

$Av = \lambda v$

If A is the original matrix, it is composed of eigenvector v and eigenvalue λ. There is one eigenvector and eigenvalue for each dimension of the parent matrix, and not all matrices can be decomposed into an eigenvector and eigenvalue. Sometimes complex (imaginary) numbers will even result.

Example 4-21 is how we calculate eigenvectors and eigenvalues in NumPy for a given matrix A:

Example 4-21. Performing eigendecomposition in NumPy

```
from numpy import array, diag
from numpy.linalg import eig, inv

A = array([
    [1, 2],
    [4, 5]
])

eigenvals, eigenvecs = eig(A)

print("EIGENVALUES")
print(eigenvals)
print("\nEIGENVECTORS")
print(eigenvecs)

"""
EIGENVALUES
[-0.46410162  6.46410162]

EIGENVECTORS
[[-0.80689822 -0.34372377]
 [ 0.59069049 -0.9390708 ]]
"""
```

So how do we rebuild matrix A from the eigenvectors and eigenvalues? Recall this formula:

$$Av = \lambda v$$

We need to make a few tweaks to the formula to reconstruct A:

$$A = Q\Lambda Q^{-1}$$

In this new formula, Q is the eigenvectors, Λ is the eigenvalues in diagonal form, and Q^{-1} is the inverse matrix of Q. Diagnal form means the vector is padded into a matrix of zeroes, and occupies the diagonal line in a similar pattern to an identity matrix.

Example 4-22 brings the example full circle in Python, starting with decomposing the matrix and then recomposing it.

Example 4-22. Decomposing and recomposing a matrix in NumPy

```
from numpy import array, diag
from numpy.linalg import eig, inv

A = array([
    [1, 2],
    [4, 5]
])

eigenvals, eigenvecs = eig(A)

print("EIGENVALUES")
print(eigenvals)
print("\nEIGENVECTORS")
print(eigenvecs)

print("\nREBUILD MATRIX")
Q = eigenvecs
R = inv(Q)

L = diag(eigenvals)
B = Q @ L @ R

print(B)

"""
EIGENVALUES
[-0.46410162  6.46410162]

EIGENVECTORS
[[-0.80689822 -0.34372377]
 [ 0.59069049 -0.9390708 ]]

REBUILD MATRIX
[[1. 2.]
 [4. 5.]]
"""
```

As you can see above, the matrix we rebuilt is the one we started with.

Conclusion

Linear algebra can be maddeningly abstract and it is full of mysteries and ideas to ponder. You may find the whole topic is one big rabbit hole, and

you would be right! However it is a good idea to continue being curious about it if you want to have a long, successful data science career. It is the foundation for statistical computing, machine learning, and other applied data science areas. Ultimately, it is the foundation for computer science in general. You can certainly get away with not knowing it for awhile but you will encounter limitations in your understanding at some point.

You may wonder how these ideas are practical as they may feel theoretical. Do not worry, we will see some practical applications throughout this book. But the theory and geometric interprations are important to have intuition when you work with data, and by understanding linear transformations visually you are prepared to take on more advanced concepts that may be thrown at you later in your pursuits.

If you want to learn more about linear programming, there is no better place than 3Blue1Brown's YouTube playlist "Essence of Linear Algebra". The linear algebra videos from PatrickJMT are helpful as well.

If you want to get more comfortable with NumPy, the O'Reilly book Python for Data (2nd edition) by Wes McKinney is a recommended read. It does not focus much on linear algebra but it does provide practical instruction on using NumPy, Pandas, and Python on datasets.

Exercises

1. Vector $\vec{v}$ has a value of `[1 2]` but then a transformation happens. $\hat{i}$ lands at `[2 0]` and $\hat{j}$ lands at `[0 1.5]`. Where does $\vec{v}$ land?

2. Vector $\vec{v}$ has a value of `[1 2]` but then a transformation happens. $\hat{i}$ lands at `[-2 1]` and $\hat{j}$ lands at `[1 -2]`. Where does $\vec{v}$ land?

3. A transformation lands $\hat{i}$ lands at `[1 0]` and $\hat{j}$ lands at `[2 2]`. What is the determinant of this transformation?

4. Can two or more linear transformations be done in single linear transformation? Why or why not?

5. Solve the system of equations for x, y, and z.

$$3x + 1y + 0z == 54$$

$$2x + 4y + 1z = 12$$

$$3x + 1y + 8z = 6$$

6. Is the matrix below linearly dependent? Why or why not?

$$\begin{bmatrix} 2 & 1 \\ 6 & 3 \end{bmatrix}$$

Chapter 5. Linear Regression

A NOTE FOR EARLY RELEASE READERS

With Early Release ebooks, you get books in their earliest form—the author's raw and unedited content as they write—so you can take advantage of these technologies long before the official release of these titles.

This will be the 5th chapter of the final book.

If you have comments about how we might improve the content and/or examples in this book, or if you notice missing material within this chapter, please reach out to the author at *thomasnield@live.com*.

One of the most practical techniques in data analysis is fitting a line through observed data points to show a relationship between two or more variables. A **regression** attempts to fit a of function to observed data to make predictions on new data. A **linear regression** fits a straight line to observed data, attempting to demonstrate a linear relationship between variables and make predictions on new data yet to be observed.

It might make more sense to see a picture rather than read a description of linear regression. Here is an example of a linear regression in Figure 5-1.

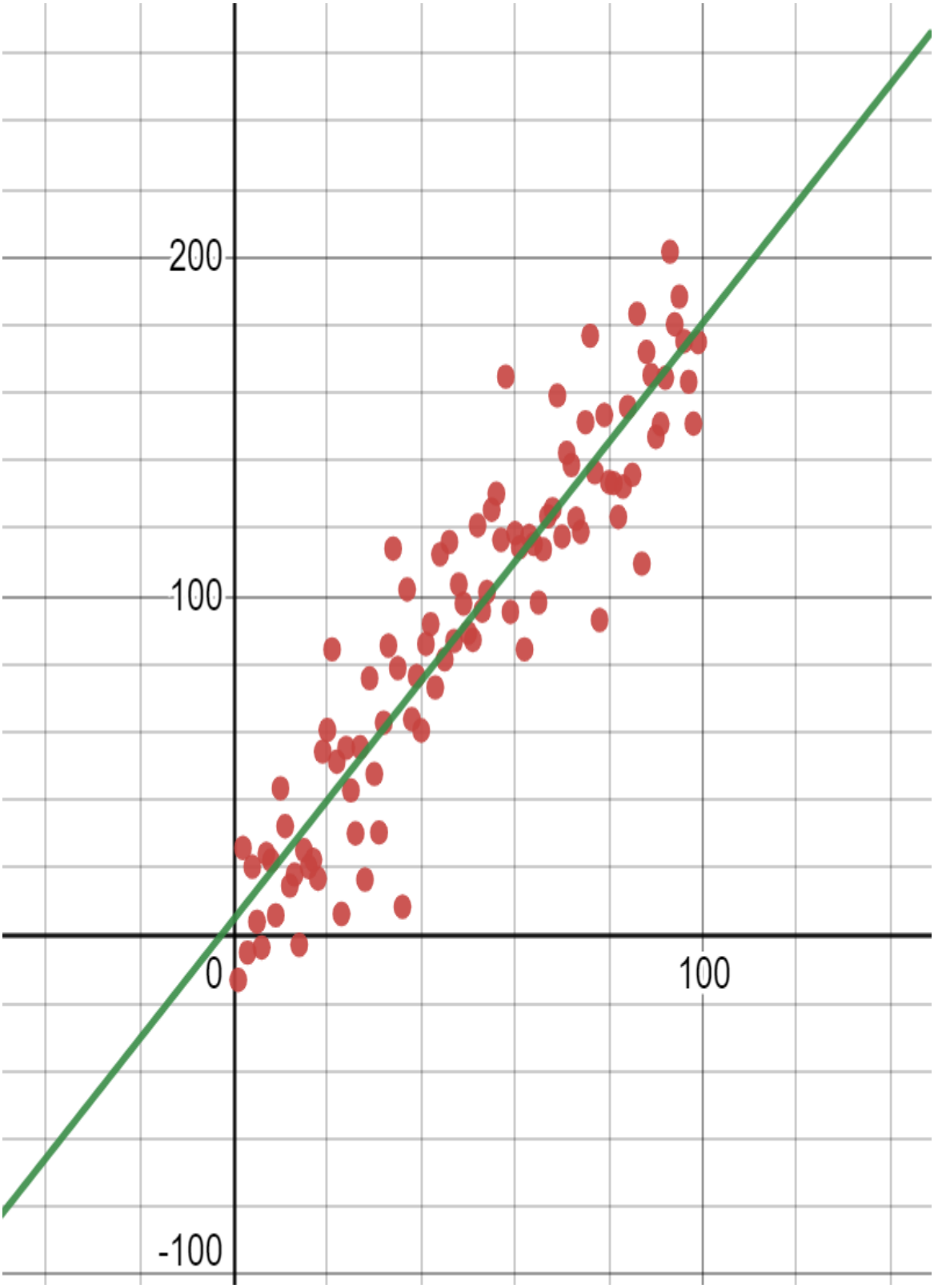


Figure 5-1. Example of a linear regression, which fits a line to observed data

Linear regression is a workhorse of data science and statistics, and not only applies concepts we learned in previous chapters but sets up new foundations for later topics like neural networks and logistic regression. This relatively simple technique has been around for over 200 years, and contemporarily is branded as a form of machine learning.

Machine learning practitioners are less likely to analyze their linear regression models in depth, and simply do a quick train-test split of the data. Statisticians, however, will question the linear regression more deeply, analyzing the prediction intervals and correlation for statistical significance. We will cover both schools of thought so readers can bridge the ever-widening gap between the two, and thus find themselves best equipped to wear both hats.

WAIT, MACHINE LEARNING IS JUST REGRESSION?

"Machine learning" is generally another name for regression models, particularly in the context of supervised learning. This is why linear regression is considered a form of machine learning. Confusingly, statisticians may refer to their regression models as *statistical learning*, whereas data science and machine learning professionals will call their models *machine learning*.

While supervised learning is often regression, unsupervised machine learning is more about clustering and anomaly detection. Reinforcement learning often pairs supervised machine learning with simulation to rapidly generate data. Of course, the data is as only good as the simulation and the simulation-to-reality gap is always an issue.

A Basic Linear Regression

I want to study the relationship between the age of a dog and the number of veterinary visits it had. In a sample we have 10 random dogs, let's plot them as shown in Figure 5-2.

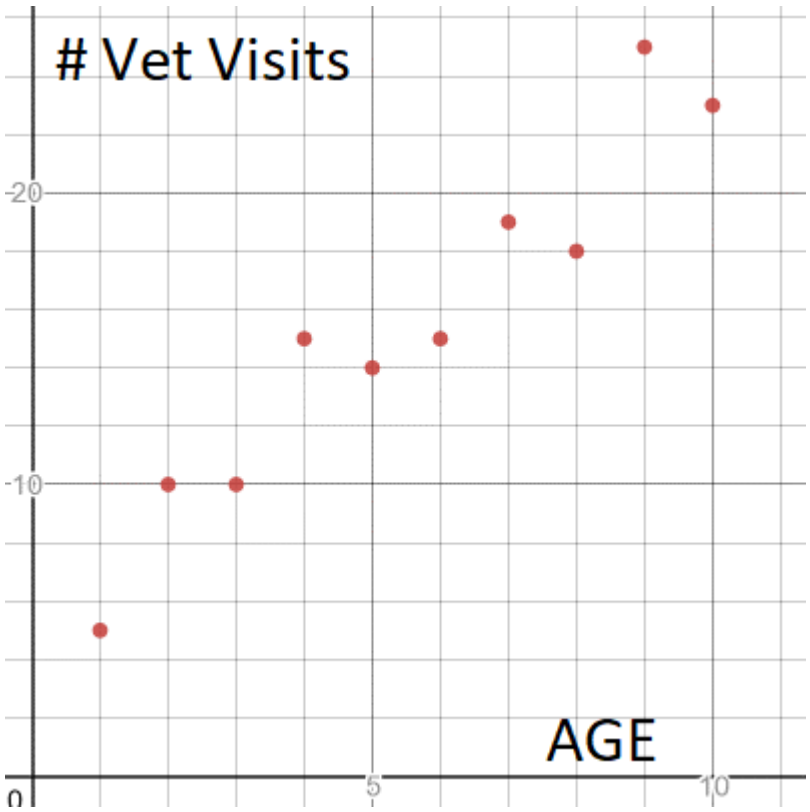


Figure 5-2. Plotting a sample of 10 dogs with their age and number of vet visits

We can clearly see there is a **linear correlation** here, meaning when one of these variables increases/decreases, the other increases/decreases in a roughly proportional amount. We could draw a line through these points to show a correlation like this in Figure 5-3.

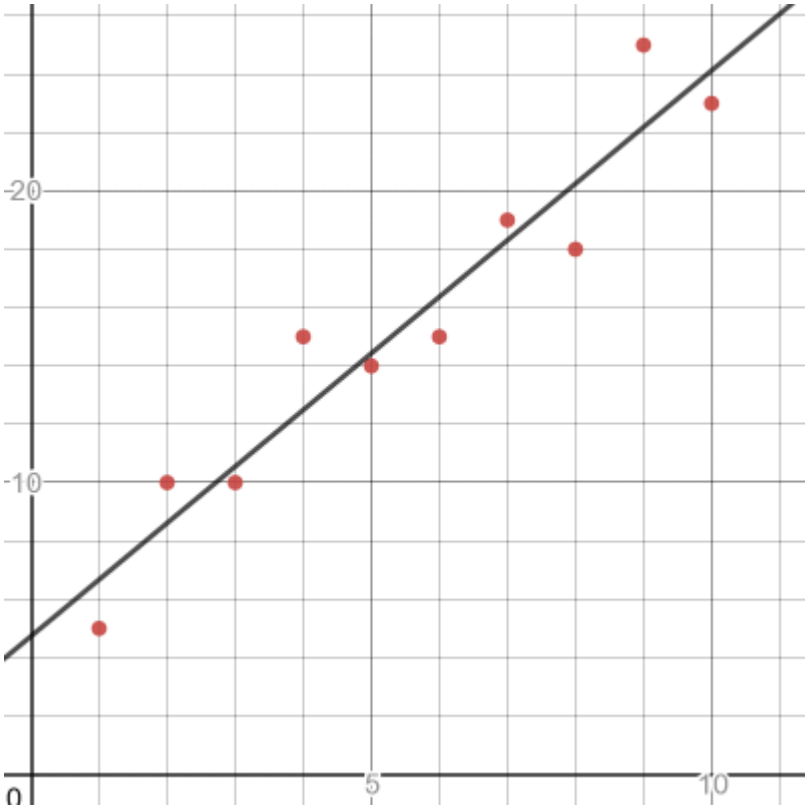


Figure 5-3. Fitting a Line Through Our Data

I will show how to calculate this fitted line later in this chapter. We will also explore how to calculate the quality of this fitted line. For now, let's focus on the benefits of performing a linear regression. It allows us to make predictions on data we have not seen before. I do not have a dog in my sample that is 8.5 years old, but I can look at this line and estimate the dog will have 21 veterinary visits in its life. I just look at the line where `x=8.5` and I see that `y=21.218` as shown in Figure 5-4.

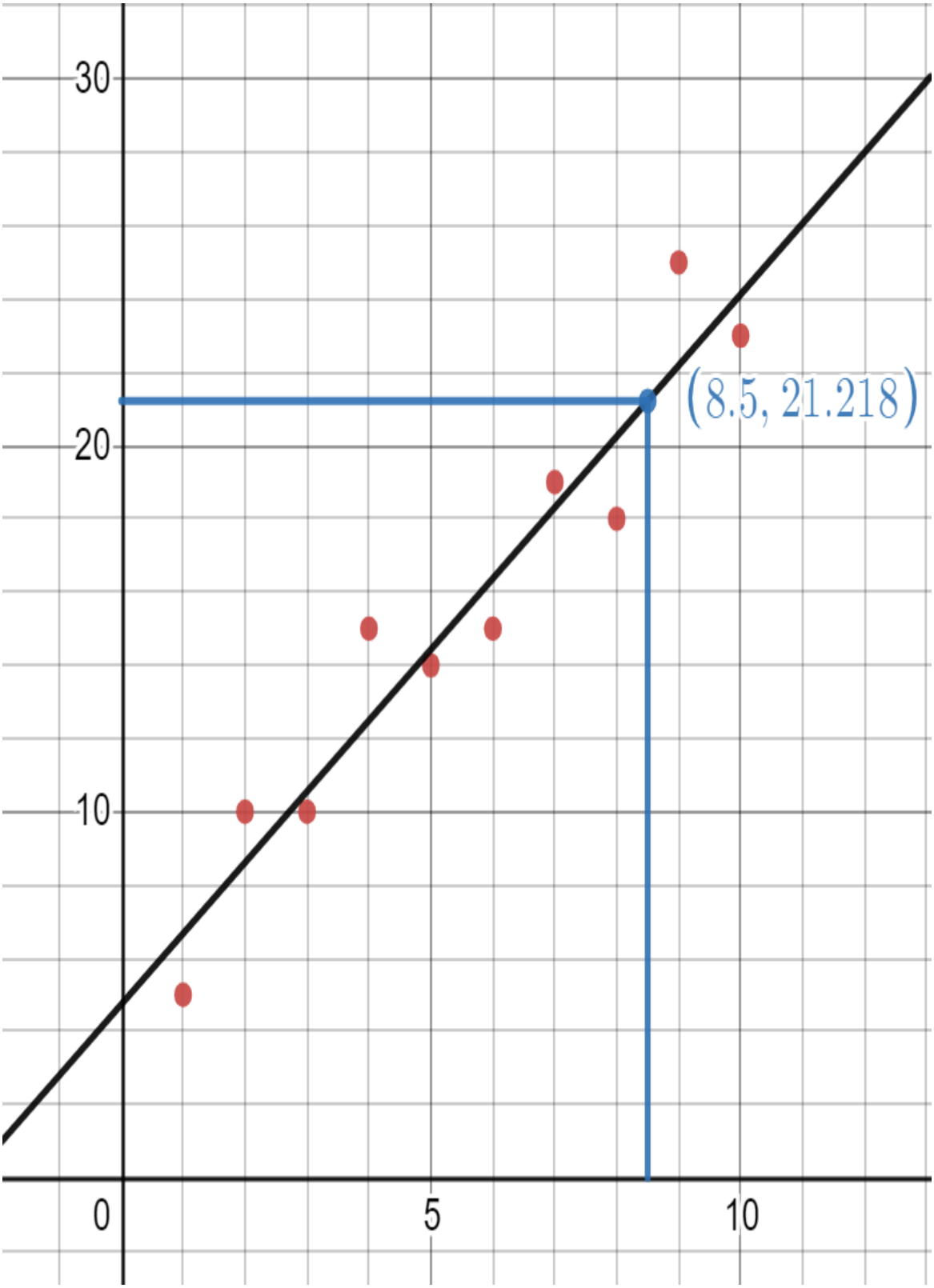


Figure 5-4. Making a prediction using a linear regression, seeing that an 8.5 year old dog is predicted to have about 21.2 vet visits

Now what are the downsides of a linear regression? I cannot expect that every outcome is going to fall EXACTLY on that line. After all, real world data is noisy and never perfect and will not follow a straight line. It may not remotely follow a straight line at all! There is going to be error around that line, where the point will fall above or below the line. We will cover this mathematically when we talk about p-values, statistical significance, and prediction intervals which describes how reliable our linear regression is. Another catch is we should not use the linear regression to make predictions outside the range of data we have, meaning we should not make predictions where `x < 0` and `x > 10` because we do not have data outside those values.

> **DON'T FORGET SAMPLING BIAS!**
>
> We should question this data and how it was sampled in order to detect bias. Was this at a single veterinary clinic? Multiple random clinics? Is there self-selection bias by using veterinary data, only polling dogs that visit the vet? If the dogs were sampled in the same geography, can that sway the data? Perhaps dogs in hot desert climates go to vets more for heat exhaustion and snake bites, and this would inflate our veterinary visits in our sample.
>
> As discussed in Chapter 3, it has become fashionable to make data an oracle for truth. However data is simply a sample from a population and we need to practice discernment on how well represented our sample is. Be just as interested (if not more) on where the data comes from and not just what the data says.

Basic Linear Regression with SciPy

We have a lot to learn regarding linear regressions in this chapter, but let's start out with some code to execute what we know so far.

There are plenty of platforms to perform a linear regression, from Excel to Python and R. But we will stick with Python in this book, starting with SciPy to do the work for us. I will show how to build a linear regression "from scratch" later in this chapter so we grasp important concepts like gradient descent and least squares.

Code Example 5-1 is how we use Scikit-Learn to perform a basic, unvalidated linear regression on the sample of 10 dogs. We pull in this data using Pandas, convert it into NumPy arrays, perform linear regression using Scikit-Learn, and use plotly to display it in a chart.

Example 5-1. Using Scikit-Learn to do a linear regression

```
import pandas as pd
import matplotlib.pyplot as plt
from sklearn.linear_model import LinearRegression

# Import points
df = pd.read_csv('https://bit.ly/3goOAnt', delimiter=",")

# Extract input variables (all rows, all columns but last column)
X = df.values[:, :-1]

# Extract output column (all rows, last column)
Y = df.values[:, -1]

# Fit a line to the points
fit = LinearRegression().fit(X, Y)

# m = 1.7867224, b = -16.51923513
m = fit.coef_.flatten()
b = fit.intercept_.flatten()
print("m = {0}".format(m))
print("b = {0}".format(b))

# show in chart
plt.plot(X, Y, 'o') # scatterplot
plt.plot(X, m*X+b) # line
plt.show()
```

First we import the data from this CSV on GitHub. We separate the two columns into *X* and *Y* datasets using Pandas. We then `fit()` the `LinearRegression` model to the input *X* data and the output *Y* data. We can then get the *m* and *b* coefficients that describe our fitted linear function.

In the plot, sure enough you will get a fitted line running through these points shown in Figure 5-5.

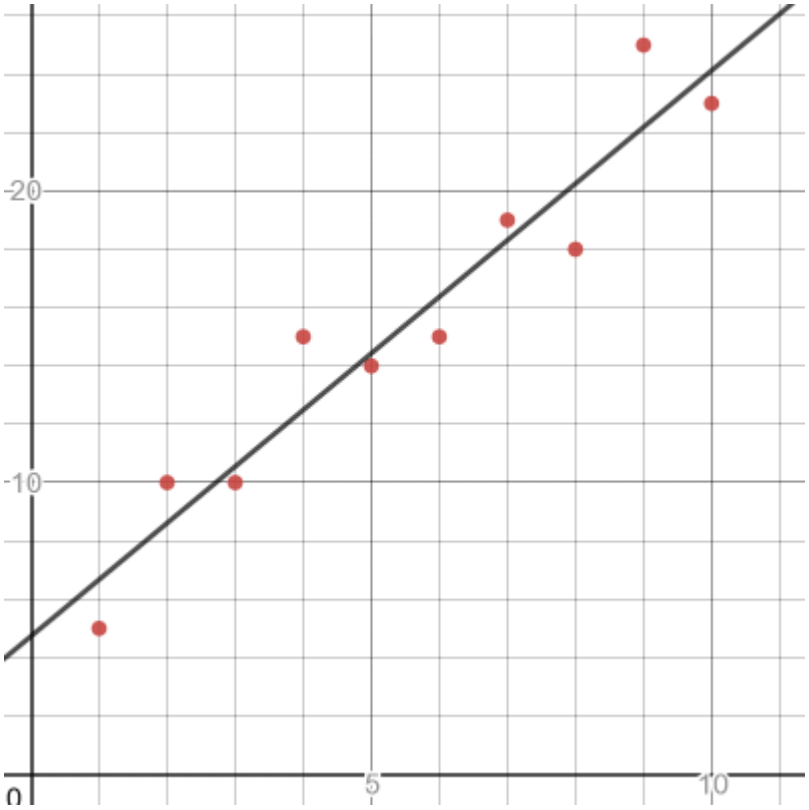


Figure 5-5. SciPy will fit a regression line to your data.

What decides the best fit line to these points? Let's discuss that next.

Residuals and Squared Errors

How do statistics tools like Scikit-Learn come up with a line that fits to these points? Well it comes down to two questions that are fundamental to machine learning training:

1) What defines a "best fit"?

2) How do we get to that "best fit"?

The first question has a pretty established answer: we minimize the squares, or more specifically the sum of the squared residuals. Let's break that down. Draw any line through the points. The **residual** is the numeric difference between the line and the points, as shown below in Figure 5-6.

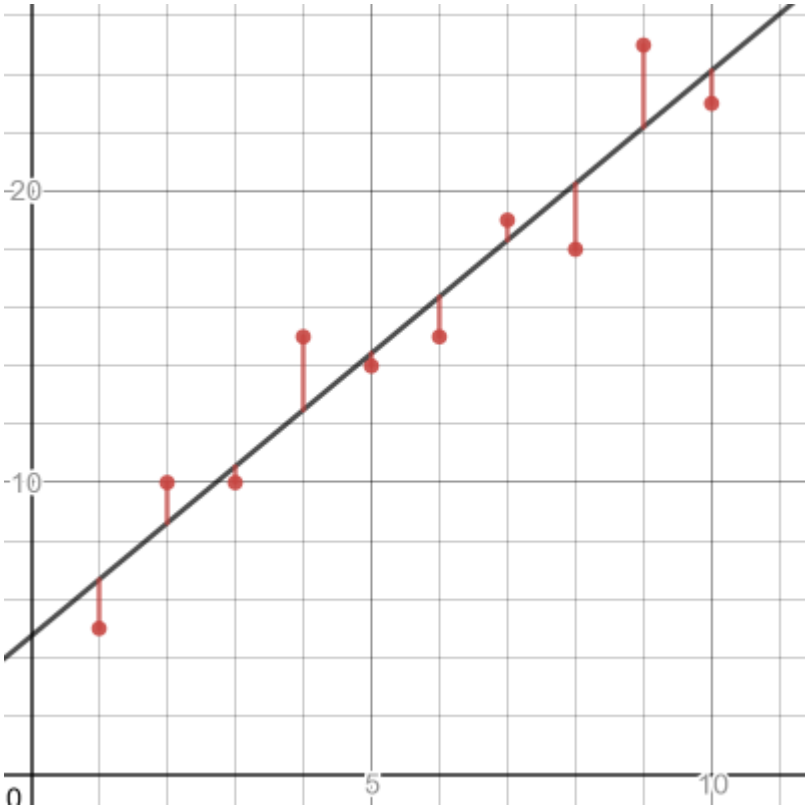


Figure 5-6. The residuals are the differences between the line and the points

Points above the line will have a positive residual, and points below the line will have a negative residual. In other words, it is the subtracted difference between the predicted y-values (derived from the line) and the actual y-values (which came from the data). Another name for residuals are **errors**, because they reflect how wrong our line is in predicting the data.

Here is how you calculate a residual `E` for a given predicted y-value and actual y-value.

![htEEDUuntk](./assets/htEEDUuntk.png)

You will often see the predicted y-value annot ![vRIWMgPlha](./assets/vRIWMgPlha.png)

Let's calculate these differences between these 10 points and the line `y = 1.93939x + 7.73333` in code Example 5-2.

Example 5-2. Calculating the residuals for a given line and data

```
import pandas as pd
```

```
# Import points
points = pd.read_csv('https://bit.ly/3goOAnt',
delimiter=",").itertuples()

# Test with a given line
m = 1.93939
b = 4.73333

# calculate sum of squares
for p in points:
    y_actual = p.y
    y_predict = m*p.x + b
    residual = y_actual - y_predict
    print(residual)
```

OUTPUT:

Example 5-3.

```
-1.67272
1.3878900000000005
-0.5515000000000008
2.5091099999999997
-0.4302799999999998
-1.3696699999999993
0.6909400000000012
-2.2484499999999983
2.812160000000002
-1.1272299999999973
```

If we are fitting a straight line through our 10 data points, we likely want to minimize these residuals in total so there is as little of a gap as possible between the line and points. But how do we measure the "total"? The best approach is to take the **sum of squares**, which simply squares each residual, or multiplies each residual by itself, and sums them. We take each actual *y* value and subtract from it the predicted *y* value taken from the line, then square and sum all those differences.

WHY NOT ABSOLUTE VALUES?

You might wonder why we have to square the residuals before summing them. Why not just add them up without squaring? That will not work because the negatives will cancel out the positives. What if we add the absolute values, where we turn all negative values into positive values? That sounds promising but absolute values are mathematically inconvenient. More specifically, absolute values do not work well with Calculus derivatives which we are going to use later for gradient descent. This is why we choose the squared residuals as our way of totaling the loss.

A visual way to think of it is shown in Figure 5-7, where we overlay a square on each residual and each side is the length of the residual. We sum the area of all these squares, and later we will learn how to find the minimum sum we can achieve by identifying the best m and b.

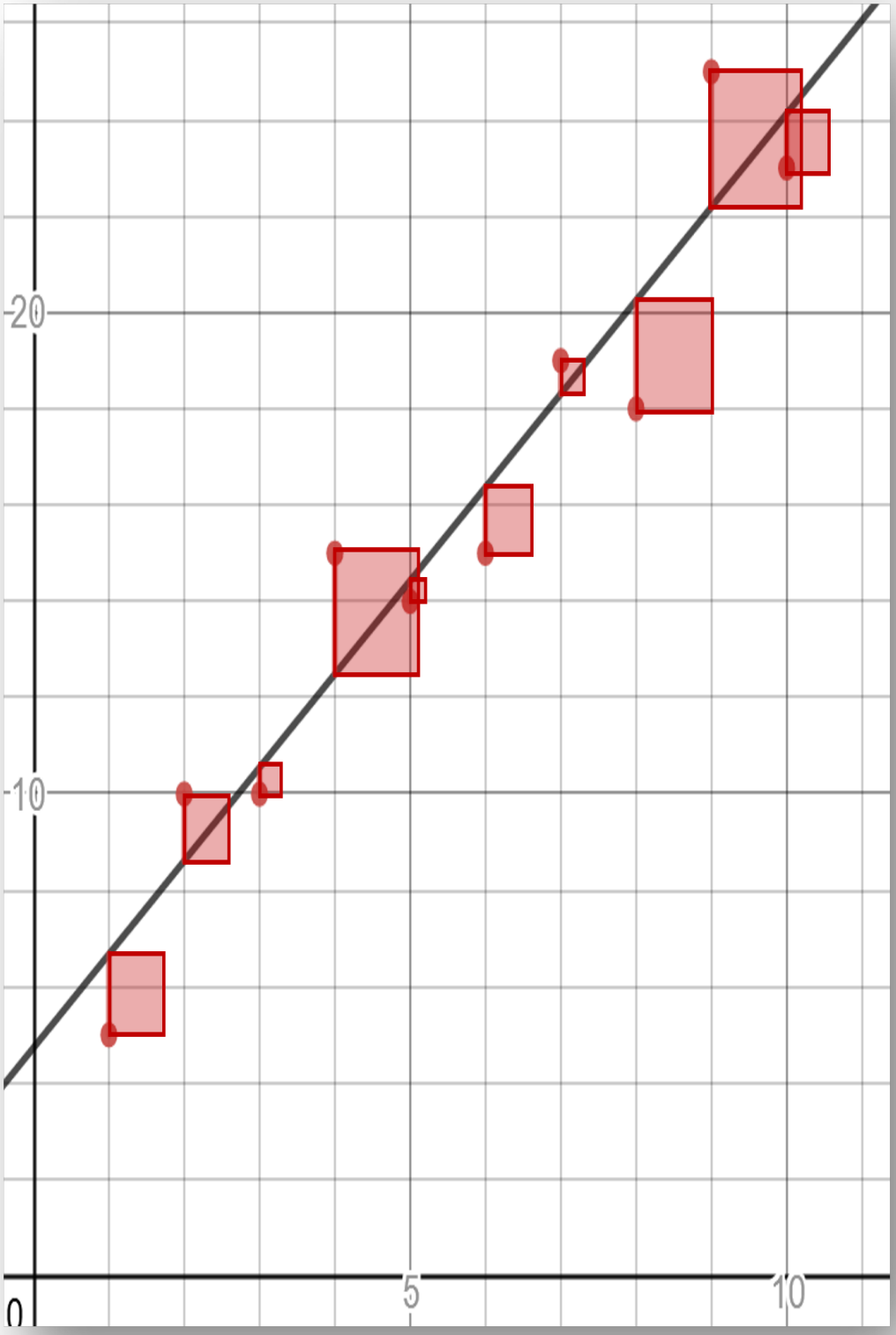

20
10
0
5
10

Figure 5-7. Visualizing the sum of squares, which would be the sum of all areas where each square has a side length equal to the residual

Let's modify our code in Example 5-4.

Example 5-4. Calculating the sum of squares for a given line and data

```
import pandas as pd

# Import points
points = pd.read_csv("https://bit.ly/2KF29Bd").itertuples()

# Test with a given line
m = 1.93939
b = 4.73333

sum_of_squares = 0.0

# calculate sum of squares
for p in points:
    y_actual = p.y
    y_predict = m*p.x + b
    residual_squared = (y_predict - y_actual)**2
    sum_of_squares += residual_squared

print("sum of squares = {}".format(sum_of_squares))
# sum of squares = 28.096969704500005
```

Next question: how do we find the *m* and *b* values that will produce the minimum sum of squares, without using a library like Scikit-Learn? Let's look at that next.

Finding the Best Fit Line

We now have a way to measure the quality of a given line against the data points: the sum of squares. The lower we can make that number the better the fit. Now how do we find the right *m* and *b* values that creates the *least* sum of squares?

There are a couple of search algorithms we can employ, which try to find the right set of values to solve a given problem. You can try to take a **brute force** approach, generating random *m* and *b* values thousands or millions of

times and choosing the ones that produce the least sum of squares. This will not work well because it will take an endless amount of time to find even a decent approximation. We will need something a little more guided. I will curate three techniques you can use: closed form, gradient descent, and stochastic gradient descent. There are other search algorithms like hill climbing that could be used, but we will stick with what's common.

MACHINE LEARNING TRAINING IS FITTING A REGRESSION

This is the heart of "training" a machine learning algorithm. We provide some data and an objective function (the sum of squares) and it will find the right coefficients *m* and *b* to fulfill that objective. Let's explore that next.

Closed Form Equation

Some readers may ask if there is a formula (called a **closed form equation**) to fit a linear regression by exact calculation. The answer is yes, but only for a simple linear regression with one input variable. This luxury does not exist for many machine learning problems with several input variables and a large amount of data that computers cannot handle. We can resort to linear algebra techniques to scale up, and we will talk about this shortly. But at a certain point you will have to resort to search algorithms like stochastic gradient descent, and is why these techniques get emphasis later in the chapter.

For a simple linear regression with only one input and one output variable, here are the closed form equations to calculate *m* and *b*. Example 5-5 shows how you can do these calculations in Python.

$$m = \frac{n\sum xy - \sum x \sum y}{n\sum x^2 - \left(\sum x\right)^2}$$

$$b = \frac{\sum y}{n} - m\frac{\sum x}{n}$$

Example 5-5. Calculating m and b for a simple linear regression

```
import pandas as pd

# Load the data
points = list(pd.read_csv('https://bit.ly/2KF29Bd',
delimiter=",").itertuples())

n = len(points)

m = (n*sum(p.x*p.y for p in points) - sum(p.x for p in points) *
    sum(p.y for p in points)) / (n*sum(p.x**2 for p in points) -
    sum(p.x for p in points)**2)

b = (sum(p.y for p in points) / n) - m * sum(p.x for p in points) /
n

print(m, b)
# 1.9393939393939394 4.7333333333333325
```

These equations to calculate *m* and *b* are derived off calculus and proofs beyond the scope of this book. But you can plug in the number of data points *n* as well as iterate the *x* and *y* values to do the operations above. Going forward, we will learn approaches that are more oriented towards contemporary techniques that cope with larger amounts of data. Closed form equations tend to not scale well.

Inverse Matrix Techniques

Going forward, I am going to replace the coefficients *m* and *b* with different names, β_1 and β_0 respectively. This is the convention you will see more often in the wild, so it might be a good time to graduate.

While we dedicated an entire chapter to linear algebra in Chapter 4, applying it can be a bit overwhelming when you are new to math and data science. This is why most examples in this book will use plain Python or Scikit-Learn. However, I will sprinkle in a linear algebra where it makes sense, just to show how linear algebra is useful. If you find this section

overwhelming feel free to move on to the rest of the chapter and come back later.

We can use transposed and inverse matrices, which we covered in Chapter 4, to fit a linear regression. Below we calculate a vector of coefficients b given a matrix of input variable values X, and a vector of output variable values y. Without going down a rabbit hole of Calculus and linear algebra proofs, here is the formula:

$$b = \left(X^T \cdot X\right)^{-1} \cdot X^T \cdot y$$

You will notice transpose and inverse operations are performed on the matrix X and combined with matrix multiplication. Here is how we perform the above operation in NumPy in Example 5-6 to get our coefficients m and b.

Example 5-6. Using inverse and transposed matrices to fit a linear regression

```
import pandas as pd
from numpy.linalg import inv
import numpy as np

# Import points
df = pd.read_csv('https://bit.ly/3goOAnt', delimiter=",")

# Extract input variables (all rows, all columns but last column)
X = df.values[:, :-1].flatten()

# Add placeholder "1" column to generate intercept
X_1 = np.vstack([X, np.ones(len(X))]).T

# Extract output column (all rows, last column)
Y = df.values[:, -1]

# Calculate coefficents for slope and intercept
b = inv(X_1.transpose() @ X_1) @ (X_1.transpose() @ Y)
print(b) # [1.93939394 4.73333333]

# Predict against the y-values
y_predict = X_1.dot(b)
```

It is not intuitive, but note above we have to stack a "column" of 1's next to our x column. The reason for this is this will generate the intercept β_0 coefficient. Since this column is all 1's it effectively generates the intercept rather than just a slope β_1.

When you have a lot of data with a lot of dimensions, computers can start to choke and produce unstable results. This is a use case for matrix decomposition which we learned about in Chapter 4 on linear algebra. In this specific case, we take our matrix X, append an additional column of 1's to generate the intercept β_0 just like before, and then decompose it into two component matrices Q and R.

$$X = Q \cdot R$$

Avoiding more Calculus rabbit holes, here is how we use Q and R to find the beta coefficient values in the matrix form b.

$$b = R^{-1} \cdot Q^T \cdot y$$

And here is how we use the QR decomposition formula above in Python using NumPy to perform a linear regression.

Example 5-7. Using QR decomposition to perform a linear regression

```
import pandas as pd
from numpy.linalg import qr, inv
import numpy as np

# Import points
df = pd.read_csv('https://bit.ly/3goOAnt', delimiter=",")

# Extract input variables (all rows, all columns but last column)
X = df.values[:, :-1].flatten()

# Add placeholder "1" column to generate intercept
X_1 = np.vstack([X, np.ones(len(X))]).transpose()

# Extract output column (all rows, last column)
Y = df.values[:, -1]

# calculate coefficents for slope and intercept
# using QR decomposition
Q, R = qr(X_1)
```

```
b = inv(R).dot(Q.transpose()).dot(Y)

print(b) # [1.93939394 4.73333333]
```

Typically, QR decomposition is the method used by many scientific libraries for linear regression because it copes with large amounts of data more easily and is more stable.

