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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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I

Getting Started

CHAPTER 1

Introduction

THANK 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.

II

Probabilistic Modelling

CHAPTER 2

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.

2.1 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 2.1.

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 chain.

2.2 THEORY

A Markov chain 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

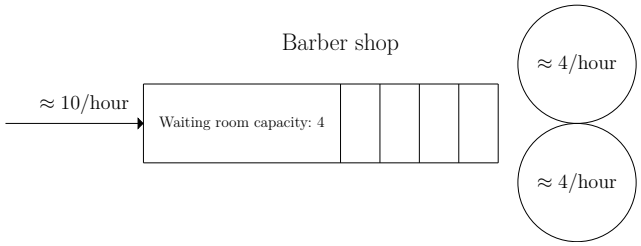

Figure 2.1 Diagrammatic representation of the barber shop as a queuing system.

hair cut. If that number is 5 this implies that 2 customers are being served and 3 are waiting. The entire state space is, in this case a finite set of integers from 0 to 6. If the system is full (all barbers and waiting room occupied) then we are in state 6 and if there is no one at the shop then we are in state 0. This is denoted mathematically as:

$$S = \{0, 1, 2, 3, 4, 5, 6\} \tag{2.1}$$

As customers arrive and leave the system goes between states as shown in Figure 2.2.

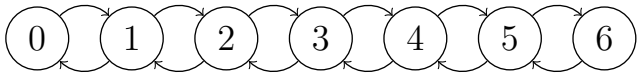

Figure 2.2 Diagrammatic representation of the state space

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 chain.
- Using rates of change from one state to another. This is called a continuous time Markov chain.

For our barber shop we will consider it as a continuous Markov chain as shown in Figure 2.3

Note that a Markov chain 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:

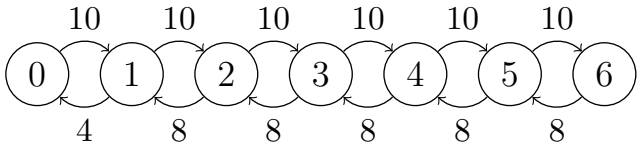

Figure 2.3 Diagrammatic representation of the state space and the transition rates

$$Q = \begin{pmatrix} -10 & 10 & 0 & 0 & 0 & 0 & 0 \\ 4 & -14 & 10 & 0 & 0 & 0 & 0 \\ 0 & 8 & -18 & 10 & 0 & 0 & 0 \\ 0 & 0 & 8 & -18 & 10 & 0 & 0 \\ 0 & 0 & 0 & 8 & -18 & 10 & 0 \\ 0 & 0 & 0 & 0 & 8 & -18 & 10 \\ 0 & 0 & 0 & 0 & 0 & 8 & -8 \end{pmatrix} \tag{2.2}$$

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:

$$P_t = e^{Qt} \tag{2.3}$$

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:

$$\pi Q = 0 \tag{2.4}$$

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

2.3 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

```python
def get_transition_rate(
    in_state, out_state, waiting_room=4, num_barbers=2,
):
    """Return the transition rate for two given states.

    Args:
        in_state: an integer
        out_state: an integer
        waiting_room: an integer (default: 4)
        num_barbers:  an integer (default: 2)

    Returns:
        A real.
    """
    arrival_rate = 10
    service_rate = 4

    capacity = waiting_room + num_barbers
    delta = out_state - in_state

    if delta == 1 and in_state < capacity:
        return arrival_rate

    if delta == -1:
        return min(in_state, num_barbers) * service_rate

    return 0
```

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

```python
import itertools
import numpy as np


def get_transition_rate_matrix(waiting_room=4, num_barbers=2):
    """Return the transition matrix Q.

    Args:
        waiting_room: an integer (default: 4)
        num_barbers: an integer (default: 2)

    Returns:
        A matrix.
    """
    capacity = waiting_room + num_barbers
    state_pairs = itertools.product(
        range(capacity + 1), repeat=2
    )

    flat_transition_rates = [
        get_transition_rate(
            in_state=in_state,
            out_state=out_state,
            waiting_room=waiting_room,
            num_barbers=num_barbers,
        )
        for in_state, out_state in state_pairs
    ]
    transition_rates = np.reshape(
        flat_transition_rates, (capacity + 1, capacity + 1)
    )
    np.fill_diagonal(
        transition_rates, -transition_rates.sum(axis=1)
    )

    return transition_rates
```

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  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]]
```

We can take the matrix exponential as discussed above. To do this, we need to use the `scipy` library. To see what would happen after .5 time units we obtain:

Python input

```
import scipy.linalg

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

We see that no matter what state (row) 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 2.4 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

```
91  def get_steady_state_vector(Q):
92      """Return the steady state vector of any given continuous
93      time transition rate matrix.
94
95      Args:
96         Q: a transition rate matrix
97
98      Returns:
99          A vector
100     """
101     state_space_size, _ = Q.shape
102     A = np.vstack((Q.T, np.ones(state_space_size)))
103     b = np.append(np.zeros(state_space_size), 1)
104     x, _, _, _ = np.linalg.lstsq(A, b, rcond=None)
105     return x
```

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

Python input

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

we get:

