Half Title Page

Title Page

LOC Page

Vince: to Riggins

Geraint: also, to Riggins

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Foreword

This is the foreword

Preface

This is the preface.

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______ Getting Started

Introduction

HANK you for starting to read this book. This book aims to bring together two fascinating topics:

- Problems that can be solved using mathematics;
- Software that is free to use and change.

What we mean by both of those things will become clear through reading this chapter and the rest of the book.

1.1 WHO IS THIS BOOK FOR?

Anyone who is interested in using mathematics and computers to solve problems will hopefully find this book helpful.

If you are a student of a mathematical discipline, a graduate student of a subject like operational research, a hobbyist who enjoys solving the travelling salesman problem or even if you get paid to do this stuff: this book is for you. We will introduce you to the world of open source software that allows you to do all these things freely.

If you are a student learning to write code, a graduate student using databases for their research, an enthusiast who programmes applications to help coordinate the neighbourhood watch, or even if you get paid to write software: this book is for you. We will introduce you to a world of problems that can be solved using your skill sets.

It would be helpful for the reader of this book to:

- Have access to a computer and be able to connect to the internet (at least once) to be able to download the relevant software.
- Be prepared to read some mathematics. Technically you do not need to understand the specific mathematics to be able to use the tools in this book. The topics covered use some algebra, calculus and probability.

1.2 WHAT DO WE MEAN BY APPLIED MATHEMATICS?

We consider this book to be a book on applied mathematics. This is not however a universal term, for some applied mathematics is the study of mechanics and involves

modelling projectiles being fired out of canons. We will use the term a bit more freely here and mean any type of real world problem that can be tackled using mathematical tools. This is sometimes referred to as operational research, operations research, mathematical modelling or indeed just mathematics.

One of the authors, Vince, used mathematics to plan the sitting plan at his wedding. Using a particular area of mathematics call graph theory he was able to ensure that everyone sat next to someone they liked and/or knew.

The other author, Geraint, used mathematics to find the best team of Pokemon. Using an area of mathematics call linear programming which is based on linear algebra he was able to find the best makeup of pokemon.

Here, applied mathematics is the type of mathematics that helps us answer questions that the real world asks.

1.3 WHAT IS OPEN SOURCE SOFTWARE

Strictly speaking open source software is software with source code that anyone can read, modify and improve. In practice this means that you do not need to pay to use it which is often one of the first attractions. This financial aspect can also be one of the reasons that someone will not use a particular piece of software due to a confusion between cost and value: if something is free is it really going to be any good?

In practice open source software is used all of the world and powers some of the most important infrastructure around. For example, one should never use any cryptographic software that is not open source: if you cannot open up and read things than you should not trust it (this is indeed why most cryptographic systems used are open source).

Today, open source software is a lot more than a licensing agreement: it is a community of practice. Bugs are fixed faster, research is implemented immediately and knowledge is spread more widely thanks to open source software. Bugs are fixed faster because anyone can read and inspect the source code. Most open source software projects also have a clear mechanisms for communicating with the developers and even reviewing and accepting code contributions from the general public. Research is implemented immediately because when new algorithms are discovered they are often added directly to the software by the researchers who found them. This all contributes to the spread of knowledge: open source software is the modern should of giants that we all stand on.

Open source software is software that, like scientific knowledge is not restricted in its use.

1.4 HOW TO GET THE MOST OUT OF THIS BOOK

The book itself is open source. You can find the source files for this book online at github.com/drvinceknight/ampwoss. There will will also find a number of *Jupyter notebooks* and *R markdown files* that include code snippets that let you follow along.

We feel that you can choose to read the book from cover to cover, writing out

the code examples as you go; or it could also be used as a reference text when faced with particular problem and wanting to know where to start.

The book is made up of 10 chapters that are paired in two 4 parts. Each part corresponds to a particular area of mathematics, for example "Emergent Behaviour". Two chapters are paired together for each chapter, usually these two chapters correspond to the same area of mathematics but from a slightly different scale that correspond to different ways of tackling the problem.

Every chapter has the following structure:

- 1. Introduction a brief overview of a given problem type. Here we will describe the problem at hand in general terms.
- 2. An Example problem. This will provide a tangible example problem that offers the reader some intuition for the rest of the discussion.
- 3. Solving with Python. We will describe the mathematical tools available to us in a programming language called Python to solve the problem.
- 4. Solving with R. Here we will do the same with the R programming language.
- 5. Brief theoretic background with pointers to reference texts. Some readers might like to delve in to the mathematics of the problem a bit further, we will include those details here.
- 6. Examples of research using these methods. Finally, some readers might even be interested in finding out a bit more of what mathematicians are doing on these problems. Often this will include some descriptions of the problem considered but perhaps at a much larger scale than the one presented in the example.

For a given reader, not all sections of a chapter will be of interest. Perhaps a reader is only interested in R and finding out more about the research. Please do take from the book what you find useful.

		_

Software

This book will involve using software, the particular interface to software we will use is to write code. There are numerous reasons why this is the correct way to do things but one of them is reproducibility.

This chapter will go over the basics of getting your computer set up to use the software discussed in this book: the programming languages R and Python. It will also briefly discuss using the command line: a particular interface to your whole computer. Finally it will give a brief introduction to R and Python.

This chapter (and indeed this whole book) is not a place to learn R and Python completely. We will cover specific tasks and how to carry them out in each language, but we will not cover the every intricacy of each language. There are numerous sources (books, websites, courses) that are available to do that. A lot of these places would argue that you should not learn multiple programming languages from one book, and instead concentrate on a single skill at a time. We agree, and the single skill to concentrate on with this book is the use of software to solve applied mathematical problems. The particular software itself is not the most important component.

2.1 SOFTWARE INSTALLATION

There are a number of different places from which you can buy your vegetables, you can grow them yourself, you can go to a market and pick fresh fruit from specific stalls, you can go to a supermarket and buy a bag of a collection of vegetables and in some places you can even get a box of vegetables regularly posted to you. Software is similar, there are a variety of places from which you can get it and a number of different forms in which it can be obtained.

If you're comfortable with using R and Python then you probably do not need to read this section and you might even use different so called "distributions" of each piece of software, but for the purpose of this book here is where we will be getting what we need:

- Python: we will use the Anaconda distribution: https://www.anaconda.com/distribution/
- R: we will be getting this directly from the Comprehensive R Archive Network (commonly referred to as CRAN): https://cran.r-project.org. We will also use another piece of software called Rstudio: https://rstudio.com.

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2.1.1 Installing Python

Installing Python and all the software we need around it is done by downloading and running the installer for the Anaconda distribution.

- 1. Go to this webpage: https://www.anaconda.com/download/.
- 2. Identify and download the version of Python 3 for your operating system (Windows, Mac OSX, Linux). Run the installer.

2.1.2 Installing R

There are actually two pieces of software we need to install to use R for the purposes of this book, first the R language itself and second an application with which we will write R code.

- 1. Go to this webpage: https://cran.r-project.org.
- 2. Identify and download the latest version of R for your operating system (Windows, Mac OSX, Linux). Run the installer.
- 3. Go to this webpage: https://rstudio.com.
- 4. Identify and download the latest version of Rstudio for your operating system (Windows, Mac OSX, Linux). Run the installer.

2.2 USING THE COMMAND LINE

There are various interfaces to using a computer, the most common one is to use a mouse and keyboard and click on programmes we want to use. Another approach is to use what is called a command line interface this is where we do not interact graphically with a computer but we type in specific commands.

We can use our command line to navigate the various directories on our computer. There are two types of operating systems that we consider here:

- Windows
- Nix: this includes OSX (the Mac operating system) and Linux

Not all commands are the same on each type of operating system. So let us start by opening our command line interface:

- Windows: after having installed Anaconda look to open the Anaconda Prompt.
 There are a number of other command line interfaces available but this is the one we recommend for the purposes of this book.
- Nix: look to open the Terminal.

This should open something that looks like and somewhat resembles a black box with some text in it. This is where we will write our commands to the computer.