> **OVERWHELMED?**
>
> If you find these linear algebra examples of linear regression overwhelming, do not worry! I just wanted to provide exposure to a practical use case for linear algebra. Going forward we will focus on other techniques you can utilize.

Gradient Descent

Gradient descent is an optimization technique that uses derivatives and iterations to minimize/maximize a set of parameters against an objective. To learn about gradient descent, let's do a quick thought experiment and then apply it on a simple example.

A Thought Experiment on Gradient Descent

Let's do a thought experiment. Imagine you are in a mountain range at night and given a flashlight. You are trying to get to the lowest point of the mountain range. You can see the slope around you before you even take a step. You step in directions where the slope visibly goes downwards. You take bigger steps for bigger slopes, and smaller steps for smaller slopes. Ultimately you will find yourself at a low point where the slope is flat, a value of 0. Sounds pretty good, right? This approach with the flashlight is known as **gradient descent**, where we step in directions where the slope goes downwards.

In machine learning, we often think of all possible sum of square losses we will encounter with different parameters as a mountainous landscape. We want to minimize our loss and we navigate the loss landscape to do it. To solve this problem gradient descent has an attractive feature: the partial

derivative is that flashlight, allowing us to see the slopes for every parameter (in this case *m* and *b*, or β_0 and β_1). We step in directions for *m* and *b* where the slope goes downwards. We take bigger steps for bigger slopes and smaller steps for smaller slopes. We can simply calculate the length of this step by taking a fraction of the slope. This fraction is known as our **learning rate**. The higher the learning rate, the faster it will run at the cost of accuracy. But the lower the learning rate, the slower it will take to train and require more iterations.

Let's Walk Before We Run

For the function $f(x) = (x-3)^2 + 4$, find the *x* value that produces the lowest point of that function. While we could solve this algebraically, let's use gradient descent to do it.

Here is visually what we are trying to do. As shown in Figure 5-8, we wan to "step" *x* towards the minimum where the slope is 0.

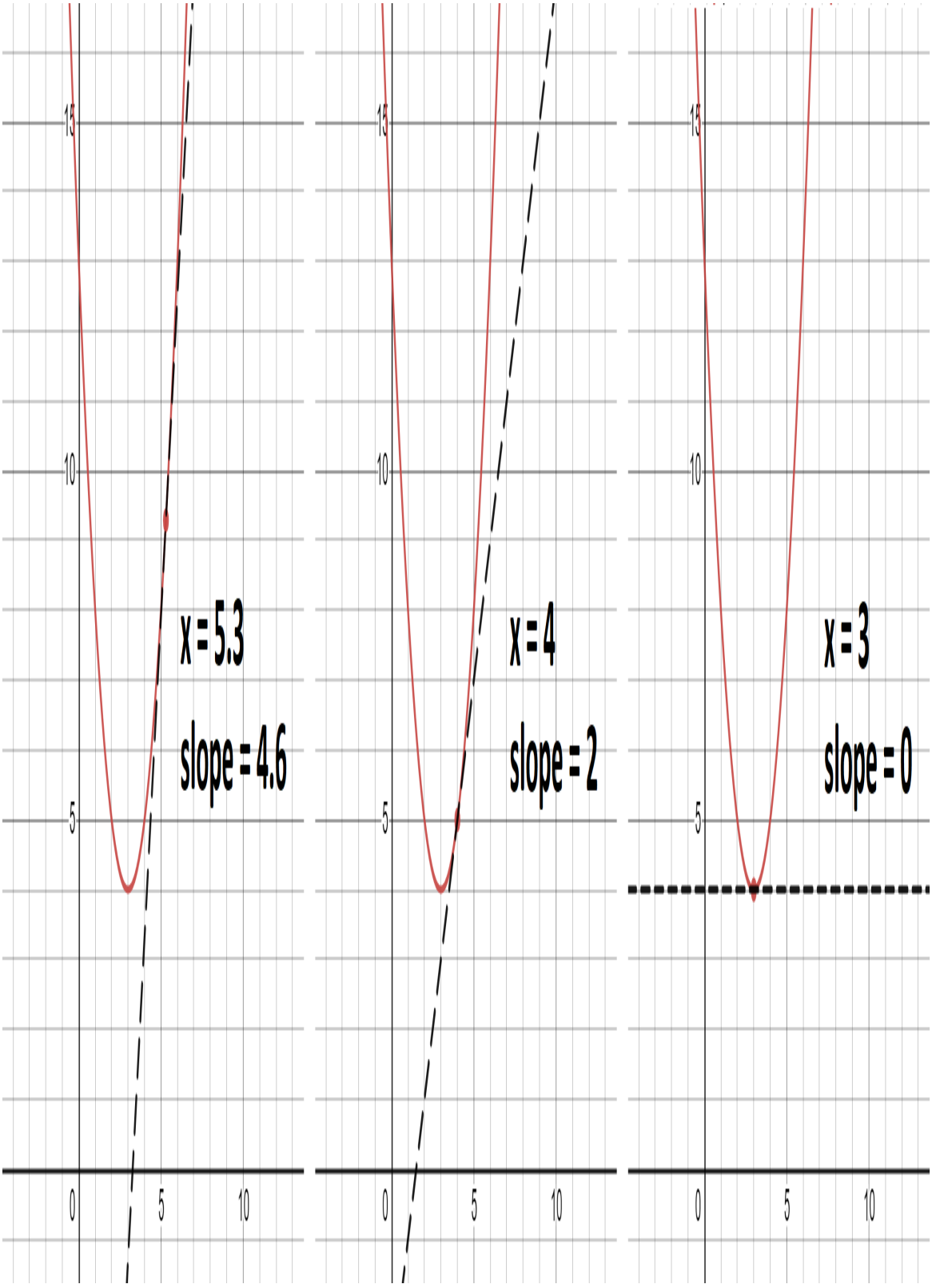


Figure 5-8. Stepping towards the local minimum where the slope approaches 0

In Example 5-8, the function `f(x)` and its derivative with respect to *x* is `dx_f(x)`. Recall we covered in Chapter 1 how to use SymPy to calculate derivatives. After finding the derivative, we then proceed to perform gradient descent.

Example 5-8. Using gradient descent to find the minimum of a parabola

```
import random


def f(x):
    return (x - 3) ** 2 + 4

def dx_f(x):
    return 2*(x - 3)

# The learning rate
L = 0.001

# The number of iterations to perform gradient descent
iterations = 100_000

 # start at a random x
x = random.randint(-15,15)

for i in range(iterations):

    # get slope
    d_x = dx_f(x)

    # update x by subtracting the (learning rate) * (slope)
    x -= L * d_x

print(x, f(x)) # prints 2.999999999999889 4.0
```

If we graph the function (as shown in Figure 5-8) we should see the lowest point of the function is clearly where `x = 3`, and the code above should get very close to that. The learning rate is used to take a fraction of the slope and subtract it from the *x* value on each iteration. Bigger slopes will result in bigger steps, and smaller slopes will result in smaller steps. After enough iterations, *x* will end up at the lowest point of the function (or close enough to it) where the slope is 0.

Gradient Descent and Linear Regression

You now might be wondering how do we use this for linear regression. Well it's the same idea except our "variables" are m and b (or β_0 and β_1) rather than x. Here's why: in a simple linear regression already know the x and y values because those are provided as the training data. The "variables" we need to solve are actually the parameters m and b, so we can find the best fit line that will then accept an x variable to predict a new y value.

How do we calculate the slopes for m and b? We need the partial derivatives for each of these. What function are we taking the derivative of? Remember we are trying to minimize loss and that will be the sum of squares. So we need to find the derivatives of our sum of squares function with respect to m and b.

I implement these two partial derivatives for m and b as shown in Example 5-9. We will learn how to do this shortly in SymPy. I then perform gradient descent to find m and b. 100,000 iterations with a learning rate of .001 will be sufficient. Note that the smaller you make that learning rate, the slower and more iterations you will need. But if you make it too high it will run fast but have a poor approximation. When someone says a machine learning algorithm is "learning" or "training", it really is just fitting a regression like this.

Example 5-9. Performing gradient descent for a linear regression

```
import pandas as pd

# Import points from CSV
points = list(pd.read_csv("https://bit.ly/2KF29Bd").itertuples())

# Building the model
m = 0.0
b = 0.0

# The learning Rate
L = .001

# The number of iterations
iterations = 100_000

n = float(len(points))  # Number of elements in X

# Perform Gradient Descent
```

```
for i in range(iterations):

    # slope with respect to m
    D_m = sum(2 * p.x * ((m * p.x + b) - p.y) for p in points)

    # slope with respect to b
    D_b = sum(2 * ((m * p.x + b) - p.y) for p in points)

    # update m and b
    m -= L * D_m
    b -= L * D_b

print("y = {0}x + {1}".format(m, b))
# y = 1.9393939393939548x + 4.733333333333227
```

Well not bad! That approximation got close to our closed form equation solution. But what's the catch? Just because we found the "best fit line" by minimizing sum of squares does not mean our linear regression is any good. Does minimizing the sum of squares guarantee a great model to make predictions? Not exactly. Now that I showed you how to fit a linear regression let's take a step back and revist the big picture, and determine whether a given linear regression is the right way to make predictions in the first place.

Gradient Descent for Linear Regression Using SymPy

If you want the SymPy code that came up with these two derivatives for the sum of squares function, for *m* and *b* respectively, here is the code in Example 5-10.

Example 5-10. Calculating partial derivatives for m and b

```
from sympy import *

m, b, i, n = symbols('m b i n')
x, y = symbols('x y', cls=Function)

sum_of_squares = Sum((m*x(i) + b - y(i)) ** 2, (i, 0, n))

d_m = diff(sum_of_squares, m)
d_b = diff(sum_of_squares, b)
print(d_m)
print(d_b)
```

```
# OUTPUTS
# Sum(2*(b + m*x(i) - y(i))*x(i), (i, 0, n))
# Sum(2*b + 2*m*x(i) - 2*y(i), (i, 0, n))
```

You will see above the two derivatives for *m* and *b* respectively printed. Note the `Sum()` function will iterate and add items together (in this case all the data points), and we treat *x* and *y* as functions that look up a value for a given point at index *i*.

In mathematical notation, where `e(x)` respresents the sum of squares loss function, here are the partial derivatives for *m* and *b*.

$$e\left(x\right) = \sum_{i=0}^{n}((mx_i + b) - y_i\Bigg)$$

$$\frac{d}{dm}e\left(x\right) = \sum_{i=0}^{n} 2\left(b + mx_i - y_i\right)x_i$$

$$\frac{d}{db}e\left(x\right) = \sum_{i=0}^{n} \left(2b + 2mx_i - 2y_i\right)$$

If you want to apply our dataset and execute a linear regression using gradient descent, you will have to perform a few additional steps as shown in Example 5-11. We will need to subsitute for the *n*, `x(i)` and `y(i)` values iterating all of our data points for the `d_m` and `d_b` derivative functions. That should leave only the *m* and *b* variables which we will search for the optimal values using gradient descent.

Example 5-11.

```
import pandas as pd
from sympy import *

# Import points from CSV
points = list(pd.read_csv("https://bit.ly/2KF29Bd").itertuples())

m, b, i, n = symbols('m b i n')
x, y = symbols('x y', cls=Function)

sum_of_squares = Sum((m*x(i) + b - y(i)) ** 2, (i, 0, n))
```

```
d_m = diff(sum_of_squares, m) \
    .subs(n, len(points) - 1).doit() \
    .replace(x, lambda i: points[i].x) \
    .replace(y, lambda i: points[i].y)

d_b = diff(sum_of_squares, b) \
    .subs(n, len(points) - 1).doit() \
    .replace(x, lambda i: points[i].x) \
    .replace(y, lambda i: points[i].y)

# compile using lambdify for faster computation
d_m = lambdify([m, b], d_m)
d_b = lambdify([m, b], d_b)

# Building the model
m = 0.0
b = 0.0

# The learning Rate
L = .001

# The number of iterations
iterations = 100_000

# Perform Gradient Descent
for i in range(iterations):

    # update m and b
    m -= d_m(m,b) * L
    b -= d_b(m,b) * L

print("y = {0}x + {1}".format(m, b))
# y = 1.939393939393954x + 4.733333333333231
```

As shown in Example 5-11, it is a good idea to call `lambdify()` on both of our partial derivative functions to convert them from SymPy to an optimized Python function. This will cause computations to perform much more quickly when we do gradient descent. The resulting Python functions are backed by NumPy, SciPy, or whatever numerical libraries SymPy detects you have available. After that, we can perform gradient descent.

Finally, if you are curious about what the loss function looks like for this simple linear regression, Example 5-12 shows the SymPy code that plugs in the `x`, `y`, and `n` values into our loss function and then plots `m` and `b` as the

input variables. Our gradient descent algorithm gets us to the lowest point in this loss landscape.

Example 5-12.

```
from sympy import *
from sympy.plotting import plot3d
import pandas as pd

points = list(pd.read_csv("https://bit.ly/2KF29Bd").itertuples())
m, b, i, n = symbols('m b i n')
x, y = symbols('x y', cls=Function)

sum_of_squares = Sum((m*x(i) + b - y(i)) ** 2, (i, 0, n)) \
    .subs(n, len(points) - 1).doit() \
    .replace(x, lambda i: points[i].x) \
    .replace(y, lambda i: points[i].y)

plot3d(sum_of_squres)
```

Overfitting and Variance

Riddle me this: if we truly wanted to minimize loss, as in reduce the sum of squares to 0, what would we do? Are there other options than linear regression? One conclusion you may arrive at is simply fit a curve that touches all the points. Heck, why not just connect the points together in segments and use that to make predictions as shown in Figure 5-9? That gives us a loss of 0!

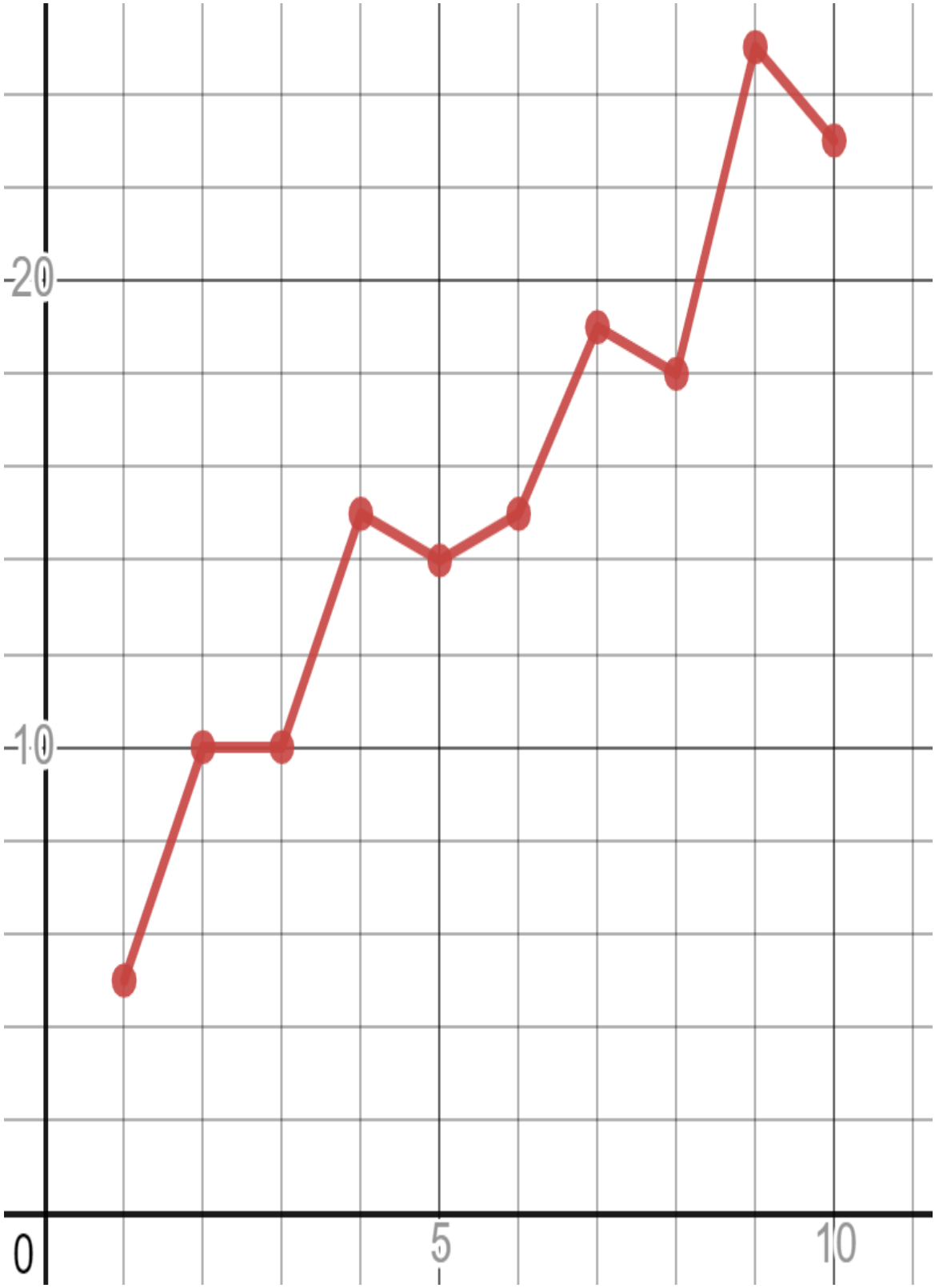


Figure 5-9. Performing a regression by simply connecting the points, resulting in zero loss.

Shoot, why did we go through all that trouble with linear regression and not do this instead? Well, remember our big picture objective is not to minimize the sum of squares but to make accurate predictions on new data. This "connect the dots" model is severely **overfit**, meaning it shaped the regression to the training data too exactly to the point it will predict poorly on new data. This simple "connect the dots" model is sensitive to outliers that are far away from the rest of the points, meaning it will have high **variance** in predictions. Because overfitting increases variance, predictions are going to be all over the place!

OVERFITTING IS MEMORIZATION

When you hear someone say a regression "memorized" the data rather than generalizing it, they are talking about overfitting.

As you can guess we want to find effective generalizations in our model rather than memorize data. Otherwise our regression simply turns into a database where we look up values.

This is why in machine learning you will find bias is added to the model, and linear regression is considered a highly biased model. This is not the same as bias in the data, which we talked about extensively in Chapter 3. **Bias in a model** means we prioritize a method (e.g. maintaining a straight line) as opposed to bending and fitting to exactly what the data says. A biased model leaves some wiggle room hoping to minimize loss on new data for better predictions, as opposed to minimizing loss on data it was trained on. I guess you could say adding bias to a model counteracts overfitting with **underfitting**, or fitting less to the training data.

As you can imagine this is a balancing act because it is two contradictory objectives. In machine learning, we basically are saying "I want to fit a regression to my data, but I don't want to fit it *too much*. I need some wiggle room for predictions on new data that will be different."

Still we cannot just apply a linear regression to some data, make some predictions with it, and assume all is okay. A linear regression can still

overfit even with the bias of a straight line. Therefore, we need to check and mitigate for both overfitting and underfitting to find the sweet spot between the two. That is if there is one at all, in which case you should abandon the model altogether. Don't p-hack, people!

Stochastic Gradient Descent

In a machine learning context, you are unlikely to do gradient descent in practice like we did earlier, where we trained on all training data (called **batch gradient descent**). In practice you are more likely to perform **stochastic gradient descent**, which will only train on one sample of the dataset on each iteration. In **mini-batch gradient descent**, multiple samples of the dataset are used (e.g. 10 or 100 data points) on each iteration.

Why only use part of the data on each iteration? Machine learning practitioners cite a few benefits. First it reduces computation significantly, as each iteration does not have to traverse the entire training dataset but only part of it. The second benefit is it reduces overfitting. By exposing the training algorithm to only part of the data on each iteration, it keeps changing the loss landscape so it does not settle in the loss minimum. After all, minimizing the loss is what causes overfitting and so we introduce some randomness to create underfitting.

Of course, our approximation becomes loose so we have to be careful. This is why we will talk about training/testing splits shortly, as well as other metrics to evaluate our linear regression's reliability.

Example 5-13 shows how to perform stochastic gradient descent in Python. If you change the sample size to be more than 1, it will perform mini-batch gradient descent.

Example 5-13. Performing stochastic gradient descent for a linear regression

```
import pandas as pd
import numpy as np

# Input data
```

```
data = pd.read_csv('https://bit.ly/2KF29Bd', header=0)

X = data.iloc[:, 0].values
Y = data.iloc[:, 1].values

n = data.shape[0]  # rows

# Building the model
m = 0.0
b = 0.0

sample_size = 1  # sample size
L = .0001  # The learning Rate
epochs = 1_000_000  # The number of iterations to perform gradient
descent

# Performing Stochastic Gradient Descent
for i in range(epochs):
    idx = np.random.choice(n, sample_size, replace=False)
    x_sample = X[idx]
    y_sample = Y[idx]

    # The current predicted value of Y
    Y_pred = m * x_sample + b

    # d/dm derivative of loss function
    D_m = (-2 / sample_size) * sum(x_sample * (y_sample - Y_pred))

    # d/db derivative of loss function
    D_b = (-2 / sample_size) * sum(y_sample - Y_pred)
    m = m - L * D_m  # Update m
    b = b - L * D_b  # Update b

    # print progress
    if i % 10000 == 0:
        print(i, m, b)

print("y = {0}x + {1}".format(m, b))
```

When I ran this, I got a linear regression of `y = 1.9382830354181135x + 4.753408787648379`. Obviously your results are going to be different, and because of stochastic gradient descent we really aren't going to converge towards a specific minimum but end up in a broader neighborhood of coefficient values.

IS RANDOMNESS BAD?

If this randomness feels uncomfortable where you get a different answer every time you run a piece of code, welcome to the world of machine learning, optimization, and stochastic algorithms! Many algorithms that do approximations are random-based, and while some are extremely useful others can be sloppy and perform poorly as you might expect.

A lot of people look to machine learning and AI as some tool that gives objective and precise answers, but that cannot be further from the truth. Machine learning can be misused as a cursory form of statistics that approximates (sometimes very liberally) based on a combination of data and random-based search strategies.

While randomness can create some powerful tools, it can also be abused. Be careful to not use seed values and randomness to p-hack a "good" result, and put effort into analyzing your data and model if it's possible.

The Correlation Coefficient

Take a look at this scatterplot in Figure 5-10 alongside its linear regression. Why might a linear regression not work too well here?

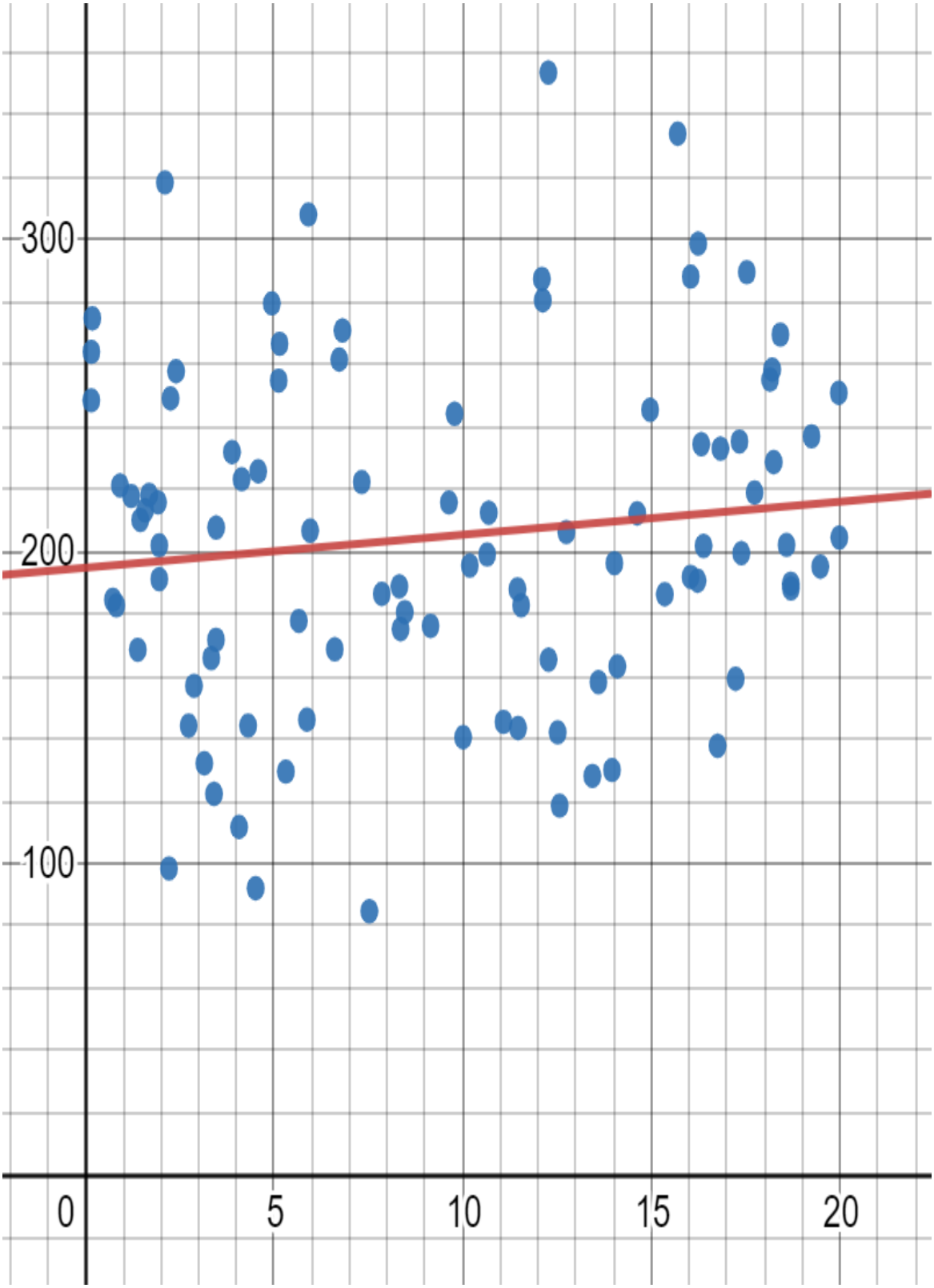


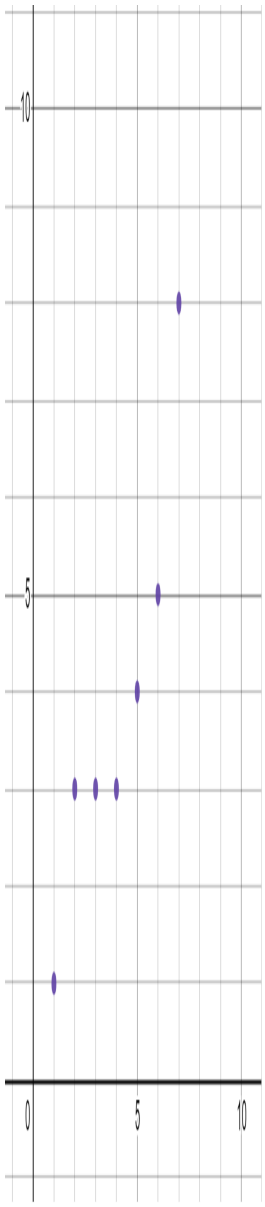
Figure 5-10. A scatterplot of data with high variance

The problem here is that the data has high variance. If the data is extremely spread out, it is going to drive up the variance to the point predictions become less accurate and useful, resulting in large residuals. Of course we can introduce a biased model, such as linear regression, to not bend and respond to the variance so easily. However the underfitting is also going to undermine our predictions because the data is so spread out. We need to numerically measure how "off" our predictions are.

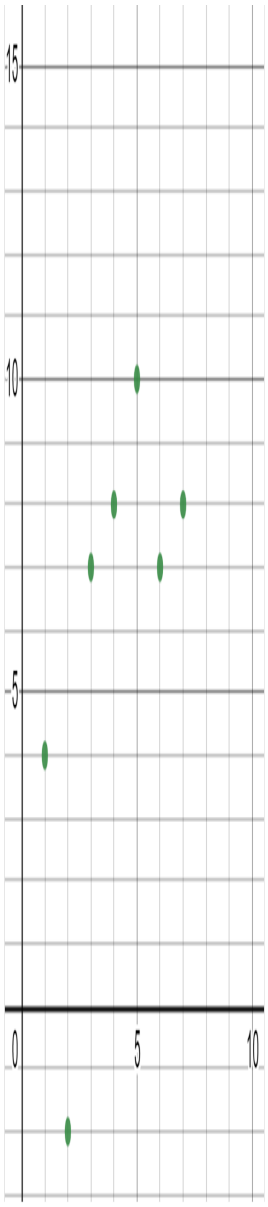
So how do you measure these residuals in aggregate? How do you also get a sense for how bad the variance in the data is? Let me introduce you to the **correlation coefficient**, also called the **Pearson correlation**, which measures the strength of the relationship between two variables as a value between -1 and 1. A correlation coefficient closer to 0 indicates there is no correlation. A correlation coefficient closer to 1 indicates a strong **positive correlation**, meaning when one variable increases the other proportionally increases. If it is closer to -1 then it indicates a strong **negative correlation**, which means as one variable increases the other proportionally decreases.

Note the correlation coefficient is often denoted as *r*. The highly scattered data in Figure 5-15 has a correlation coefficient of 0.1201. Since it is much closer to 0 than 1, we can infer it has little correlation.

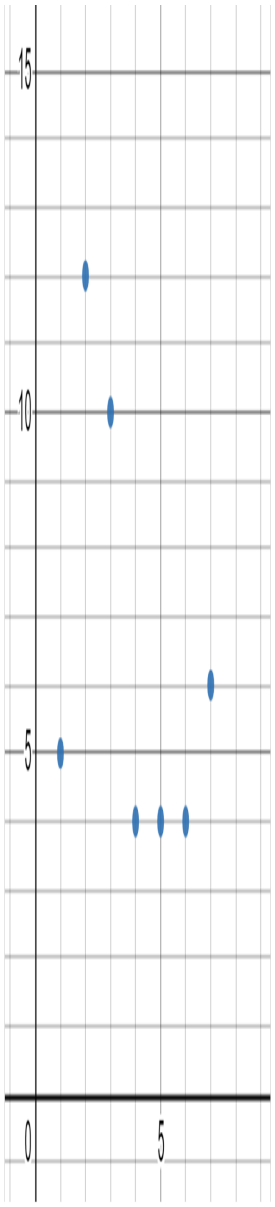
Here are three other scatterplots in Figure 5-11 showing their correlation coefficients. Notice that the more the points follow a line, the stronger the correlation. More dispersed points result in weaker correlations.



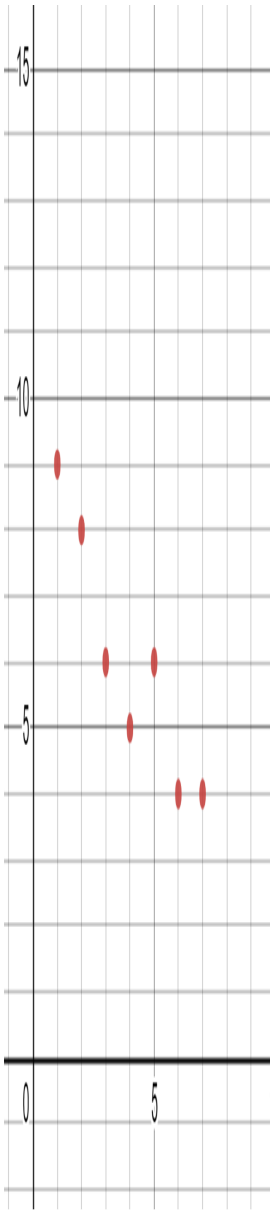
PEARSON CORRELATION: .923133



PEARSON CORRELATION: .643237



PEARSON CORRELATION: -.44984



PEARSON CORRELATION: -.9267

Figure 5-11. Correlation coefficients for four scatterplots

As you can imagine, the correlation coefficient is useful to see if there is a possible relationship between two variables. If there is a strong positive/negative relationship, it will be useful in our linear regression. If there is not a relationship, they may just add noise and hurt model accuracy.

How do we use Python to calculate the correlation coefficient? Let's use our simple 10-point dataset we used earlier. A quick and easy way to analyze correlations for all pairs of variables is using Pandas' `corr()` function. It makes it easy to see the correlation coefficient between every pair of variables in a dataset, which in this case will only be *x* and *y*. This is known as a **correlation matrix**. Take a look in Example 5-14.

Example 5-14. Using Pandas to see the correlation coefficent between every pair of variables

```
import pandas as pd

# Read data into Pandas dataframe
df = pd.read_csv('https://bit.ly/2KF29Bd', delimiter=",")

# Print correlations between variables
correlations = df.corr(method='pearson')
print(correlations)

# OUTPUT:
#           x         y
# x  1.000000  0.957586
# y  0.957586  1.000000
```

As you can see the correlation coefficient `.957586` between *x* and *y* indicates a strong positive correlation between the two variables. You can ignore the parts of the matrix where *x* or *y* are set to themselves and have a value of `1.0`. Obviously when *x* or *y* is set to itself the correlation will be perfect at 1.0, because their values match themselves exactly. When you have more than two variables, the correlation matrix will show a larger grid because there are more variables to pair and compare.

If you change the code to use a different dataset with a lot of variance, where the data is spread out, you will see that correlation coefficient

decreases. This again indicates a weaker correlation.

CALCULATING THE CORRELATION COEFFICIENT

For those that are mathematically curious how the correlation coefficient is calculated, here is the formula:

$$r = \frac{n\sum xy - (\sum x)(\sum y)}{\sqrt{n\sum x^2 - (\sum x^2)}\sqrt{n\sum y^2 - (\sum y^2)}}$$

If you want to see this fully implemented in Python, I like to use one-line `for` loops to do those summations. Example 5-15 shows a correlation coefficient implemented from scratch in Python.

Example 5-15. Calculating correlation coefficient from scratch in Python

```
import pandas as pd
from math import sqrt

# Import points from CSV
points =
list(pd.read_csv("https://bit.ly/2KF29Bd").itertuples())
n = len(points)

numerator = n * sum(p.x * p.y for p in points) - \
            sum(p.x for p in points) * sum(p.y for p in points)

denominator = sqrt(n*sum(p.x**2 for p in points) - sum(p.x for p
in points)**2) \
              * sqrt(n*sum(p.y**2 for p in points) - sum(p.y for
p in points)**2)

corr = numerator / denominator

print(corr)

# OUTPUT:
# 0.9575860952087218
```

Statistical Significance

Here is another aspect to a linear regression you must consider: is my data correlation coincidental? In Chapter 3 we studied hypothesis testing and p-values, and we are going to extend those ideas here with a linear regression.

THE STATSMODEL LIBRARY

While we are not going to introduce yet another library in this book, it is worth mentioning that `statsmodel` is noteworthy if you want to do statistical analysis.

https://www.statsmodels.org/stable/regression.html

Scikit-Learn and other machine learning libraries do not provide tools for statistical significance and confidence intervals for reasons we will discuss in another sidebar. We are going to code those techniques ourselves. But know this library exists and it is worth checking out!

Let's start with a fundamental question: is it possible I see a linear relationship in my data due to random chance? How can we be 95% sure the correlation between these two variables is real, not coincidental? If this sounds like a hypothesis test from Chapter 3, it's because it is! We need to express not just the correlation coefficient, but quantify how confident we are that the correlation coefficient did not occur by chance.

Rather than estimating a mean like we did in Chapter 3 with the drug testing example, we are estimating the population correlation coefficient based on a sample. We denote the population correlation coefficient with the Greek symbol ρ ("Rho") while our sample correlation coefficient is r. Just like we did in Chapter 3, we will have a null hypothesis H_0 and alternative hypothesis H_1.

$$H_0 : \rho = 0 \text{ (implies no relationship)}$$

$$H_1 : \rho \neq 0 \text{ (relationship is present)}$$

Our null hypothesis H_0 is that there is no relationship between two variables, or more technically the correlation coefficient is 0. The alternative hypothesis H_1 is there is a relationship, and it can be a positive or negative correlation. This is why the alternative hypothesis is defined as $\rho \neq 0$ to support both a positive and negative correlation.

Let's return to our dataset of 10 points as shown in Figure 5-12. How likely is it we would see these data points by chance? And they happen to produce what looks like a linear relationship?

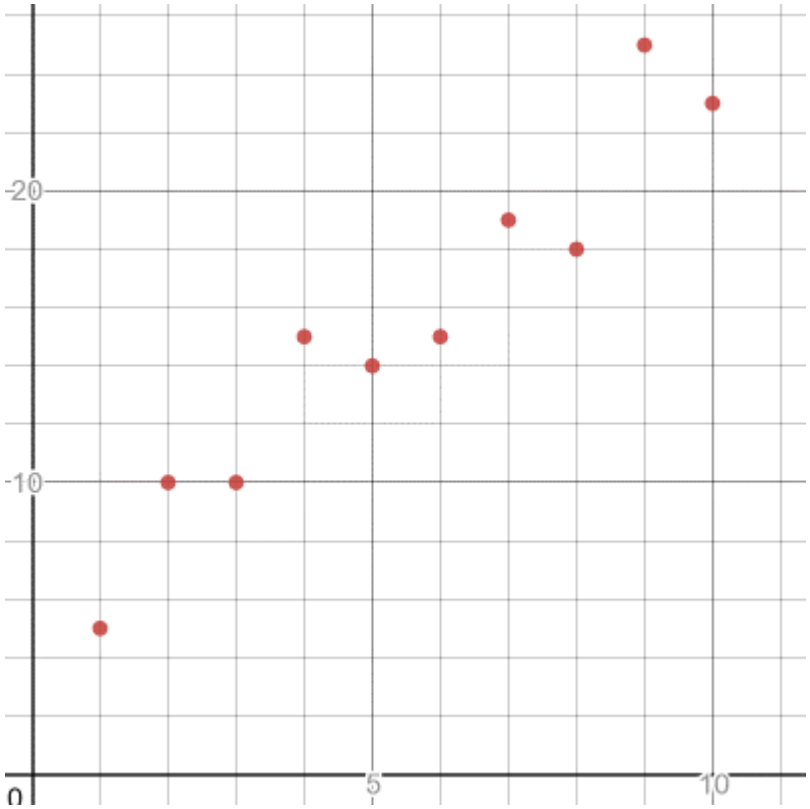


Figure 5-12. How likely would we see this data, which seems to have a linear correlation, by random chance?

We already calculated the correlation coefficient for this dataset earlier in Example 5-14, which is 0.957586. That's a strong and compelling positive correlation. But again we need to evaluate if this was by random luck. Let's pursue our hypothesis test with 95% confidence using a two-tailed test, exploring if there is a relationship between these two variables.

We talked about the T-distribution in Chapter 3, which has fatter tails to capture more variance and uncertainty. We use a T-distribution rather than a normal distribution to do hypothesis tesing with linear regression. First, let's plot a T-distribution with a 95% critical value range as shown in Figure 5-13. We account for the fact there are 10 records in our sample and therefore we have 9 degrees of freedom (10 - 1 = 9).