For example to list the contents of the directory we are currently in:

On nix:

	Cli input
	ls
•	15
	On Windows
	Cli input
	CII Input
:	dir
	It is also possible to get the page of the directory we are suggested in
	It is also possible to get the name of the directory we are currently in:
	On nix:
	Cli input
3	pwd
_	
	On Windows
	On windows
	Cli input
	cd
_	
	Finally we can also use the command line to move to another directory. The
C	command for this are the same on Nix and on Windows.
	minume for this are the same on this and on willdows.
	Cli input
	-

The command line is an important tool to learn to use when doing tasks:

cd <name_of_subdirectory>

• If we want to scale the tasks, a commonly heard phrase is that 'mouse clicks do not scale' highlighting that to repeat a task many times when using a graphical interface is inefficient.

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• If we want someone else to be able to repeat the tasks, we can use screenshots of graphical interfaces but there will always be a level of ambiguity whereas the commands used in the command line are precise.

We can use our two programming languages right within the command line interface (we will actually be using a different tool that we will describe shortly).

To use Python, simply type the following and press Enter:

```
Cli input _______
```

This should make something like the following appear:

```
Python 3.7.1 | packaged by conda-forge | (default, Nov 13 2018, 10:30:07)

[Clang 4.0.1 (tags/RELEASE_401/final)] :: Anaconda, Inc. on darwin

Type "help", "copyright", "credits" or "license" for more information.

>>>
```

The >>> is a prompt ready to accept a Python command. Let us start with the following:

```
Python input >>> 2 + 2
```

When you press Enter, this will give:

```
Python output

4
```

This particular way of using Python is called a REPL which stands for: 'Read Eval Print Loop' which indicates that it takes a command, evaluates it and waits for the next one.

To quit Python's REPL type the following (note that (), more about that later):

```
Python input

>>> quit()
```

We can do the same for R. To start R's REPL, in your command line type the following and press Enter:

```
Cli input

R
```

This should make something like the following appear:

```
_____ Cli output _____
    R version 3.5.1 (2018-07-02) -- "Feather Spray"
15
    Copyright (C) 2018 The R Foundation for Statistical Computing
16
    Platform: x86_64-apple-darwin13.4.0 (64-bit)
17
18
    R is free software and comes with ABSOLUTELY NO WARRANTY.
19
    You are welcome to redistribute it under certain conditions.
20
    Type 'license()' or 'licence()' for distribution details.
21
22
      Natural language support but running in an English locale
23
24
    R is a collaborative project with many contributors.
25
    Type 'contributors()' for more information and
26
    'citation()' on how to cite R or R packages in publications.
27
28
    Type 'demo()' for some demos, 'help()' for on-line help, or
29
    'help.start()' for an HTML browser interface to help.
30
    Type 'q()' to quit R.
31
32
33
```

The > is a prompt ready to accept an R command. Let us start with the following:

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		R input
34	> 2 + 2	
34	7 2 1 2	

When you press Enter, this will give:

```
R output

4
```

To quit R's REPL type the following:

```
R input > q()
```

This will bring up a further prompt asking you to save some information about what you just did. You can type n for now:

```
R input

> Save workspace image? [y/n/c]: n
```

These two REPLs are not unique and also not the most efficient way of using the languages, however they can at times be useful if you just want to type a very short command or perhaps check something quickly.

Another approach is to save a collection of commands in a plain text file and pass it to the interpreter at the command line.

For example, if we had a number of Python commands in main.py we could run this at the command line using:

```
Cli input

python main.py
```

Similarly for a file with a number of R commands main.R:

Cli input

Rscript main.R

These are just a few of many ways to use Python and R. An important notion to understand is that Python and R are not the particular tools that we use to interface to them. On a day to day basis the authors of this book will use both of the above approaches as well as the next ones, we recommend readers take time to experiment and understand the particular use cases for which each tool works best for them.

The two tools we recommend to use in this book are:

- For Python: the Jupyter notebook, a tool that behaves similarly to a REPL, runs in the web browser and is very popular in research.
- For R: RStudio, an integrated development environment with a lot of helpful features.

The best way to start the Jupyter notebook is to type the following in your command line:

Jupyter notebook

This will create a *notebook server* that runs on your computer and should open a page that looks like Note that despite running in a web browser this does not need the internet to run.

We can create a new notebook and write and run code in the cells.

To start Rstudio, locate the application on your computer and double click on it. This will open an application that looks like

Rstudio includes its on REPL, so we can type and run single commands there but we can also write in a file that we can run

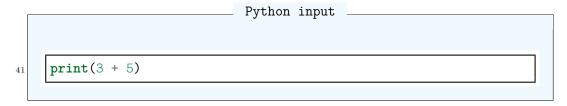
In the next sections we will cover some basics of Python and R.

2.3 BASIC PYTHON

This section gives a very brief overview of some introductory aspects of Python, there are excellent resources available for learning Python and we recommend the reader goes there if they feel they need an in depth understanding of the language

In the previous section, we saw how to get Python to perform a single calculation:

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which will give:

```
Python output

8
```

We can also assign values to a variable:

```
Python input

a = 3
b = 5
c = a + b
print(c)
```

This makes a point at 3 etc...

which will give:

```
Python output

8
```

There are a number of different types of variables in Python, here is a very brief list of some of them:

- Integers int for example 2, 4, -459060.
- Floats float for example 2.0, 3.4, -3.459060.
- Strings str for example "two", "hello world", "3450".
- Booleans bool for example True or False.

Based on the values of a variable it is possible to construct Booleans:

```
Python input

is_a_larger_than_b = a > b
```

The variable is_a_larger_than_b will be the boolean variable False.

This is an important concept as boolean variable allow us to use conditional statements that let us write code that does specific things based on the value of variables. For example the following code will add 5 to the smallest variable:

```
Python input
     a = 3
49
     b = 5
50
     if a < b:
51
         a = a + 3
52
     elif a > b:
53
         b = b + 5
54
     else:
55
          a = a + 3
56
         b = b + 3
57
     print(a, b)
58
```

which gives:

```
Python output

6 5
```

If you are experimenting by typing the code as you go change the value of a or b to see how the behaviour changes. What happens if they are equal?

It is also possible to use these conditional statements to repeat code. For example the following code will repeatedly add 1 to the smallest variable until it becomes equal to the largest one:

```
Python input

a = 3
b = 5
while a != b:
    if a < b:
        a = a + 1
else:
    b = b + 1
```

It is important to be able to reuse code, this is done using a programming concept called a *function*, which acts similarly to a mathematical function.

The following code, creates a function that takes two variables as input and outputs the largest number and the smallest increased by 3.

```
def add_3_to_smallest(a, b):

"""This function adds 3 to the smallest of a or b."""

if a < b:

return a + 3, b

return a, b + 3
```

Once we have defined the function, the following is how we use it:

```
Python input

print(add_3_to_smallest(a=5, b=-42))
```

which gives:

```
Python output

(5, -39)
```

Python has a type of variable that is in fact a collection of pointers to other variables. This is called a list. Here for example is a collection of strings:

```
Python input

tennis_players = [
    "Federer",
    "S. Williams",
    "V. Williams",
    "King",
]
```

There are a number of things that can be done with lists but one particular aspect is that they are a sub type of something called an iterable in Python which means we can iterate over them. We do this in Python using a **for** loop. For example, the following code will iterate over the list and print all the values:

```
Python input

for name in tennis_players:
    print(name)
```

which gives:

```
Python output

Federer
S. Williams
V. Williams
King
```

We will often want to iterate over a set of integers, Python has a range command that can create such a set with ease. The following code will print every 3 integers from 30 to 50:

```
Python input

for integer in range(30, 50, 3):
    print(integer)
```

which will give:

```
Python output

30
33
36
91
92
42
45
48
```

A final important aspect of Python is that of libraries. The code examples above are from the so called 'standard library' but Python has numerous libraries specific to given problems. A lot of these libraries came bundled with the anaconda distribution but if you want to download one that is not you can always do so as long as you have an internet connection.

For example, to download a library for studying queueing systems ciw open your command line interface and type the following:

```
95 pip install ciw
```

Once you restart your python interpreter, for example if you are using a Jupyter notebook then restart the Kernel, you can then run the following to make ciw available to you:

```
Python input

import ciw
```

2.4 BASIC R

This section gives a very brief overview of some introductory aspects of R, there are excellent resources available for learning R [1] and we recommend the reader goes there if they feel they need an in depth understanding of the language

In the previous section, we saw how to get R to perform a single calculation:

```
Print(3 + 5)
```

which will give:

We can also assign values to a variable:

```
R input

a <- 3
b <- 5
c <- a + b
print(c)
```

which will give:

An important difference between R and Python is that in R the base structure is in fact a vector, even if it only contains a single variable. We can use the ${\tt c}$ command to concatenate these base structures together:

```
R input

print(c(a, 4))
```

giving:

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```
R output

[1] 3 4
```

There are a number of different types of variables in R, here is a very brief list of some of them:

- Integers integer for example 2, 4, -459060.
- Floats double for example 2.0, 3.4, -3.459060.
- Strings character for example "two", "hello world", "3450".
- Booleans logical for example TRUE or FALSE.

Based on the values of a variable it is possible to construct Booleans:

```
R input

[is_a_larger_than_b <- a > b]
```

The variable is a larger than b will be the boolean variable FALSE.

This is an important concept as boolean variable allow us to use conditional statements that let us write code that does specific things based on the value of variables. For example the following code will add 5 to the smallest variable:

```
R input
      a <- 3
107
      b <- 5
108
      if (a < b) {
109
        a < -a + 3
110
      } else if (a > b) {
111
        b < -b + 3
112
      } else {
113
        a < -a + 3
114
        b < -b + 3
115
116
      print(c(a, b))
117
```

which gives:

If you are experimenting by typing the code as you go, change the value of a or b to see how the behaviour changes. What happens if they are equal?

R is a so called "vectorized" language which means that there is often a more appropriate approach to doing things repeatedly using vectors. This applies to the if statement in that there exists a ifelse statement that applies to vectors of booleans. For example:

```
R input

booleans <- c(FALSE, TRUE, FALSE, FALSE)

print(ifelse(booleans, "cat", "dog"))
```

which gives:

```
R output

[1] "dog" "cat" "dog" "dog"
```

It is also possible to use conditional statements to repeat code. For example the following code will repeatedly add 1 to the smallest variable until it becomes equal to the largest one:

```
_____ R input _
      a <- 3
122
      b <- 5
123
      while (a != b) {
124
        if (a < b) {
125
          a < -a + 1
126
        }
127
        else {
128
          b < -b + 1
129
        }
130
131
```

It is important to be able to reuse code, this is done using a programming concept called a *function*, which acts similarly to a mathematical function.

The following code creates a function that takes two variables as input and outputs the largest number and the smallest increased by 3.

```
R input
     add 3 to smallest <- function(a, b) {
132
        # This function adds 3 to the smallest of a or b.
133
        if (a < b) {
134
          return(c(a + 3, b))
135
        }
136
        else {
137
          return(c(a, b + 3))
138
139
140
```

Note that R will implicitly return the last computed expression without the need for a return statement. So the above can also be written as:

```
R input
      add 3 to smallest <- function(a, b) {
141
        # This function adds 3 to the smallest of a or b.
142
        if (a < b) {
143
          c(a + 3, b)
144
        }
145
        else {
146
          c(a, b + 3)
147
        }
148
149
```

Once we have defined the function, the following is how we use it:

```
R input

print(add_3_to_smallest(a = 5, b = -42))
```

which gives:

```
R output

[1] 5 -39
```

It is possible to iterate over elements inside R vectors:

```
tennis_players <- c("Federer",
"S. Williams",
"V. Williams",
"King")
```

The following will print all the names contained in the vector:

```
for (name in tennis_players) {
    print(name)
}
```

which gives:

```
R output

[1] "Federer"
[1] "S. Williams"
[1] "V. Williams"
[1] "King"
```

We will often want to iterate over a vector of integers, R has a seq command that can create such a vector with ease. The following code will print every 3 integers from 30 to 50:

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```
R input

for (i in seq(30, 50, 3)) {
 print(i)
}
```

which will give:

```
R output

[1] 30
[1] 33
[1] 36
[1] 39
[1] 42
[1] 45
[1] 45
[1] 48
```

A final important aspect of R is that of packages. The code examples above are from the so called 'base R' but R has numerous packages specific to given problems. If you want to download and use one you can always do so as long as you have an internet connection.

For example, to download a very common collection of data science tools called tidyverse we use the following line of code inside of an R session:

```
R input

install.packages("simmer")
```

Once this package is installed it is loaded using

```
R input

library(simmer)
```

2.5 A NOTE ON HOW CODE IS DISPLAYED IN THIS BOOK

FURTHER READING

- Becskei, A. and Serrano, L. (2000). Engineering stability in gene networks by autoregulation. *Nature*, 405: 590–593.
- Rosenfeld, N., Elowitz, M.B., and Alon, U. (2002). Negative auto-regulation speeds the response time of transcription networks. *J. Mol. Biol.*, 323: 785–793.
- Savageau, M.A. (1976). Biochemical Systems Analysis: A study of Function and Design in Molecular Biology. Addison-Wesley. Chap. 16.
- Savageau, M.A. (1974). Comparison of classical and auto-genous systems of regulation in inducible operons. *Nature*, 252: 546–549.

Probabilistic Modelling

Markov Chains

Many real world situations have some level of unpredictability through randomness: the flip of a coin, the number of orders of coffee in a shop, the winning numbers of the lottery. However, mathematics can in fact let us make predictions about what we expect to happen. One tool used to understand randomness is Markov chains, an area of mathematics sitting at the intersection of probability and linear algebra.

3.1 PROBLEM

Consider a barber shop. The shop owners have noticed that customers will not wait if there is no room in their waiting room and will choose to take their business elsewhere. The Barber shop would like to make an investment so as to avoid this situation. They know the following information:

- They currently have 2 barber chairs (and 2 barbers).
- They have waiting room for 4 people.
- They usually have 10 customers arrive per hour.
- Each Barber takes about 15 minutes to serve a customer so they can serve 4 customers an hour.

This is represented diagrammatically in Figure 3.1.

They are planning on reconfiguring space to either have 2 extra waiting chairs or another barber's chair and barber.

The mathematical tool used to model this situation is a Markov Processes.

3.2 THEORY

A Markov Process is a model of a sequence of random events that is defined by a collection of **states** and rules that define how to move between these states.

For example, in the barber shop a single number is sufficient to describe the status of the shop. If that number is 1 this implies that 1 customer is currently having their

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Figure 3.1 Diagrammatic representation of the barber shop as a queuing system.

hair cut. If that number is 5 this implies that 2 customers are being served and 3 are waiting. Thus the state space for this particular Markov Process is:

$$S = \{0, 1, 2, 3, 4, 5, 6\} \tag{3.1}$$

As customers arrive and leave the system goes between states as shown in Figure 3.2.



Figure 3.2 Diagrammatic representation of the state space

The rules that govern how to move between these states can be defined in two ways:

- Using probabilities of changing state (or not) in a well defined time period. This is called a discrete Markov process.
- Using rates of change from one state to another. This is called a continuous time Markov process.

For our barber shop we will consider it as a continuous Markov process as shown in Figure 3.3

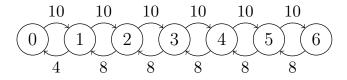


Figure 3.3 Diagrammatic representation of the state space and the transition rates

Note that a Markov process assumes the rates follow an exponential distribution. One interesting property of this distribution is that it is considered memoryless which means that if a customer has been having their hair cut for 5 minutes this does not change the rate at which their service ends. This distribution is quite common in the real world and therefore a common assumption.