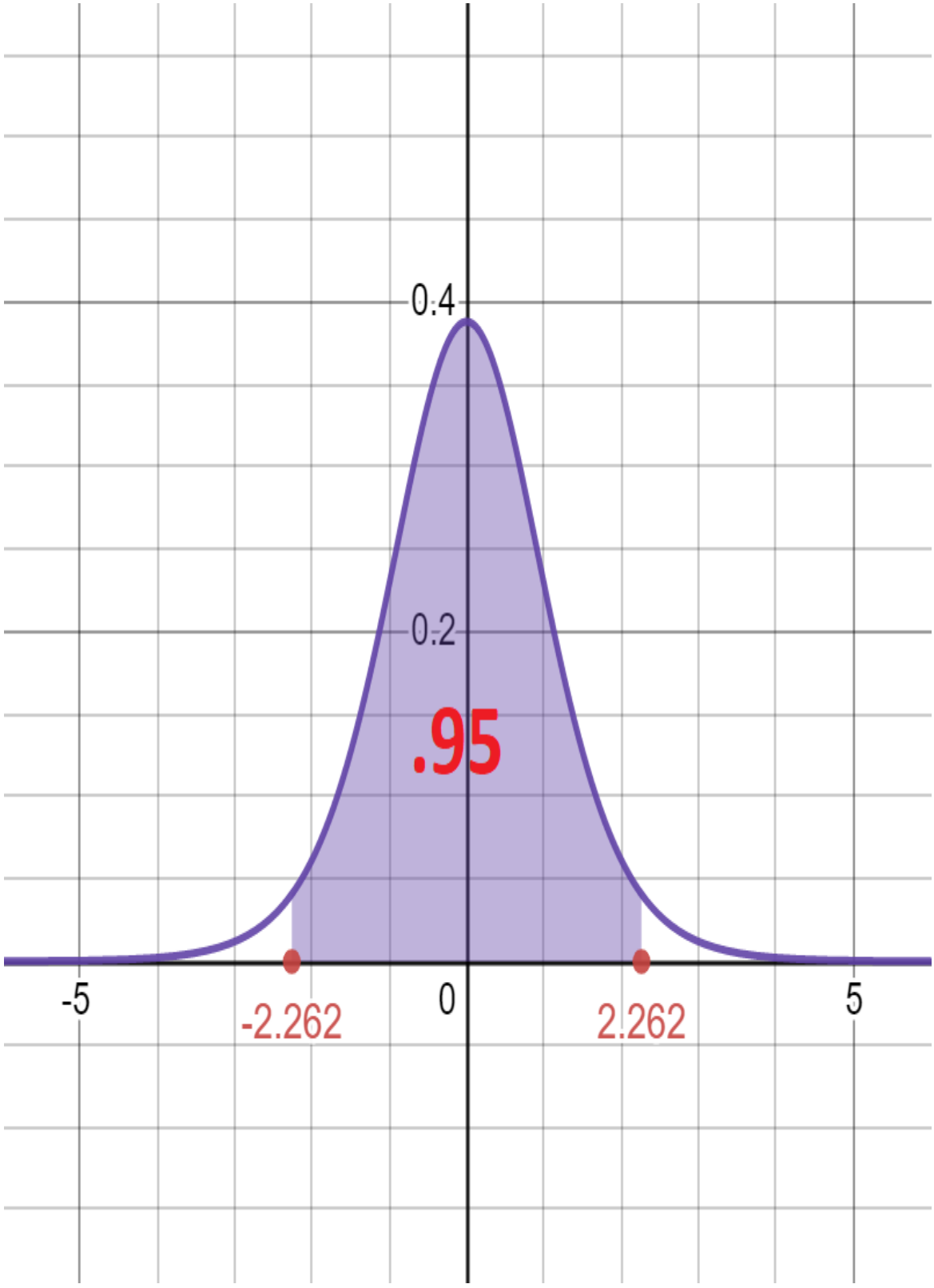


Figure 5-13. A T-Distribution with 9 degrees of freedom, as there are 10 records and we subtract 1.

The critical value is approximately ± 2.262, and we can calculate that in Python as shown in Example 5-16. This captures 95% of the center area of our T-distribution.

Example 5-16. Calculating the critical value from a T-distribution

```
from scipy.stats import t

n = 10
lower_cv = t(n-1).ppf(.025)
upper_cv = t(n-1).ppf(.975)

print(lower_cv, upper_cv)
# -2.262157162740992 2.2621571627409915
```

If our test value happens to fall outside this range of (-2.262, 2.262) then we can reject our null hypothesis and say our correlation is real (not coincidental) with at least 95% confidence. To calculate the test value *t*, we need to use this formula below. Again *r* is the correlation coefficient and *n* is the sample size.

$$t = \frac{r}{\sqrt{\frac{1-r^2}{n-2}}}$$

$$t = \frac{.957586}{\sqrt{\frac{1-.957586^2}{10-2}}} = 9.39956$$

Let's put the whole test together in Python as shown in Example 5-17. If our test value falls outside the critical range of 95% confidence, we accept that our correlation was not by chance.

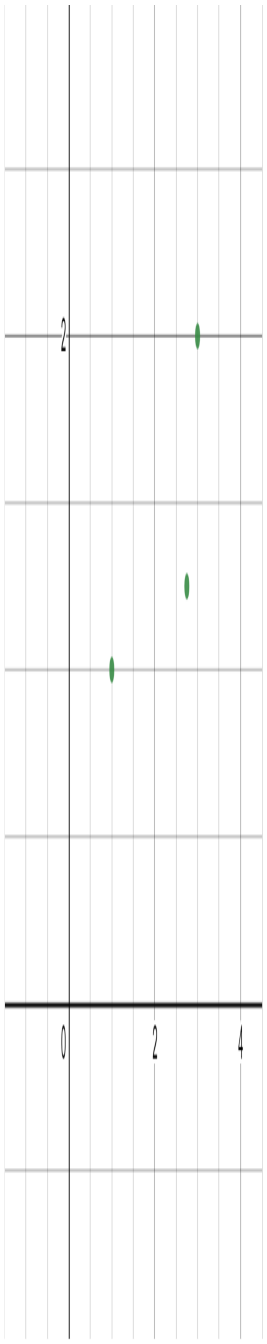
Example 5-17. Testing significance for linear-looking data

```
from scipy.stats import t
from math import sqrt

# sample size
n = 10

lower_cv = t(n-1).ppf(.025)
upper_cv = t(n-1).ppf(.975)
```

```
# correlation coefficient
# derived from data https://bit.ly/2KF29Bd
r = 0.957586

# Perform the test
test_value = r / sqrt((1-r**2) / (n-2))

print("TEST VALUE: {}".format(test_value))
print("CRITICAL RANGE: {}, {}".format(lower_cv, upper_cv))

if test_value < lower_cv or test_value > upper_cv:
    print("CORRELATION PROVEN, REJECT H0")
else:
    print("CORRELATION NOT PROVEN, FAILED TO REJECT H0 ")

# Calculate p-value
if test_value > 0:
    p_value = 1.0 - t(n-1).cdf(test_value)
else:
    p_value = t(n-1).cdf(test_value)

# Two-tailed, so multiply by 2
p_value = p_value * 2
print("P-VALUE: {}".format(p_value))
```

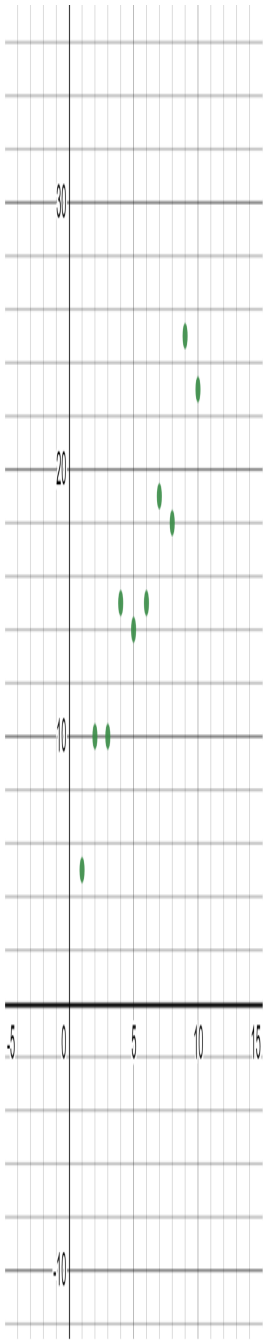
The test value above is approximately 9.39956, which is definitely outside the range of (-2.262, 2.262) so we can reject the null hypothesis and say our correlation is real. That's because the p-value is remarkably significant: .000005976. This is well below our .05 threshold, so this is virtually not coincidence there is a correlation. I'll confess I actually fabricated this dataset, and it makes sense the p-value is so small because the points strongly resemble a line. It is highly unlikely these points randomly arranged themselves near a line this closely by chance.

Figure 5-14 shows some other datasets with their correlation coefficients and p-values. Analyze each one of them. Which one is likely the most useful for predictions? What are the problems with the other ones?



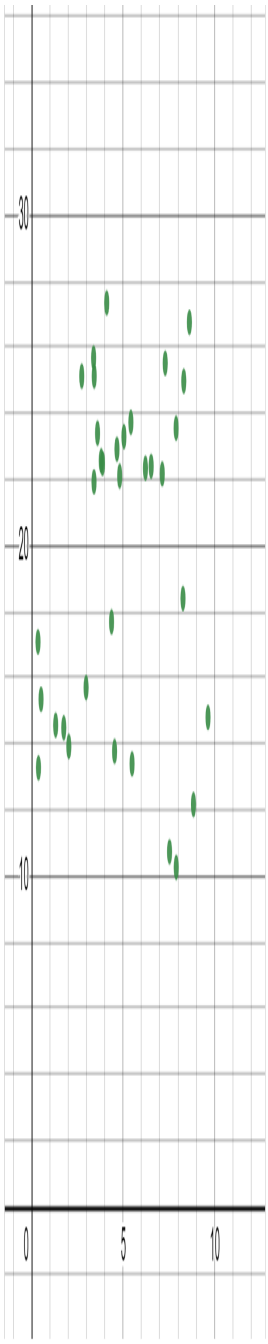
r 0.771454

p-value 0.34913



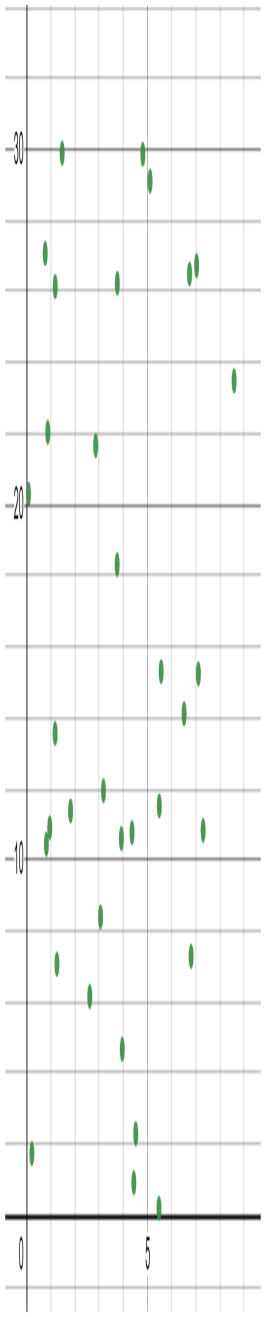
r 0.957586095

p-value 0.000005976



r 0.100984708

p-value 0.569732057



r 0.037875905

p-value 0.831544971

Figure 5-14. Different datasets and their correlation coefficients and p-values

Now that you've had a chance to work through the analysis on the datasets from Figure Figure 5-14, let's walk through the findings. The left figure has a high positive correlation, but it only has 3 points. The lack of data drives up the p-value significantly to .34913 and increases the likelihood the data happened by chance. This makes sense because having just 3 data points makes it likely to see a linear pattern, but it's not much better than having 2 points that will simply connect a line between the two points. This brings up an important rule-of-thumb: having more data will decrease your p-value, especially if that data gravitates towards a line.

The second figure is what we just covered. It only has 10 data points, but it forms a linear pattern so nicely, we not only have a strong positive correlation but also an extremely low p-value. When you have a p-value this low, you can bet you are measuring an engineered and tightly controlled process, not something socological or natural.

The right two figures in Figure 5-14 perform poorly for a linear model. Their correlation coefficient is close to 0 indicating no correlation, and the p-values unsurprisingly indicate randomness played a role.

The rule of thumb is this: the more data you have that consistently resembles a line, the more significant the p-value for your correlation will be. The more scattered or sparse the data, the more the p-value will increase and thus indicate your correlation occurred by random chance.

Coefficient of Determination

Let's learn an important metric you will see a lot in statistics and machine learning regressions. The **coefficient of determination**, called r^2, measures how much variation in one variable is explainable by the variation of the other variable. It is also the square of the correlation coefficient r. As r approaches a perfect correlation (-1 or 1), the r^2 approaches 1. Essentially, r^2 shows how much two variables interact with each other.

Let's continue looking at our data from Figure 5-12. In Example 5-18, take our dataframe code from earlier that calculates the correlation coefficient and then simply square it. That will multiply each correlation coefficient by itself.

Example 5-18. Creating a correlation matrix in Pandas

```
import pandas as pd

# Read data into Pandas dataframe
df = pd.read_csv('https://bit.ly/2KF29Bd', delimiter=",")

# Print correlations between variables
coeff_determination = df.corr(method='pearson') ** 2
print(coeff_determination)

# OUTPUT:
#           x         y
# x  1.000000  0.916971
# y  0.916971  1.000000
```

A coefficient of determination of .916971 is interpreted as "91.6971% of the variation in *x* is explained by *y* (and vice versa), and the remaining 8.3029% is noise caused by other uncaptured variables." 0.916971 is a pretty good coefficient of determination, showing that *x* and *y* explain each other's variance. But there could be other variables at play making up that remaining 0.083029. Remember, correlation does not equal causation, so there could be other variables contributing to the relationship we are seeing.

CORRELATION IS NOT CAUSATION!

It is important to note that while we put a lot of emphasis on measuring correlation and building metrics around it, please note *correlation is not causation!* You probably have heard that mantra before but I want to expand on why statisticians say it.

Just because we see a correlation between x and y does not mean x causes y. It could actually be y causes x! Or maybe there is a third uncaptured variable z that is causing x and y. It could be that x and y do not cause each other at all and the correlation is just coincidental, hence why it is important we measure the statistical significance.

Now I have a more pressing question for you. Can computers discern between correlation and causation? The answer is a resounding "NO!" Computers only have concept of correlation but not causation. Let's say I load a dataset to Scikit-Learn showing gallons of water consumed and my water bill. My computer, or any program including Scikit-Learn, does not have any notion of whether more water usage causes a higher bill, or a higher bill causes more water usage. An "AI" system could easily conclude the latter, as nonsensical as that is. This is why many machine learning projects require a human in the loop to inject common sense.

In computer vision, this happens too. Computer vision often uses a regression on the numeric pixels to predict a category. If I train a computer vision system to recognize cows using pictures of cows, it can easily make correlations with the field rather than cows. Therefore if I show a picture of an empty field, it will label the grass as cows! This again is because computers have no concept of causality (the cow shape should cause the label "cow") and instead gets lost in correlations we are not interested in.

Standard Error of the Estimate

One way to measure the overall error of a linear regression is the **SSE, or sum of squared error**. We learned about this earlier where we square each residual and sum them. If $\hat{y}$ (pronounced "y-hat") is each predicted value from the line and y represents each actual y value from the data, here is the calculation:

$$SSE = \sum \left(y - \hat{y}\right)^2$$

However, all of these squared values are hard to interpret so we can use some square root logic to scale things back into their original units. We will also average all of them, and this is what the **standard error of the**

estimate (S_e) does. If n is the number of data points, Example 5-19 shows how we calculate the standard error S_e in Python.

$$S_e = \frac{\sum (y - \hat{y})^2}{n - 2}$$

Example 5-19. Calculating the standard error of the estimate

```
Here is how we calculate it in Python:

import pandas as pd
from math import sqrt

# Load the data
points = list(pd.read_csv('https://bit.ly/2KF29Bd',
delimiter=",").itertuples())

n = len(points)

# Regression line
m = 1.939
b = 4.733

# Calculate Standard Error of Estimate
S_e = sqrt((sum((p.y - (m*p.x +b))**2 for p in points))/(n-2))

print(S_e)
# 1.87406793500129
```

Why $n - 2$ instead of $n - 1$, like we have done in so many variance calculations in Chapter 3? Without going too deep into mathematical proofs, this is because a linear regression has two variables, not just one, so we have to increase the uncertainty by one more in our degrees of freedom.

You will notice the standard error of the estimate looks remarkably similar to the standard deviation we studied in Chapter 3. This is not by accident. That is because it is the standard deviation for a linear regresison.

Prediction Intervals

As mentioned earlier, our data in a linear regression is a sample from a population. Therefore our regression is only as good as our sample. Our linear regression line also has a normal distribution running along it. Effectively, this makes each predicted *y* value a sample statistic just like the mean. As a matter of fact, the "mean" is shifting along the line.

Remember when we talked statistics in Chapter 2 about variance and standard deviation? The concepts apply here too. With a linear regression, we hope that data follows a normal distribution in a linear fashion. A regression line serves as the shifting "mean" of our bell curve and the spread of the data around the line reflects the variance/standard deviation, as shown in Figure 5-15.

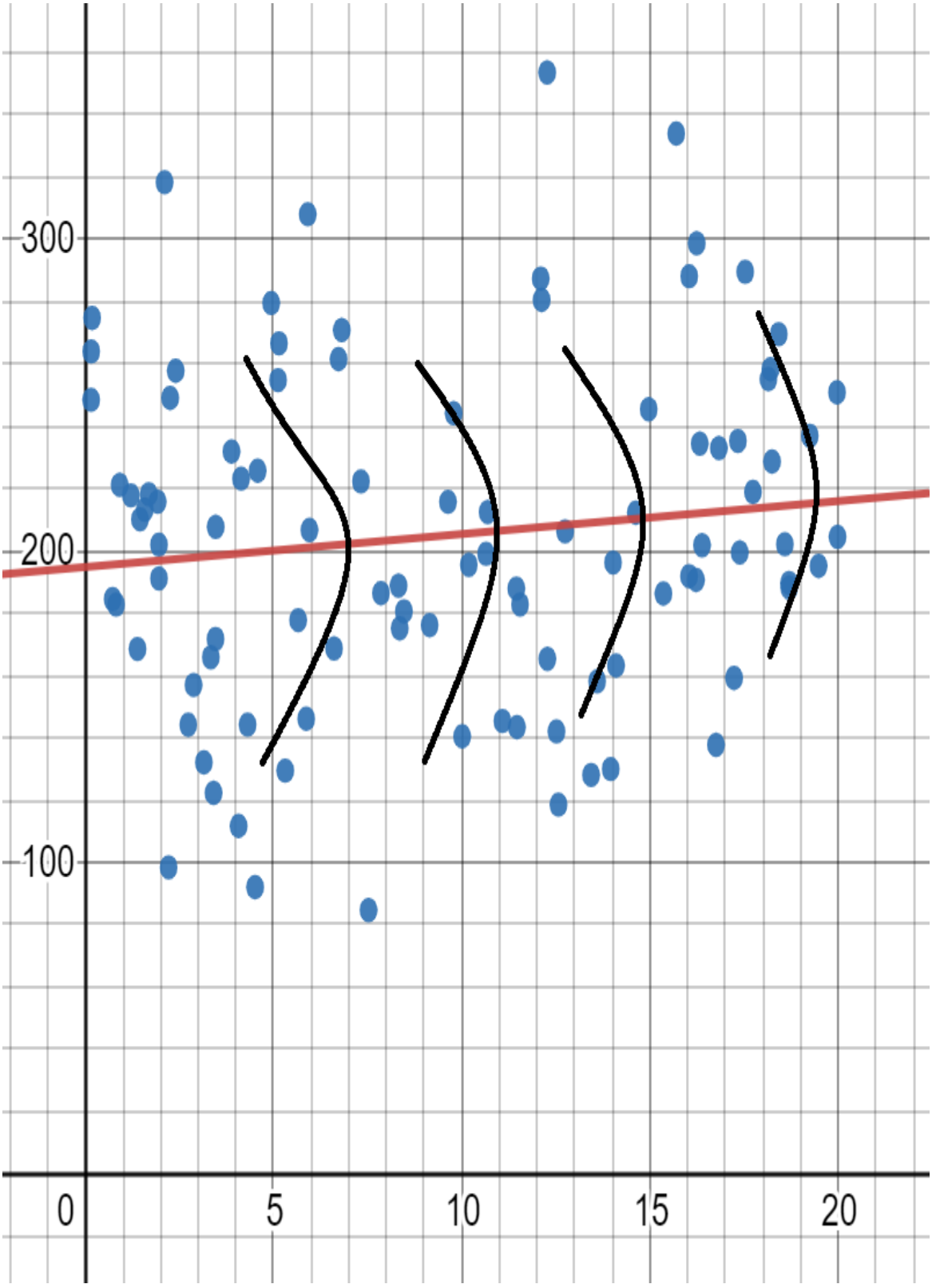


Figure 5-15. A linear regression assumes a normal distribution is following the line

When we have a normal distribution following a linear regression line, it is known as a **bivariate normal distribution**. This makes sense because we have not just one variable but a second one steering a distribution as well. There is a confidence interval around each *y* prediction and this is known as a **prediction interval**.

Let's bring back some context with our veterinary example, estimating the age of a dog and number of vet visits. I want to know the prediction interval for number of vet visits with 95% confidence for a dog that is 8.5 years old. What this prediction interval looks like is shown in Figure 5-16. We are 95% confident that an 8.5 year old dog will have had between 16.462 and 25.966 veterinary visits.

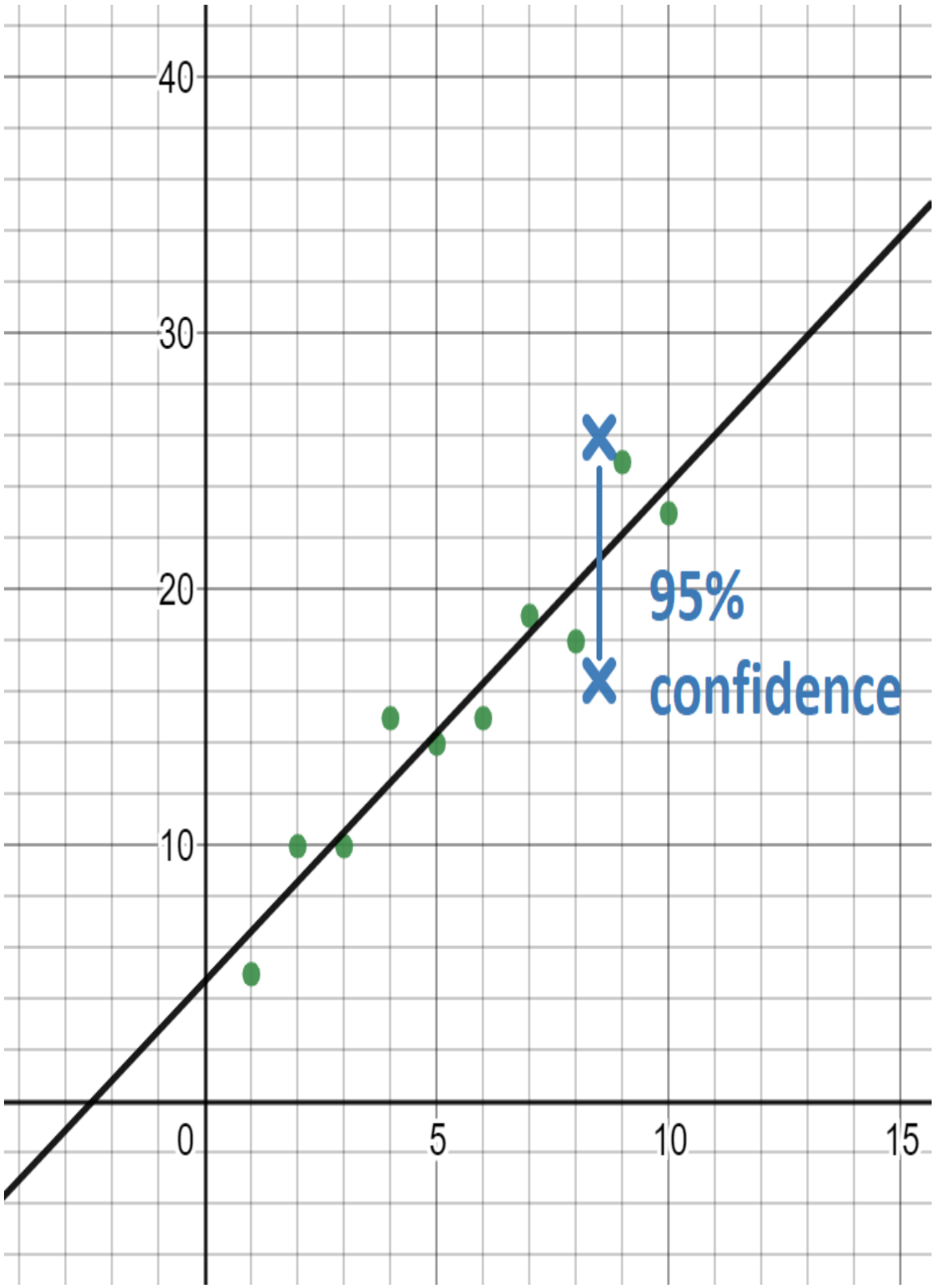


Figure 5-16. A prediction interval for a dog that is 8.5 years old with 95% confidence

How do we calculate this? We need to get the margin of error, and plus/minus it around the predicted y-value. It's a beastly equation that involves a critical value from the t-distribution as well as the standard error of the estimate. Let's take a look:

$$E = t_{.025} * S_e * \sqrt{1 + \frac{1}{n} + \frac{n(x_0 + \overline{x})^2}{n\left(\sum x^2\right) - \left(\sum x\right)^2}}$$

The x-value we are interested in is specified as x_0, which in this case is 8.5. Here is how we solve this in Python shown in Example 5-20.

Example 5-20. Calculating a prediction interval of vet visits for a dog that's 8.5 years old

```
import pandas as pd
from scipy.stats import t
from math import sqrt

# Load the data
points = list(pd.read_csv('https://bit.ly/2KF29Bd',
delimiter=",").itertuples())

n = len(points)

# Linear Regression Line
m = 1.939
b = 4.733

# Calculate Prediction Interval for x = 8.5
x_0 = 8.5
x_mean = sum(p.x for p in points) / len(points)

t_value = t(n - 2).ppf(.975)

standard_error = sqrt(sum((p.y - (m * p.x + b)) ** 2 for p in
points) / (n - 2))

margin_of_error = t_value * standard_error * \
                  sqrt(1 + (1 / n) + (n * (x_0 - x_mean) ** 2) / \
                       (n * sum(p.x ** 2 for p in points) - sum(p.x
for p in points) ** 2))

predicted_y = m*x_0 + b
```

```
# Calculate prediction interval
print(predicted_y - margin_of_error, predicted_y + margin_of_error)
# 16.462516875955465 25.966483124044537
```

Oy vey! That's a lot of calculation, and unfortunately SciPy and other mainstream data science libraries do not do this. But if you are inclined towards statistical analysis, this is very useful information. We not only create a prediction based on a linear regression (e.g. a dog that's 8.5 years old will have 21.2145 vet visits), but we are actually able to say something much less absolute: there's a 95% likelihood an 8.5 year old dog will visit the vet between 16.46 and 25.96 times. Brilliant, right? And it's a much safer claim because it captures a range rather than a single value, and thus accounts for uncertainty.

CONFIDENCE INTERVALS FOR THE PARAMETERS

When you think about it, the linear regression line itself is a sample statistic, and there is a linear regression line for the whole population we are trying to infer. This means parameters like m and b have their own distributions, and we can model confidence intervals around m and b individually to reflect the population's slope and y-intercept. This is beyond the scope of this book but it's worth noting this type of analysis can be done.

You can find resources to do these calculations from scratch but it might just be easier to use Excel's regression tools or libraries for Python. We will talk about specialized libraries for Python at the end of this chapter.

Train/Test Splits

This analysis I just did with the correlation coefficient, statistical significance, and coefficient of determination unfortunately is not done often by machine learning practioners. Sometimes they are dealing with so

much data they do not have the time or technical ability to. For example a 128x128 pixel image is at least 16,384 variables. Do you have time to do statistical analysis on each of those pixel variables? Probably not! Unfortuantely this leads many data scientists to not learn these statistical metrics at all.

In an obscure online forum, I once read a post saying statistical regression is a scalpel, while machine learning is a chainsaw. When operating with massive amounts of data and variables, you cannot sift through all of that with a scalpel. You have to resort to a chainsaw and while you lose explainability and precision, you at least can scale to make broader predictions on more data. That being said, statisical concerns like sampling bias and overfitting do not go away. But there are a few practices that can be employed for quick-and-dirty validation.

WHY ARE THERE NO CONFIDENCE INTERVALS AND P-VALUES IN SCIKIT-LEARN?

Scikit-Learn does not support confidence intervals and P-values, as these two techniques are open problems for higher-dimensional data. This only emphasizes the gap between statisticans and machine learning practitioners. As one of the maintainers of Scikit-Learn, Gael Varoquaux, said "… in general computing correct p-values requires assumptions on the data that are not met by the data used in machine learning (no multicollinearity, enough data compared to the dimensionality) … P-values are something that are expected to be well checked (they are a guard in medical research). Implementing them is asking for trouble… We can give p-values only in very narrow settings [with few variables]."

If you want to go down the rabbit hole, there are some interesting discussions on Github:

https://github.com/scikit-learn/scikit-learn/issues/6773

https://github.com/scikit-learn/scikit-learn/issues/16802

As mentioned before, `statsmodel` is a library that provides helpful tools for statistical analysis. Just know it will likely not scale to larger dimensional models because of the aforementioned reasons.

https://www.statsmodels.org/stable/regression.html

A basic technique machine learning practioners will use to mitigate overfitting is a practice called the **train/test split**, where typically 1/3 of the data is set aside for testing and the other 2/3 is used for training (other ratios can be used as well). The **training dataset** is used to fit the linear regression, while the **testing dataset** is used to measure the linear regression's performance on data it has not seen before. This technique is generally used for all supervised machine learning including logistic regression and neural networks. Figure 5-17 shows a visalization of how we break up our data into 2/3 for training and 1/3 for testing.

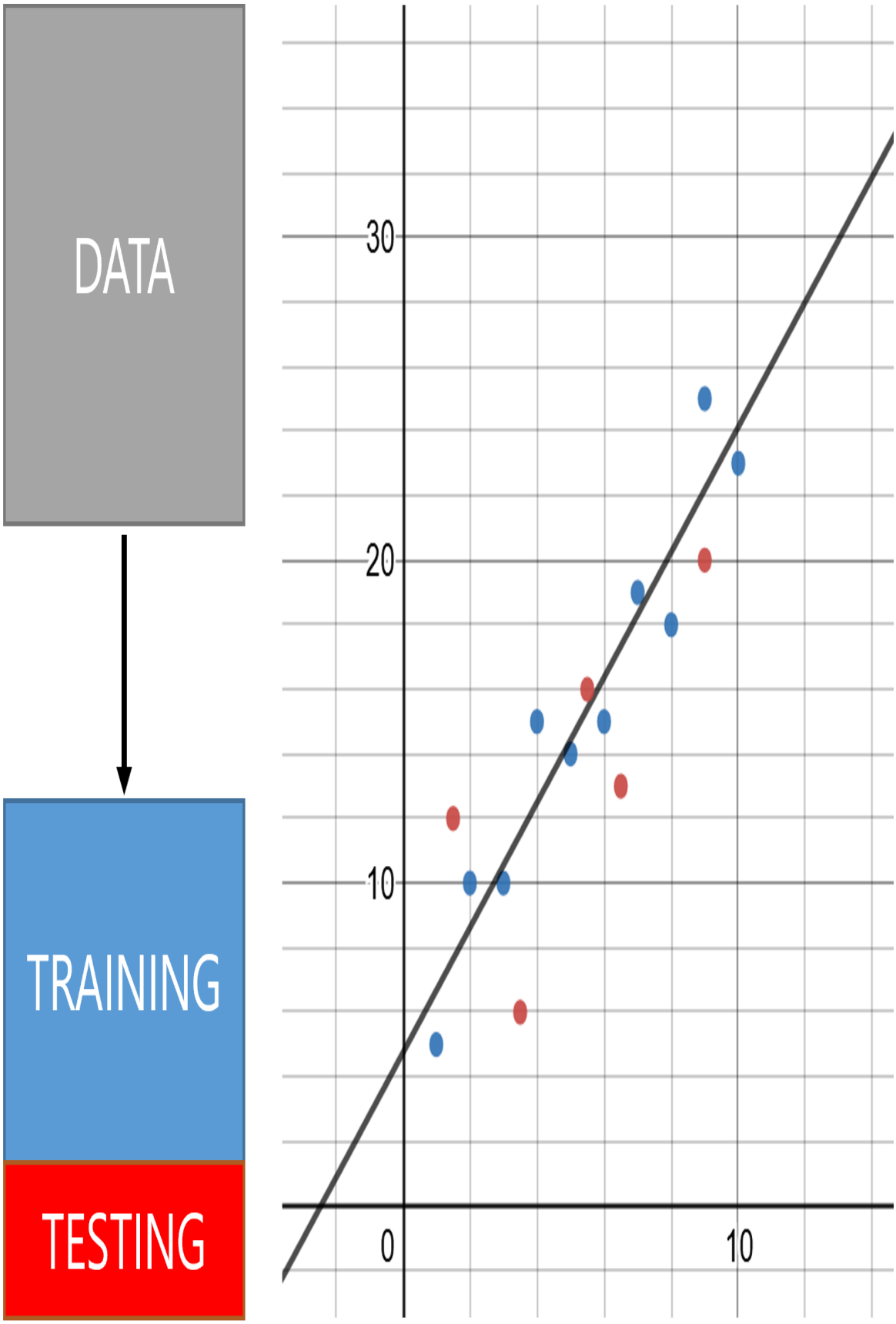

DATA
TRAINING
TESTING
30
20
10
0
10

Figure 5-17. Splitting into training/testing data. The line is fitted to the training data (blue) using least squares, while the test data (red) is analyzed afterwards to see how off the predictions are on data that was not seen before

Example 5-21 shows how to perform a train/test split using Scikit-Learn, where 1/3 of the data is set aside for testing, and the other 2/3 is used for training.

> **TRAINING IS FITTING A REGRESSION**
>
> Remember that "fitting" a regression is synonymous with "training". The latter word is used by machine learning practitioners.

Example 5-21. Doing a train/test split on linear regression

```
import pandas as pd
from sklearn.linear_model import LinearRegression
from sklearn.model_selection import train_test_split

# Load the data
df = pd.read_csv('https://bit.ly/3cIH97A', delimiter=",")

# Extract input variables (all rows, all columns but last column)
X = df.values[:, :-1]

# Extract output column (all rows, last column)
Y = df.values[:, -1]

# Separate training and testing data
# This leaves a third of the data out for testing
X_train, X_test, Y_train, Y_test = train_test_split(X, Y,
test_size=1/3)

model = LinearRegression()
model.fit(X_train, Y_train)
result = model.score(X_test, Y_test)
print("R^2: %.3f" % result)
```

Notice that the `train_test_split()` will take our dataset (*X* and *Y* columns), shuffle it, and then return our training and testing datasets based on our testing dataset size. We use the `LinearRegression`'s `fit()` function to fit on the training data `X_train` and `Y_train`. Then we use

the `score()` function on testing datasets `X_test` and `Y_test` to evalute the r^2, giving us a sense how the regression performs on data it has not seen before. The higher the r^2 is for our test dataset, the better. Having that number higher indicates the regression performs well on data it has not seen before.

USING R-SQUARE FOR TESTING

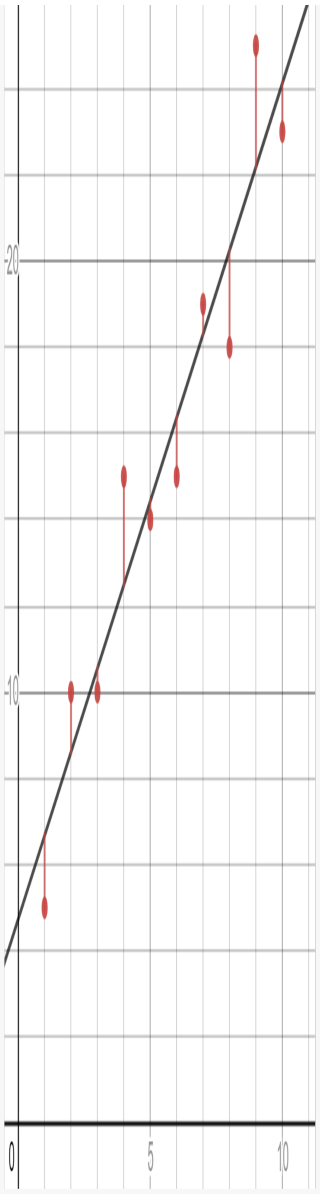
Note the r^2 is calculated a little bit different here as we have a predefined linear regression from training. We are comparing the testing data to a regression line built from training data. The objective is still the same: being closer to 1.0 is desirable to show the regression correlation is strong even with the training data, while being closer to 0.0 indicates the test dataset performs poorly. Here is how it is calculated, where y_i is each actual y-value, $\widehat{y_i}$ is each predicted y-value, and $\overline{y}$ is the average y-value for all data points.

$$r^2 = 1 - \frac{\sum \left(y_i - \widehat{y_i}\right)^2}{\sum \left(y_i - \overline{y}\right)^2}$$

Figure 5-18 shows different r^2 values from different linear regressions.

$R^2 = 1.0$

(PERFECT!)



$R^2 = 0.917$

(GOOD!)

$R^2 = 0.071$

(POOR!)

Figure 5-18. An R-square applied to different testing datasets with a trained linear regression

We can also alternate the testing dataset across each 1/3 fold. This is known as **cross-validation** and is often considered the gold standard of validation techniques. Figure 5-19 shows how each 1/3 of the data takes a turn being the testing dataset.

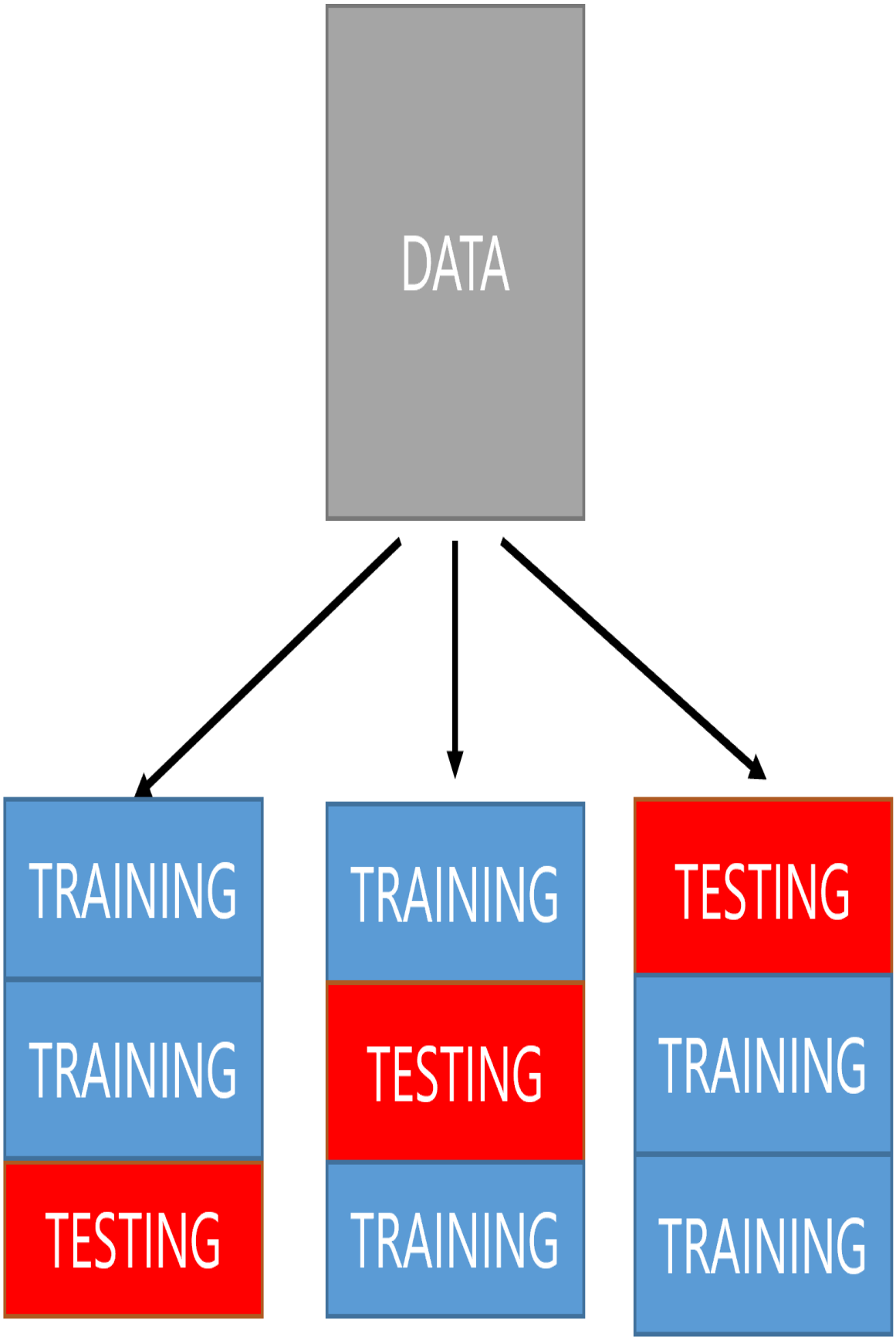

DATA
TRAINING
TRAINING
TESTING
TRAINING
TESTING
TRAINING
TESTING
TRAINING
TRAINING

Figure 5-19. A visualization of cross-validation with three folds

The code in Example 5-22 shows a cross-validation performed across three folds, and then the scoring metric (in this case the mean sum of squares (MSE)) is averaged alongside its standard deviation to show how consistently each test performed.

Example 5-22. Using 3-fold cross validation for a linear regression

```
import pandas as pd
from sklearn.linear_model import LinearRegression
from sklearn.model_selection import KFold, cross_val_score

df = pd.read_csv('https://bit.ly/3cIH97A', delimiter=",")

# Extract input variables (all rows, all columns but last column)
X = df.values[:, :-1]

# Extract output column (all rows, last column)\
Y = df.values[:, -1]

# Perform a simple linear regression
kfold = KFold(n_splits=3, random_state=7, shuffle=True)
model = LinearRegression()
results = cross_val_score(model, X, Y, cv=kfold)
print(results)
print("MSE: mean=%.3f (stdev-%.3f)" % (results.mean(),
results.std()))
```

DO TRAINING/TEST SPLITS HAVE TO BE THIRDS?

We do not have to fold our data by thirds. You can use **k-fold validation** to split on any proportion. Typically 1/3, 1/5, or 1/10 are commonly used for the proportion of test data, but 1/3 is the most common.

Generally, the *k* you choose has to result in a test dataset that has a large enough sample for the problem. You also need enough alternating/shuffled test datasets to provide a fair estimate of performance on data that was not seen before. Modestly sized datasets can use *k* values of 3, 5, or 10. **Leave-one-out-cross-validation (LOOCV)** will alternate each individual data record as the only sample in the test dataset, and this can be helpful when the whole dataset is small.

When you get concerned about variance in your model, one thing you can do is rather than doing a simple train/test split or cross-validation, you can use **random fold validation** to repeatedly shuffle and train/test split your data an unlimited number of times and aggregate the testing results. In Example 5-23 there are 10 iterations of randomly sampling a 1/3 of the data for testing and the other 2/3 for training. Those 10 testing results are then averaged alongside its standard deviation to see how consistently the test datasets perform.

What's the catch? It's computationally very expensive as we are training the regression many times.

Example 5-23. Using a random-fold validation for a linear regression

```
import pandas as pd
from sklearn.linear_model import LinearRegression
from sklearn.model_selection import cross_val_score, ShuffleSplit

df = pd.read_csv('https://bit.ly/38XwbeB', delimiter=",")

# Extract input variables (all rows, all columns but last column)
X = df.values[:, :-1]
```

```
# Extract output column (all rows, last column)\
Y = df.values[:, -1]

# Perform a simple linear regression
kfold = ShuffleSplit(n_splits=10, test_size=.33, random_state=7)
model = LinearRegression()
results = cross_val_score(model, X, Y, cv=kfold)

print(results)
print("mean=%.3f (stdev-%.3f)" % (results.mean(), results.std()))
```

So when you are crunched for time or your data is too voluminous to statstically analyze, a training/testing split is going to provide a way to measure how well your linear regression will perform on data it has not seen before.

TRAIN/TEST SPLITS ARE NOT GUARANTEES

It is important to note that just because you apply machine learning best practices of splitting your training and testing data, it does not mean your model is going to perform well. You can easily over-tune your model and p-hack your way into a good test result, only to find it does not work well out in the real-world. This is why holding out another dataset called the **validation set** is sometimes necessary, especially if you are comparing different models or configurations. That way your tweaks on the training data to get better performance on the testing data does not leak info into the training. You can use the validation dataset as one last stopgap to see if p-hacking caused you to overfit to your testing dataset.

Even then, your whole dataset (including training, testing, and validation) could have been biased to begin with, and no split is going to mitigate that. Andrew Ng discussed this as a large problem with machine learning during his Q&A with DeepLearning.AI and Stanford HAI. He walked through an example showing why machine learning has not replaced radiologists (*https://spectrum.ieee.org/andrew-ng-xrays-the-ai-hype*).

Multiple Linear Regression

We put almost exclusive focus on doing linear regression on one input variable and one output variable in this chapter. However the concepts we learned here should largely apply to multivariable linear regression. Metrics like r^2, standard error, and confidence intervals can be used but it gets harder with the more data/variables you have. Example 5-24 is an example

of a linear regression with two input variables and one output variable using Scikit-Learn.

Example 5-24. A linear regressoin with two input variables

```
import pandas as pd
from sklearn.linear_model import LinearRegression

# Load the data
df = pd.read_csv('https://bit.ly/2X1HWH7', delimiter=",")

# Extract input variables (all rows, all columns but last column)
X = df.values[:, :-1]

# Extract output column (all rows, last column)\
Y = df.values[:, -1]

# Training
fit = LinearRegression().fit(X, Y)

# Print coefficients
print("Coefficients = {0}".format(fit.coef_))
print("Intercept = {0}".format(fit.intercept_))
print("z = {0} + {1}x + {2}y".format(fit.intercept_, fit.coef_[0],
fit.coef_[1]))
```

There is a degree of precariousness when a model becomes so inundated with variables it starts to lose explainability, and this is when machine learning practices start to come in and treat the model as as black box. I hope that you are convinced statistical concerns do not go away, and data becomes increasingly sparse the more variables you add. But if you step back and analyze the relationships between each pair of variables using a correlation matrix, and seek understanding on how each pair of variables interact, it will only help your efforts creating a productive machine learning model.

Conclusions

We covered a lot in this chapter. We attempted to go beyond a cursory understanding of linear regression and making train/test splits our only validation. I wanted to show you both the scalpel (statistics) and the chainsaw (machine learning) so you can judge which is best for a given

problem you encounter. There are a lot of metrics and analysis methods available in linear regressoin alone, and we covered a number of them to understand whether a linear regression is reliable for predictions. You may find yourself in positions to do regressions fast and dirty (via machine learning) or meticulously analyze and comb your data using statistical tools. Which approach you use is situational, and if you want to learn more about statistical tools available for Python check out the `statsmodel` library.

https://www.statsmodels.org/stable/regression.html

Throughout the rest of this book I scale back on doing detailed statistical analysis of the models we create, and take a more machine-learning oriented approach using train/test splits as well as confusion matrices. In <<ch06> covering logistic regression, we will still apply the R^2 and statistical significance. But I hope that this chapter convinced you there are ways to analyze data meaningfully, and the investment can make the difference between a successful project and a rushed one.

Exercises

A dataset of two variables, *x* and *y*, is provided here: *https://bit.ly/3C8JzrM*.

1. Perform a simple linear regression to find the *m* and *b* values that minimizes the loss (sum of squares).
2. Calculate the correlation coefficient and statistical significance of this data. Is the correlation useful?
3. If I predict where `x = 50`, what is the 95% prediction interval for the predicted value of *y*?
4. Start your regression over and do a train/test split. Feel free to experiment with cross-validation and random-fold validation. Does the linear regression perform well and consistently on the testing data? Why or why not?

Chapter 6. Logistic Regression and Classification

A NOTE FOR EARLY RELEASE READERS

With Early Release ebooks, you get books in their earliest form—the author's raw and unedited content as they write—so you can take advantage of these technologies long before the official release of these titles.

This will be the 6th chapter of the final book.

If you have comments about how we might improve the content and/or examples in this book, or if you notice missing material within this chapter, please reach out to the author at *thomasnield@live.com*.

In this chapter we are going to cover **logistic regression**, a type of regression that predicts a probability of an outcome given one or more independent variables. This in turn can be used for **classification**, which is predicting categories rather than real numbers as we did with linear regression.

Logistic regression is easy to implement, and fairly resilient against outliers and other data challenges. Many machine learning problems can best be solved with logistic regression, offering more practicality and performance than other types of supervised machine learning.

Just like we did in Chapter 5 when we covered linear regression, we will attempt to walk the line between statistics and machine learning, using tools and analysis from both disciplines. Logistic regression will integrate many concepts we have learned from this book, from probability to linear regression. If you are new to these topics, it may be worth refreshing your memory by completing a few of the end of chapter exercises from earlier chapters before reading this chapter.

My suggestion here is a bit wordy, but if you feel that a working knowledge is necessary for this chapter, I think a similar cue would be helpful for your reader.

Understanding Logistic Regression

Imagine there was a small industrial accident and you are trying to understand the impact of chemical exposure. You have 11 patients that were exposed for differing numbers of hours to this chemical. Some have shown symptoms (value of *1*) and others have not shown

symptoms (value of *0*). Let's plot them in Figure 6-1, where the x-axis is hours of exposure and the y-axis is whether or not (1 or 0) they have showed symptoms.

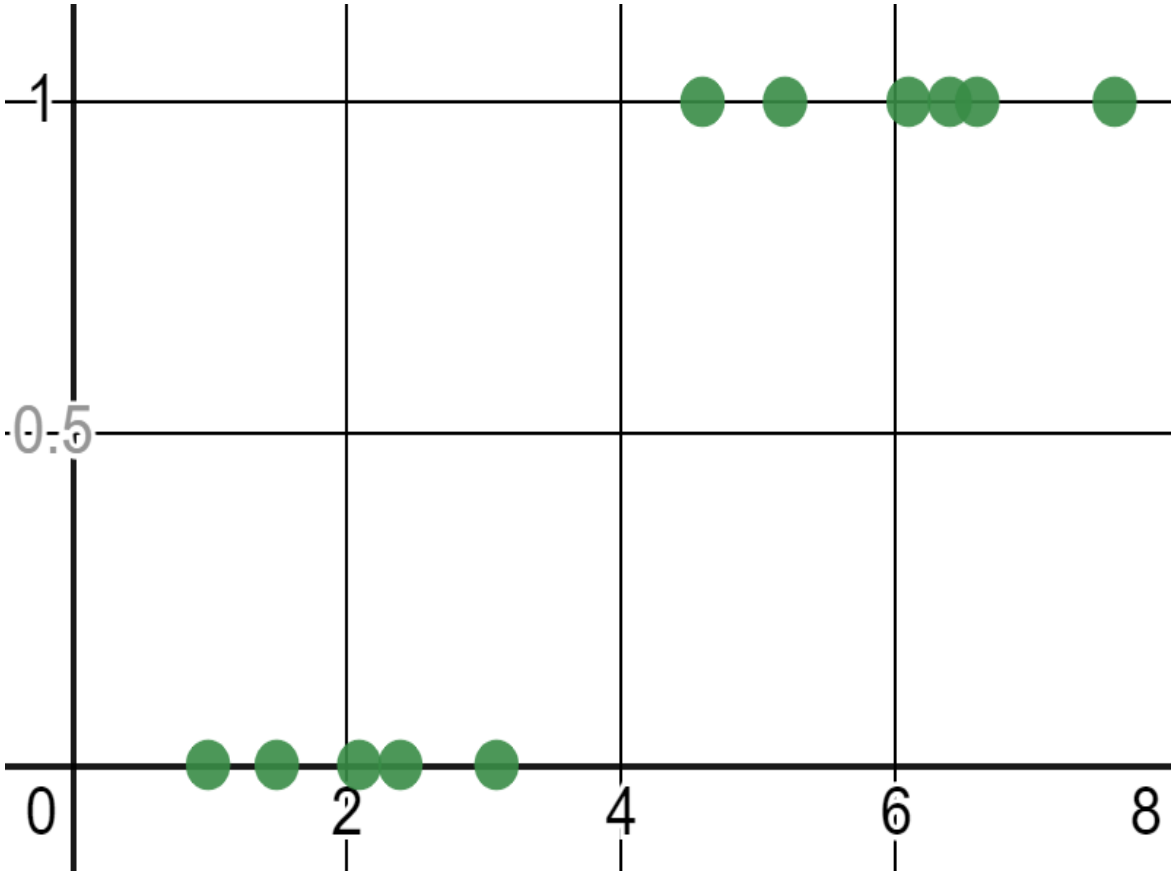


Figure 6-1. Plotting whether patients showed symptoms (1) or not (0) over x hours of exposure.

At what length of time do patients start showing symptoms? Well it is easy to see at almost distinctly 4 hours, we immediately transition from patients not showing symptoms (0) to showing symptoms (1). In Figure 6-2, we see the same data depicted with these points.

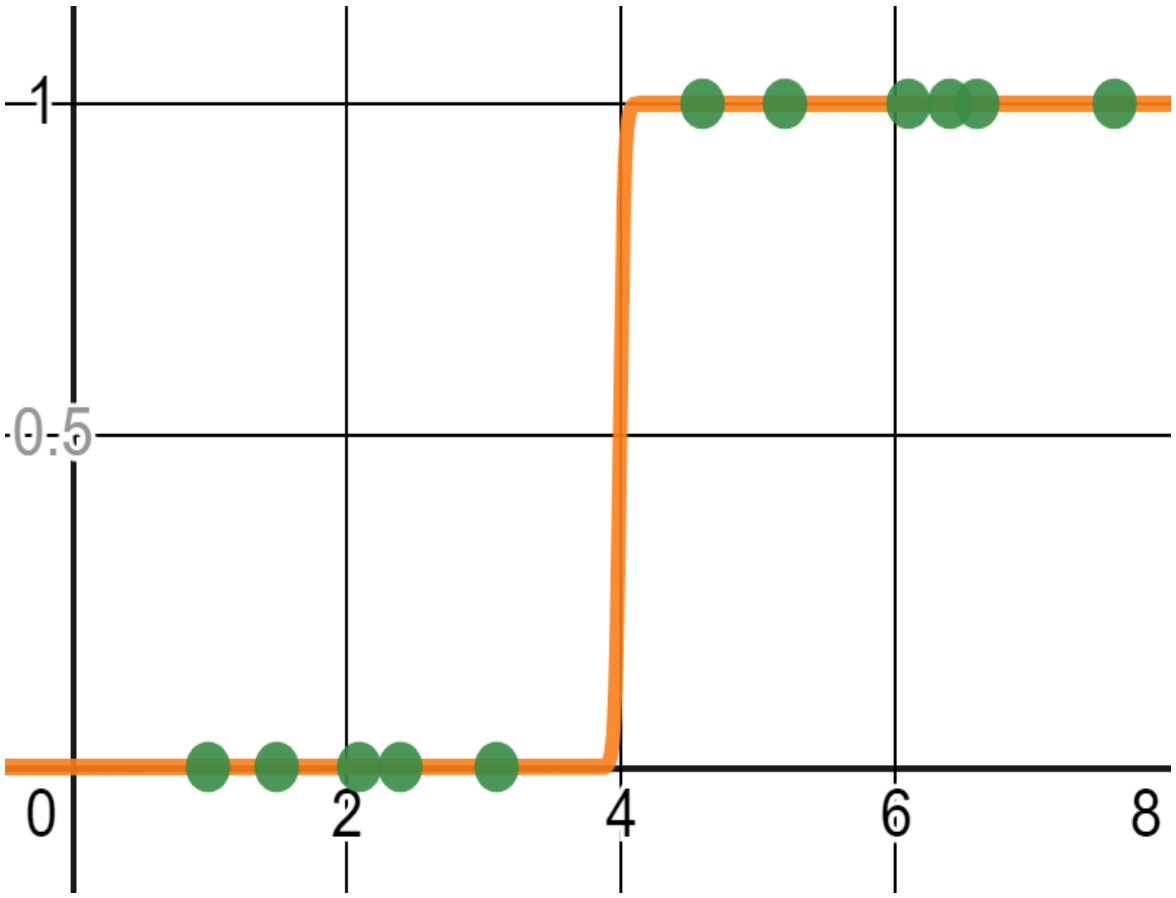


Figure 6-2. After 4 hours, we see a clear jump where patients start showing symptoms

Doing a cursory analysis on this sample, we can say that there is nearly 0% probability a patient exposed for less than 4 hours will show symptoms, but there is 100% probability for greater than 4 hours. Between these two groups, there is an immediate jump to showing symptoms at approximately 4 hours.

Of course, nothing is ever this clear-cut in the real world. Let's say you gathered more data, where the middle of the range has a mix of patients showing symptoms versus not showing symptoms as shown in Figure 6-3.

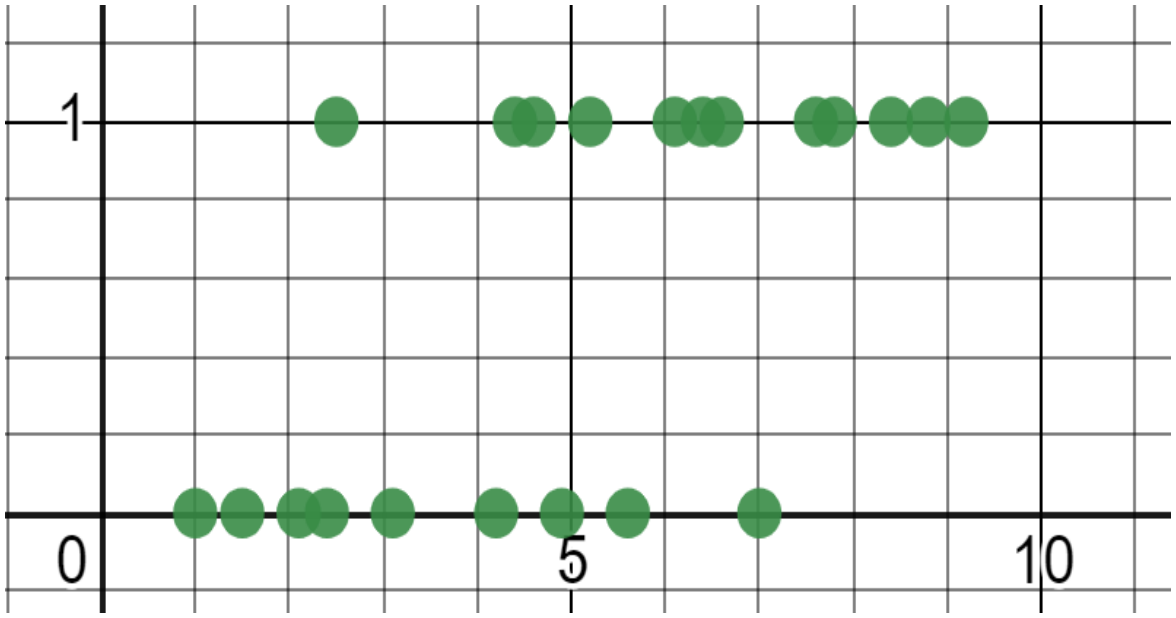


Figure 6-3. A mix of patients who show symptoms (1) and do not show symptoms (0) exist in the middle.

The way to interpret this is the probability of patients showing symptoms gradually increases with each hour of exposure. Let's visualize this with a **logistic function**, or an S-shaped curve where the output variable is squeezed between 0 and 1, as shown in Figure 6-4.

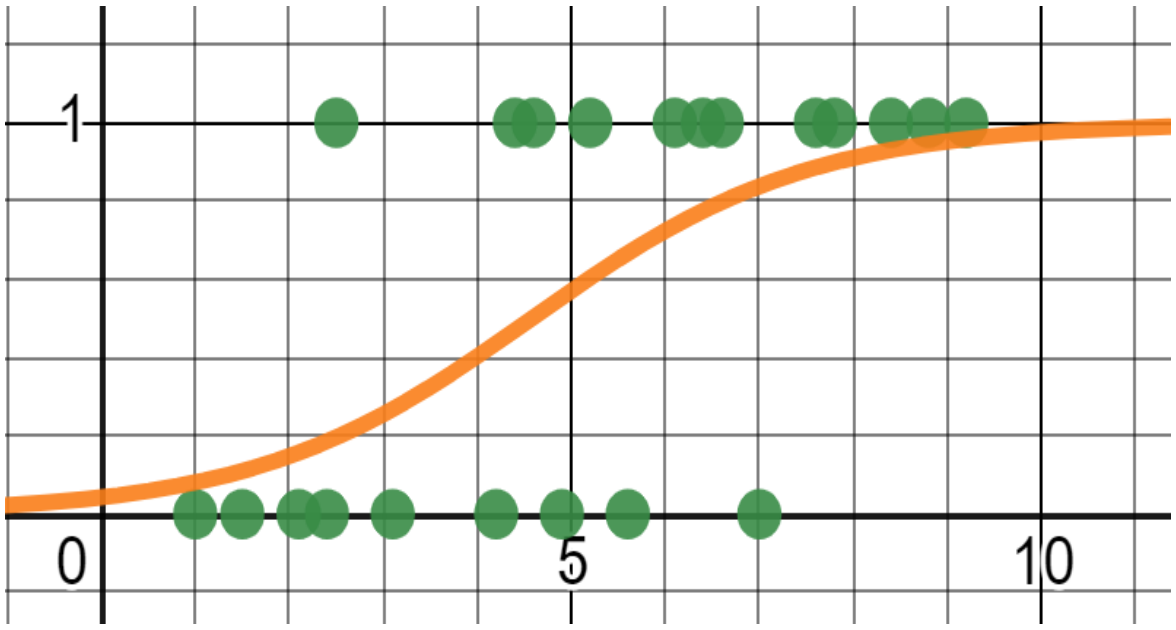


Figure 6-4. Fitting a logistic function to the data

Because of this overlap of points in the middle, there is no distinct cutoff when patients show symptoms, but rather a gradual transition from 0% probability to 100% probability ("0" and "1"). This example demonstrates how a **logistic regression** results in a curve

indicating a probability of belonging to the true category (a patient showed symptoms) across an independent variable (hours of exposure).

We can repurpose a logistic regression to not just predict a probability for given input variables, but also add a threshold to predict whether it belongs to that category. For example, if I get a new patient and find they have been exposed for 6 hours, I predict a 71.1% chance they will show symptoms as traced in Figure 6-5. If my threshold is at least 50% probability to show symptoms, I will simply classify that he will show symptoms.

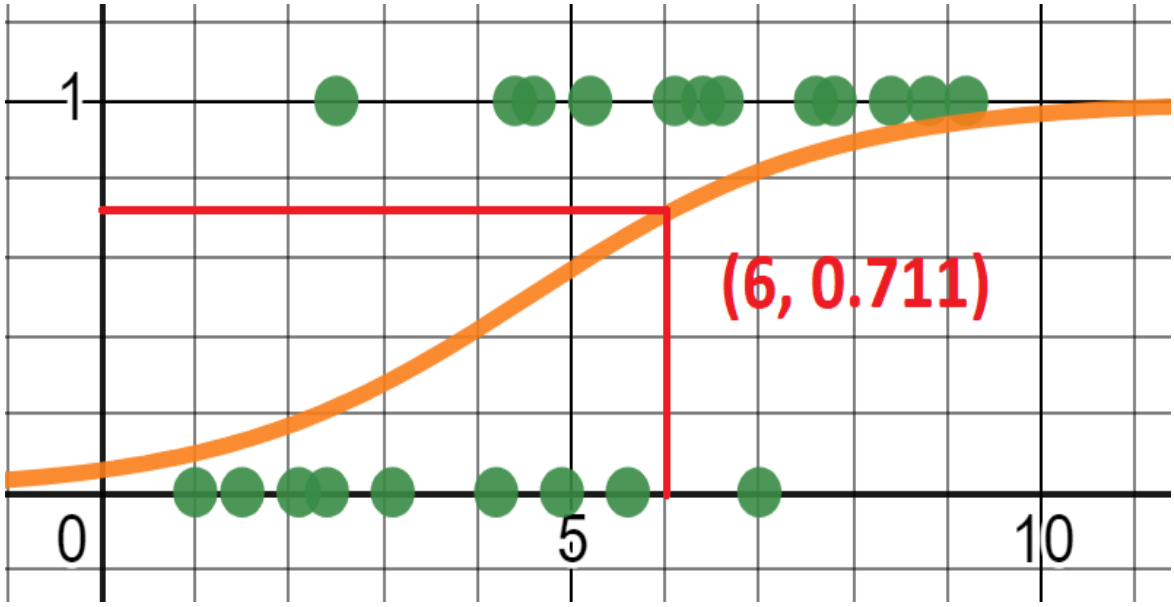


Figure 6-5. We can expect a patient exposed for 6 hours to be 71.1% likely to have symptoms, and because that's greater than a threshold of 50% we predict they will show symptoms

Performing a Logistic Regression

So how do we perform a logistic regression? Let's first take a look at the logistic function and explore the math behind it.

Logistic Function

The **logistic function** is an S-shaped curve (also known as a **sigmoid curve**) that, for a given set of input variables, produces an output variable between 0 and 1. Because the output variable is between 0 and 1 it can be used to represent a probability.

Here is the logistic function that outputs a probablity y for one input variable x.

$$y = \frac{1.0}{1.0 + e^{-(\beta_0 + \beta_1 x)}}$$

In this chapter, you may also see me express the y variable as p instead, indicating it is a probability.

$$p = \frac{1.0}{1.0 + e^{-(\beta_0 + \beta_1 x)}}$$

Note this formula uses Euler's number e which we covered in Chapter 1. The x variable is the independent/input variable. β_0 and β_1 are the coefficients we need to solve for.

β_0 and β_1 are packaged inside an exponent resembling a linear function, which you may recall looks identical to $y = mx + b$ or $y = \beta_0 + \beta_1 x$. This is not a coincidence and logistic regression actually has a close relationship to linear regression, which we will discuss later in this chapter. β_0 indeed is the intercept (which we call b in a simple linear regression) and β_1 is the slope for x (which we call m in a simple linear regression). This linear function in the exponent is known as the log-odds function, but for now just know this whole logistic function produces this S-shaped curve we need to output a shifting probability across an x value.

To declare the logistic function in Python, use the `exp()` function from the `math` package to declare the e exponent as shown in Example 6-1.

Example 6-1. The logistic function in Python for one independent variable

```
import math

def predict_probability(x, b0, b1):
    p = 1.0 / (1.0 + math.exp(-(b0 + b1 * x)))
    return p
```

Let's plot to see what it looks like, and assume $\beta_0 = -2.823$ and $\beta_1 = 0.62$. We will use SymPy in Example 6-2 and the outputted graph is shown in Figure 6-6.

Example 6-2. Using SymPy to plot a logistic function

```
from sympy import *
b0, b1, x = symbols('b0 b1 x')

p = 1.0 / (1.0 + exp(-(b0 + b1 * x)))

p = p.subs(b0,-2.823)
p = p.subs(b1, 0.620)
print(p)

plot(p)
```

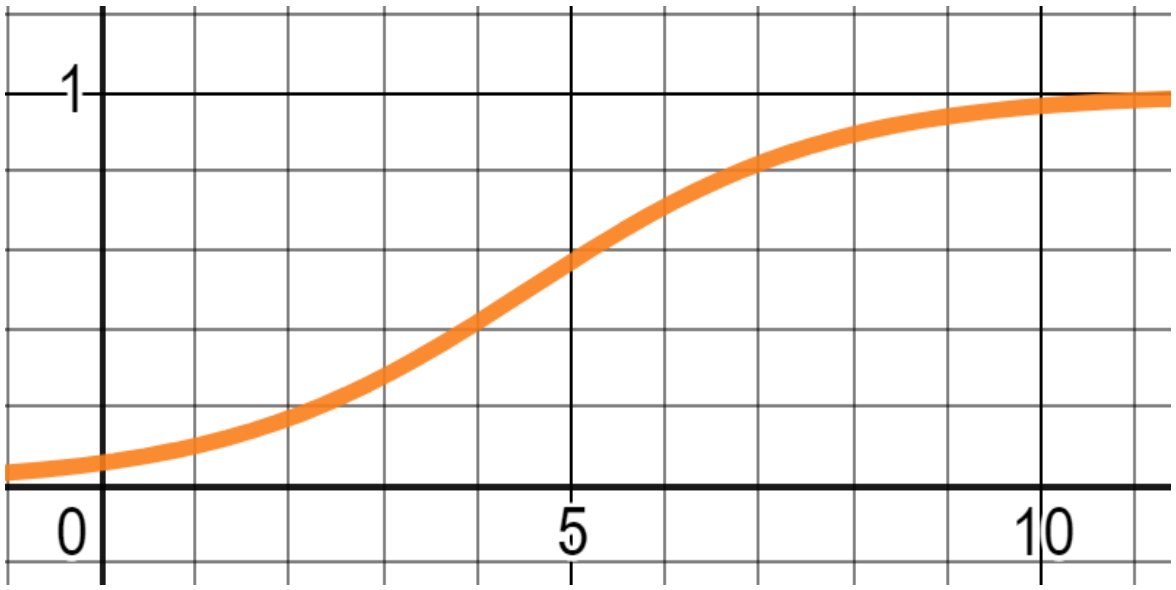


Figure 6-6. A logistic function

In some textbooks, you may alternatively see the logistic function declared like this.

$$p = \frac{e^{\beta_0+\beta_1 x}}{1 + e^{\beta_0+\beta 1 x}}$$

Do not fret about it, because it is the same function just algebraically expressed differently. Note like linear regression we can also extend logistic regression to more than one input variable ($x_1, x_2, \ldots x_n$), as shown in this formula. We just add more β_x coefficients.

$$p = \frac{1}{1 + e^{-(\beta_0+\beta_1 x_1+\beta_2 x_2+\ldots\beta_n x_n)}}$$

Fitting the Logistic Curve

How do you fit the logistic curve to a given training dataset? First, the data can have any mix of decimal, integer, and binary variables but the output variable must be binary (0 or 1). When we actually do prediction, the output variable will be 0 and 1 resembling a probability.

The data provides our input and output variable values, but we need to solve for the β_0 and β_1 coefficients to fit our logistic function. Recall how we used least squares in Chapter 5. However, this does not apply here. Instead we use **maximum likelihood estimation** which, as the name suggests, maximizes the likelihood a given logistic curve would output the observed data.

To calculate the maximum likelihood estimation, there really is no closed form equations like in linear regression. We can still use stochastic gradient descent, or have a library do it for us. Let's cover both of these approaches starting with the library SciPy.

Using SciPy

The nice thing about SciPy is the models often have a standardized set of functions and API's, meaning in many cases you can copy/paste your code and can then reuse it between models. In Example 6-3 you will see a logistic regression performed on our patient data. If you compare it to our linear regression code in Chapter 5, you will see it has nearly identical code in importing, separating, and fitting our data. The main difference is I use a `LogistricRegression()` for my model instead of a `LinearRegression()`.

Example 6-3. Using a plain logistic regression SciPy

```
import pandas as pd
from sklearn.linear_model import LogisticRegression

# Load the data
df = pd.read_csv('https://bit.ly/33ebs2R', delimiter=",")

# Extract input variables (all rows, all columns but last column)
X = df.values[:, :-1]

# Extract output column (all rows, last column)
Y = df.values[:, -1]

# Perform logistic regression
# Turn off penalty
model = LogisticRegression(penalty='none')
model.fit(X, Y)

# print beta1
print(model.coef_.flatten()) # 0.69267212

# print beta0
print(model.intercept_.flatten()) # -3.17576395
```

> **MAKING PREDICTIONS**
>
> To make specific predictions, use the `predict()` and `predict_prob()` functions on the `model` object in ScipPy, regardless if it is a `LogisticRegression` or any other type of classification model. The `predict()` function will predict a specific class (e.g. True 1.0 or False 1.0) while the `predict_prob()` will output probabilities for each class.

After running the model in SciPy, I get a logistic regression where $\beta_0 = -3.17576395$ and $\beta_1 = 0.69267212$. When I plot this it should look pretty good as shown in Figure 6-7.

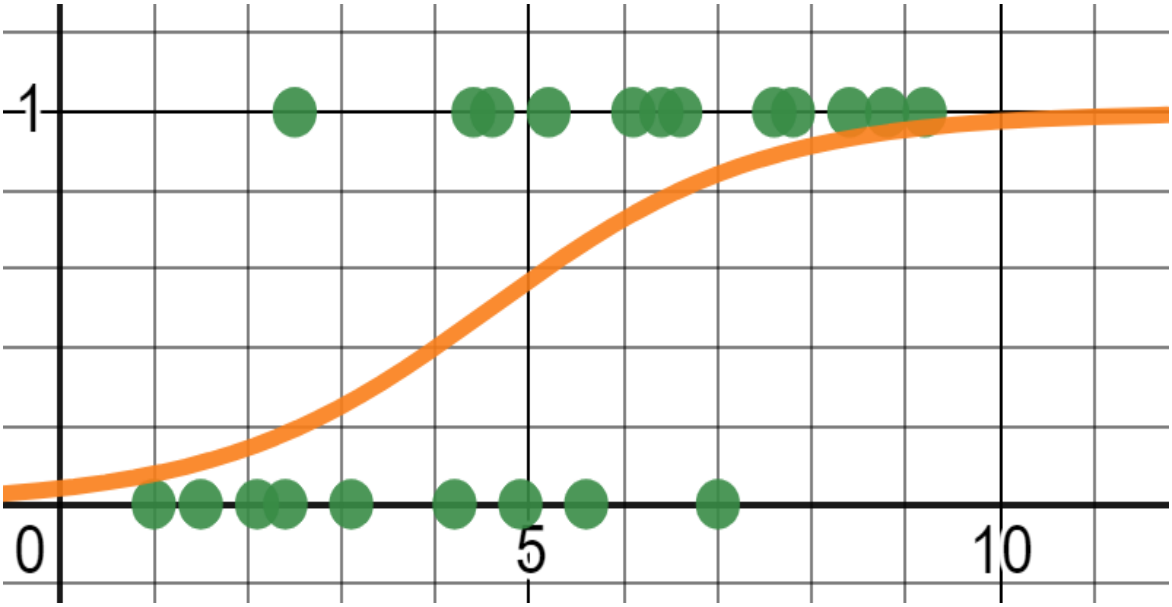


Figure 6-7. Plotting the Scikit-Learn logistic regression

There are a couple of things to note here. When I created the `LogisticRegression()` model, I specified no `penalty` argument which chooses a regularization technique like `l1` or `l2`. While this is beyond the scope of this book, I have included brief insights in the Learning about SciPy Parameters box so that you have helpful references on hand.

DESMOS GRAPH FOR LOGISTIC REGRESSION

While Python plotting libraries can get the job done with visualizations, I used Desmos quite a bit in this chapter. You can find the Desmos graph for this logistic regression here. Feel free to play with it!

https://www.desmos.com/calculator/uilb8gyqwj

Finally I am going to `flatten()` the coefficient and intercept which come out as multidimensional matrices but with one element. Flattening means collapsing a matrix of numbers into lesser dimensions, particularly when there are fewer elements than there are dimensions. For example, I use `flattent()` here to take a single number nested into a 2-dimensional matrix, and pull it out as a single value. I then have my β_0 and β_1 coefficients.

LEARNING ABOUT SCIPY PARAMETERS

SciPy offers a lot of options in its regresssion and classification models. Unfortunately there is not enough bandwidth or pages to cover them as this is not a book focusing exclusively on machine learning.

However the SciPy docs are well-written and the page on logistic regression is found here.

https://scikit-learn.org/stable/modules/generated/sklearn.linear_model.LogisticRegression.html

If a lot of terms are unfamiliar, such as regularization and `l1` and `l2` penalties, there are other great O'Reilly books exploring these topics. One of the more helpful texts I have found is **Hands-On Machine Learning with Scikit-Learn, Keras, and TensorFlow** by Aurélien Géron.

https://learning.oreilly.com/library/view/hands-on-machine-learning/9781492032632/

Regarding regularization, including L1 and L2, Josh Starmer has two great videos.

https://www.youtube.com/watch?v=Q81RR3yKn30

https://www.youtube.com/watch?v=NGf0voTMlcs

Using Maximum Likelihood and Gradient Descent

As we have done throughout this book, I aim to provide insights on building techniques from scratch even if libraries can do it for us. To fit a logistic regression ourselves, there are several ways but all methods typically turn to maximum likelihood estimation (MLE). MLE maximizes the likelihood a given logistic curve would output the observed data. It is different than sum of squares, but we can still apply gradient descent or stochastic gradient descent to solve it.

I'll try to streamline the mathematical jargon and minimize the linear algebra here. Essentially the idea is to find the β_0 and β_1 coefficients that brings our logistic curve to those points as closely as possible, indicating it is most likely to have produced those points. If you recall in Chapter 2 when we studied probability, we combine probabilities (or likelihoods) of multiple events by multiplying them together. In this application, we are calculating the likelihood we would see all these points for a given logistic regression curve.

Applying the idea of joint probabilities, each patient has a likelihood they would show symptoms *based on the fitted logistic function* as shown in Figure 6-8.