These states and rates can be represented mathematically using a transition matrix Q where Q_{ij} represents the rate of going from state i to state j. In this case we have:

$$Q = \begin{pmatrix} -10 & 10 & 0 & 0 & 0 & 0 & 0 \\ 4 & -14 & 10 & 0 & 0 & 0 & 0 \\ 0 & 8 & -18 & 10 & 0 & 0 & 0 \\ 0 & 0 & 8 & -18 & 10 & 0 & 0 \\ 0 & 0 & 0 & 8 & -18 & 10 & 0 \\ 0 & 0 & 0 & 0 & 8 & -18 & 10 \\ 0 & 0 & 0 & 0 & 0 & 8 & -8 \end{pmatrix}$$
(3.2)

You will see that Q_{ii} are negative and ensure the rows of Q sum to 0. This gives the total rate of change leaving state i.

We can use Q to understand the probability of being in a given state after t time unis. This is can be represented mathematically using a matrix P_t where $(P_t)_{ij}$ is the probability of being in state j after t time units having started in state i. We can use Q to calculate P_t using the matrix exponential:

$$P_t = e^{Qt} (3.3)$$

What is also useful is understanding the long run behaviour of the system. This allows us to answer questions such as "what state are we most likely to be in on average?" or "what is the probability of being in the last state on average?".

This long run probability distribution over the state can be represented using a vector π where π_i represents the probability of being in state i. This vector is in fact the solution to the following matrix equation:

$$\pi Q = 0 \tag{3.4}$$

In the upcoming sections we will demonstrate all of the above concepts.

3.3 SOLVING WITH PYTHON

The first step we will take is to write a function to obtain the transition rates between two given states:

```
Python input
```

```
def get_transition_rate(
175
          in_state,
176
          out_state,
177
         waiting_room=4,
178
         number of barbers=2,
179
          arrival_rate=10,
180
          service rate=4,
181
     ):
182
          """Return the transition rate for two given states.
183
184
          Args:
185
              in_state: an integer denoting the current state
186
              out_state: an integer denoting the next state
187
              waiting_room: an integer denoting the size of the
188
                              waiting room (default: 4)
189
              number_of_barbers: an integer denoting the number of
190
                                    barber and chairs (default: 2)
191
              arrival_rate: a real number denoting the number of
192
                              individuals per unit time that arrive at
193
                              the barber shop (default: 10)
194
              service_rate: a real number denoting the number of
195
                              individuals per unit time that a single
196
                              barber can serve (default: 4)
197
198
          Returns:
199
              A real.
200
          11 11 11
201
          capacity = waiting room + number of barbers
202
203
         delta = out_state - in_state
204
          if delta == 1 and in state < capacity:</pre>
205
              return arrival_rate
206
207
          if delta == -1:
208
              return min(in state, number of barbers) * service rate
209
210
          return 0
211
```

Next, we write a function that creates an entire transition rate matrix Q for a given problem. We will use the numpy to handle all the linear algebra and the itertools library for some iterations:

```
Python input

import itertools
import numpy as np
```

Now we define the function:

Python input

```
def get_transition_rate_matrix(
214
          waiting_room=4,
215
         number of barbers=2,
216
          arrival_rate=10,
217
          service rate=4,
218
     ):
219
          """Return the transition matrix Q.
220
221
          Args:
222
              waiting_room: an integer denoting the size of the
223
                              waiting room (default: 4)
224
              number_of_barbers: an integer denoting the number of
                                   barber and chairs (default: 2)
226
              arrival rate: a real number denoting the number of
227
                              individuals per unit time that arrive at
228
                              the barber shop (default: 10)
229
              service_rate: a real number denoting the number of
230
                              individuals per unit time that a single
231
                              barber can serve (default: 4)
232
233
          Returns:
234
              A matrix.
235
236
          capacity = waiting_room + number_of_barbers
237
          state_pairs = itertools.product(
238
              range(capacity + 1), repeat=2
239
240
          flat transition rates = [
241
242
              get transition rate(
                  in_state=in_state,
243
                  out_state=out_state,
244
                  waiting_room=waiting_room,
245
                  number_of_barbers=number_of_barbers,
246
                  arrival_rate=arrival_rate,
247
                  service rate=service rate,
248
              )
249
              for in state, out state in state pairs
250
251
          transition_rates = np.reshape(
252
              flat transition rates, (capacity + 1, capacity + 1)
253
254
255
         np.fill_diagonal(
              transition_rates, -transition_rates.sum(axis=1)
256
          )
257
258
         return transition rates
259
```

Using this we can obtain the matrix Q for our default system:

```
Python input

Q = get_transition_rate_matrix()

print(Q)
```

which gives:

```
_____Python output _____
            10
                 0
                                  0]
262
         4 -14
                10
                      0
                          0
                                  0]
263
             8 -18
                                  0]
                    10
                          0
                              0
264
                                  0]
             0
                 8 -18
                        10
                              0
                                  0]
             0
                 0
                      8 -18
                            10
266
                          8 -18
                                 10]
267
                          0
                                 -8]]
268
```

We can take the matrix exponential as discussed above. To do this, we need to use the scipy library:

```
Python input
import scipy.linalg
```

To see what would happen after .5 time units we obtain:

```
Python input

print(scipy.linalg.expm(Q * 0.5).round(5))
```

which gives:

```
Python output

[[0.10492 0.21254 0.20377 0.17142 0.13021 0.09564 0.0815 ]
[0.08501 0.18292 0.18666 0.1708 0.14377 0.1189 0.11194]
[0.06521 0.14933 0.16338 0.16478 0.15633 0.14751 0.15346]
[0.04388 0.10931 0.13183 0.15181 0.16777 0.18398 0.21142]
[0.02667 0.07361 0.10005 0.13422 0.17393 0.2189 0.27262]
[0.01567 0.0487 0.07552 0.11775 0.17512 0.24484 0.32239]
[0.01068 0.03668 0.06286 0.10824 0.17448 0.25791 0.34914]]
```

To see what would happen after 500 time units we obtain:

```
Python input

print(scipy.linalg.expm(Q * 500).round(5))
```

which gives:

```
Python output
     [[0.03431 0.08577 0.10722 0.13402 0.16752 0.2094
                                                        0.26176]
279
      [0.03431 0.08577 0.10722 0.13402 0.16752 0.2094
280
                                                         0.26176]
      [0.03431 0.08577 0.10722 0.13402 0.16752 0.2094
                                                         0.26176]
281
      [0.03431 0.08577 0.10722 0.13402 0.16752 0.2094
                                                         0.26176]
282
      [0.03431 0.08577 0.10722 0.13402 0.16752 0.2094
                                                         0.26176]
283
      [0.03431 0.08577 0.10722 0.13402 0.16752 0.2094
                                                         0.26176]
284
      [0.03431 0.08577 0.10722 0.13402 0.16752 0.2094
                                                         0.26176]]
```

We see that no matter what state (column) the system is in, after 500 time units the probabilities are all the same. We could in fact stop our analysis here, however our choice of 500 time units was arbitrary and might not be the correct amount for all possible scenarios, as such we will continue to aim to solve the underlying equation 3.4 directly.

To do this we will solve the underlying system using a numerically efficient algorithm called least squares optimisation (available from the numpy library):

Python input _ def get_steady_state_vector(Q): 286 """Return the steady state vector of any given continuous 287 time transition rate matrix. 288 289 Args: 290 Q: a transition rate matrix 291 292 Returns: 293 A vector 294 295 state space size, = Q.shape 296 A = np.vstack((Q.T, np.ones(state_space_size))) 297 b = np.append(np.zeros(state_space_size), 1) 298 x, _, _, = np.linalg.lstsq(A, b, rcond=None) 299 return x 300

So if we now see the steady state vector for our default system:

```
Python input

print(get_steady_state_vector(Q).round(5))
```

we get:

```
Python output

[0.03431 0.08577 0.10722 0.13402 0.16752 0.2094 0.26176]
```

We can see that the shop is expected to be empty approximately 3.4% of the time and full 26.2% of the time.