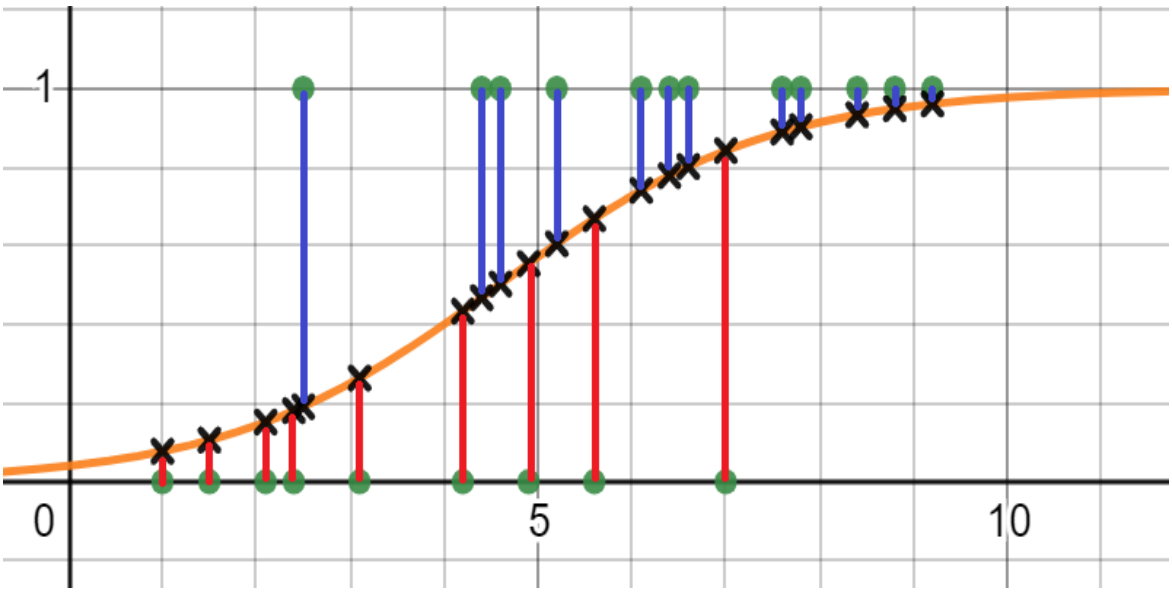


Figure 6-8. Every input value has a corresponding likelihood on the logistic curve

We fetch each likelihood off the logistic regression curve above or below each point. If the point is below the logistic regression curve, we need to subtract the resulting probability from 1.0 because we want to maximize the false cases too.

Given coefficients $\beta_0 = -3.17576395$ and $\beta_1 = 0.69267212$, Example 6-4 shows how we calculate the joint likelihood for this data in Python.

Example 6-4. Calculating the joint likelihood of observing all the points for a given logistic regression

```
import math
import pandas as pd

patient_data = pd.read_csv('https://bit.ly/33ebs2R', delimiter=",").itertuples()

b0 = -3.17576395
b1 = 0.69267212

def logistic_function(x):
    p = 1.0 / (1.0 + math.exp(-(b0 + b1 * x)))
    return p

# Calculate the joint likelihood
joint_likelihood = 1.0

for p in patient_data:
    if p.y == 1.0:
        joint_likelihood *= logistic_function(p.x)
    elif p.y == 0.0:
        joint_likelihood *= (1.0 - logistic_function(p.x))

print(joint_likelihood) # 4.7911180221699105e-05
```

Here's a mathematical trick we can do to compress that `if` expression. When you set any number to the power of 0, it will always be 1. Take a look at this formula and note the handling of true (1) and false (0) cases in the exponents.

$$\text{joint likelihood} = \prod_{i=1}^{n} \left(\frac{1.0}{1.0 + e^{-(\beta_0 + \beta_1 x_i)}} \right)^{y_i} \times \left(\frac{1.0}{1.0 + e^{-(\beta_0 + \beta_1 x_i)}} \right)^{1.0 - y_i}$$

To do this in Python, compress everything inside that for `for` loop into Example 6-5:

Example 6-5. Compressing the joint likelihood calculation without an `if` expression

```
for p in patient_data:
    joint_likelihood *= logistic_function(p.x) ** p.y * \
                        (1.0 - logistic_function(p.x)) ** (1.0 - p.y)
```

What exactly did I do? Notice that there are two halves to this expression, one for when $y = 1$ and the other where $y = 0$. When any number is raised to exponent *0* it will result in *1*. Therefore, whether *y* is `1` or `0` it will cause the opposite condition on the other side to evaluate to *1* and have no effect. We get to express our `if` expression but do it completely in a mathematical expression. We cannot do derivatives on expressions that use `if`, so this will be helpful.

Note that computers can get overwhelmed multiplying several small decimals together, known as **floating point underflow**. This means that as decimals get smaller and smaller, which can happen in multiplication, the computer runs into limitations keeping track of that many decimal places. Joel Grus' O'Reilly book *Data Science From Scratch* shares a clever mathematical hack to get around this. You can take the `log()` of each decimal you are mulitiplying, and instead add them together. This is thanks to the additive properties of logarithms we covered in Chapter 1. You can then call the `exp()` function to convert the total sum back to get the product.

Let's revise our code to use logarithmic addition instead of multiplication. Note that the `log()` function will default to base *e* and while any base technically works, this is preferable because e^x is the derivative of itself and will computationally be more efficient.

Example 6-6. Using logarithmic addition

```
# Calculate the joint likelihood
joint_likelihood = 0.0

for p in patient_data:
    joint_likelihood += math.log(logistic_function(p.x) ** p.y * \
                                 (1.0 - logistic_function(p.x)) ** (1.0 - p.y))

joint_likelihood = math.exp(joint_likelihood)
```

To express the Python code above in proper mathematical notation, here is the expression.

$$\text{joint likelihood} = \sum_{i=1}^{n} log\left(\left(\frac{1.0}{1.0 + e^{-(\beta_0 + \beta_1 x_i)}}\right)^{y_i} \times \left(1.0 - \frac{1.0}{1.0 + e^{-(\beta_0 + \beta_1 x_i)}}\right)^{1.0 - y_i}\right)$$

Would you like to calculate the partial derivatives for β_0 and β_1 in the above expression? I didn't think so. It's a beast. Goodness, expressing that function in SymPy alone is a mouthful! Look at this in Example 6-7.

Example 6-7. Expressing a joint likelihood for logistic regression in SymPy

```
joint_likelihood = Sum(log((1.0 / (1.0 + exp(-(b + m * x(i)))))**y(i) * \
        (1.0 - (1.0 / (1.0 + exp(-(b + m * x(i))))))**(1-y(i))), (i, 0, n))
```

So let's just let SymPy do the partial derivatives for us, for β_0 and β_1 respectively. We will then immediately compile and use them for gradient decsent, as shown in Example 6-8.

Example 6-8. Using Gradient Descent on Logistic Regression

```
from sympy import *
import pandas as pd

points = list(pd.read_csv("https://tinyurl.com/y2cocoo7").itertuples())

b1, b0, i, n = symbols('b1 b0 i n')
x, y = symbols('x y', cls=Function)
joint_likelihood = Sum(log((1.0 / (1.0 + exp(-(b0 + b1 * x(i))))) ** y(i) \
        * (1.0 - (1.0 / (1.0 + exp(-(b0 + b1 * x(i)))))) ** (1 - y(i))), (i, 0,
n))

# Partial derivative for m, with points substituted
d_b1 = diff(joint_likelihood, b1) \
                   .subs(n, len(points) - 1).doit() \
                   .replace(x, lambda i: points[i].x) \
                   .replace(y, lambda i: points[i].y)

# Partial derivative for m, with points substituted
d_b0 = diff(joint_likelihood, b0) \
                   .subs(n, len(points) - 1).doit() \
                   .replace(x, lambda i: points[i].x) \
                   .replace(y, lambda i: points[i].y)

# compile using lambdify for faster computation
d_b1 = lambdify([b1, b0], d_b1)
d_b0 = lambdify([b1, b0], d_b0)

# Perform Gradient Descent
b1 = 0.01
b0 = 0.01
L = .01

for j in range(10_000):
    b1 += d_b1(b1, b0) * L
    b0 += d_b0(b1, b0) * L

print(b1, b0)
# 0.6926693075370812 -3.175751550409821
```

After calculating the partial derivatives for β_0 and β_1, we substitute the x and y values as well as the number of data points n. Then we use `lambdify()` to compile the derivative function for efficiency (it uses NumPy behind-the-scenes). After that we perform gradient descent like we did in Chapter 5, but since we are trying to maximize rather than minimize, we add each adjustment to β_0 and β_1 rather than subtract like in least squares.

As you can see in Example 6-8, we got $\beta_0 = -3.175751550409821$ and $\beta_1 = 0.6926693075370812$. This is highly comparable to the coefficient values we got in SciPy earlier.

As we learned to do in Chapter 5, we can also utilize stochastic gradient descent and only sample one or a handful of records on each iteration. This would extend the benefits of increasing computational speed and performance as well as prevent overfitting. It would be redundant to cover it again here, so we will keep moving on.

Multivariable Logistic Regression

Let's try an example that uses logistic regression on multiple input variables. Here's a sample of a few records from a dataset containing some employment retention data (full dataset is here: *https://bit.ly/3aqsOMO)*.

SEX	AGE	PROMOTIONS	YEARS_EMPLOYED	DID_QUIT
1	32	3	7	0
1	34	2	5	0
1	29	2	5	1
0	42	4	10	0
1	43	4	10	0

Figure 6-9. Sample of employment retention data

There are 54 records in this dataset. Let's say we want to use it to predict whether other employees are going to quit. Logistic regression can achieve this. Recall we can support more than one input variable as shown in this formula.

$$y = \frac{1}{1 + e^{-(\beta_0 + \beta_1 x_1 + \beta_2 x_2 + ... \beta_n x_n)}}$$

I will create β coefficients for each of the variables `sex`, `age`, `promotions` and `years_employed`. The output variable `did_quit` is binary, and that is going to drive the logistic regression outcome we are predicting. Because we are dealing with multiple

dimensions, it is going to be hard to visualize the curvy hyperplane that is our logistic curve. So we will steer clear from visualization.

Let's make it interesting. We will use Scikit-Learn but make an interactive shell we can test new employees with. Here is the code in Example 6-9 and when we run it, a logistic regression will be performed and then we can type in new employees to predict whether they quit or not. What can go wrong? I am sure nothing. We are only making predictions on people's personal attributes and making decisions accordingly. I'm sure it will be fine.

(**if it was not clear, I'm being very tongue-in-cheek**).

Example 6-9. Doing a multivariable logistic regression on employee data

```
import pandas as pd
from sklearn.linear_model import LogisticRegression

employee_data = pd.read_csv("https://tinyurl.com/y6r7qjrp")

# grab independent variable columns
inputs = employee_data.iloc[:, :-1]

# grab dependent "did_quit" variable column
output = employee_data.iloc[:, -1]

# build logistic regression
fit = LogisticRegression(penalty='none').fit(inputs, output)

# Print coefficients:
print("COEFFICIENTS: {0}".format(fit.coef_.flatten()))
print("INTERCEPT: {0}".format(fit.intercept_.flatten()))

# Interact and test with new employee data
def predict_employee_will_stay(sex, age, promotions, years_employed):
    prediction = fit.predict([[sex, age, promotions, years_employed]])
    probabilities = fit.predict_proba([[sex, age, promotions, years_employed]])
    if prediction == [[1]]:
        return "WILL LEAVE: {0}".format(probabilities)
    else:
        return "WILL STAY: {0}".format(probabilities)

# Test a prediction
while True:
    n = input("Predict employee will stay or leave {sex},{age},{promotions},{years
employed}: ")
    (sex, age, promotions, years_employed) = n.split(",")
    print(predict_employee_will_stay(int(sex), int(age), int(promotions),
int(years_employed)))
```

Figure 6-10 is a screenshot of my Python shell in PyCharm, testing a given employee to see if they are predicted to quit. The employee is a sex "1", age is 34, had 1 promotion, and has been at the company for 5 years. Sure enough the prediction is "WILL LEAVE".

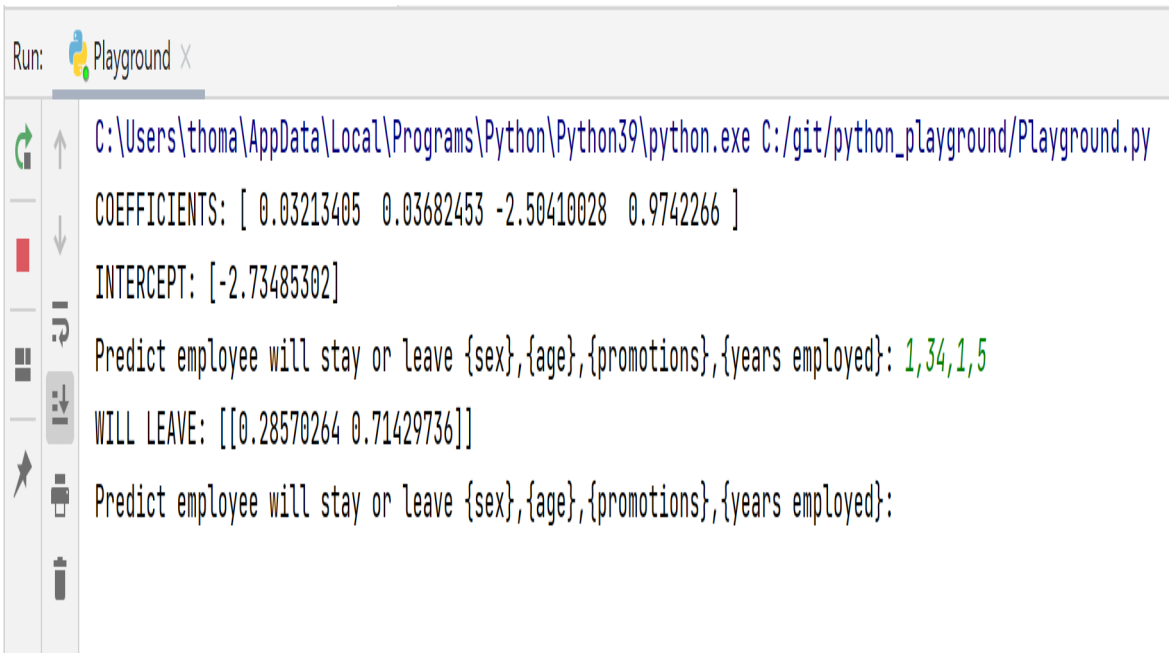


Figure 6-10. Making a prediction whether a 34-year-old employee with 1 promotion and 5 years employment will quit

Note that the `predict_proba()` function will output two values, the first being the probability of 0 (false) and the second being 1 (true).

You will notice that in the coefficients for `sex`, `age`, `promotions`, and `years employed` are displayed in that order. By the weight of the coefficients, you can see that `sex` and `age` play very little role in the prediction (they both have a weight near 0). However `promotions` and `years_employed` have significant weights of `-2.504` and `.97`. Here's a secret with this toy dataset: I fabricated it so that an employee quits if they do not get a promotion roughly every 2 years. Sure enough my logistic regression picked up this pattern and you can try it out with other employees as well.

Of course, real life is not always this clean. An employee who has been at a company for 8 years and never got a promotion is likely comfortable with their role and not leave anytime soon. If that is the case, variables like age then might play a role and get weighted. Then of course, we can get concerned about other relevant variables that are not being captured. See the warning callout *Be Careful Making Classifications on People!* to learn more.

BE CAREFUL MAKING CLASSIFICATIONS ON PEOPLE!

A quick and surefire way to shoot yourself in the foot is to collect data on people and use it to make predictions haphazardly. Not only can data privacy concerns come about, but legal and PR issues can emerge if the model is found to be discriminatory. Input variables like race and gender can become weighted from ML training. After that, undesirable outcomes are inflicted on those demographics like not being hired or being denied loans. More extreme applications include being falsely flagged by surveillance systems or being denied criminal parole. Note too that seemingly benign variables like commute time have been found to correlate with discriminatory variables.

At the time of writing, a number of articles have been citing machine learning discrimination as an issue.

https://www.theregister.com/2021/07/16/facial_recognition_failure/

https://www.nytimes.com/2020/06/24/technology/facial-recognition-arrest.html

As data privacy laws continue to evolve, it is advisable to err on the side of caution and engineer personal data carefully. Think about what automated decisions will be propagated and how that can cause harm.

Finally on this employee retention example, think about where this data came from. Over what period of time did this sample come from? How far back do we go looking for employees who quit? What constitutes an employee who stayed? Are they current employees at this point in time? How do we know they are not about to quit, making them a false negative? Data scientists easily fall into traps only analyzing what data says, but not questioning where it came from.

The best way to get answers to these questions is understand what the predictions are being used for. Is it to decide when to give people promotions to retain them? Can this create a circular bias promoting people with a set of attributes? Will that bias be re-affirmed when those promotions start becoming the new training data?

These are all important questions, and perhaps even inconvenient ones that cause unwanted scope creep into the project. If scrutiny is not welcome by your team or leadership on a project, consider how a misguided project will impact your career. In this case, you might be more empowered in a different role where curiosity is an asset.

Understanding the Log-Odds

At this point, it is time to discuss the logistic regression and what it is mathematically made of. This can be a bit dizzying so take your time here. If you get overwhelmed you can always revisit this section later.

Starting in the 1900's, it has always been an interest to mathematicians to take a linear function and scale its output to fall between 0 and 1, and therefore be useful for predicting probability. The log-odds, also called the logit function, lends itself to logistic regression for this purpose.

Remember earlier I pointed out the exponent value $\beta_0 + \beta_1 x$ is a linear function? Look below at our logistic function again:

$$p = \frac{1.0}{1.0 + e^{-(\beta_0 + \beta_1 x)}}$$

This linear function being raised to *e* is known as the **log-odds** function, which takes the logarithm of the odds for the event of interest. Your response might be "Wait, I don't see any `log()` or odds. I just see a linear function!" Bear with me, I will show the hidden math.

As an example, let's use our logistic regression from earlier where $\beta_0 = -3.17576395$ and $\beta_1 = 0.69267212$. What is the probability of showing symptoms after 6 hours, where $x = 6$? We already know how to do this: plug these values into our logistic function.

$$p = \frac{1.0}{1.0 + e^{-(-3.17576395 + 0.69267212(6))}} = 0.727161542928554$$

We plug in these values and output a probability of .72716. But let's look at this from an odds perspective. Recall in Chapter 2 we learned how to calculate odds from a probability:

$$\text{odds} = \frac{p}{1 - p}$$

$$\text{odds} = \frac{.72716}{1 - .72716} = 2.66517246407876$$

So at 6 hours, a patient is 2.66517 times more likely to show symptoms than not show symptoms.

When we wrap the odds function in a natural logarithm (a logarithm with base *e*), we call this the **logit function**. The output of this formula is what we call the **log-odds**, named… shockingly… because we take the logarithm of the odds.

$$\text{logit} = log\left(\frac{p}{1 - p}\right)$$

$$\text{logit} = log\left(\frac{.72716}{1 - .72716}\right) = 0.98026877$$

Our log-odds at 6 hours is 0.9802687. What does this mean and why do we care? When we are in "log-odds land" it is easier to compare one set of odds against another. We treat anything greater than 0 as favoring odds an event will happen, whereas anything less than 0 is against an event. A log-odds of -1.05 is linearly the same distance from 0 as 1.05. In plain odds though, the equivalents are .3499 and 2.857 respectively, which is not as interpretable. That is the convenience of log-odds.

ODDS AND LOGS

Logarithms and odds have an interesting relationship. Odds are against an event when it is between 0.0 and 1.0, but anything greater than 1.0 favors the event and extends into positive infinity. This lack of symmetry is awkward. However, logarithms rescale an odds so that it is completely linear, where a log-odds of 0.0 means fair odds. A log-odds of -1.05 is linearly the same distance from 0 as 1.05, and thus make comparing odds much easier.

Josh Starmer has a great video talking about this relationship between odds and logs here:

https://www.youtube.com/watch?v=ARfXDSkQf1Y

Recall I said the linear function in our logistic regression formula $\beta_0 + \beta_1 x$ is our log-odds function. Check this out:

$$\log\ \text{odds} = \beta_0 + \beta_1 x$$

$$\log\ \text{odds} = -3.17576395 + 0.69267212(6)$$

$$\log\ \text{odds} = 0.98026877$$

It's the same value 0.98026877 as our previous calculation, the odds of our logistic regression at x = 6 and then taking the `log()` of it! So what is the link? What ties all this together? Given a probability from a logistic regression *p* and input variable *x*, it is this:

$$log\left(\frac{p}{1-p}\right) = \beta_0 + \beta_1 x$$

Let's plot the log-odds line alongside the logistic regression, as shown in Figure 6-11.

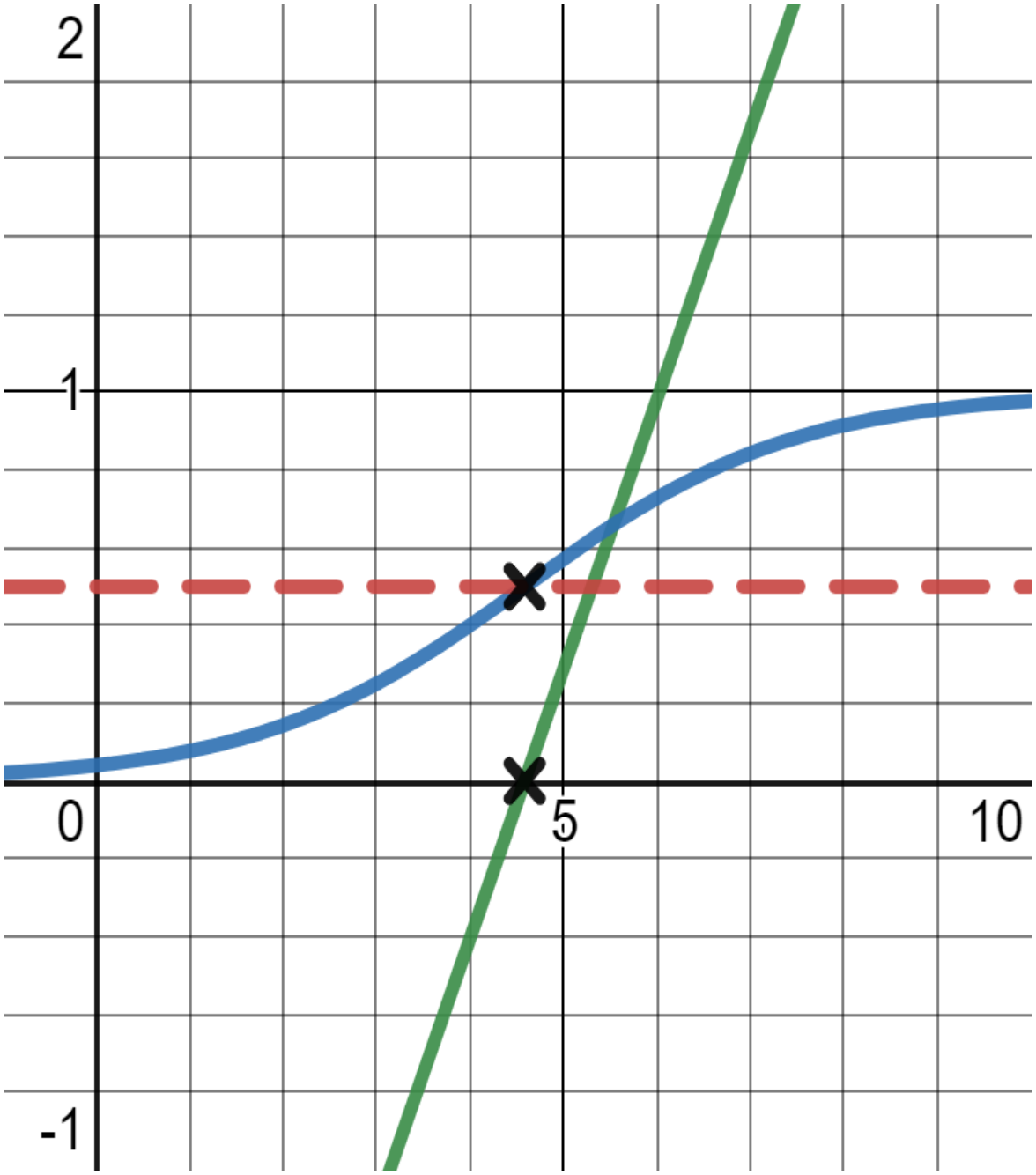


Figure 6-11. The log-odds line is converted into a logistic function that outputs a probability. Graph is available here: https://www.desmos.com/calculator/y29ujzvwc1

Every logistic regression is actually a linear function behinds the scenes, and that linear function is a log-odds function. Note in Figure 6-11 that when the log-odds is 0.0 on the line, then the probability of the logistic curve is at 0.5. This makes sense because when our odds are fair at 1.0, the probability is going to be 0.50 as shown in the logistic regression, and the log-odds are going to be 0 as shown by the line.

Another benefit we get looking at the logistic regression from an odds perspective is we can compare the effect between one x value and another. Let's say I want to understand how much my odds change between 6 hours and 8 hours of exposure to the chemical. I can take the odds at 6 hours and then 8 hours, and then ratio the two odds against each other in an **odds ratio**. This is not to be confused with a plain odds which, yes is a ratio, but it is not an odds ratio.

Let's first find the probabilities of symptoms for 6 hours and 8 hours respectively.

$$p = \frac{1.0}{1.0 + e^{-(\beta_0 + \beta_1 x)}}$$

$$p_6 = \frac{1.0}{1.0 + e^{-(-3.17576395 + 0.69267212(6))}} = 0.727161542928554$$

$$p_8 = \frac{1.0}{1.0 + e^{-(-3.17576395 + 0.69267212(8))}} = 0.914167258137741$$

Now let's convert those into odds, which we will declare as o_x .

$$o = \frac{p}{1 - p}$$

$$o_6 = \frac{0.727161542928554}{1 - 0.727161542928554} = 2.66517246407876$$

$$o_8 = \frac{0.914167258137741}{1 - 0.914167258137741} = 10.6505657200694$$

Finally, set the two odds against each other as an odds ratio, where the odds for 8 hours is the numerator and the odds for 6 hours is in the denominator. We get a value of approximately 3.996, meaning that our odds of showing symptoms increases by nearly a factor of 4 with an extra 2 hours of exposure.

$$\text{odds ratio} = \frac{10.6505657200694}{2.66517246407876} = 3.99620132040906$$

You will find this odds ratio value of 3.996 holds across any two hour range, like 2 hours to 4 hours, 4 hours to 6 hours, 8 hours to 10 hours… etc. As long as its a 2-hour gap you will find that odds ratio stays consistent. It will differ for other range lengths.

R-Squared

We covered quite a few statistical metrics for linear regression in Chapter 5, and we will try to do the same for logistic regression. We still worry about many of the same problems as in linear regression, including overfitting and variance. As a matter of fact, we can borrow and

adapt several metrics from linear regression and apply them to logistic regression. Let's start with R^2.

Just like linear regression, there is an R^2 for a given logistic regression. If you recall from Chapter 5, the R^2 indicates how well a given independent variable explains a dependent variable. Applying this to our chemical exposure problem, it makes sense we want to measure how much chemical exposure hours explains showing symptoms.

There is not really a consensus on the best way to calculate the R^2 on a logistic regression, but a popular technique known as McFadden's Pseudo R^2 closely mimics the R^2 used in linear regression. We will use this technique in the following examples and here is the formula:

$$R^2 = \frac{(\log\ \text{likelihood}) - (\log\ \text{likelihood fit})}{(\log\ \text{likelihood})}$$

We will learn how to calculate the "log likelihood fit" and "log likelihood" so we can calculate the R^2.

We cannot use residuals here like in linear regression, but we can project the outcomes back onto the logistic curve as shown in Figure 6-12, and look up their corresponding likelihoods between 0.0 and 1.0.

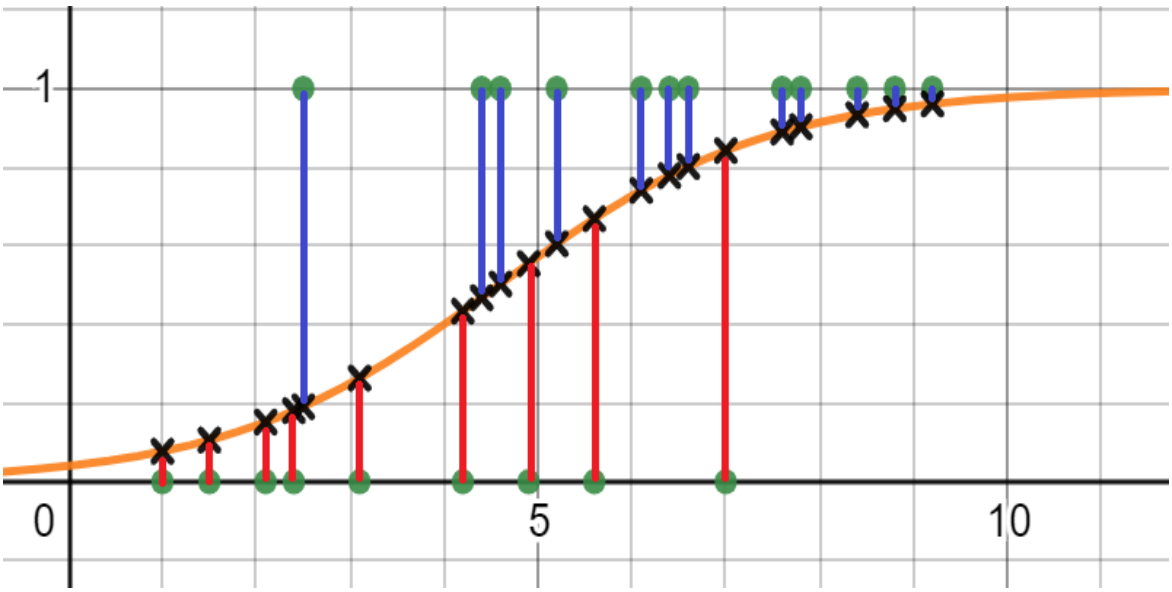


Figure 6-12. Projecting the output values back onto the logistic curve

We can then take the `log()` of each of those likelihoods and sum them together. This will be the log likelihood of the fit. Just like we did calculating maximum likelihood, we will convert the "false" likelihoods by subtracting from 1.0.

Example 6-10. Calculating the log-likelihood of the fit

```
from math import log, exp
import pandas as pd

patient_data = pd.read_csv('https://bit.ly/33ebs2R', delimiter=",").itertuples()

b0 = -3.17576395
b1 = 0.69267212

def logistic_function(x):
    p = 1.0 / (1.0 + exp(-(b0 + b1 * x)))
    return p

# Sum the log-likelihoods
log_likelihood_fit = 0.0

for p in patient_data:
    if p.y == 1.0:
        log_likelihood_fit += log(logistic_function(p.x))
    elif p.y == 0.0:
        log_likelihood_fit += log(1.0 - logistic_function(p.x))

print(log_likelihood_fit) # -9.946161673231583
```

Using some clever binary multipication and Python comprehensions, we can consolidate that `for` loop and `if` expression into one line that returns the `log_likelihood_fit`. Similar to what we did in the maximum likelihood formula, we can use some binary subtraction between the true and false cases to mathematically eliminate one or the other. In this case we multiply by 0 and therefore apply either the true or false case, but not both, to the sum accordingly.

Example 6-11. Consolidating our log likelihood logic into a single line

```
log_likelihood_fit = sum(log(logistic_function(p.x)) * p.y +
                         log(1.0 - logistic_function(p.x)) * (1.0 - p.y)
                         for p in patient_data)
```

If we were to express the likelihood of the fit in mathematic notation, this is what it would look like. Note that $f(x_i)$ is the logistic function for a given input variable x_i.

$$\log\ \text{likelihood fit} = \sum_{i=1}^{n} \left(log\left(f\left(x_i\right)\right) \times y_i\right) + \left(log\left(1.0 - f\left(x_i\right)\right) \times \left(1 - y_i\right)\right)$$

As calculated above in Example 6-10 or Example 6-11, we have -9.9461 as our log-likelihood of the fit. We need one more datapoint to calculate the R^2: the log-likelihood that estimates without using any input variables, and simply uses the number of true cases divided by all cases (effectively leaving only the intercept). Note we can count the number of symptomatic cases by summing all the y-values together $\sum y_i$, because only the 1's and not the 0's will count into the sum. Here is the formula:

$$\log\ \text{likelihood} = \frac{\sum y_i}{n} \times y_i + \left(1 - \frac{\sum y_i}{n}\right) \times \left(1 - y_i\right)$$

Here is the expanded Python equivalent of this formula applied in Example 6-12.

Example 6-12. Log of likelihood of patients

```
import pandas as pd
from math import log, exp

patient_data = list(pd.read_csv('https://bit.ly/33ebs2R',
delimiter=",").itertuples())

likelihood = sum(p.y for p in patient_data) / len(patient_data)

log_likelihood = 0.0

for p in patient_data:
    if p.y == 1.0:
        log_likelihood += log(likelihood)
    elif p.y == 0.0:
        log_likelihood += log(1.0 - likelihood)

print(log_likelihood) # -14.341070198709906
```

To consolidate this logic and reflect the formula, we can compress that `for` loop and `if` expression into a single line, using some binary multiplication logic to handle both true and false cases:

Example 6-13. Consolidating the log likelihood into a single line

```
log_likelihood = sum(log(likelihood)*p.y + log(1.0 - likelihood)*(1.0 - p.y) \
        for p in patient_data)
```

Finally, just plug these values in and get your R^2:

$$R^2 = \frac{(\log\ \text{likelihood}) - (\log\ \text{likelihood fit})}{(\log\ \text{likelihood})}$$

$$R^2 = \frac{-0.5596 - (-9.9461)}{-0.5596} R^2 = 0.306456$$

And here is the Python code shown in Example 6-14, calculating the R^2 in its entirety.

Example 6-14. Calculating the R^2 for a logistic regression

```
import pandas as pd
from math import log, exp

patient_data = list(pd.read_csv('https://bit.ly/33ebs2R',
delimiter=",").itertuples())

# Declare fitted logistic regression
b0 = -3.17576395
b1 = 0.69267212

def logistic_function(x):
    p = 1.0 / (1.0 + exp(-(b0 + b1 * x)))
    return p
```

```
# calculate the log likelihood of the fit
log_likelihood_fit = sum(log(logistic_function(p.x)) * p.y +
                         log(1.0 - logistic_function(p.x)) * (1.0 - p.y)
                         for p in patient_data)

# calculate the log likelihood without fit
likelihood = sum(p.y for p in patient_data) / len(patient_data)

log_likelihood = sum(log(likelihood) * p.y + log(1.0 - likelihood) * (1.0 - p.y) \
        for p in patient_data)

# calculate R-Square
r2 = (log_likelihood - log_likelihood_fit) / log_likelihood

print(r2)  # 0.306456105756576
```

Okay so we got an $R^2 = .306456$, so does hours of chemical exposure explain whether someone shows symptoms? As we learned in Chapter 5 on linear regression, a poor fit will be closer to an R^2 of 0.0 and a greater fit will be closer to 1.0. Therefore we can conclude that hours of exposure is mediocre for predicting symptoms, as the R^2 is 0.30645. There must be other variables that help better predict if someone will show symptoms besides time of exposure. This makes sense because we have a large mix of patients showing symptoms versus not showing symptoms for most of our observed data, as shown in Figure 6-13.

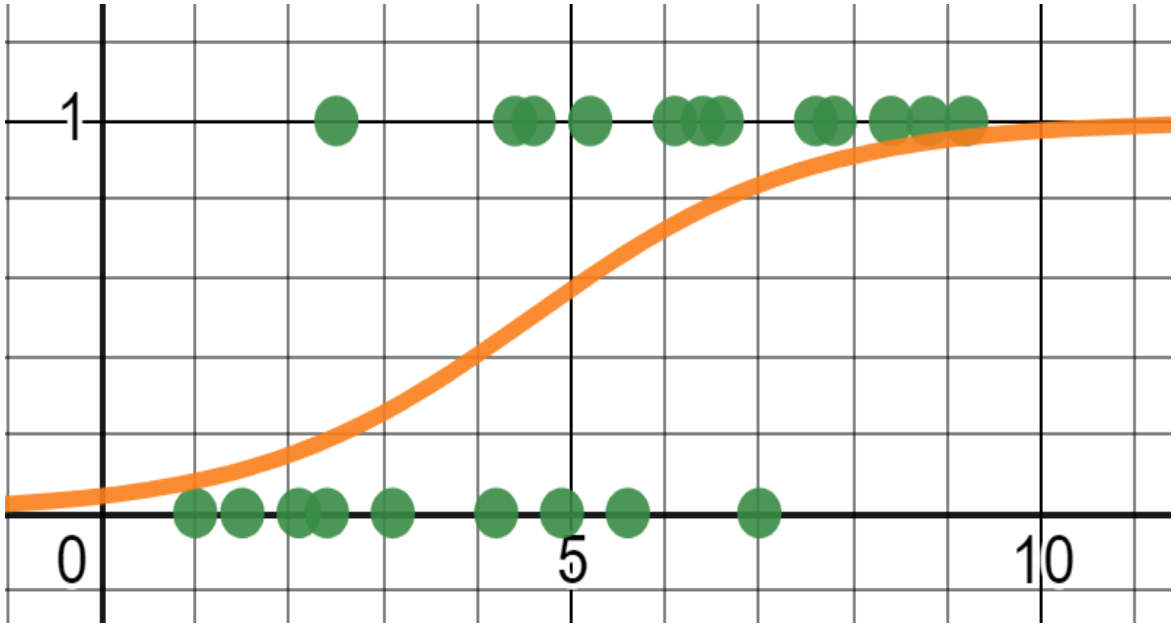


Figure 6-13. Our data has a mediocre R^2 of 0.30645, because there is a lot of variance in the middle of our curve

But if we did have a clean divide in our data, where 1 and 0 outcomes are cleanly separated as shown below in Figure 6-14, we would have a perfect R^2 of 1.0.

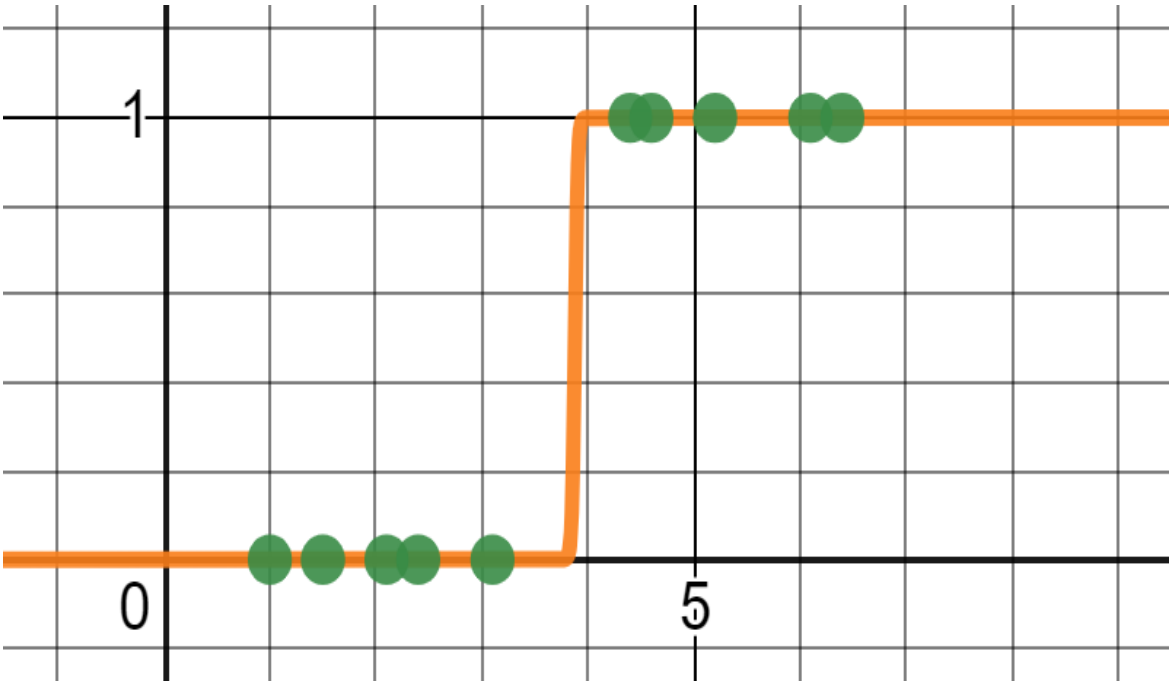


Figure 6-14. This logistic regression has a perfect R^2 of 1.0 because there is a clean divide in outcomes predicted by hours of exposure.

P-Values

Just like linear regression, we are not done just because we have an R^2. We need to investigate how likely we would have seen this data by chance rather than because of an actual relationship. This means we need a P-Value.

To do this, we will need to learn a new probability distribution called the **Chi-Square Distribution**, annotated as chi^2 Distribution. It is continuous and used in several areas of statistics, including this one!

If we take each value in a standard normal distribution (mean of 0 and standard deviation of 1) and square it, that will give us the chi^2 distribution with 1 degree of freedom. For our purposes, the degrees of freedom will depend on how many parameters n are in our logistic regression, which will be $n - 1$. You can see examples of different degrees of freedom in Figure 6-15. Since we have two parameters (hours of exposure and whether symptoms were shown), our degrees of freedom will be 1 because $2 - 1 = 1$.

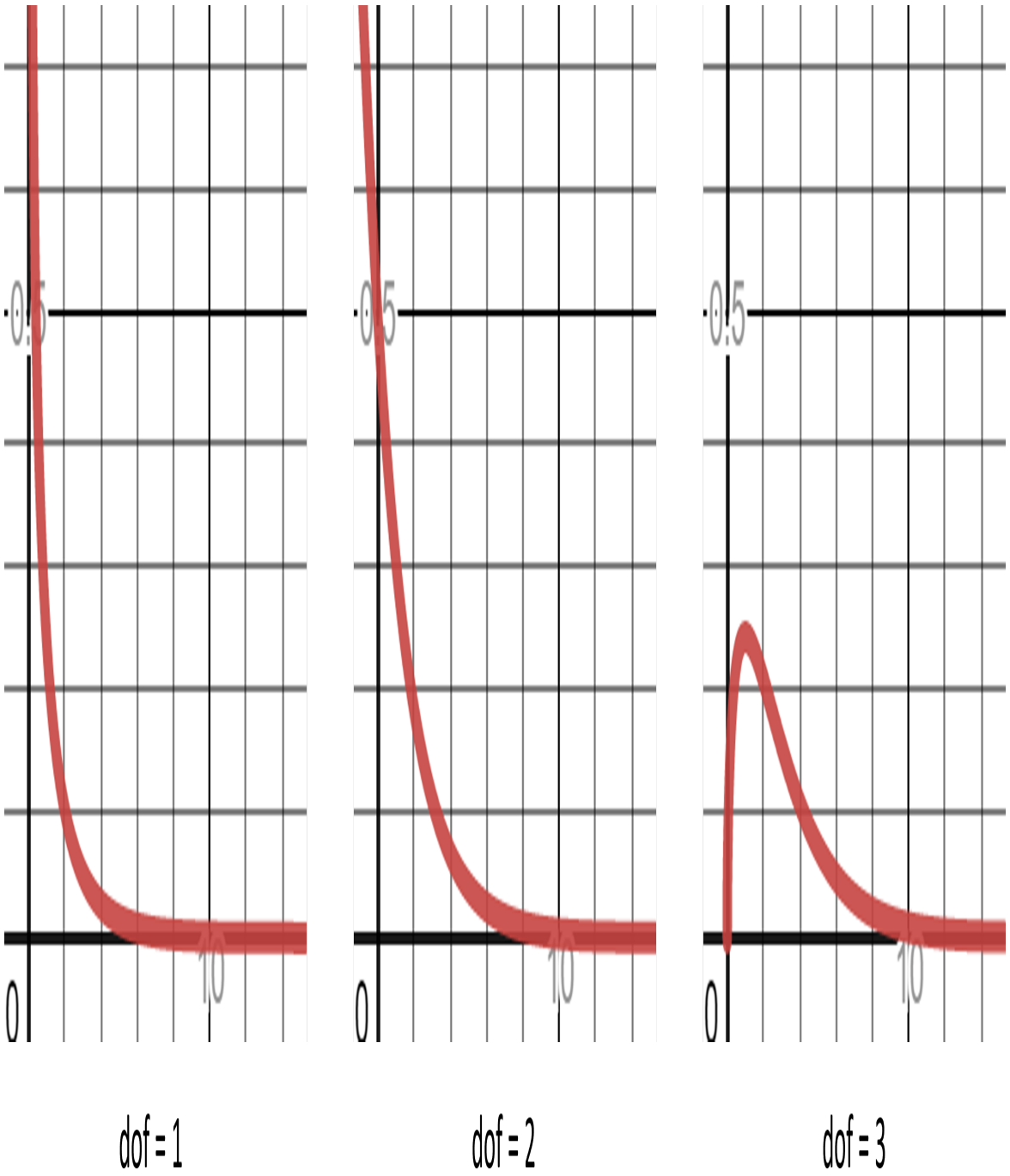


Figure 6-15. A χ^2 Distribution with differing degrees of freedom.

We will need the *log likelihood fit* and *log likelihood* as calculated in the previous subsection on R^2. Here is the formula that will produce the χ^2 value we need to look up.

$$\chi^2 = 2\,(\log\ \text{likelihood}\ \text{fit}) - (\log\ \text{likelihood})$$

We then take that value and look up the probability from the χ^2 distribution. That will give us our p-value.

$$\text{p-value} = \text{chi}(2((\log\ \text{likelihood fit}) - (\log\ \text{likelihood}))$$

Here is our p-value for a given fitted logistic regression. We use SciPy's `chi2` module to use the chi-square distribution.

Example 6-15. Calculating a p-value for a given logistic regression

```
import pandas as pd
from math import log, exp
from scipy.stats import chi2

patient_data = list(pd.read_csv('https://bit.ly/33ebs2R',
delimiter=",").itertuples())

# Declare fitted logistic regression
b0 = -3.17576395
b1 = 0.69267212

def logistic_function(x):
    p = 1.0 / (1.0 + exp(-(b0 + b1 * x)))
    return p

# calculate the log likelihood of the fit
log_likelihood_fit = sum(log(logistic_function(p.x)) * p.y +
                         log(1.0 - logistic_function(p.x)) * (1.0 - p.y)
                         for p in patient_data)

# calculate the log likelihood without fit
likelihood = sum(p.y for p in patient_data) / len(patient_data)

log_likelihood = sum(log(likelihood) * p.y + log(1.0 - likelihood) * (1.0 - p.y) \
                     for p in patient_data)

# calculate p-value
chi2_input = 2 * (log_likelihood_fit - log_likelihood)
p_value = chi2.pdf(chi2_input, 1) # 1 degree of freedom (n - 1)

print(p_value)  # 0.0016604875618753787
```

So we have a p-value of 0.00166, and if our threshold for signifiance is .05, we say this data is statistically significant and was not by random chanc e.

Train/Test Splits

As covered in Chapter 5 on linear regression, we can use train/test splits as a way to validate machine learning algorithms. This is the more "machine learning" approach to assessing the performance of a logistic regression, and we still have to be concerned about problems like overfitting and variance.

While it is a good idea to rely on traditional statistical metrics like R^2 and p-values, when you are dealing with more variables this becomes less practical. This is where train/test splits come in handy once again. To review, Figure 6-16 visualizes a 3-fold cross validation alternating a testing dataset.

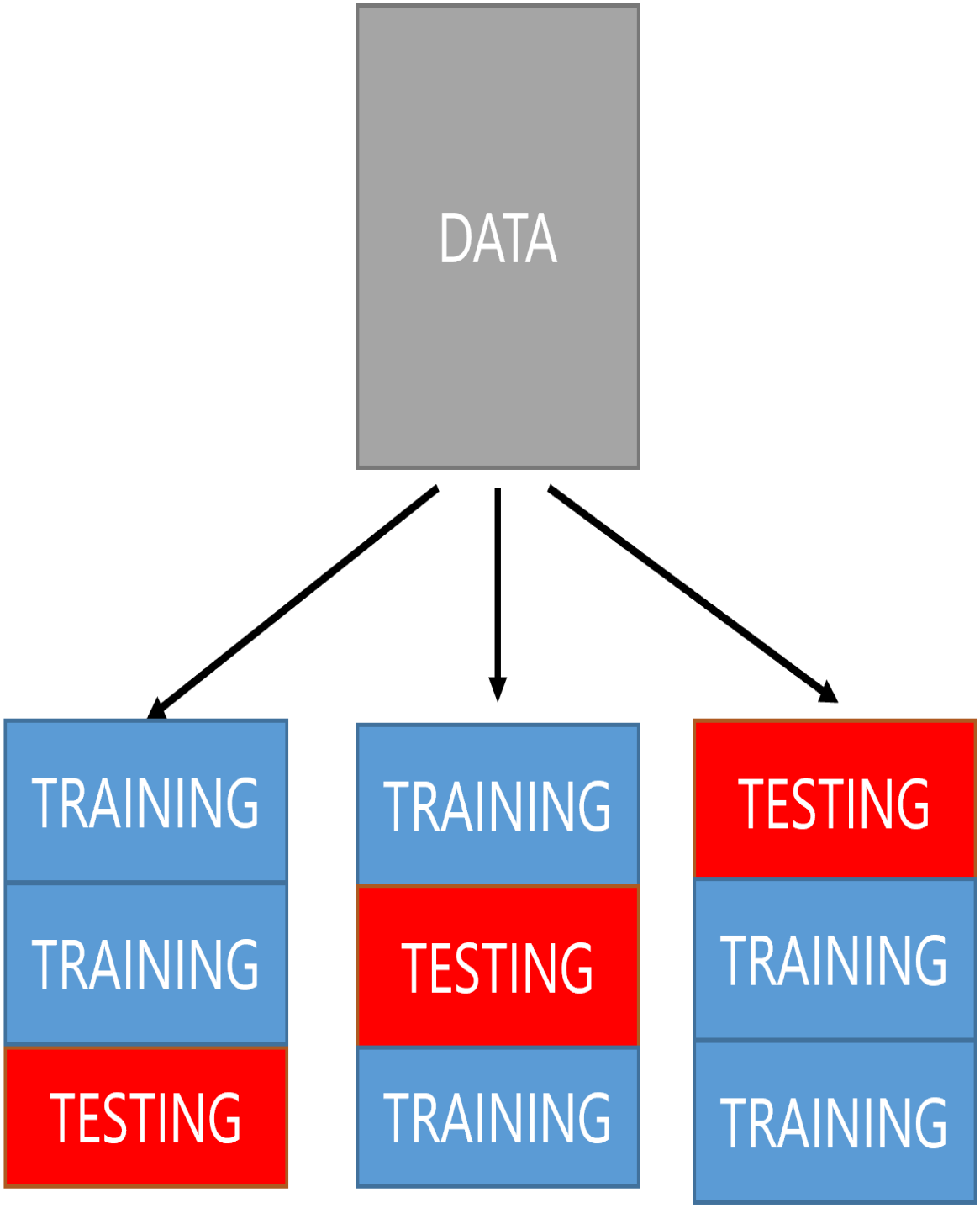


Figure 6-16. A 3-fold cross validation, alternating each third of the dataset as a test dataset.

In Example 6-16 we perform a logistic regression on the employee retention dataset, but we split the data into thirds. We then alternate each third as the test data. Finally, summarize the three accuracies as an average and standard deviation.

Example 6-16. Performing a logistic regression with 3-fold cross validation

```
import pandas as pd
from sklearn.linear_model import LogisticRegression
from sklearn.model_selection import KFold, cross_val_score

# Load the data
df = pd.read_csv("https://tinyurl.com/y6r7qjrp", delimiter=",")

X = df.values[:, :-1]
Y = df.values[:, -1]

# "random_state" is the random seed, which we fix to 7
kfold = KFold(n_splits=3, random_state=7, shuffle=True)
model = LogisticRegression(penalty='none')
results = cross_val_score(model, X, Y, cv=kfold)

print("Accuracy Mean: %.3f (stdev=%.3f)" % (results.mean(), results.std()))
```

That out of the way, let's talk about why accuracy is a bad measure for classification.

Confusion Matrices

Suppose a model observed people with the name "Michael" quit their job. The reason why first and last name are captured as input variables is indeed questionable, as it is doubtful someone's name has any impact on whether they quit. However, to simplify the example, let's go with it. The model then predicts that any person named "Michael" will quit their job.

Now this is where accuracy falls apart. I have 100 employees, including one named "Michael" and another named "Samantha". Michael is wrongly predicted to quit, and it is Samantha that ends up quitting. What's the accuracy of my model? It is 98% because there were only 2 wrong predictions out of 100 employees as visualized in Figure 6-17.

Figure 6-17. The employee named "Michael" is predicted to quit, but its actually another employee that does, giving us 98% accuracy

Especially for imbalanced data where the event of interest (e.g. a quitting employee) is rare, the accuracy metric is horrendously misleading for classification problems. If you ever have a vendor, consultant, or data scientist try to sell you a classification system on claims of accuracy, ask for a confusion matrix.

A **confusion matrix** is a grid that breaks out the predictions against the actual outcomes showing the true positives, true negatives, false positives (type I error), and false negatives (type II error). Here is a confusion matrix presented in Figure 6-18.

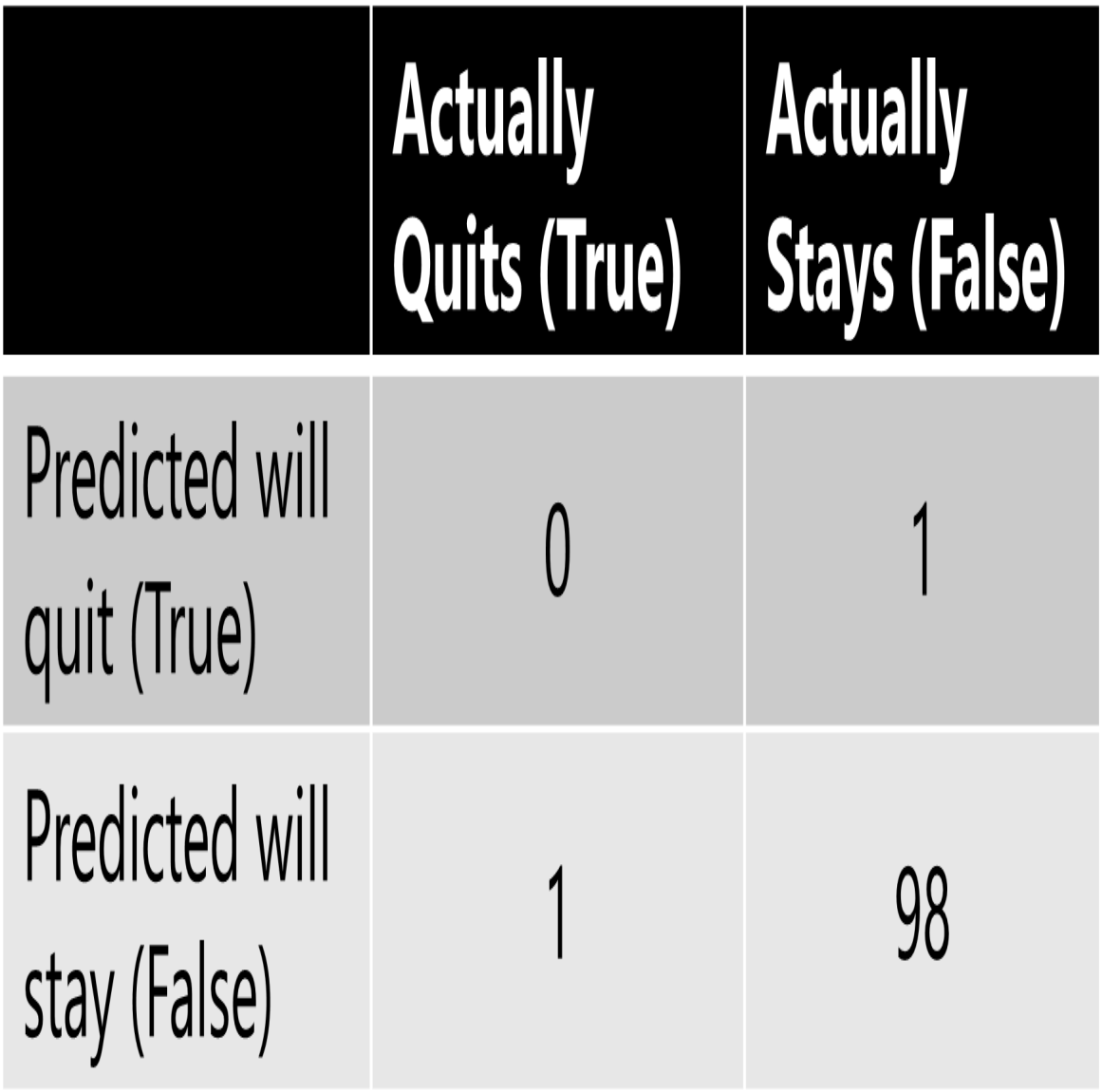


Figure 6-18. A simple confusion matrix

Generally, we want the diagonal values (top-left to bottom-right) to be higher because these reflect correct classifications. We want to evaluate how many employees who were predicted to quit actually did quit (true positives). Conversely, we also want to evaluate how many employees who were predicted to stay actually did stay (true negatives).

The other cells reflect wrong predictions, where an employee predicted to quit ended up staying (false positive), and where an employee predicted to stay ends up quitting (false

negative).

What we need to do is dice up that accuracy metric into more specific accuracy metrics targeting different parts of the confusion matrix. Let's look at Figure 6-19 which adds some useful measures.

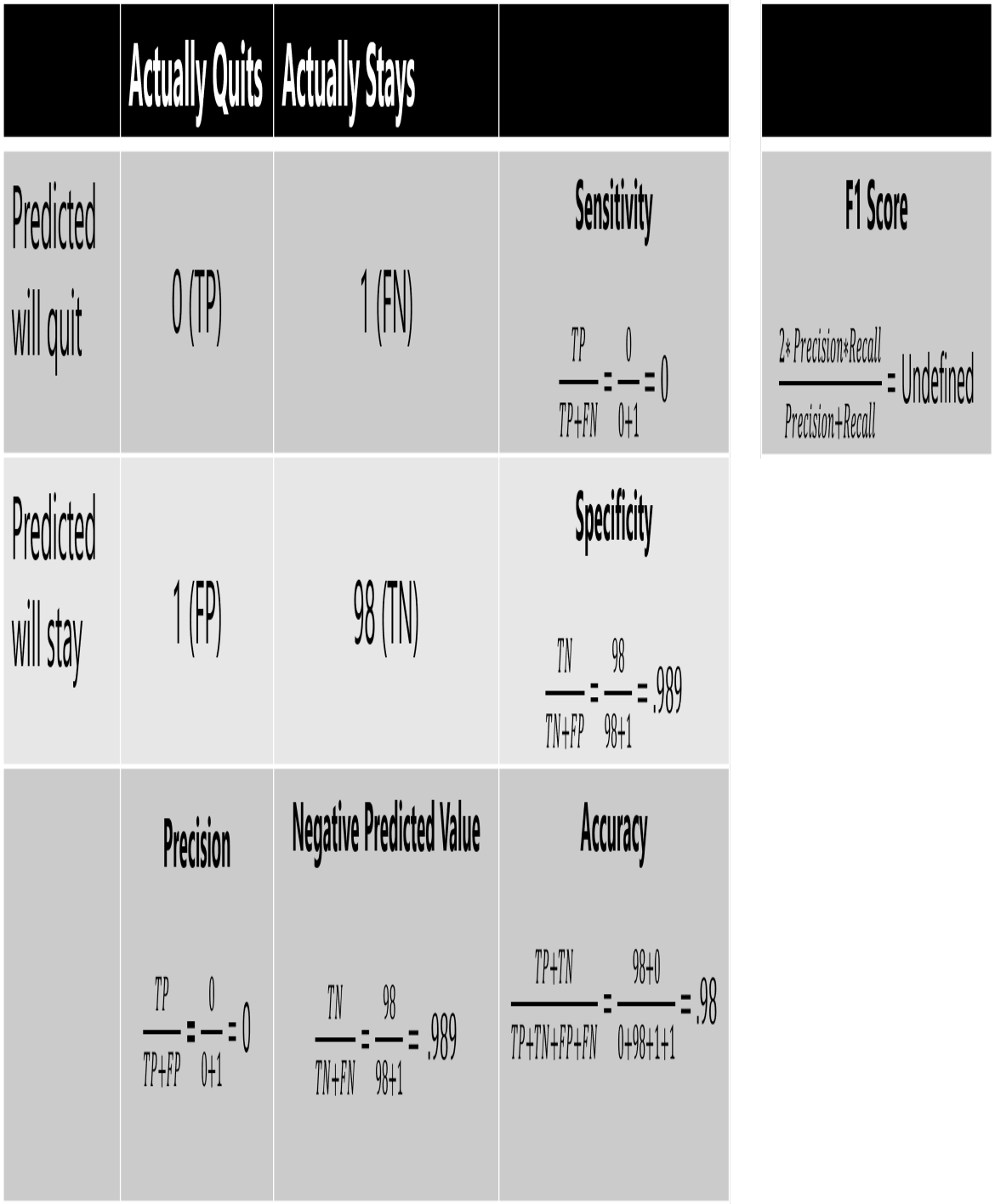


Figure 6-19. Adding useful metrics to the confusion matrix

From the confusion matrix, we can derive all sorts of useful metrics beyond just accuracy. We can easily see that precision (how accurate positive predictions were) and sensitivity (rate of identified positives) are 0, meaning this machine learning model fails entirely at positive predictions.

Example 6-17 shows how to use the confusion matrix API in SciPy on a logistic regression with a train/test split. Note that the confusion matrix is only applied to the test dataset.

Example 6-17. Creating a confusion matrix for a test dataset in SciPy

```
import pandas as pd
from sklearn.linear_model import LogisticRegression
from sklearn.metrics import confusion_matrix
from sklearn.model_selection import train_test_split

# Load the data
df = pd.read_csv('https://bit.ly/3cManTi', delimiter=",")

# Extract input variables (all rows, all columns but last column)
X = df.values[:, :-1]

# Extract output column (all rows, last column)\
Y = df.values[:, -1]

model = LogisticRegression(solver='liblinear')

X_train, X_test, Y_train, Y_test = train_test_split(X, Y, test_size=.33,
random_state=10)
model.fit(X_train, Y_train)
prediction = model.predict(X_test)

"""
The confusion matrix evaluates accuracy within each category.
[[truepositives falsenegatives]
 [falsepositives truenegatives]]

The diagonal represents correct predictions,
so we want those to be higher
"""
matrix = confusion_matrix(y_true=Y_test, y_pred=prediction)
print(matrix)
```

Bayes Theorem and the Confusion Matrix

Do you recall Bayes Theorem in Chapter 2? You can use Bayes Theorem to bring in outside information to further validate findings on a confusion matrix. Figure 6-20 shows a confusion matrix of 1000 patients tested for a disease.

	TESTS POSITIVE	TESTS NEGATIVE
AT RISK	198	2
NOT AT RISK	50	750

Figure 6-20. A confusion matrix for a medical test, identifying a disease

We are told that for patients that have a health risk, 99% will be identified successfully (sensitivity). Using the confusion matirix, we can see that mathematically checks out.

$$\text{sensitivity} = \frac{198}{198 + 2} = .99$$

But what if we flip the condition? What percentage of those who tested positive have the health risk (precision)? While we are flipping a conditional probability, we do not have to use Bayes Theorem here because the confusion matrix gives us all the numbers we need.

$$\text{precision} = \frac{198}{198 + 50} = .798$$

Okay so 79.8% is not terrible, and that's the percentage of people who tested positive that actually have the disease. But ask yourself this… what are we assuming about our data? Is it representative of the population?

We do some quick research and found 1% of the population actually has the disease. There is an opportunity to use Bayes Theorem here. We can account for the proportion of the population that actually has the disease, and incorporate that into our confusion matrix findings. We then discover something significant.

$$P\left(\text{At Risk if Positive}\right) = \frac{P(\text{Positive if At Risk}) \times P(\text{At Risk})}{P(\text{Positive})}$$

$$P\left(\text{At Risk if Positive}\right) = \frac{.99 \times .01}{.248}$$

$$P(\text{At Risk if Positive}) = .0339$$

When we account for the fact only 1% of the population is at risk, and 20% of our test patients are at risk, the probability of being at risk given a positive test is 3.39%! How did it drop from 99%? This just shows how easily we can get duped by probabilities that are only high in a specific population like the vendor's 1000 test patients. So if this test only has a 3.39% probability of successfully identifying a true positive, we probably should not use it.

Reciever Operator Characteristics (ROC)/Area Under Curve (AUC)

When we are evaluating different machine learning configurations, we may end up with dozens, hundreds, or thousands of confusion matrices. These can be tedious to review, so we can summarize all of them with a **receiver operator characteristic (ROC) curve** as shown in Figure 6-21. This allows us to see each testing instance (each represented by a black dot) and find an agreeable balance between true positives and false positives.

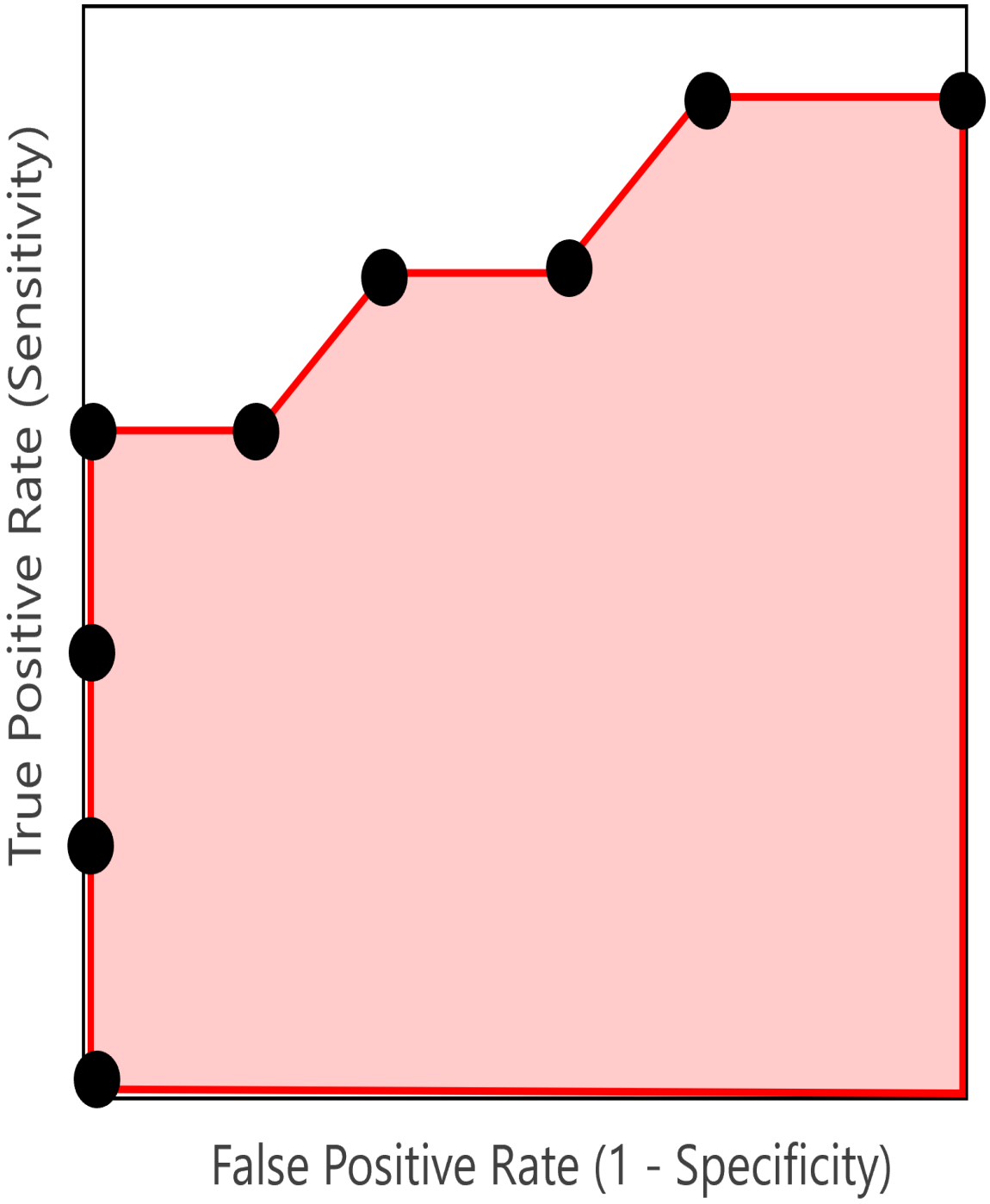


Figure 6-21. A receiver operator characteristic (ROC) curve

We can also compare different machine learning models by creating separate ROC curves for each. For example, if in Figure 6-22 our red curve represents a logistic regression and the blue curve represents a decision tree, we can see the performance of them side-by-side. The **area under the curve (AUC)** is a good metric for choosing which model to use. Since the red curve (logistic regression) has a greater area, this suggests it is a superior model.

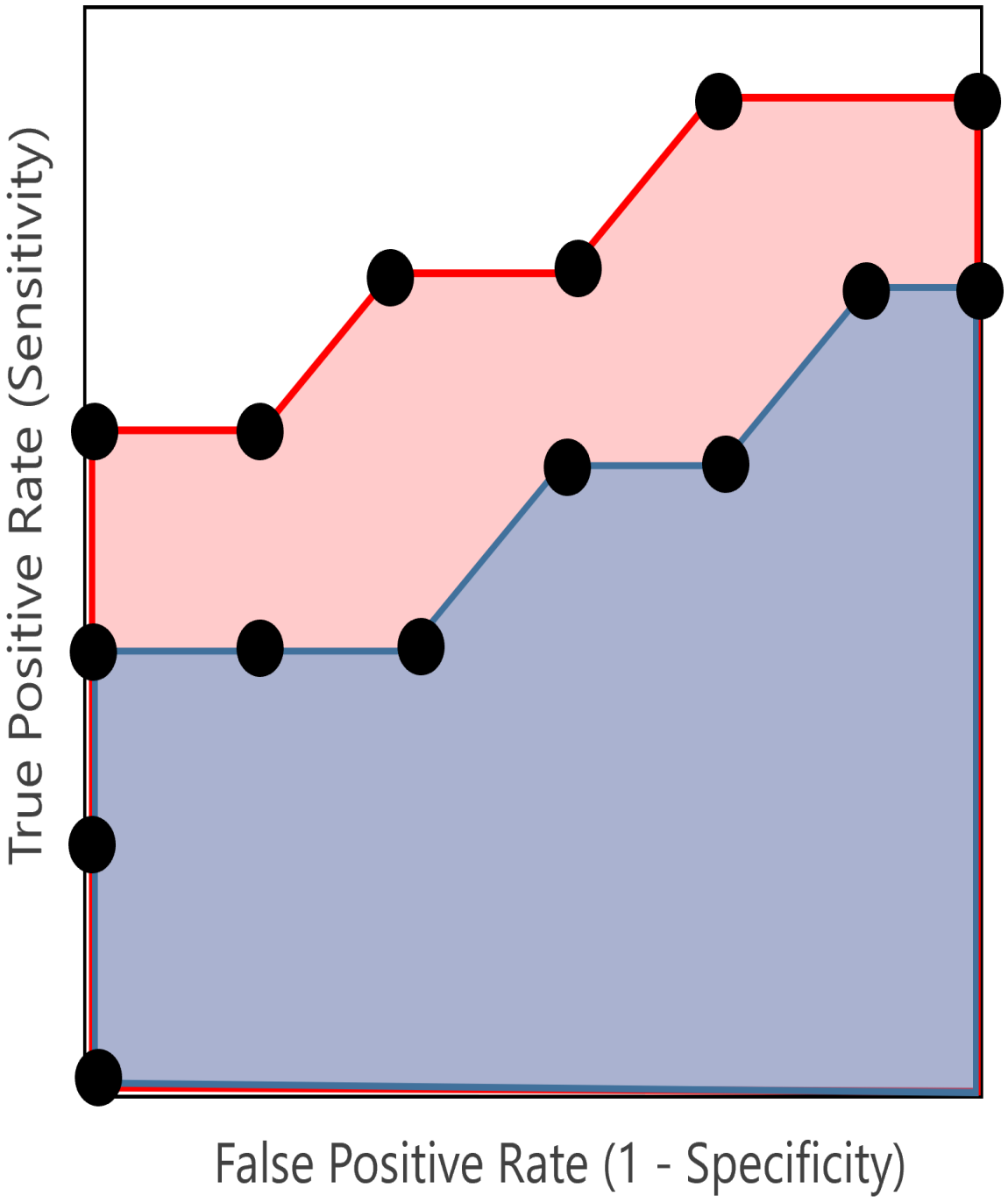


Figure 6-22. Comparing two models by their area under the curve (AUC) with their respective ROC curves

To use the AUC as a scoring metric, change the `scoring` parameter in the Scikit-Learn API to use `roc_auc` as shown for a cross-validation in Example 6-18.

Example 6-18. Using the AUC as the Scikit-Learn parameter.

```
# put Scikit_learn model here
```

```
results = cross_val_score(model, X, Y, cv=kfold, scoring='roc_auc')
print("AUC: %.3f (%.3f)" % (results.mean(), results.std()))
# AUC: 0.791 (0.051)
```

Class Imbalance

There is one last thing to cover before we close this chapter. As we saw earlier when discussing confusion matrices, **class imbalance**, which happens when data is not equally represented across every outcome class, is a problem in machine learning. Unfortunately many problems of interest are imbalanced such as disease prediction, security breaches, fraud detection, and so on. Class imbalance is still an open problem with no great solution. However, there are a few techniques you can try.

First you can do obvious things like collect more data or try different models, as well as utilize confusion matrices and ROC/AUC curves. All of this will help track poor predictions and pro-actively catch errors.

Another common technique is to duplicate samples in the minority class until it is equally represented in the dataset. You can do this in Scikit-Learn as shown in Example 6-19 when doing your train-test splits. Pass the `stratify` option with the column containing the class values, and it will attempt to equally represent the data of each class.

Example 6-19. Using the "stratify" option in Scikit-Learn to balance classes in the data

```
X, Y = ...
X_train, X_test, Y_train, Y_test =  \
        train_test_split(X, Y, test_size=.33, stratify=Y)
```

There are also a family of algorithms called SMOTE, which generate synthetic samples of the minority class.

What would be most ideal is to tackle the problem in a way that uses anomaly detection models, which are deliberately designed for seeking out a rare event. These seek outliers however, and are not necessarily a classification since they often are unsupervised algorithms. All these techniques are beyond the scope of this book but are worth mentioning as they **might** provide better solutions to a given problem.

Conclusions

Logistic regression is the workhorse model for predicting probabilities and classifications on data. As we learned, logistic regressions can predict more than one category rather than just a true/false. You just build a separate logistic regression modeling whether or not it belongs to that category, and the model that produces the highest probability is the one that wins. You may discover that Scikit-Learn, for the most part, will do this for you and detect when your data has more than two classes.

In this chapter, we covered not just how to fit a logistic regression using gradient descent and Scikit-Learn, but also statistical and machine learning approaches to validation. On the statistical front we covered the R^2 and p-value, and in machine learning we explored train/test splits, confusion matrices, and ROC/AUC.

If you want to learn more about logistic regression, probably the best resource to jump-start further is Josh Starmer's StatQuest playlist on Logistic Regression. I have to credit Josh's work in assisting this chapter, particularly in how to calculate R^2 and p-values for logistic regression. If for nothing else, watch his videos for the fantastic opening jingles!

https://youtu.be/yIYKR4sgzI8

As always, you will find yourself walking between the two worlds of statistics and machine learning. Many books and resources right now cover logistic regression from a machine learning perspective, but try to seek out proper statistics resources too. There are advantages and disadvantages to both schools of thought, and you can only win by being adaptable to both!

Exercises

A dataset of three input variables `RED`, `GREEN`, and `BLUE` as well as an output variable `LIGHT_OR_DARK_FONT_IND`, is provided here: *https://bit.ly/3BO7fSc*. It will be used to predict whether a light/dark font (0/1 respectively) will work for a given background color (specified by RGB values).

1. Perform a logistic regression on the above data, using 3-fold cross validation.
2. Calculate the average and standard deviation of the AUC across the 3-fold cross validation.
3. Pick a few different background colors (you can use an RGB tool like this one: *https://bit.ly/3FHywrZ)* and see if the logistic regression sensibly chooses a light (0) or dark (1) font for each one.
4. The Space Shuttle Challenger tragedy occurred on January 28, 1986. Data on the temperature and number of O-ring failures is stored here: *https://bit.ly/3iUHo3I*. Figure out how to transform the data so it is suitable for a logistic regression, and after performing the regression calculate the R^2 and p-value.

Chapter 7. Neural Networks

A NOTE FOR EARLY RELEASE READERS

With Early Release ebooks, you get books in their earliest form—the author's raw and unedited content as they write—so you can take advantage of these technologies long before the official release of these titles.

This will be the 7th chapter of the final book.

If you have comments about how we might improve the content and/or examples in this book, or if you notice missing material within this chapter, please reach out to the author at *thomasnield@live.com*.

A regression and classification technique that has enjoyed a renaissance over the past 10 years are neural networks. In the simplest definition, a **neural network** is a multi-layered regression containing layers of weights, biases, and nonlinear functions that reside between input variables and output variables. **Deep learning** is a popular variant of neural networks that utilizes multiple "hidden" (or middle) layers of nodes containing weights and biases. Each node resembles a linear function before being passed to a nonlinear function (called an activation function). Just like linear regression which we learned about in Chapter 5, optimization techniques like stochastic gradient descent are used to find the optimal weight and bias values to minimize the residuals.

Neural networks offer exciting solutions to problems previously difficult for computers to solve. From identifying objects in images to processing words in audio, neural networks have created tools that affect our everyday lives. This includes virtual assistants and search engines, as well as photo tools in our iPhones.

Given the media hoopla and bold claims dominating news headlines about neural networks, it may be surprising that have been around since the 1950's. The reason for their sudden popularity after 2010 is due to the growing availability of data and computing power. The ImageNet challenge between 2011 and 2015 was probably the largest driver of the renaissance, boosting performance on classifying 1000 categories on 1.4 million images to an accuracy of 96.4%.

However, like any machine learning technique it only works on narrowly defined problems. Even projects to create "self-driving" cars do not use end-to-end deep learning, and primarily use hand-coded rule systems with convoluted neural networks acting as a "label maker" for identifying objects on the road. We will discuss this later in

this chapter to understand where neural networks are actually used. But first we will build a simple neural network in NumPy, and then use Scikit-Learn to explore library implementations.

When to Use Neural Networks and Deep Learning

Neural networks and deep learning can be used for classification and regression, so how does it size up to linear regression, logistic regression, and other types of machine learning? You might have heard the expression "when all you have is a hammer, everything starts to look like a nail." There are advantages and disadvantages that are situational for each type of algorithm. Linear regression and logistic regression, as well as gradient boosted trees (which we did not cover in this book), do a pretty fantastic job easily making predictions on structured data. Think of "structured data" as data that easily is populated in a table, with rows and columns. But perceptual problems like image classification are much less structured, as we are trying to find fuzzy correlations between groups of pixels to identify shapes and patterns, not rows of data in a table. Trying to predict the next 4-5 words in a sentence being typed, or deciphering the words being said in an audio clip, are also perceptual problems and examples of neural networks being used for natural language processing.