The final function we will write is one that uses all of the above to just return the probability of the shop being full.

```
Python input
```

```
def get_probability_of_full_shop(
303
          waiting_room=4,
304
         number_of_barbers=2,
305
          arrival_rate=10,
306
          service_rate=4,
307
     ):
308
          """Return the probability of the barber shop being full.
309
310
          Args:
311
              waiting_room: an integer denoting the size of
312
                              the waiting room (default: 4)
313
314
              number_of_barbers: an integer denoting the number
315
                                    of barber and chairs
316
                                    (default: 2)
317
318
              arrival_rate: a real number denoting the number of
319
                              individuals per unit time that arrive
320
                              at the barber shop (default: 10)
321
322
              service_rate: a real number denoting the number of
323
                              individuals per unit time that a single
324
                              barber can serve (default: 4)
325
326
          Returns:
327
              A real.
328
          11 11 11
329
          Q = get_transition_rate_matrix(
330
331
              waiting_room=waiting_room,
              number_of_barbers=number_of_barbers,
332
              arrival rate=arrival rate,
333
              service_rate=service_rate,
334
335
         pi = get_steady_state_vector(Q)
336
         return pi[-1]
337
```

We can now confirm the previous probability calculated probability of the shop being full:

```
____ Python input _____
     print(round(get_probability_of_full_shop(), 6))
338
     which gives:
                      _____Python output _____
     0.261756
339
     If we were too have 2 extra space in the waiting room:
                       _____ Python input _____
     print(round(get_probability_of_full_shop(waiting_room=6), 6))
340
     which gives:
                 _____Python output _____
     0.23557
341
     This is a slight improvement however, increasing the number of barbers has a
  substantial effect:
                             \_ Python input \_
     print(
342
         round(get_probability_of_full_shop(number_of_barbers=3), 6)
343
344
                           ___ Python output __
     0.078636
345
```

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In fact the only way to lower the probability of the shop being full below the 10% threshold is to have barbers work at the faster rate of 4.6 customers per time unit:

```
Python input
      print(
346
          round(
347
               get_probability_of_full_shop(
348
                    waiting_room=20, service_rate=4.6
349
               ),
350
               6,
351
           )
352
353
```

```
Python output

0.094487
```

3.4 SOLVING WITH R

The first step we will take is write a function to obtain the transition rates between two given states:

R input

```
#' Return the transition rate for two given states.
355
     # '
356
     #' Oparam in state an integer denoting the current state
357
     #' Oparam out_state an integer denoting the next state
358
     #' @param waiting_room an integer denoting the size of
359
                 the waiting room (default: 4)
360
     #' @param number_of_barbers an integer denoting the number
361
                of barber and chairs (default: 2)
362
     #' Oparam arrival_rate a real number denoting the number
363
     # "
                of individuals per unit time that arrive at
364
                the barber shop (default: 10)
365
     #' Oparam service_rate a real number denoting the number
366
                 of individuals per unit time that a single barber
367
                 can serve (default: 4)
368
369
     #' @return A real
370
     get_transition_rate <- function(</pre>
371
                                        in state,
372
                                        out_state,
373
                                        waiting room = 4,
374
                                        number_of_barbers = 2,
375
                                        arrival rate = 10,
376
                                        service_rate = 4) {
377
       capacity <- waiting room + number_of_barbers</pre>
378
       delta <- out_state - in_state
379
       if (delta == 1) {
381
          if (in_state < capacity) {</pre>
382
            return(arrival_rate)
383
384
       }
385
386
       if (delta == -1) {
387
          return(min(in_state, number_of_barbers) * service_rate)
389
       return(0)
390
391
```

We will not actually use this function but a vectorized version of this:

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```
vectorized_get_transition_rate <- Vectorize(
   get_transition_rate,
   vectorize.args = c("in_state", "out_state")
)</pre>
```

This function can now take a vector of inputs for the in_state and out_state variables which will allow us to simplify the following code that creates the matrices:

R input

```
#' Return the transition rate matrix Q
396
      # '
397
      #' @param waiting_room an integer denoting the size of the
398
                waiting room (default: 4)
399
      #' @param number_of_barbers an integer denoting the number of
400
                barber and chairs (default: 2)
401
      #' Oparam arrival rate a real number denoting the number of
402
                 individuals per #' unit time that arrive at the
403
                barber shop (default: 10)
404
      #' Oparam service_rate a real number denoting the number of
405
                 individuals per unit time that a single barber
406
                 can serve (default: 4)
407
408
      #' @return A matrix
409
     get_transition_rate_matrix <- function(</pre>
410
                                                waiting_room = 4,
411
                                                number_of_barbers = 2,
412
                                                arrival rate = 10,
413
                                                service_rate = 4) {
414
       max state <- waiting room + number of barbers</pre>
415
416
       Q <- outer(0:max state,
417
          0:max_state,
418
         vectorized get transition rate,
419
         waiting_room = waiting_room,
420
         number of barbers = number of barbers,
421
          arrival rate = arrival rate,
          service_rate = service_rate
423
424
       row_sums <- rowSums(Q)</pre>
425
426
       diag(Q) <- -row_sums</pre>
427
       Q
428
429
```

Using this we can obtain the matrix Q for our default system:

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```
R input

Q <- get_transition_rate_matrix()
print(Q)
```

which gives:

```
R output
            [,1] [,2] [,3] [,4] [,5] [,6] [,7]
432
      [1,]
             -10
                    10
                           0
                                 0
433
      [2,]
               4
                   -14
                          10
                                        0
                                 0
                                              0
                                                    0
434
      [3,]
                     8
                         -18
                                10
                                       0
                                                   0
               0
435
      [4,]
                     0
                           8
                              -18
                                     10
               0
436
      [5,]
                     0
                           0
                                 8
                                     -18
                                            10
437
      [6,]
                           0
                                 0
                                        8
                                           -18
                                                  10
438
      [7,]
                                                  -8
439
```

One immediate thing we can do with this matrix is take the matrix exponential discussed above. To do this, we need to use an R library call expm:

```
R input

library(expm, warn.conflicts = FALSE, quietly = TRUE)
```

To be able to make use of the nice %>% "pipe" operator we are also going to load the dplyr library:

```
R input

library(dplyr, warn.conflicts = FALSE, quietly = TRUE)
```

Now if we wanted to see what would happen after .5 time units we obtain:

```
R input

[print((Q * .5) %>% expm %>% round(5))
```

which gives:

```
R output
              [,1]
                      [,2]
                               [,3]
                                       [,4]
                                                [,5]
                                                        [,6]
                                                                 [,7]
443
     [1,] 0.10492 0.21254 0.20377 0.17142 0.13021 0.09564 0.08150
444
     [2,] 0.08501 0.18292 0.18666 0.17080 0.14377 0.11890 0.11194
445
     [3,] 0.06521 0.14933 0.16338 0.16478 0.15633 0.14751 0.15346
446
     [4,] 0.04388 0.10931 0.13183 0.15181 0.16777 0.18398 0.21142
447
     [5,] 0.02667 0.07361 0.10005 0.13422 0.17393 0.21890 0.27262
448
     [6,] 0.01567 0.04870 0.07552 0.11775 0.17512 0.24484 0.32239
449
     [7,] 0.01068 0.03668 0.06286 0.10824 0.17448 0.25791 0.34914
450
```

After 500 time units we obtain:

```
R input

print( (Q * 500) %>% expm %>% round(5))
```

which gives:

```
R output
              [,1]
                      [,2]
                               [,3]
                                       [,4]
                                                [,5]
                                                       [,6]
                                                                [,7]
452
     [1,] 0.03431 0.08577 0.10722 0.13402 0.16752 0.2094 0.26176
453
     [2,] 0.03431 0.08577 0.10722 0.13402 0.16752 0.2094 0.26176
454
     [3,] 0.03431 0.08577 0.10722 0.13402 0.16752 0.2094 0.26176
455
     [4,] 0.03431 0.08577 0.10722 0.13402 0.16752 0.2094 0.26176
456
     [5,] 0.03431 0.08577 0.10722 0.13402 0.16752 0.2094 0.26176
457
     [6,] 0.03431 0.08577 0.10722 0.13402 0.16752 0.2094 0.26176
458
     [7,] 0.03431 0.08577 0.10722 0.13402 0.16752 0.2094 0.26176
459
```

We see that no matter what state (row) we are in, after 500 time units the probabilities are all the same. We could in fact stop our analysis here, however our choice of 500 time units was arbitrary and might not be the correct amount for all possible scenarios, as such we will continue to aim to solve the underlying equation 3.4 directly.