In this chapter, we will primarily focus on simple neural networks, with only 1-2 hidden layers.

VARIANTS OF NEURAL NETWORKS

Variants of neural networks include convolutional neural networks, which is often used for image recognition. Long-short Term Memory (LSTM) is used for predicting on time-series, or forecasting. Recurrent neural networks are often used for text-to-speech applications.

IS USING A NEURAL NETWORK OVERKILL?

Using neural networks for the upcoming example is probably overkill, as a logistic regression would probably be more practical. Even a formulaic approach can be used. However, I have always been a fan of understanding complex techniques by applying them to simple toy problems. So with that in mind, try not to use neural networks where simpler models will be more practical. We will break this rule in this chapter for the sake of understanding the technique.

A Simple Neural Network

Here is a simple toy example to get a feel for neural networks. I want to predict whether a font should be light (1) or dark (0) for a given color background. Here is a few examples of different background colors in Figure 7-1. The top row looks best with light font, and the bottom row looks best with dark font.

Figure 7-1. Light background colors look best with dark font, and dark background colors look best with light font

In computer science one way to represent a color is with RGB values, or the "red", "green", and "blue" values. Each of these values are between 0 and 255 and express how these three colors are mixed to create the desired color. For example, if we express the RGB as `(red, green, blue)` then dark orange would have an RGB of `(255,140,0)` and pink would be `(255,192,203)`. Black would be `(0,0,0)` and white would be `(255,255,255)`.

From a machine learning and regression perspective, we have three numeric input variables `red`, `green`, and `blue` to capture a given background color. We need to fit a function to these input variables and output whether a light (1) or dark (0) font should be used for that background color.

REPRESENTING COLORS THROUGH RGB

There are hundreds of color picker palettes online to experiment with RGB values. W3 Schools has one here.

https://www.w3schools.com/colors/colors_rgb.asp

Note this example is not far from how neural networks work recognizing images, as each pixel is often modeled as three numeric RGB values. In this case we are just focusing on one "pixel" as a background color.

Let's start high level and put all the implementation details aside. We are going to approach this topic like an onion, starting with a higher understanding and peeling away slowly into the details. For now this is why we simply label "mystery math" on a process that takes inputs and produces outputs. We have three numeric input variables R, G, and B which are processed by this mystery math. Then it outputs a prediction between 0 and 1 as shown in Figure 7-2.

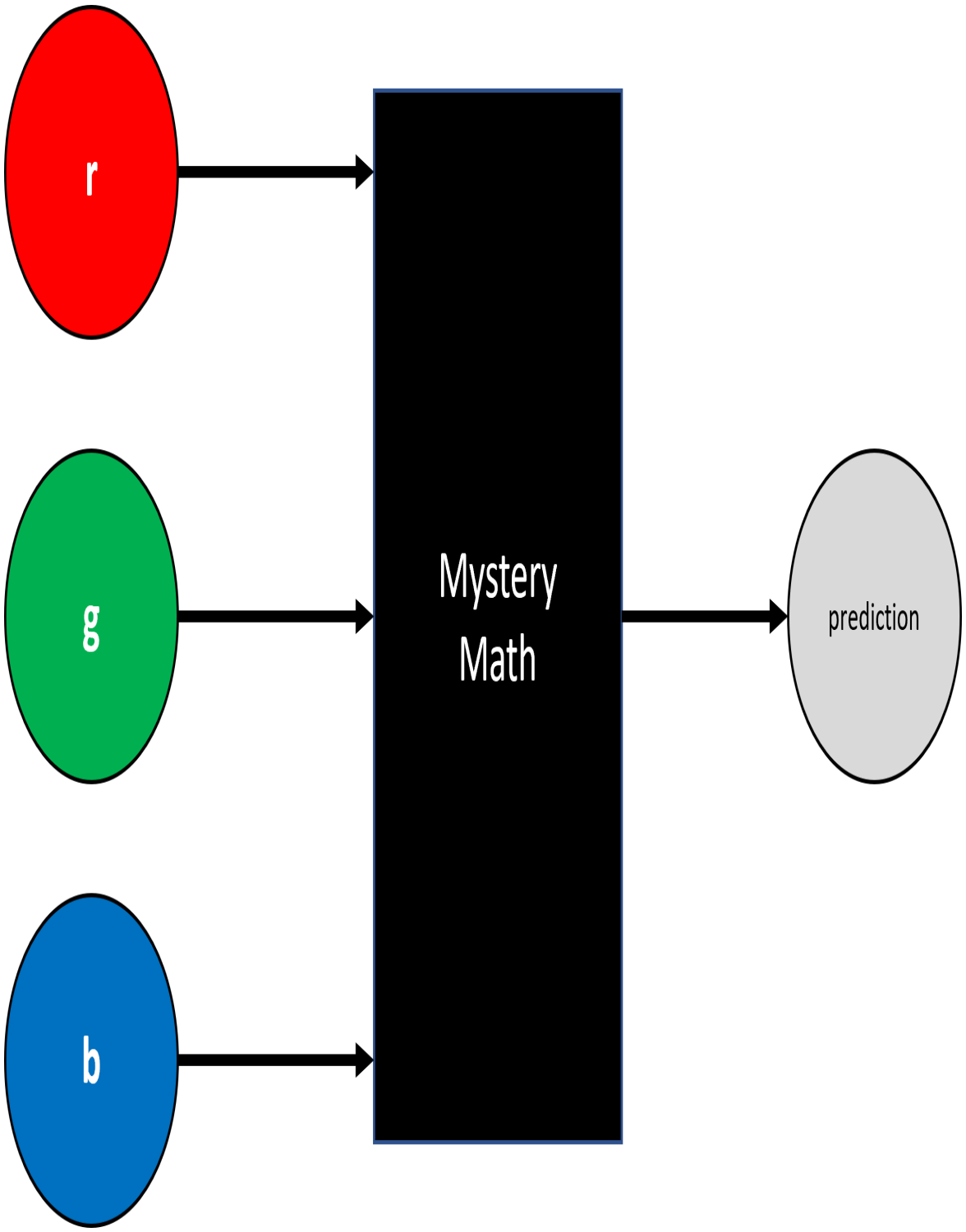


Figure 7-2. We have three numeric RGB values used to make a prediction for a light or dark font.

This prediction output expresses a probability. Once we replace RGB with their numerical values, we see that less than 0.5 will suggest a dark font whereas greater than 0.5 will suggest a light font as demonstrated in Figure 7-3.

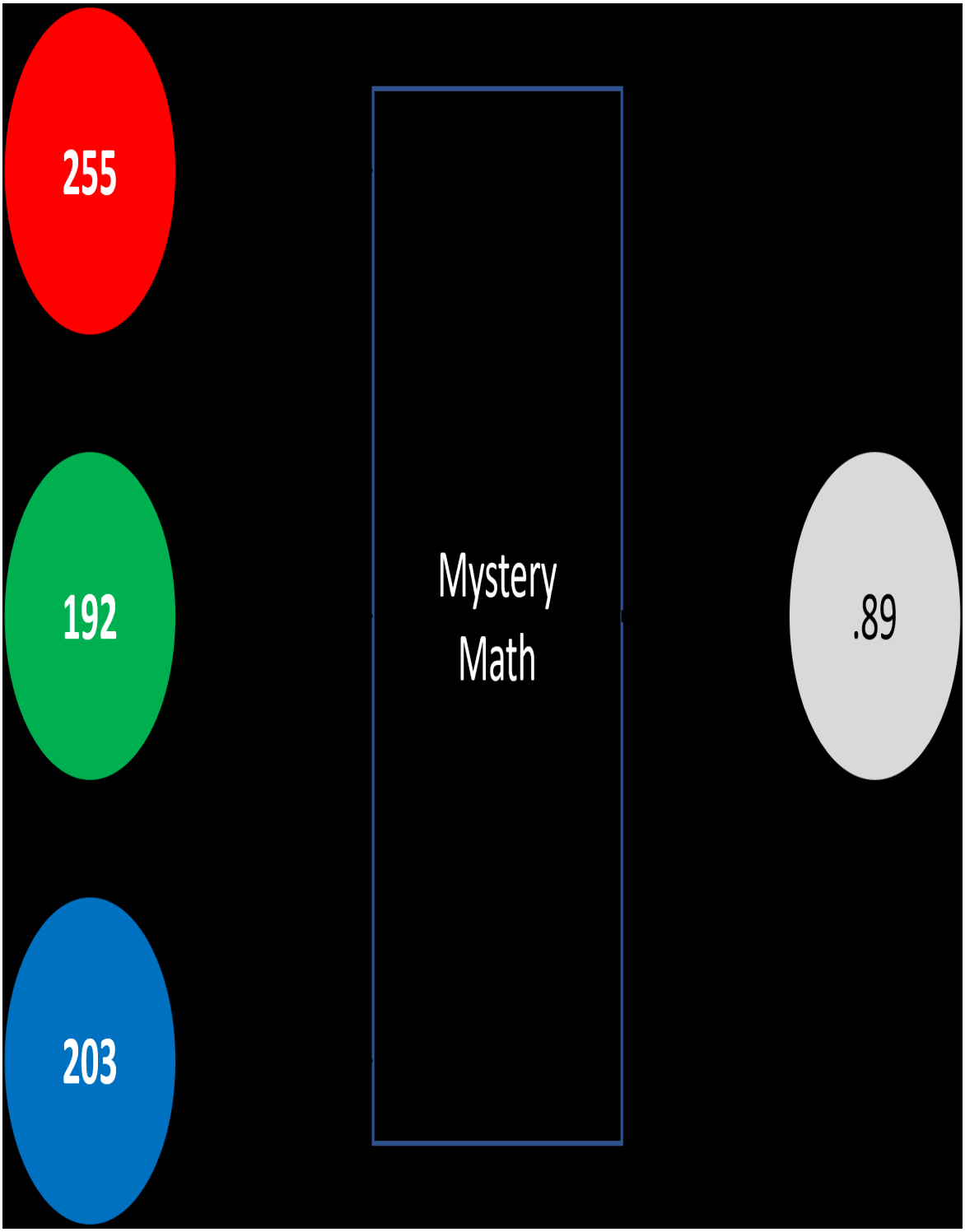


Figure 7-3. If we input a background color of pink (255,192,203) then the mystery math recommends a light font because the outputted probability .89 is greater than 0.5.

So what is going on inside that mystery math black box? Let's take a look in Figure 7-4.

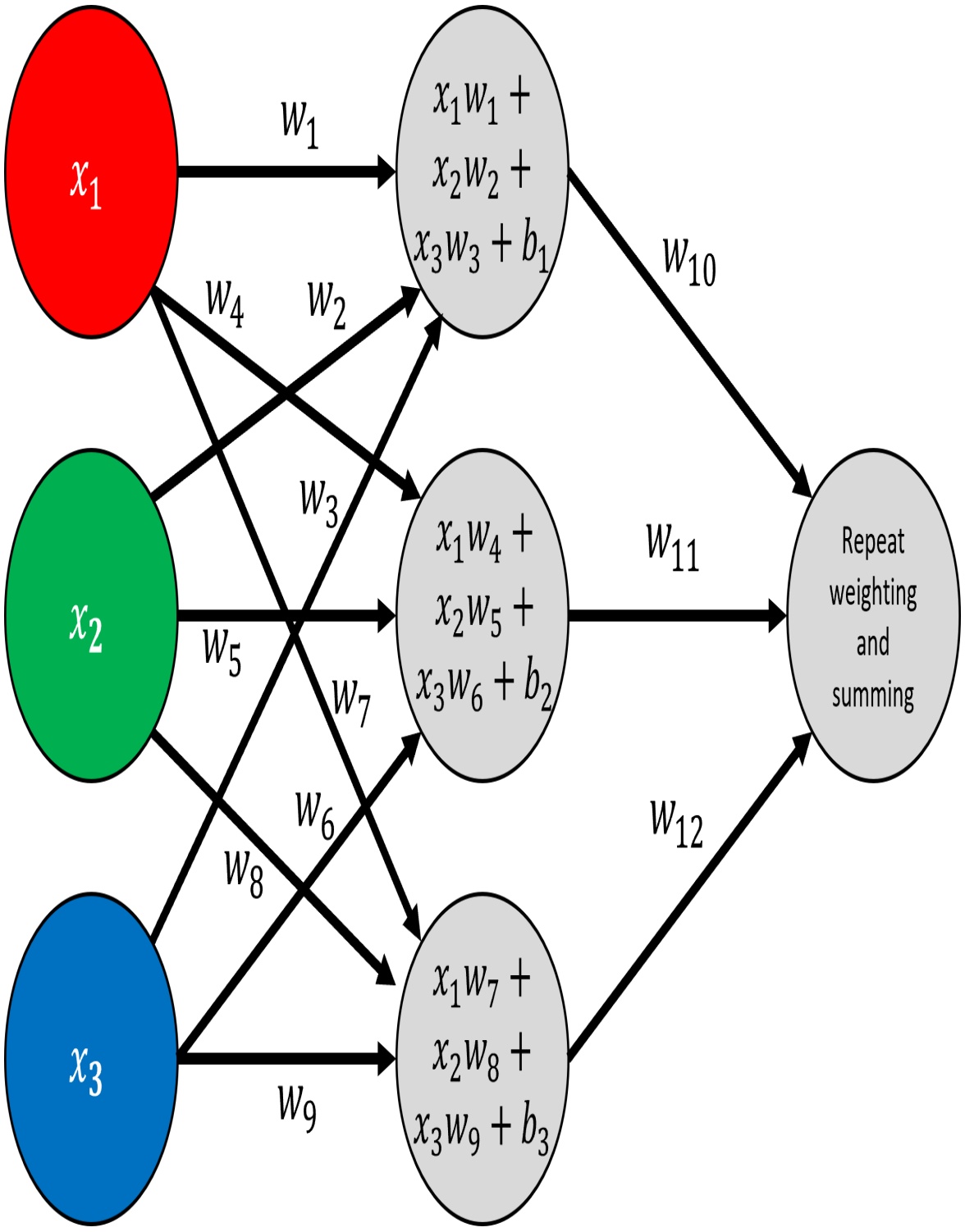


Figure 7-4. The hidden layer of the neural network applies weight and bias values to each input variable, and the output layer applies another set of weights and biases to that output.

We are missing another piece to this neural network, the activation functions, but we will get to that shortly. Let's first understand what's going on here. The first layer on the left is simply an input of the three variables, which in this case are the red, green, and

blue values. In the hidden (middle) layer, notice that we produce three **nodes**, or functions of weights and biases, between the inputs and outputs. Each node essentially is a linear function with slopes w_i and intercepts b_i, being multiplied and summed with input variables x_i. There is a weight w_i between each input node and hidden node, and another set of weights between each hidden node and output node. Each hidden and output node gets an additional bias b_i added.

Notice the output node repeats the same operation, taking the resulting weighted and summed outputs from the hidden layer and making them inputs into the final layer, where another set of weights and biases will be applied. I put "repeat weighting and summing" instead of the mathematical expressions because the expressions nested from the hidden layer is too long to display in the graphic. But here is the expression for the final node, and note how the outputs from the hidden layer become inputs to the final layer.

$$\begin{aligned}\text{output} = w_{10}\left(x_1w_1 + x_2w_2 + x_3w_3 + b_1\right)\\ +w_{11}\left(x_1w_4 + x_2w_5 + x_3w_6 + b_2\right)\\ +w_{12}\left(x_1w_7 + x_2w_8 + x_3w_9 + b_3\right) + b_4\end{aligned}$$

In a nutshell, this is a regression just like linear or logistic regression, but with many more parameters to solve for. The weight and bias values are analagous to the `m` and `b`, or β_1 and β_0, parameters in a linear regression. We do use stochastic gradient descent and minimize loss just like linear regression, but we need an additional tool called backpropogation to untangle the weight w_i and bias b_i values and calculate their partial derivatives using the chain rule. We will get to that later in this chapter, but for now let's assume we have the weight and bias values optimized. We need to talk about activation functions first.

Activation Functions

Let's bring in the activation functions next. An **activation function** is a nonlinear function that transforms or compresses the weighted and summed values in a node, helping the neural network separate the data effectively so it can be classified. Let's take a look at Figure 7-5. If you do not have the activation functions, your hidden layers will not be productive and will perform no better than a linear regression.

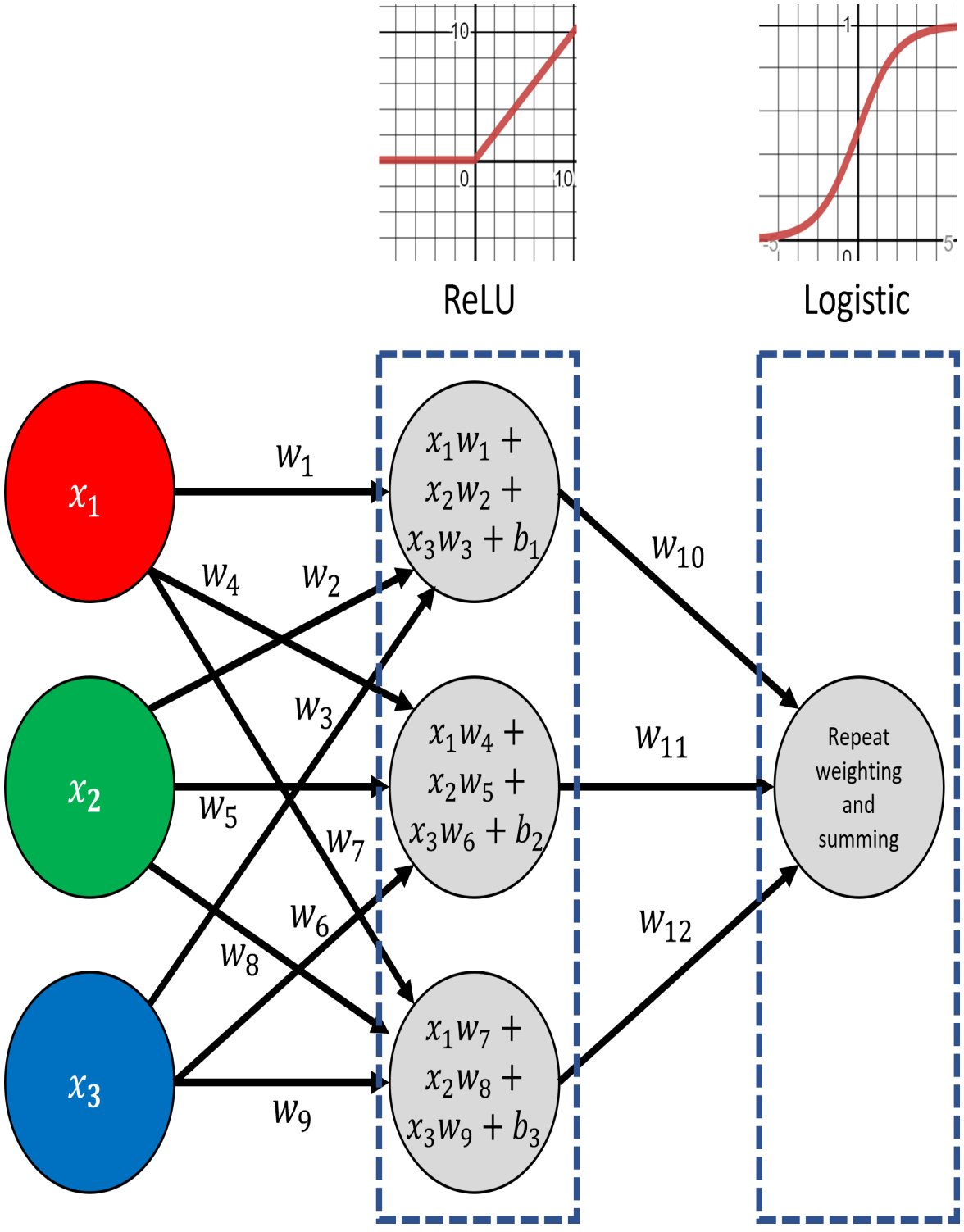


Figure 7-5. Applying Activation Functions

The **ReLU activation function** will zero out any negative outputs from the hidden nodes. If the weights, biases, and inputs multiply and sum to a negative number, it will

be converted to 0. Otherwise the output is left alone. Here is the graph for ReLU (Figure 7-6) using SymPy (Example 7-1).

Example 7-1. Plotting the ReLU function

```
from sympy import *

# plot relu
x = symbols('x')
relu = Max(0, x)
plot(relu)
```

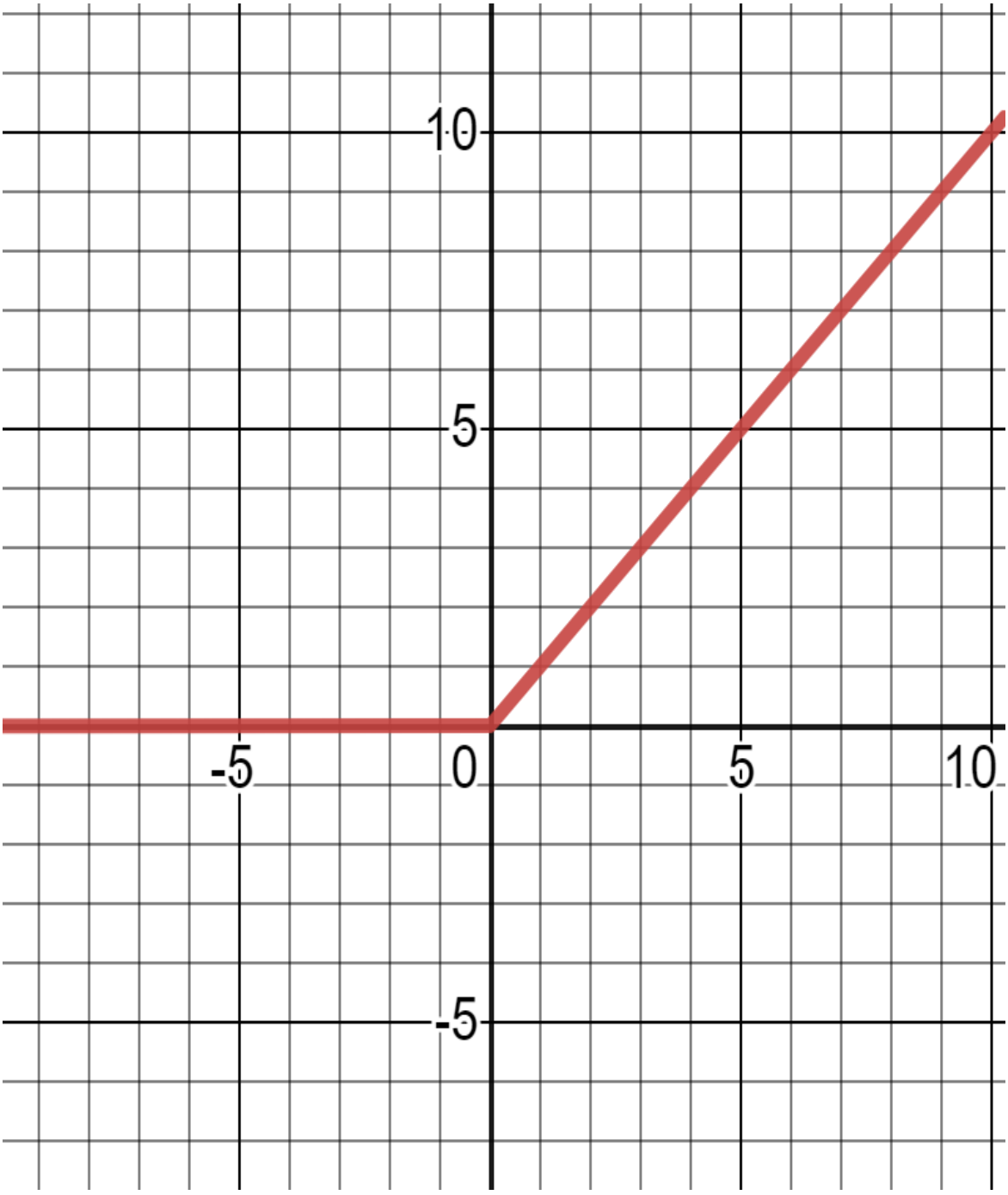


Figure 7-6. Graph for ReLU function

ReLU is short for “rectified linear unit”, but that is just a fancy way of saying “turn negative values into 0.” ReLU has gotten popular for middle layers in neural networks and deep learning because of its speed and mitigation of the vanishing gradient problem. Vanishing gradients occur when the partial derivative slopes get so small they prematurely approach 0 and bring training to a screeching halt.

The output layer has an important job: it takes the piles of math from the hidden layers of the neural network and turns them into an interpretable result, such as presenting classification predictions. The output layer for this particular neural network uses the **logistic activation function**, which is a simple sigmoid curve. If you read Chapter 6, the logistic (or sigmoid) function should be familiar, and demonstrates that logistic regression is acting as a layer in our neural network. The output node weights, biases, and sums each of the incoming values from the hidden layer. After that, it passes that resulting value through the logistic function so it outputs a number between 0 and 1. Much like logistic regression in Chapter 6, this represents a probability that the given color inputted into the neural network recommends a light font. If it is greater than or equal to .5, the neural network is suggesting a light font, but less than that will advise a dark font.

Here is the graph for the logistic function (Figure 7-7) using SymPy (Example 7-2).

Example 7-2. Logistic activation function in SymPy

```
from sympy import *

# plot logistic
x = symbols('x')
logistic = 1 / (1 + exp(-x))
plot(logistic)
```

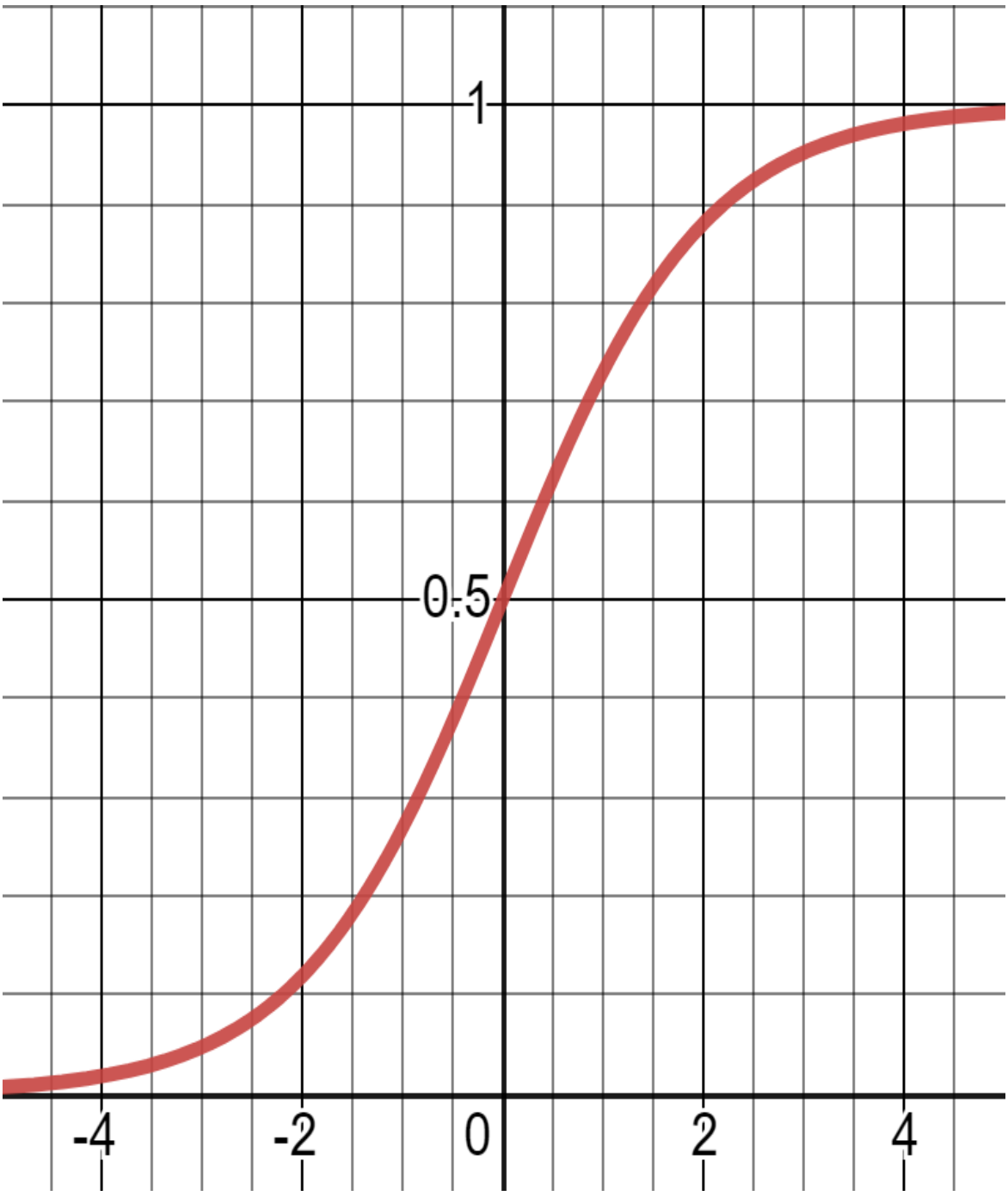


Figure 7-7. Logistic activation function

Note that when we pass a node's weighted, biased, and summed value through an activation function, we now call that an **activated output** meaning it has been filtered through the activation function. When the activated output leaves the hidden layer, the signal is ready to be fed into the next layer. The activation function could have strengthened, weakened, or left the signal as-is. This is where the brain and synapse metaphor for neural networks comes from. S Given the potential for complexity, you

might be wondering if there are other activation functions. Some common ones as shown in Table 7-1.

Table 7-1. Common Activation Functions

Name	Typical Layer Used	Description	Notes
Linear	Output	Leaves values as-is	Not commonly used

Logistic	Output	S-shaped sigmoid curve	Compresses values between 0 and 1, often assists binary classifcation
Tangent Hyperbolic	Hidden	tanh, S-shaped sigmoid curve between -1 and 1	Assists in “centering” data by bringing mean close to 0
ReLU	Hidden	Turns negative values to 0	Popular activation faster than sigmoid and tanh, mitigates vanishing gradient problems and computationally cheap
Leaky ReLU	Hidden	Multiplies negative values by .01	Controversial variant of ReLU that marginalizes rather than eliminates negative values
Softmax	Output	Ensures all output nodes add up to 1.0	Useful for multiple classifications and rescaling outputs so they add up to 1.0

This is not a comprehensive list of activation functions, and in theory any function could be an activation function in a neural network.

While this neural network seemingly supports two classes (light or dark font) it actually is modeled towards one class: whether or not a font should be light (1) or not (0). If you wanted to support multiple classes, you can add more output nodes for each class. For instance, if you are trying to recognize handwritten digits 0-9, there would be 10 output nodes representing the probability a given image is each of those numbers. You might consider using softmax as the output activation when you have multiple classes as well. Figure 7-8 shows an example of taking a pixellated image of a digit, where the pixels are broken up as individual neural network inputs and then passed through two middle layers, and then an output layer with 10 nodes representing probabilities for 10 classes (for the digits 0-9).

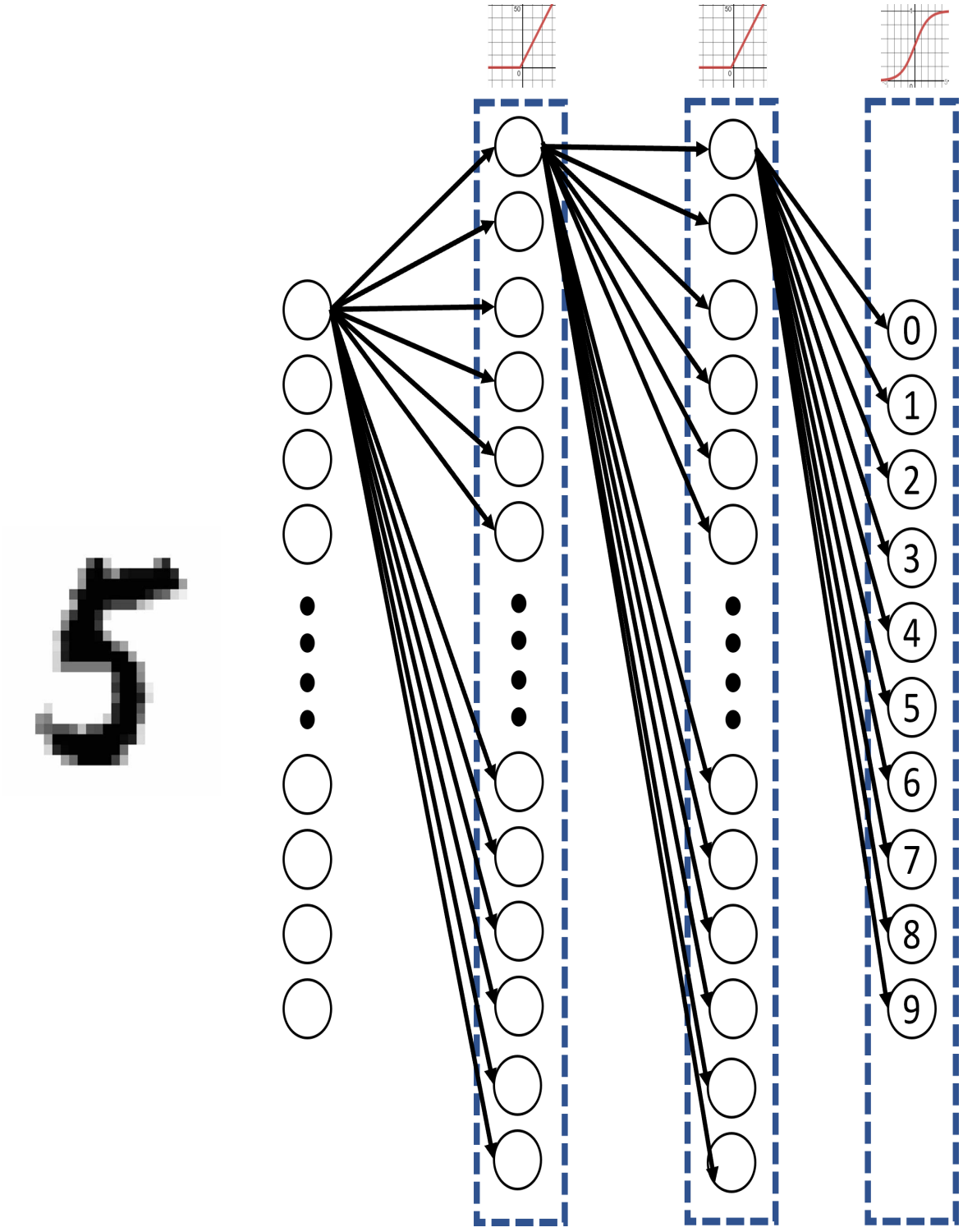


Figure 7-8. A neural network that takes each pixel as an input and predicts what digit the image contains

An example of using the MNIST dataset on a neural network can be found in the Appendix.

I DON'T KNOW WHAT ACTIVATION FUNCTION TO USE!

If you are unsure what activations to use, current best practices gravitate towards ReLU for middle layers and logistic (sigmoid) for output layer. If you have multiple classifications in the output, use softmax for the output layer.

Forward Propogation

Let's capture what we have learned so far using NumPy. Note I have not optimized the parameters (our weight and bias values) yet. We are going to initalize those with random values.

Example 7-3 is the Python code to create a simple feed-forward neural network that is not optimized yet. By "feed-forward", this means we are simply inputting a color into the neural network and seeing what it outputs. The weights and biases are randomly initialized and will be optimized later in this chapter, so do not expect a useful output yet.

Example 7-3. A simple forward propagation network with random weight and bias values.

```
import numpy as np
import pandas as pd
from sklearn.model_selection import train_test_split

all_data = pd.read_csv("https://tinyurl.com/y2qmhfsr")

# Extract the input columns, scale down by 255
all_inputs = (all_data.iloc[:, 0:3].values / 255.0)
all_outputs = all_data.iloc[:, -1].values

# Split train and test data sets
X_train, X_test, Y_train, Y_test = train_test_split(all_inputs, all_outputs,
test_size=1/3)
n = X_train.shape[0] # number of training records

# Build neural network with weights and biases
# with random initialization
w_hidden = np.random.rand(3, 3)
w_output = np.random.rand(1, 3)

b_hidden = np.random.rand(3, 1)
b_output = np.random.rand(1, 1)

# Activation functions
relu = lambda x: np.maximum(x, 0)
logistic = lambda x: 1 / (1 + np.exp(-x))

# Runs inputs through the neural network to get predicted outputs
def forward_prop(X):
    Z1 = w_hidden @ X + b_hidden
```

```
    A1 = relu(Z1)
    Z2 = w_output @ A1 + b_output
    A2 = logistic(Z2)
    return Z1, A1, Z2, A2

# Calculate accuracy
test_predictions = forward_prop(X_test.transpose())[3] # grab only output
layer, A2
test_comparisons = np.equal((test_predictions >= .5).flatten().astype(int),
Y_test)
accuracy = sum(test_comparisons.astype(int) / X_test.shape[0])
print("ACCURACY: ", accuracy)
```

A couple of things to note here. The dataset containing the RGB input values as well as output value (1 for light and 0 for dark) are contained at *https://tinyurl.com/y2qmhfsr*. I am scaling down the input columns R, G, and B values by a factor of 1/255 so they are between 0 and 1. This will help the training later so the number space is compressed.

Note I also separated `2/3` of the data for training and `1/3` for testing using Scikit-Learn, which we learned how to do in Chapter 5. `n` is simply the number of training data records.

Now bring your attention to these lines of code as shown in Example 7-4.

Example 7-4. The weight matrices and bias vectors in NumPy

```
# Build neural network with weights and biases
# with random initialization
w_hidden = np.random.rand(3, 3)
w_output = np.random.rand(1, 3)

b_hidden = np.random.rand(3, 1)
b_output = np.random.rand(1, 1)
```

These are declaring our weights and biases for both the hidden and output layers of our neural network. This may not be obvious yet but matrix multiplication is going to make our code powerfully simple using linear algebra and NumPy.

The weights and biases are going to be initialized as random values between 0 and 1. Let's look at the weight matrices first. When I ran the code I got these matrices.

$$W_{hidden} = \begin{bmatrix} 0.034535 & 0.5185636 & 0.81485028 \\ 0.3329199 & 0.53873853 & 0.96359003 \\ 0.19808306 & 0.45422182 & 0.36618893 \end{bmatrix}$$

$$W_{output} = \begin{bmatrix} 0.82652072 & 0.30781539 & 0.93095565 \end{bmatrix}$$

Note above that w_{hidden} is the weights in the hidden layer. The first row represents the first node weights w_1, w_2, and w_3. The second row is the second node with weights w_4,

w_5, and w_6. The third row is the third node with weights w_7, w_8, and w_9.

The output layer only has one node, meaning its matrix only has one row with weights w_{10}, w_{11}, and w_{12}.

See a pattern here? Each node is represented as a row in a matrix. If there are 3 nodes there are 3 rows. If there is 1 node there is 1 row. Each column holds a weight value for that node.