To be able to do this, we will make use of the versatile **pracma** package which includes a number of numerical analysis functions for efficient computations.

```
R input
     library(pracma, warn.conflicts = FALSE, quietly = TRUE)
460
461
      #' Return the steady state vector of any given continuous time
462
      #' transition rate matrix
463
464
      #' @param Q a transition rate matrix
465
466
      #' @return A vector
467
     get steady state vector <- function(Q){</pre>
468
        state_space_size <- dim(Q)[1]</pre>
469
        A \leftarrow rbind(t(Q), 1)
470
        b <- c(integer(state space size), 1)</pre>
471
        mldivide(A, b)
472
473
```

This is making use of pracma's mldivide function which chooses the best numerical algorithm to find the solution to a given matrix equation Ax = b.

So if we now see the steady state vector for our default system:

```
R input

print(get_steady_state_vector(Q))
```

we get:

```
R output
                  [,1]
475
      [1,] 0.03430888
476
      [2,] 0.08577220
477
      [3,] 0.10721525
478
      [4,] 0.13401906
479
      [5,] 0.16752383
480
      [6,] 0.20940479
481
      [7,] 0.26175598
482
```

We can see that the shop is expected to be empty approximately 3.4% of the time and full 26.2% of the time.

The final piece of this puzzle is to create a single function that uses all of the above to just return the probability of the shop being full.

```
R input
     #' Return the probability of the barber shop being full
483
484
     #' @param waiting_room an integer denoting the size of the
485
                waiting room (default: 4)
486
         Oparam number_of_barbers an integer denoting the number of
487
                barber and chairs (default: 2)
488
     #' Oparam arrival_rate a real number denoting the number of
489
     # '
                individuals per #' unit time that arrive at the
490
     #'
                barber shop (default: 10)
491
         Oparam service_rate a real number denoting the number of
492
                individuals per unit time that a single barber can
493
                serve (default: 4)
494
495
     #' @return A real
496
     get_probability_of_full_shop <- function(</pre>
497
                                                  waiting_room = 4,
498
                                                  number of barbers = 2,
499
                                                  arrival_rate = 10,
500
                                                  service rate = 4) {
501
       pi <- get_transition_rate_matrix(</pre>
502
         waiting_room = waiting_room,
503
         number of barbers = number of barbers,
504
         arrival_rate = arrival_rate,
505
          service rate = service rate
506
       ) %>%
507
          get_steady_state_vector()
508
509
       capacity <- waiting_room + number_of_barbers</pre>
510
       pi[capacity + 1]
511
512
```

Now we can run this code efficiently with both scenarios:

```
Print(get_probability_of_full_shop(waiting_room = 6))
```

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which decreases the probability of a full shop to:

```
R output

[1] 0.2355699
```

but adding another barber and chair:

```
R input

print(get_probability_of_full_shop(number_of_barbers = 3))
```

gives:

```
R output

516

[1] 0.0786359
```

In fact even with room for 20 people to wait the only way 2 barbers would be able to have a less than 10% of the shop being full is to find a way to each serve .6 more of a customer per hour:

```
Print(

get_probability_of_full_shop(

waiting_room = 20,

service_rate = 4.6)

)
```

```
R output

[1] 0.09448688
```

3.5 RESEARCH

TBA

Discrete Event Simulation

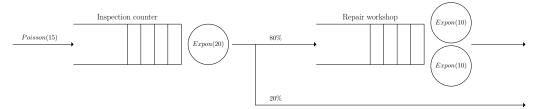
OMPLEX situations further compounded by randomness appear throughout our daily lives. For example, data flowing through a computer network, patients being treated at an emergency services, and daily commutes to work. Mathematics can be used to understand these complex situations so as to make predications which in turn can be used to make improvements. One tool used to do this is to let a computer create a dynamic virtual representation of the scenario in question, the particular type we are going to cover here is called Discrete Event Simulation.

4.1 PROBLEM

Consider the following situation: a bicycle repair shop would like reconfigure their set-up in order to guarantee that all bicycles processed by the repair shop take a maximum of 30 minutes. Their current set-up is as follows:

- Bicycles arrive randomly at the shop at a rate of 15 per hour.
- They wait in line to be seen at an inspection counter, manned by one member
 of staff who can inspect one bicycle at a time. On average an inspection takes
 around 3 minutes.
- After inspection it is found that around 20% of bicycles do not need repair, and they are then ready for collection.
- After inspection is is found that around 80% of bicycles go on to be repaired. These then wait in line outside the repair workshop, which is manned by two members of staff who can each repair one bicycle at a time. On average a repair takes around 6 minutes.
- After repair the bicycles are ready for collection.

A diagram of the system is shown below:



We can also assume that there is infinite capacity at the bicycle repair shop for waiting bicycles. The shop will hire and extra member of staff in order to meet their target of a maximum throughout of 30 minutes. They would like to know if they should work on the inspection counter or in the repair workshop?

4.2 THEORY

A number of the events that govern the behaviour of the bicycle shop above are probabilistic. For example the times that bicycles arrive at the shop, the duration of the inspection and repairs, and whether the bicycle would need to go on to be repaired or not. When a number of these probabilistic events are arranged in a complex system such as the bicycle shop, using analytical methods to manipulate these probabilities becomes difficult. One method to deal with this is *simulation*.

Consider one probabilistic event, rolling a die. A die has six sides numbered 1 to 6, each side is equally likely to land. Therefore the probability of rolling a 1 is $\frac{1}{6}$, the probability of rolling a 2 is $\frac{1}{6}$, and so on. This means that that if we roll the die a large number of times, we would except $\frac{1}{6}$ of those rolls to be a 1. This is called the law of large numbers.

Now imagine we have an event in which we do not know the analytical probability of it occurring. Consider rolling a weighted die, in this case a die in which the probability of obtaining one number is much greater than the others. How can we estimate the probability of obtaining a 5 on this die?

Rolling the weighted die once does not give us much information. However due to the law of large numbers, we can roll this die a number of times, and find the proportion of those rolls which gave a 5. The more times we roll the die, the closer this proportion approaches the underlying probability of obtaining a 5.

For a complex system such as the bicycle shop, we would like to estimate the proportion of bicycles that take longer than 30 minutes to be processed. As it is a complex system it is difficult to work this out analytically. So we would like to observe this system a number of times and record the overall proportions of bicycles spending longer than 30 minutes in the shop, which will converge to the true underlying proportion. However unlike rolling a weighted die, it it costly to observe this shop over a number of days with identical conditions. In this case it is costly in terms of time, as the repair shop already exists. However some scenarios, for example the scenario where the repair shop hires and additional member of staff, do not yet exist, so observing this this would be costly in terms of money also. We can however build a virtual representation of this complex system on a computer, and observe a virtual day of work much more quickly and much less costly on the computer, similar to a video game.

In order to do this, the computer needs to be able to generate random outcomes of each of the smaller events that make up the large complex system. Generating random events are essentially doing things to random numbers, that need to be generated.

Computers are deterministic, therefore true randomness is not always possible. They can however generate pseudorandom numbers: sequences of numbers that look like random numbers, but are entirely determined from the previous numbers in the sequence. Most programming languages have methods of doing this.

In order to simulate an event we can again manipulate the law of large numbers. Let $X \sim U(0,1)$, a uniformly pseudorandom variable between 0 and 1. Let R be the outcome of a roll of an unbiased die. Then R can be defined as:

$$R = \begin{cases} 1 & \text{if } 0 \le X < \frac{1}{6} \\ 2 & \text{if } \frac{1}{6} \le X < \frac{2}{6} \\ 3 & \text{if } \frac{2}{6} \le X < \frac{3}{6} \\ 4 & \text{if } \frac{3}{6} \le X < \frac{4}{6} \\ 5 & \text{if } \frac{4}{6} \le X < \frac{5}{6} \\ 6 & \text{if } \frac{5}{6} \le X < 1 \end{cases}$$

$$(4.1)$$

The bicycle repair shop is a system made up of interactions of a number of other simpler random events. This can be thought of as many interactions of random variables, each generated using pseudorandom numbers.