Let's look at the biases too. Since there is one bias per node, there's going to be 3 rows of biases for the hidden layer, and 1 row of biases for the output layer. There's only 1 bias per node so there will only be 1 column.

$$B_{hidden} = \begin{bmatrix} 0.41379442 \\ 0.81666079 \\ 0.07511252 \end{bmatrix}$$

$$B_{output} = [0.58018555]$$

Now let's compare these matrix values to our visualized neural network as shown in Figure 7-9.

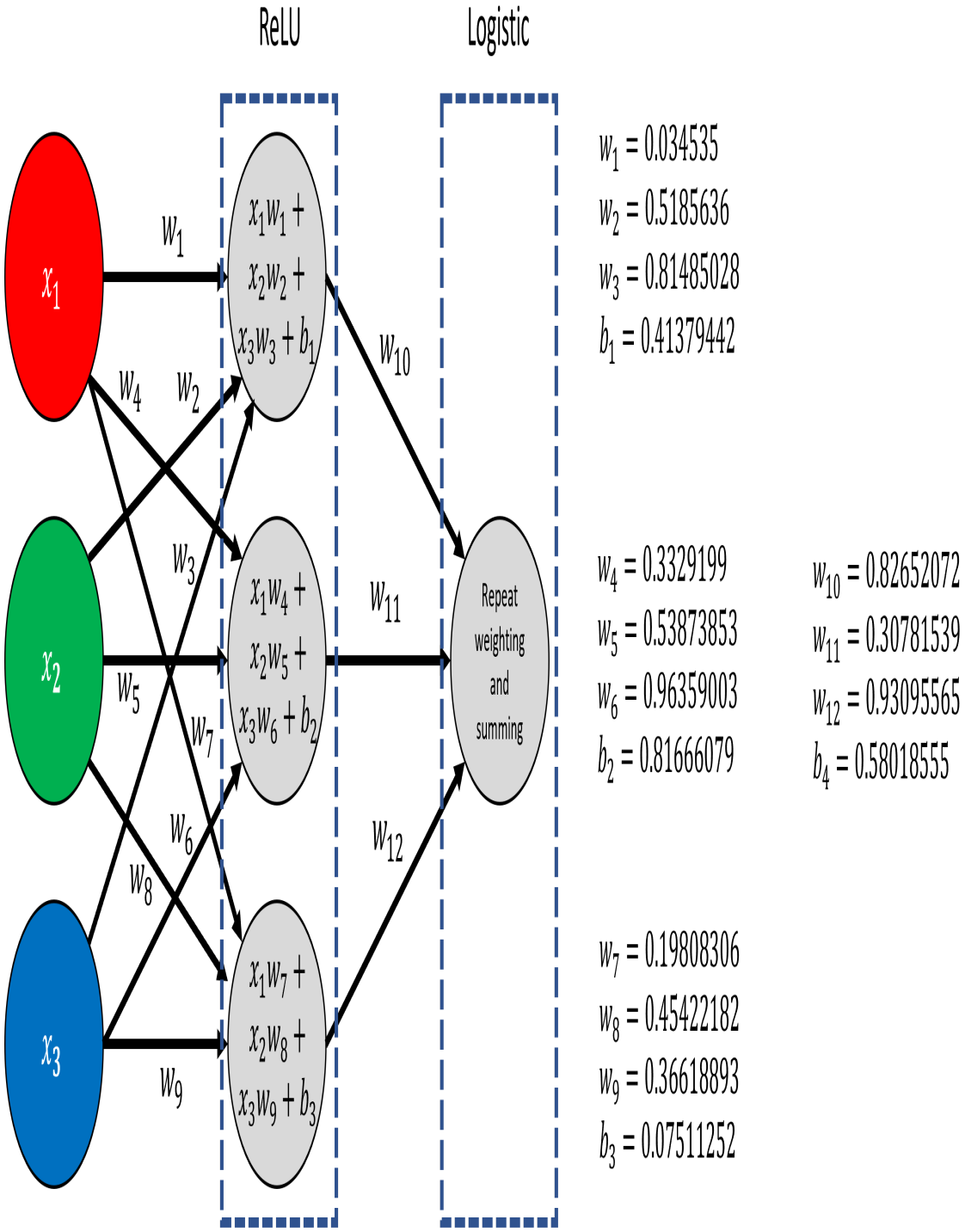


Figure 7-9. Visualizing our neural network against the weight and bias matrix values.

So besides being esoterically compact, what is the benefit of these weights and biases in these matrix form? Let's bring our attention to these lines of code in Example 7-5.

Example 7-5. The activation functions and forward propagation function for our neural network.

```
# Activation functions
relu = lambda x: np.maximum(x, 0)
logistic = lambda x: 1 / (1 + np.exp(-x))

# Runs inputs through the neural network to get predicted outputs
def forward_prop(X):
    Z1 = w_hidden @ X + b_hidden
    A1 = relu(Z1)
    Z2 = w_output @ A1 + b_output
    A2 = logistic(Z2)
    return Z1, A1, Z2, A2
```

This code above is important because it concisely executes our entire neural network using matrix multiplication and matrix-vector multiplication. It runs a color of three RGB inputs through the weights, biases, and activation functions in just a few lines of code.

I first declare the `relu()` and `logistic()` activation functions, which literally take a given input value and returns the output value from the curve. The `forward_prop()` function executes our entire neural network for a given color input `X` containing the R,G, and B values. It returns the matrix outputs from 4 stages: `Z1`, `A1`, `Z2`, and `A2`.

The hidden layer is represented by `Z1` and `A1`. `Z1` is the weights and biases applied to `X`. Then `A1` takes that output from `Z1` and pushes it through the activation `ReLU` function. `Z2` takes the output from `A1` and applies the output layer weights and biases. That output is in turn pushed through the activation function, the logistic curve, and becomes `A2`. The final stage `A2` is the prediction probability from the output layer, returning a value between 0 and 1. We call it `A2` because it is the "activated" output from layer 2.

Let's break this down in more detail starting with `Z1`.

$$Z_1 = W_{hidden}X + B_{hidden}$$

First we perform matrix-vector multiplication between W_{hidden} and the input color `X`. We multiply each row of W_{hidden} (each row being a set of weights for a node) with the vector `X` (the RGB color input values). We then add the biases to that result.

$$Z_1 = W_{hidden} X + B_{hidden}$$

$$Z1 = \begin{bmatrix} 0.034535 & 0.5185636 & 0.81485028 \\ 0.3329199 & 0.53873853 & 0.96359003 \\ 0.19808306 & 0.45422182 & 0.36618893 \end{bmatrix} \begin{bmatrix} 0.82652072 \\ 0.30781539 \\ 0.93095565 \end{bmatrix} + \begin{bmatrix} 0.41379442 \\ 0.81666079 \\ 0.07511252 \end{bmatrix}$$

$$Z1 = \begin{bmatrix} 0.946755221909086 \\ 1.33805678888247 \\ 0.644441873391768 \end{bmatrix} + \begin{bmatrix} 0.41379442 \\ 0.81666079 \\ 0.07511252 \end{bmatrix}$$

$$Z_1 = \begin{bmatrix} 1.36054964190909 \\ 2.15471757888247 \\ 0.719554393391768 \end{bmatrix}$$

Figure 7-10. Applying the hidden layer weights and biases to an input X using matrix-vector multiplication, as well as vector addition

That Z_1 vector is the raw output from the hidden layer, but we still need to pass it through the activation function to turn Z_1 into A_1. Easy enough. Just pass each value in

that vector through the ReLU function and it will give us A_1. Because all the values are positive, it should not have an impact.

$$A_1 = ReLU\left(Z_1\right)$$

$$A_1 = \begin{bmatrix} ReLU(1.36054964190909) \\ ReLU(2.15471757888247) \\ ReLU(0.719554393391768) \end{bmatrix} = \begin{bmatrix} 1.36054964190909 \\ 2.15471757888247 \\ 0.719554393391768 \end{bmatrix}$$

Now let's take that hidden layer output A_1 and pass it through the final layer to get Z_2 and then A_2. A_1 becomes the input into the output layer.

$$Z_2 = W_{output}A_1 + B_{output}$$

$$Z_2 = \begin{bmatrix} 0.82652072 & 0.3078159 & 0.93095565 \end{bmatrix} \begin{bmatrix} 1.36054964190909 \\ 2.15471757888247 \\ 0.719554393391768 \end{bmatrix} + \begin{bmatrix} 0.58018555 \end{bmatrix}$$

$$Z_2 = \begin{bmatrix} 2.45765202842636 \end{bmatrix} + \begin{bmatrix} 0.58018555 \end{bmatrix}$$

$$Z_2 = \begin{bmatrix} 3.03783757842636 \end{bmatrix}$$

Finally pass this single value in Z_2 through the activation function to get A_2. This will produce a prediction of approximately `0.95425`.

$$A_2 = logistic\left(Z_2\right)$$

$$A_2 = logistic\left(\begin{bmatrix} 3.0378364795204 \end{bmatrix}\right)$$

$$A_2 = logistic\left(\begin{bmatrix} 3.0378364795204 \end{bmatrix}\right)$$

$$A_2 = 0.954254478103241$$

That executes our entire neural network, although we have not trained it yet. But take a moment to appreciate that we have taken all these input values, weights, biases, and nonlinear functions and turned it all into a single value that will provide a prediction.

Again, `A2` is the final output that makes a prediction whether that background color need a light (1) or dark (1) font. Even though our weights and biases have not been optimized yet, let's calculate our accuracy as shown in Example 7-6. Take the test dataset `X_test`, transpose it, and pass it through the `forward_prop()` function but only grab the `A2` vector with the predictions for each test color. Then compare the predictions to the actuals, and calculate the percentage of correct predictions.

Example 7-6. Calculating Accuracy

```
# Calculate accuracy
test_predictions = forward_prop(X_test.transpose())[3]  # grab only A2
test_comparisons = np.equal((test_predictions >= .5).flatten().astype(int),
Y_test)
accuracy = sum(test_comparisons.astype(int) / X_test.shape[0])
print("ACCURACY: ", accuracy)
```

When I run the whole code in Example 7-3, I roughly got anywhere from 55% to 67% accuracy. Remember the weights and biases are randomly generated so answers will vary. While this may seem high given the parameters were randomly generated, remember that the output predictions are binary: light or dark. Therefore a random coin flip might as well produce this outcome for each prediction, so this number should not be surprising.

> **DO NOT FORGET TO CHECK FOR IMBALANCED DATA!**
>
> As discussed in Chapter 6, do not forget to analyze your data to check for imbalanced classes. This whole background color dataset is a little imbalanced. 512 colors have output of 0 and 833 have an output of 1. This can skew accuracy and might be why our random weights and biases gravitate higher than 50% accuracy. If the data is extremely imbalanced (as in 99% of the data is one class), then remember to use confustion matrices to track the false positives and false negatives.

Alright, does everything structurally make sense so far? Feel free to review everything up to this point before moving on. We just have one final piece to cover: optimizing the weights and biases. Hit the espresso machine or nitro coffee bar, because this is the most involved Calculus we will be doing in this book!

Backpropogation

Before we start using stochastic gradient descent to optimize our neural network, a challenge we have is figuring out how to change each of the weight and bias values accordingly even though they all are tangled together to create the output variable, which then is used to calculate the residuals. How do we find the derivative of each weight w_i and bias b_i variable? We need to first learn the chain rule.

The Chain Rule

Put aside the neural network for a moment and let's learn the chain rule with a simple algebraic example. Let's say you are given two functions:

$$y = x^2 + 1$$

$$z = y^3 - 2$$

Notice above the two functions are linked, because the `y` is the output variable in the first function but is the input variable in the second. This means we can substitute the first function `y` into the second function `z` like this:

$$z = \left(x^2 + 1\right)^3 - 2$$

So what is the derivative for `z` with respect to `x`? We already have the subsitution expressing `z` in terms of `x`. Let's use SymPy to calculate that in Example 7-7.

Example 7-7. Finding the derivative of z with respect to x

```
from sympy import *

z = (x**2 + 1)**3 - 2
dz_dx = diff(z, x)
print(dz_dx)

# 6*x*(x**2 + 1)**2
```

So our derivative for `z` with respect to `x` is $6x\left(x^2 + 1\right)^2$.

$$\frac{dz}{dx}\left(\left(x^2 + 1\right)^3 - 2\right)$$

$$= 6x\left(x^2 + 1\right)^2$$

But look at this. Let's start over and take a different approach. If we take the derivatives of the `y` and `z` functions separately, and then multiply them together, this also produces the derivative of `z` with respect to `x`! Let's try it.

$$\frac{dy}{dx}\left(x^2 + 1\right) = 2x$$

$$\frac{dz}{dy}\left(y^3 - 2\right) = 3y^2$$

$$\frac{dz}{dx} = (2x)\left(3y^2\right) = 6xy^2$$

Alright, $6xy^2$ may not look like $6x\left(x^2 + 1\right)^2$, but that's only because we have not subsituted the `y` function yet. Do that so the entire $\frac{dz}{dx}$ derivative is expressed in terms of `x` without `y`.

$$\frac{dz}{dx} = 6xy^2 = 6x\left(x^2 + 1\right)^2$$

Now we see we got the same derivative function $6x\left(x^2+1\right)^2$!

What we have witnessed here is the **chain rule**, which says that for a given function `y` (with input variable `x`) composed into another function `z` (with input variable `y`), we can find the derivative of `z` with respect to `x` by multiplying the two respective derivatives together.

$$\frac{dz}{dx} = \frac{dz}{dy} \times \frac{dy}{dx}$$

Example 7-8 shows the SymPy code that makes this comparison, showing the derivative from the chain rule is equal to the derivative of the subsituted function.

Example 7-8. Calculating the derivative dz/dx with and without the chain rule, but still getting the same answer

```
from sympy import *

x, y = symbols('x y')

# derivative for first function
# need to underscore y to prevent variable clash
_y = x**2 + 1
dy_dx = diff(_y)

# derivative for second function
z = y**3 - 2
dz_dy = diff(z)

# Calculate derivative with and without
# chain rule, substitute y function
dz_dx_chain = (dy_dx * dz_dy).subs(y, _y)
dz_dx_no_chain = diff(z.subs(y, _y))

# Prove chain rule by showing both are equal
print(dz_dx_chain) # 6*x*(x**2 + 1)**2
print(dz_dx_no_chain) # 6*x*(x**2 + 1)**2
```

The chain rule is a key part of training a neural network with the proper weights and biases. Rather than untangle the derivative of each node in a nested onion fashion, we can multiply the derivatives across each node instead which is mathematically a lot easier.

Calculating the Weight and Bias Derivatives

We are not quite ready to apply stochastic gradient descent to train our neural network yet. We have to get the partial derivatives with respect to the weights W_i and biases B_i, and we now have the chain rule to help us.

While the process is largely the same, there is a complication using stochastic gradient descent on neural networks. The nodes in one layer feed their weights and biases into the next layer, which then applies another set of weights and biases. This creates an onion-like nesting we need to untangle starting with the output layer.

During gradient descent, we need to figure out which weights and biases should be adjusted, and by how much, to reduce the overall cost function. The cost for a single prediction is going to be the squared output of the neural network A_2 minus the prediction Y.

$$C = (A_2 - Y)^2$$

But let's peel back a layer. That activated output A_2 is just Z_2 with the activation function.

$$A_2 = sigmoid\left(Z_2\right)$$

Z_2 in turn is the output weights and biases applied to activation output A_1, which comes from the hidden layer.

$$Z_2 = W_2 A_1 + B_2$$

A_1 is built off Z_1 which is passed through the ReLU activation function.

$$A_1 = ReLU\left(Z_1\right)$$

Finally, Z_1 is the input `X` values weighted and biased by the hidden layer.

$$Z_1 = W_1 X + B_1$$

We need to find the weights and biases contained in the W_1, B_1, W_2, and B_2 matrices and vectors that will minimize our loss. By nudging their slopes, we can change the weights and biases that have the most impact in minimizing loss. However, each little nudge on a weight or bias is going to propogate all the way to the loss function on the outer layer. This is where the chain rule can help us figure out this impact.

Let's focus on finding the relationship on a weight from the output layer W_2, and the cost function C. A change in the weight W_2 results in a change to the unactivated output Z_2. That then changes the activated output A_2, which changes the cost function C. Using the chain rule, we can define the derivative of C with respect to W_2 as this.

$$\frac{dC}{dW_2} = \frac{dZ_2}{dW_2} \frac{dA_2}{dZ_2} \frac{dC}{dA_2}$$

When we multiply these three gradients together, we get a measure of how much a change to W_2 will change the cost function C.

Now we will calculate these three derivatives. Let's use SymPy to calculate the derivative of the cost function with respect to `A2` in Example 7-9.

Example 7-9. Calculating the derivative of the cost function with respect to A2.

```
from sympy import *

A2, y = symbols('A2 Y')
C = (A2 - Y)**2
dC_dA2 = diff(C, A2)
print(dC_dA2) # 2*A2 - 2*Y
```

$$\frac{dC}{dA_2} = 2A_2 - 2y$$

Next let's get the derivative of A_2 with respect to Z_2. Remember that $A2$ is the output of an activation function, in this case the logistic function. So we really are just taking the derivative of a sigmoid curve.

Example 7-10. Finding the derivative of A_2 with respect to Z_2

```
from sympy import *

Z2 = symbols('Z2')

logistic = lambda x: 1 / (1 + exp(-x))

A2 = logistic(Z2)
dA2_dZ2 = diff(A2, Z2)
print(dA2_dZ2) # exp(-Z2)/(1 + exp(-Z2))**2
```

$$\frac{dA_2}{dZ_2} = \frac{e^{-Z_2}}{(1 + e^{-Z_2})^2}$$

The derivative of Z_2 with respect to a w_2 is going to work out to just be A_1, as it is just a linear function and going to return the slope.

Example 7-11. Derivative of Z_2 with respect to W_2

```
from sympy import *

A1, W2, B2 = symbols('A1, W2, B2')

Z2 = A1*W2 + B2
dZ2_dW2 = diff(Z2, W2)
print(dZ2_dW2) # A1
```

$$\frac{dZ_2}{dW_1} = A_1$$

Putting it all together here is the derivative to find how much a change in a weight in W_2 affects the cost function C.

$$\frac{dC}{dw_2} = \frac{dZ_2}{dw_2}\frac{dA_2}{dZ_2}\frac{dC}{dA_2} = (A_1)\left(\frac{e^{-Z_2}}{(1+e^{-Z_2})^2}\right)(2A_2 - 2y)$$

When we run an input `X` with the three input R, G, and B values we will have values for A_1, A_2, Z_2, and y.

> **DON'T GET LOST IN THE MATH!**
>
> It is easy to get lost in the math at this point and forget what you were trying to achieve in the first place, which is finding the derivative of the cost function with respect to a weight (W_2) in the ouput layer. When you find yourself in the weeds and forgetting what you were trying to do, then step back, take a breath, get a coffee, and remind yourself what you were trying to accomplish. If you cannot, you should start over from the beginning and work your way to the point you got lost.

However this is just one component of the neural network, the derivative for W_2. Here are the SymPy calculations in Example 7-12 for the rest of the partial derivatives we will need for chaining.

Example 7-12. Calculating all the partial derivatives we will need for our neural network

```
from sympy import *

W1, W2, B1, B2, A1, A2, Z1, Z2, X, Y = \
    symbols('W1 W2 B1 B2 A1 A2 Z1 Z2 X Y')

# Calculate derivative of cost function with respect to A2
C = (A2 - Y)**2
dC_dA2 = diff(C, A2)
print("dC_dA2 = ", dC_dA2) # 2*A2 - 2*Y

# Calculate derivative of A2 with respect to Z2
logistic = lambda x: 1 / (1 + exp(-x))
_A2 = logistic(Z2)
dA2_dZ2 = diff(_A2, Z2)
print("dA2_dZ2 = ", dA2_dZ2) # exp(-Z2)/(1 + exp(-Z2))**2

# Calculate derivative of Z2 with respect to A1
_Z2 = A1*W2 + B2
dZ2_dA1 = diff(_Z2, A1)
print("dZ2_dA1 = ", dZ2_dA1) # W2

# Calculate derivative of Z2 with respect to W2
dZ2_dW2 = diff(_Z2, W2)
print("dZ2_dW2 = ", dZ2_dW2) # A1
```

```
# Calculate derivative of Z2 with respect to B2
dZ2_dB2 = diff(_Z2, B2)
print("dZ2_dB2 = ", dZ2_dB2) # 1

# Calculate derivative of A1 with respect to Z1
relu = lambda x: Max(x, 0)
_A1 = relu(Z1)

d_relu = lambda x: x > 0 # Slope is 1 if positive, 0 if negative
dA1_dZ1 = d_relu(Z1)
print("dA1_dZ1 = ", dA1_dZ1) # Z1 > 0

# Calculate derivative of Z1 with respect to W1
_Z1 = X*W1 + B1
dZ1_dW1 = diff(_Z1, W1)
print("dZ1_dW1 = ", dZ1_dW1) # X

# Calculate derivative of Z1 with respect to B1
dZ1_dB1 = diff(_Z1, B1)
print("dZ1_dB1 = ", dZ1_dB1) # 1
```

Notice that ReLU was calculated manually rather than using SymPy. This is because derivatives work with smooth curves, not jagged corners which exists on ReLU. But it's easy to hack around that simply by declaring the slope to be 1 for positive numbers, and 0 for negative numbers. This makes sense because negative numbers have a flat line with slope 0. But positive numbers are left as-is with a 1-to-1 slope.

These partial derivatives can be chained together to create new partial derivatives with respect to the weights and biases. Let's get all four partial derivatives for the weights in W_1, W_2, B_1, and B_2 with respect to the cost function. We already walked through $\frac{dC}{dw_2}$. Let's show it alongside the other three chained derivatives we need.

$$\frac{dC}{dW_2} = \frac{dZ_2}{dW_2}\frac{dA_2}{dZ_2}\frac{dC}{dA_2} = (A_1)\left(\frac{e^{-Z_2}}{(1+e^{-Z_2})^2}\right)(2A_2 - 2y)$$

$$\frac{dC}{dB_2} = \frac{dZ_2}{dB_2}\frac{dA_2}{dZ_2}\frac{dC}{dA_2} = (1)\left(\frac{e^{-Z_2}}{(1+e^{-Z_2})^2}\right)(2A_2 - 2y)$$

$$\frac{dC}{dW_1} = \frac{dC}{DA_2}\frac{DA_2}{dZ_2}\frac{dZ_2}{dA_1}\frac{dA_1}{dZ_1}\frac{dZ_1}{dW_1} = (2A_2 - 2y)\left(\frac{e^{-Z_2}}{(1+e^{-Z_2})^2}\right)(W_2)(Z_1 > 0)(X)$$

$$\frac{dC}{dB_1} = \frac{dC}{DA_2}\frac{DA_2}{dZ_2}\frac{dZ_2}{dA_1}\frac{dA_1}{dZ_1}\frac{dZ_1}{dB_1} = (2A_2 - 2y)\left(\frac{e^{-Z_2}}{(1+e^{-Z_2})^2}\right)(W_2)(Z_1 > 0)(1)$$

We will use these chained gradients to calculate the slope for the cost function C with respect to W_1, B_1, W_2, and B_2.

Stochastic Gradient Descent

We are now ready to integrate the chain rule to perform stochastic gradient descent. To keep things simple, we are going to only sample one training record on every iteration. Batch and mini-batch gradient descent are commonly used in neural networks and deep learning, but there's enough linear algebra and Calculus to juggle just one sample per iteration.

Let's take a look at our full implementation of our neural network, with backpropogated stochastic gradient descent, in Example 7-13.

Example 7-13. Implementing a Neural Network using Stochastic Gradient Descent

```
import numpy as np
import pandas as pd
from sklearn.model_selection import train_test_split

all_data = pd.read_csv("https://tinyurl.com/y2qmhfsr")

# Learning rate controls how slowly we approach a solution
# Make it too small, it will take too long to run.
# Make it too big, it will likely overshoot and miss the solution.
L = 0.05

# Extract the input columns, scale down by 255
all_inputs = (all_data.iloc[:, 0:3].values / 255.0)
all_outputs = all_data.iloc[:, -1].values

# Split train and test data sets
X_train, X_test, Y_train, Y_test = train_test_split(all_inputs, all_outputs,
test_size=1 / 3)
n = X_train.shape[0]

# Build neural network with weights and biases
# with random initialization
w_hidden = np.random.rand(3, 3)
w_output = np.random.rand(1, 3)

b_hidden = np.random.rand(3, 1)
b_output = np.random.rand(1, 1)

# Activation functions
relu = lambda x: np.maximum(x, 0)
logistic = lambda x: 1 / (1 + np.exp(-x))

# Runs inputs through the neural network to get predicted outputs
def forward_prop(X):
    Z1 = w_hidden @ X + b_hidden
    A1 = relu(Z1)
```

```
    Z2 = w_output @ A1 + b_output
    A2 = logistic(Z2)
    return Z1, A1, Z2, A2

# Derivatives of Activation functions
d_relu = lambda x: x > 0
d_logistic = lambda x: np.exp(-x) / (1 + np.exp(-x)) ** 2

# returns slopes for weights and biases
# using chain rule
def backward_prop(Z1, A1, Z2, A2, X, Y):
    dC_dA2 = 2 * A2 - 2 * Y
    dA2_dZ2 = d_logistic(Z2)
    dZ2_dA1 = w_output
    dZ2_dW2 = A1
    dZ2_dB2 = 1
    dA1_dZ1 = d_relu(Z1)
    dZ1_dW1 = X
    dZ1_dB1 = 1

    dC_dW2 = dC_dA2 @ dA2_dZ2 @ dZ2_dW2.T

    dC_dB2 = dC_dA2 @ dA2_dZ2 * dZ2_dB2

    dC_dA1 = dC_dA2 @ dA2_dZ2 @ dZ2_dA1

    dC_dW1 = dC_dA1 @ dA1_dZ1 @ dZ1_dW1.T

    dC_dB1 = dC_dA1 @ dA1_dZ1 * dZ1_dB1

    return dC_dW1, dC_dB1, dC_dW2, dC_dB2


# Execute gradient descent
for i in range(100_000):
    # randomly select one of the training data
    idx = np.random.choice(n, 1, replace=False)
    X_sample = X_train[idx].transpose()
    Y_sample = Y_train[idx]

    # run randomly selected training data through neural network
    Z1, A1, Z2, A2 = forward_prop(X_sample)

    # distribute error through backpropogation
    # and return slopes for weights and biases
    dW1, dB1, dW2, dB2 = backward_prop(Z1, A1, Z2, A2, X_sample, Y_sample)

    # update weights and biases
    w_hidden -= L * dW1
    b_hidden -= L * dB1
    w_output -= L * dW2
    b_output -= L * dB2

# Calculate accuracy
test_predictions = forward_prop(X_test.transpose())[3]  # grab only A2
```

```
test_comparisons = np.equal((test_predictions >= .5).flatten().astype(int),
Y_test)
accuracy = sum(test_comparisons.astype(int) / X_test.shape[0])
print("ACCURACY: ", accuracy)
```

There is a lot going on here, but it builds on everything else we learned in this chapter. We perform 100,000 iterations of stochastic gradient descent. Splitting the training and testing data by `2/3` and `1/3` respectively, I get approximately 97-99% accuracy in my test dataset depending on how the randomness works out. This means after training, my neural network correctly identifies 97-99% of the test data with the right light/dark font predictions.

The `backward_prop()` function is key here, implementing the chain rule to take the error in the output node (the squared residual), and then divides it up and distributes it backwards to the output and hidden weights/biases to get the slopes with respect to each weight/bias. We then take those slopes and nudge the weights/biases in the `for` loop respectively, multiplying with the learning rate `L` just like we did in Chapter 5 and Chapter 6. We do some matrix-vector multiplication to distribute the error backwards based on the slopes, and we transpose matrices and vectors when needed so the dimensions between rows and columns match up.

If you want to make the neural network a bit more interactive, here's a snippit of code in Example 7-14 where we can type in different background colors (through an R,G, and B value) and see if it predicts a light or dark font. Append it to the bottom of the previous code Example 7-13 and give it a try!

Example 7-14. Adding an interactive shell to our neural network

```
# Interact and test with new colors
def predict_probability(r, g, b):
    X = np.array([[r, g, b]]).transpose() / 255
    Z1, A1, Z2, A2 = forward_prop(X)
    return A2

def predict_font_shade(r, g, b):
    output_values = predict_probability(r, g, b)
    if output_values > .5:
        return "DARK"
    else:
        return "LIGHT"

while True:
    col_input = input("Predict light or dark font. Input values R,G,B: ")
    (r, g, b) = col_input.split(",")
    print(predict_font_shade(int(r), int(g), int(b)))
```

Building your own neural network from scratch is a lot of work and math, but it gives you insight into their true nature. By working through the layers, the Calculus, and the

linear algebra, we get a stronger sense of what deep learning libraries like Tensorflow do behind the scenes.

As you have gathered from reading this entire chapter, there are a lot of moving parts to make a neural network tick. It can be helpful to put a breakpoint in different parts of the code to see what each matrix operation is doing. You can also port the code into a Jupyter Notebook (or use Google's Collab service) to get more visual insight into each step.

3BLUE1BROWN ON BACKPROPOGATION

3Blue1Brown has some classic videos talking about backpropagation and the Calculus behind neural networks.

https://youtu.be/Ilg3gGewQ5U

https://youtu.be/tIeHLnjs5U8

Using Scikit-Learn

There is some limited amount of neural network functionality in Scikit-Learn. If you are serious about deep learning you will probably want to study Tensorflow and get a computer with a strong GPU (there's a great excuse to get that gaming computer you always wanted!). But Scikit-Learn does have some convenient models available, including the `MLPClassifier`, which stands for "multi-layer perceptron classifier." This is a neural network designed for classifcation, and uses a logistic output activation by default.

Example 7-15 is a Scikit-Learn version of the background color classification application we developed. The `activation` argument specifies the hidden layer

Example 7-15. Using Scikit-Learn Neural Network Classifier

```
import pandas as pd
# load data
from sklearn.model_selection import train_test_split
from sklearn.neural_network import MLPClassifier

df = pd.read_csv('https://bit.ly/3GsNzGt', delimiter=",")

# Extract input variables (all rows, all columns but last column)
# Note we should do some linear scaling here
X = (df.values[:, :-1] / 255.0)

# Extract output column (all rows, last column)
Y = df.values[:, -1]

# Separate training and testing data
```

```
X_train, X_test, Y_train, Y_test = train_test_split(X, Y, test_size=1/3)

nn = MLPClassifier(solver='sgd',
                   hidden_layer_sizes=(3, ),
                   activation='relu',
                   max_iter=100_000,
                   learning_rate_init=.05)

nn.fit(X_train, Y_train)

# Print weights and biases
print(nn.coefs_ )
print(nn.intercepts_)

print("Training set score: %f" % nn.score(X_train, Y_train))
print("Test set score: %f" % nn.score(X_test, Y_test))
```

Running this code above I get about 99.3% accuracy on my test data.

> **MNIST EXAMPLE USING SCIKIT-LEARN**
>
> To see a Scikit-Learn example predicting handwritten digits using the MNIST dataset, turn to Appendix A.

Limitations of Neural Networks and Deep Learning

For all of its strengths, neural networks struggle with certain types of tasks. This flexibility with layers, nodes, and activation functions makes it flexible fitting to data in a nonlinear manner… probably too flexible. Why? It can overfit to the data. Andrew Ng, a pioneer in deep learning education and the former head of Google Brain, mentioned this as a problem in a press conference in 2021. Asked why machine learning has not replaced radiologists yet, this was his answer:

It turns out that when we collect data from Stanford Hospital, then we train and test on data from the same hospital, indeed, we can publish papers showing [the algorithms] are comparable to human radiologists in spotting certain conditions.

It turns out [that when] you take that same model, that same AI system, to an older hospital down the street, with an older machine, and the technician uses a slightly different imaging protocol, that data drifts to cause the performance of AI system to degrade significantly. In contrast, any human radiologist can walk down the street to the older hospital and do just fine.

So even though at a moment in time, on a specific data set, we can show this works, the clinical reality is that these models still need a lot of work to reach production.

—Andrew Ng

[1] *https://spectrum.ieee.org/andrew-ng-xrays-the-ai-hype*

In other words, the machine learning overfitted to the Stanford hospital training and testing dataset. When taken to other hospitals with different machinery, the performance degraded significantly due to the overfitting.

The same challenges occur with autonomous vehicles and "self-driving" car startups. It is not just enough to train a neural network on one stop sign, but it has to be trained on countless combinations of conditions around that stop sign: good weather, rainy weather, night and day, with graffiti, blocked by a tree, in different locales, etc. In traffic scenarios, think of all the different types of vehicles, pedestrians, pedestrians dressed in costumes, and infinite number of edge cases that will be encountered! There is simply no effective way to capture every type of event that is encountered on the road just by having more weights and biases in a neural network.

This is why autonomous vehicles themselves do not use neural networks in an end-to-end manner. Instead, different software and sensor modules are broken up where one module may use a neural network to draw a box around an object. Then another module will use a different neural network to classify the object in that box, such as a pedestrian. From there, traditional rule-based logic will attempt to predict the path of the pedestrian and hardcoded logic will choose from different conditions on how to react. The machine learning was limited to label-making activity, not the tactics and maneuvers of the vehicle. On top of that, basic sensors like radar will simply stop if an unknown object is detected in front of the vehicle, and this is just another piece of the software stack that does not use machine learning or deep learning.

This might be surprising given all the media headlines about neural networks and deep learning beating humans in games like Chess and Go, or even besting pilots in combat flight simulations. It is important to remember in reinforcement learning environments like these that simulations are closed-worlds, where infinite amounts of labelled data can

be generated and learned through a virtual finite world. However the real world is not a simulation where we can generate unlimited amounts of data (and no, this is not a philosphy book so we will pass on discussions whether we live in a simulation). Collecting data in the real world is expensive and hard! On top of that, the real world is filled with infinite unpredictability and rare events. All these factors drive machine learning practitioners to resort to data entry labor to label pictures of traffic objects and other data. Autonomous vehicle startups often have to pair this kind of data entry work with simulated data, because the miles needed to generate training data is too astronomical to gather simply by driving a fleet of vehicles millions of miles.

These are all reasons why AI research likes to use board games and video games, because labelled data can be generated easily and cleanly. Francis Chollet, a renowned engineer at Google who developed Keras for Tensorflow (and also wrote a great book Deep Learning with Python), shared some insight on this:

> *The thing is, once you pick a measure, you're going to take whatever shortcut is available to game it. For instance, if you set chess-playing as your measure of intelligence (which we started doing in the 1970s until the 1990s), you're going to end up with a system that plays chess, and that's it. There's no reason to assume it will be good for anything else at all. You end up with tree search and minimax, and that doesn't teach you anything about human intelligence. Today, pursuing skill at video games like Dota or StarCraft as a proxy for general intelligence falls into the exact same intellectual trap…*
>
> *If I set out to 'solve' Warcraft III at a superhuman level using deep learning, you can be quite sure that I will get there as long as I have access to sufficient engineering talent and computing power (which is on the order of tens of millions of dollars for a task like this). But once I'd have done it, what would I have learned about intelligence or generalization? Well, nothing. At best, I'd have developed engineering knowledge about scaling up deep learning. So I don't really see it as scientific research because it doesn't teach us anything we didn't already know. It doesn't answer any open question. If the question was, 'Can we play X at a superhuman level?,' the answer is definitely, 'Yes, as long as you can generate a sufficiently dense sample of training situations and feed them into a sufficiently expressive deep learning model.' We've known this for some time.*
>
> —Francois Chollet

[2] *https://www.theverge.com/2019/12/19/21029605/artificial-intelligence-ai-progress-measurement-benchmarks-interview-francois-chollet-google*

In other words, we have to be careful to not conflate an algorithm's performance in a game with broader capabilities that have yet to be solved. Machine learning, neural networks, and deep learning all work narrowly on defined problems. It cannot broadly

reason or choose its own tasks, or ponder objects it has not seen before. Like any coded application, it only does what it was programmed to do.

Solve the problem. With whatever tool it takes. There should be no partiality to neural networks or any other tool in the box. With all of this in mind, using a neural network might not be the best option for the task in front of you. It is important to always consider what you are striving to resolve without making any tool at your disposal the primary objective. The use of deep learning has to be strategic and warranted. There are certainly use cases, but in most of your everyday work you will likely have more success with simpler and more biased models like linear regression, logistic regression, or traditional rule-based systems. But if you find yourself having to classify objects in images, and you have the budget and labor to build that dataset, then deep learning is going to be your best bet.

IS AN AI WINTER COMING?

Are neural networks and deep learning useful? Absolutely! And it is definitely worth learning.

That being said, there is a good chance you have seen media, politicians, and tech celebrities hail deep learning as some general artifical intelligence that can match, if not outperform, human intelligence and even destined to control the world. This is simply not true. Neural networks are *loosely* inspired by the human brain, but are by no means a replication of them. Their capabilities are nowhere near on par with what you see in movies like *The Terminator*, *Westworld*, or *WarGames*. Instead, neural networks and deep learning work narrowly on specific problems, like recognizing dog and cat photos after being optimized on thousands of images. As stated earlier, it cannot reason or choose its own tasks, or contemplate uncertainty or objects it has not seen before. It only does what it was programmed to do.

This disconnect may have inflated investment and expectations, resulting in a bubble that could burst. This would bring about another "AI winter," where disillusionment and disappointment dry up funding in AI research. In North America, Europe, and Japan AI winters have happened multiple times since the 1960's. There's a good chance another AI winter is around the corner, but it does not mean neural networks and deep learning will lose usefulness. They will continue to be applied in the problems they are good at: computer vision, audio, natural language, and a few other domains. Maybe you can discover new ways to use them! Use what works best whether its linear regression, logistic regression, a traditional rule-based software, or a neural network. There is much more power in the simplicity of the right tool for the task you are facing.

Conclusions

Neural networks and deep learning offer some exciting applications, and we just scratched the surface in this one short chapter. From recognizing images to processing natural language, there continues to be groundbreaking use cases in applying neural networks and its different flavors of deep learning.

From scratch, we learned how to structure a simple neural network with one hidden layer to predict whether or not a light or dark font should be used against a background

color. We also applied some advanced Calculus concepts to calculate partial derivatives of nested functions, and applied it to stochastic gradient descent to train our neural network. We touched on libraries like Scikit-Learn. Whiel we do not have the bandwidth in this book to talk about Tensorflow and more advanced applications, there are great resources out there to expand your knowledge.

3Blue1Brown has a fantastic playlist on neural networks and backpropogation, and it is worth watching multiple times. Josh Starmer's StatQuest playlist on neural networks is helpful as well, particularly in visualizing neural networks as manifold manipulation. Another great video about manifold theory and neural networks can be found here on The Art of the Problem. Finally when you are ready to deep-dive, check out Aurélien Géron's book by O'Reilly and Francois Chollet's Deep Learning with Python.

If you made it to the end of this chapter and feel you absorbed everything within reason, congrats! You have effectively learned not just probability, statistics, calculus, and linear algebra but you applied it to practical applications like linear regression, logistic regression, and neural networks. We will talk about how you can proceed going forward in the next chapter, and start a new phase of your professional growth.

About the Author

Thomas Nield is the founder of Nield Consulting Group as well as an instructor at O'Reilly Media and University of Southern California. He enjoys making technical content relatable and relevant to those unfamiliar or intimidated by it. Thomas regularly teaches classes on data analysis, machine learning, mathematical optimization, and practical artificial intelligence. He's authored two books, including *Getting Started with SQL* (O'Reilly) and *Learning RxJava* (Packt).