In this case the fundemental random event that need to be generated are:

- time each bicycle arrives to the repair shop,
- the time each bicycle spends at the inspection counter,
- whether each bicycle needs to go on the the repair workshop,
- the time each those bicycles spends at the repair shop.

As the simulation progresses these events will be generated, and will interact together as described in Section 4.1. The proportion of customers spending longer than 30 minutes in the shop can then be counted. This proportion itself is a random variable, and so just like the weighted die, running this simulation once does not give us much information. But we can run the simulation many times and take an average proportion, to smooth out any variability.

The process outlined above is a particular implementation of Monte Carlo simulation called discrete event simulation, which generates pseudorandom numbers and observes their interactions. In practice there are two main approaches to simulating complex probabilistic systems such as this one: the event scheduling approach, and process based simulation. It just so happens that the main implementations in Python and R use each of these approaches, so you will see both approaches used here.

4.2.1 Event Scheduling Approach

When using the event scheduling approach, we can think of the 'virtual representation' of the system as being the facilities that the bicycles use, and let entities (the bicycles) interact with these facilities. It is these facilities that determine how the entities behave.

In a simulation that uses an event scheduling approach, a key concept is that events occur that cause further events to occur in the future, either immediately or after a delay, such as after some time in service. In the bicycle shop examples of such events include a bicycle joining a queue, a bicycle beginning service, and a bicycle finishing service. At each event the event list is updated, and the clock then jumps forward to the next event in this updated list.

4.2.2 Process Based Simulation

When using process based simulation, we can think of the 'virtual representation' of the system as being the sequence of actions that each entity (the bicycles) must take, and these sequences of actions might contain delays as a number of entities seize and release a finite amount of resources. It is the sequence of actions that determine how the entities behave.

For the bicycle repair shop an example of one possible sequence of actions would be:

 $arrive \rightarrow seize \ inspection \ counter \rightarrow delay \rightarrow release \ inspection \ counter \rightarrow seize$ $repair \ shop \rightarrow delay \rightarrow release \ repair \ shop \rightarrow leave$

The scheduled delays in this sequence of events correspond to the time spend being inspected and the time spend being repaired. Waiting in line for service at these facilities are not included in the sequence of events; that is implicit by the 'seize' and 'release' actions, as an entity will wait for a free resource before seizing one. Therefore in process based simulations, in addition to defining a sequence of events, resource types and their numbers also need to be defined.

4.3 SOLVING WITH PYTHON

In this book we will use the Ciw library in order to conduct discrete event simulation. Ciw uses the event scheduling approach, which means we must define the system's facilities, and then let customers loose to interact with them.

In this case there are two facilities to define: the inspection desk and the repair workshop. Let's order these as so. For each of these we need to define:

- the distribution of times between consecutive bicycles arriving,
- the distribution of times the bicycles spend in service,
- the number of servers available,
- the probability of routing to each of the other facilities after service.

In this case we will assume that the time between consecutive arrivals follow a exponential distribution, and that the service times also follow exponential distributions. These are common assumptions for this sort of queueing system.

In Ciw, these are defined in a Network object, created using the ciw.create_network function. The code below uses this function to create a Network object that defines the current bicycle repair shop:

```
import ciw

N = ciw.create_network(
    arrival_distributions=[ciw.dists.Exponential(15), ciw.dists.NoArrivals()],
    service_distributions=[ciw.dists.Exponential(20), ciw.dists.Exponential(10)],
    number_of_servers=[1, 2],
    routing=[[0.0, 0.8], [0.0, 0.0]]

)
```

This function takes arguments that are used to define each of the four properties we listed above. Each of these arguments take in a list of properties, for each facility respectively in their order. Arguments asking for for distributions take in Ciw objects defining those distributions, ciw.dists.Exponential for exponential distributions, and ciw.dists.NoArrivals for when there are no external arrivals at the repair workshop (all bicycles arriving there are routed from the inspection desk). The number_of_servers argument takes a list of integers (1 server at the inspection desk, 2 at the repair workshop). The routing argument defines how bicycles are routed after service: from the inspection desk there is zero probability of returning to the inspection desk, and a probability of 0.8 of being routed to the repair workshop; from the repair workshop bicycles are not routed anywhere, they leave the system.

Now this we have defined the system, we need to use this to build the virtual representation of the system: in Ciw this is a Simulation object:

```
Python input

ciw.seed(0)
Q = ciw.Simulation(N)
```

Notice here a random seed is set. This is because there is some element of randomness when initialising this object, and in order to ensure reproducible results we force the pseudorandom number generator to produce the same sequence of pseudorandom numbers each time. Now we have a virtual representation of the system, we can run this for one eight hour working day:

```
Python input

Q.simulate_until_max_time(8)
```

Note that the simulation always begins with an empty system, so the first bicycle to arrive will never wait for service. Depending on the situation this may be an unwanted feature, though not in this case as it is reasonable to assume that the bicycle shop will begin the day with no customers. Now we'll count the number of bicycles that have finished service, and count the number of those whose entire journey through the system lasted longer than 0.5 hours:

```
Python input
     left individuals = Q.nodes[-1].all individuals
534
     number_over_30mins = 0
535
     for ind in left_individuals:
536
         throughput = 0
537
         for record in ind.data_records:
538
              throughput += record.exit date - record.arrival date
539
          if throughput > 0.5:
540
              number over 30mins += 1
541
     print(number over 30mins / len(left individuals))
542
```

The first line here obtains a list of all the individuals who have left the system, that is reach the final (index -1) node. Each individual will have a data record for each facility they visited. This contains many pieces of information about their time at that facility, the ones relevant here are their arrival_date and their exit_date, the difference of which gives their total time spent at that facility. Summing the total time spent at every facility gives their overall throughput in the system.

This piece of code gives

```
Python output

0.26126126126126126
```

meaning 26.13% of all bicycles spent longer than half an hour at the repair shop. However this particular day may have contained a number of extreme events.

For a more accurate proportion this experiment should be repeated, and an average proportion taken. In order to do so, let's write a function that performs the above experiment, so that we can eventually repeat the function call.

```
Python input
     def find percentage over 30mins(n inspectors, n repairers, seed)
544
          """Returns the percentage of bicycles spending over 30 minutes
545
          at the repair shop in one run of the simulation.
546
547
          Args:
548
              n_inspectors: the number of servers at the inspection desk
549
              n_repairers: the number of servers in the repair workshop
550
              seed: the seed for the pseudorandom number generator
551
552
          Returns:
553
              A real.
554
555
         N = ciw.create_network(
556
              arrival_distributions=[ciw.dists.Exponential(15), ciw.dists.NoArrivals()],
557
              service_distributions=[ciw.dists.Exponential(20), ciw.dists.Exponential(10)],
558
              number of servers=[n inspectors, n repairers],
559
              routing=[[0.0, 0.8], [0.0, 0.0]]
560
         )
561
562
         ciw.seed(seed)
563
          Q = ciw.Simulation(N)
564
          Q.simulate until max time(24)
565
566
          left individuals = Q.nodes[-1].all individuals
567
         number_over_30mins = 0
568
          for ind in left_individuals:
569
              throughput = 0
570
              for record in ind.data_records:
571
                  throughput += record.exit_date - record.arrival_date
572
              if throughput > 0.5:
573
                  number_over_30mins += 1
574
          return number_over_30mins / len(left_individuals)
575
```

This can be used to find the average proportion over 100 trials:

```
percentage_over_30 = []
for trial in range(100):
    percentage_over_30.append(find_percentage_over_30mins(1, 2, trial))
print(sum(percentage_over_30) / len(percentage_over_30))
```

which gives:

```
Python output

0.15935355368513382
```

that is, on average 15.94% of bicycles will spend longer than 30 minutes at the repair shop.

Now consider the two possible future scenarios we wish top compare: hiring an extra member of staff to serve at the inspection desk, or hiring an extra member of staff at the repair workshop. Which scenario yields a smaller proportion of bicycles spending over 30 minutes at the shop? Let's investigate. First look at the situation where the additional member of staff works at the inspection desk:

```
Python input

percentage_over_30 = []
for trial in range(100):
    percentage_over_30.append(find_percentage_over_30mins(2, 2, trial))
print(sum(percentage_over_30) / len(percentage_over_30))
```

which gives:

```
Python output

0.038476805648229126
```

that is 3.85% of bicycles.

Now look at the situation where the additional member of staff works at the repair workshop:

```
percentage_over_30 = []
for trial in range(100):
    percentage_over_30.append(find_percentage_over_30mins(1, 3, trial))
print(sum(percentage_over_30) / len(percentage_over_30))
```

which gives:

```
Python output

0.10359146418929761
```

that is 10.36% of bicycles.

Therefore an additional member of staff at the inspection desk would be more beneficial than an additional member of staff at the repair workshop.

4.4 SOLVING WITH R

In this book we will use the Simmer package in order to conduct discrete event simulation. Simmer uses the process based approach, which means we must define the each bicycle's sequence of actions, and then generate a number of bicycles with these sequences.

In Simmer these sequences of actions are made up of called trajectories. The diagram below shows the branched trajectories than a bicycle would take at the repair shop:

These are defined in simmer by:

```
R input
     library(simmer)
591
592
     bicycle <-
593
        trajectory("Inspection") %>%
594
        seize("Inspector") %>%
595
        timeout(function() {rexp(1, 20)}) %>%
596
        release("Inspector") %>%
597
        branch(
598
          function() (runif(1) < 0.8), continue=c(F),</pre>
599
          trajectory("Repair") %>%
600
            seize("Repairer") %>%
601
            timeout(function() {rexp(1, 10)}) %>%
602
            release("Repairer"),
603
          trajectory("Out")
604
605
```

Here we define a bicycle object which is made up of Simmer trajectorys. You will see that this sequence of event matches those in Figure ??. First the bicycle seizes an "Inspector" resource (yet to be defined), pauses for some service time, sampled from an exponential distribution with parameter 20, then releases the "Inspector" resource, so that resource is free to be seized by another bicycle. Then trajectory branches on the condition that an uniformly pseudorandom variable lies above or lies 0.8: if below begin the "Repair" sub-trajectory, otherwise the "Out" sub-trajectory which does not have any actions. The "Repair trajectory first seizes a "Repairer" resource (again, yet to be defined), pauses for some service time, sampled from an exponential distribution with parameter 10, then releases the "Repairer" resource. Once there are no actions left in the sequence the bicycle leaves the system.

These trajectories are not very useful alone, we are yet to define the resources used, or a way to generate bicycles with these trajectories. This is done in the code below, where a repair_shop is defined:

```
repair_shop <-
simmer("Repair Shop") %>%
add_resource("Inspector", 1) %>%
add_resource("Repairer", 2) %>%
add_generator("Bicycle", bicycle, function() {rexp(1, 15)})
```

Here we have added one resource labelled "Inspector", and two resources labelled

"Repairer". Finally we have added a generator which generates a number of the bicycle objects that we defined earlier. This generator also takes in a function to sample the delays between generating new bicycle objects, that is the inter-arrival times.

Now we have a virtual representation of the system, we can run this for one eight hour working day:

```
Rinput -
     set.seed(seed)
611
     repair_shop %>% run(until=8)
612
```

Note that the simulation always begins with an empty system, so the first bicycle to arrive will never wait for service. Depending on the situation this may be an unwanted feature, though not in this case as it is reasonable to assume that the bicycle shop will begin the day with no customers. Now we'll count the number of bicycles that have finished service, and count the number of those whose entire journey through the system lasted longer than 0.5 hours:

```
R input
     recs <- repair_shop %>% get_mon_arrivals()
613
     throughput = recs$end time - recs$start time
614
     print(mean(throughput > 0.5))
615
```

The first line here obtains a data frame of information about all the arrivals to the system. This data frame will have columns containing a limited number of pieces of information about the arrivals, however much more information can be recorded and monitored by adding monitoring actions to the trajectories. The relevant columns here are the start time and end time, the difference of which gives their total time spent in the system, the throughput. A new vector is created containing throughput information. We then calculate the proportion of entries in that vector over half an hour by taking the mean of a vector of boolean values checking this condition (this works because the booleans TRUE and RFALSE have numeric values of 1 and 0 respectively).

This piece of code gives

```
R output
     [1] 0.02777778
616
```

meaning 27.78% of all bicycles spent longer than half an hour at the repair shop. However this particular day may have contained a number of extreme events. For a more accurate proportion this experiment should be repeated, and an average proportion taken. In order to do so, let's write a function that performs the above experiment, so that we can eventually repeat the function call.

```
R input
     #' Returns the percentage of bicycles spending over 30 minutes
617
         at the repair shop in one run of the simulation.
618
     # '
619
     #' @param n_inspectors the number of servers at the inspection desk
620
     #' Oparam n_repairers the number of servers in the repair works \mathsf{hop}
621
     #' Oparam seed the seed for the pseudorandom number generator
622
623
     #' @return A real
624
     find_percentage_over_30mins <- function(n_inspectors, n_repairers, seed) {</pre>
625
       bicycle <-
626
          trajectory("Inspection") %>%
627
          seize("Inspector") %>%
628
          timeout(function() {rexp(1, 20)}) %>%
629
          release("Inspector") %>%
630
         branch(
631
            function() (runif(1) < 0.8), continue=c(F),</pre>
632
            trajectory("Repair") %>%
633
              seize("Repairer") %>%
634
              timeout(function() {rexp(1, 10)}) %>%
635
              release("Repairer"),
636
            trajectory("Out")
637
          )
638
639
       repair shop <-
640
          simmer("Repair Shop") %>%
641
          add_resource("Inspector", n_inspectors) %>%
642
          add resource ("Repairer", n repairers) %>%
643
          add_generator("Bicycle", bicycle, function() {rexp(1, 15)})
644
645
       set.seed(seed)
646
       repair_shop %>% run(until=8)
647
       recs <- repair shop %>% get mon arrivals()
648
       throughput = recs$end_time - recs$start_time
649
       return(mean(throughput > 0.5))
650
651
```

This can be used to find the average proportion over 100 trials:

```
R input
     percentage_over_30 <- c()</pre>
652
     for (seed in 1:100) {
653
       percentage over 30[seed] <- find percentage over 30mins(1, 2, seed)
654
655
     print(mean(percentage_over_30))
656
```

which gives:

```
R output
   [1] 0.1551579
657
```

that is, on average 15.52% of bicycles will spend longer than 30 minutes at the repair shop.

Now consider the two possible future scenarios we wish top compare: hiring an extra member of staff to serve at the inspection desk, or hiring an extra member of staff at the repair workshop. Which scenario yields a smaller proportion of bicycles spending over 30 minutes at the shop? Let's investigate. First look at the situation where the additional member of staff works at the inspection desk:

```
Rinput -
     percentage over 30 <- c()</pre>
658
     for (seed in 1:100) {
659
       percentage over 30[seed] <- find percentage over 30mins(2, 2, seed)
660
661
     print(mean(percentage_over_30))
662
```

which gives:

```
R output -
     [1] 0.04115338
663
```

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that is 4.12% of bicycles.

Now look at the situation where the additional member of staff works at the repair workshop:

```
percentage_over_30 <- c()
for (seed in 1:100) {
   percentage_over_30[seed] <- find_percentage_over_30mins(1, 3, seed)
}
print(mean(percentage_over_30))
```

which gives:

```
R output

[1] 0.1000899
```

that is 10.01% of bicycles.

Therefore an additional member of staff at the inspection desk would be more beneficial than an additional member of staff at the repair workshop.

4.5 RESEARCH

TBA

Bibliography

[1] Hadley Wickham. Advanced r. Chapman and Hall/CRC, 2014.

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