Python output

```
107 [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(
    waiting_room=4, num_barbers=2
):
    """Return the probability of the barber shop being full.

    Args:
        waiting_room: an integer (default: 4)
        num_barbers: an integer (default: 2)

    Returns:
        A real.
    """
    Q = get_transition_rate_matrix(
        waiting_room=waiting_room, num_barbers=num_barbers,
    )
    pi = get_steady_state_vector(Q)
    return pi[-1]
```

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

Python input

```
print(round(get_probability_of_full_shop(), 6))
```

which gives:

Python output

```
0.261756
```

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))
```

which gives:

Python output

```
0.23557
```

This is a slight improvement however, increasing the number of barbers has a substantial effect:

Python input

```
print(round(get_probability_of_full_shop(num_barbers=3), 6))
```

Python output

```
0.078636
```

2.4 SOLVING WITH R

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

R input

```r
#' Return the transition rate for two given states.
#'
#' @param in_state an integer
#' @param out_state an integer
#' @param waiting_room an integer (default: 4)
#' @param num_barbers an integer  (default: 2)
#'
#' @return A real
get_transition_rate <- function(in_state,
                                out_state,
                                waiting_room = 4,
                                num_barbers = 2){
  arrival_rate <- 10
  service_rate <- 4

  capacity <- waiting_room + num_barbers
  delta <- out_state - in_state

  if (delta == 1) {
    if (in_state < capacity) {
      return(arrival_rate)
    }
  }

  if (delta == -1) {
    return(min(in_state, num_barbers) * service_rate)
  }
  return(0)
}
```

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

R input

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

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
#'
#' @param waiting_room an integer (default: 4)
#' @param num_barbers an integer (default: 2)
#'
#' @return A matrix
get_transition_rate_matrix <- function(waiting_room = 4,
                                       num_barbers = 2){
  max_state <- waiting_room + num_barbers

  Q <- outer(0:max_state,
    0:max_state,
    vectorized_get_transition_rate,
    waiting_room = waiting_room,
    num_barbers = num_barbers
  )
  row_sums <- rowSums(Q)

  diag(Q) <- -row_sums
  Q
}
```

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

R input

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

which gives:

R output

```
     [,1] [,2] [,3] [,4] [,5] [,6] [,7]
[1,]  -10   10    0    0    0    0    0
[2,]    4  -14   10    0    0    0    0
[3,]    0    8  -18   10    0    0    0
[4,]    0    0    8  -18   10    0    0
[5,]    0    0    0    8  -18   10    0
[6,]    0    0    0    0    8  -18   10
[7,]    0    0    0    0    0    8   -8
```

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`.

To be able to make use of the nice %>% "pipe" operator we are also going to load the `magrittr` library. Now if we wanted to see what would happen after .5 time units we obtain:

R input

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

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

which gives:

R output

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

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]
[1,] 0.03431 0.08577 0.10722 0.13402 0.16752 0.2094 0.26176
[2,] 0.03431 0.08577 0.10722 0.13402 0.16752 0.2094 0.26176
[3,] 0.03431 0.08577 0.10722 0.13402 0.16752 0.2094 0.26176
[4,] 0.03431 0.08577 0.10722 0.13402 0.16752 0.2094 0.26176
[5,] 0.03431 0.08577 0.10722 0.13402 0.16752 0.2094 0.26176
[6,] 0.03431 0.08577 0.10722 0.13402 0.16752 0.2094 0.26176
[7,] 0.03431 0.08577 0.10722 0.13402 0.16752 0.2094 0.26176
```

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 2.4 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

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

#' Return the steady state vector of any given continuous time
#' transition rate matrix
#'
#' @param Q a transition rate matrix
#'
#' @return A vector
get_steady_state_vector <- function(Q){
  state_space_size <- dim(Q)[1]
  A <- rbind(t(Q), 1)
  b <- c(integer(state_space_size), 1)
  mldivide(A, b)
}
```

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

```r
print(get_steady_state_vector(Q))
```

we get:

R output

```
           [,1]
[1,] 0.03430888
[2,] 0.08577220
[3,] 0.10721525
[4,] 0.13401906
[5,] 0.16752383
[6,] 0.20940479
[7,] 0.26175598
```

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

```r
#' Return the probability of the barber shop being full
#'
#' @param waiting_room (default: 4)
#' @param num_barbers (default: 2)
#'
#' @return A real
get_probability_of_full_shop <- function(waiting_room = 4,
                                         num_barbers = 2){
  arrival_rate <- 10
  service_rate <- 4
  pi <- get_transition_rate_matrix(
    waiting_room = waiting_room,
    num_barbers = num_barbers
    ) %>%
    get_steady_state_vector()

  capacity <- waiting_room + num_barbers
  pi[capacity + 1]
}
```

Now we can run this code efficiently with both scenarios:

R input

```r
print(get_probability_of_full_shop(waiting_room = 6))
```

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(num_barbers = 3))
```

gives:

R output

```
[1] 0.0786359
```

2.5 RESEARCH

TBA

CHAPTER 3

Discrete Event Simulation

Complex 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 predictions 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.

3.1 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 in Figure 3.1

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 time in the system of 30 minutes. They would like to know if they should work on the inspection counter or in the repair workshop?

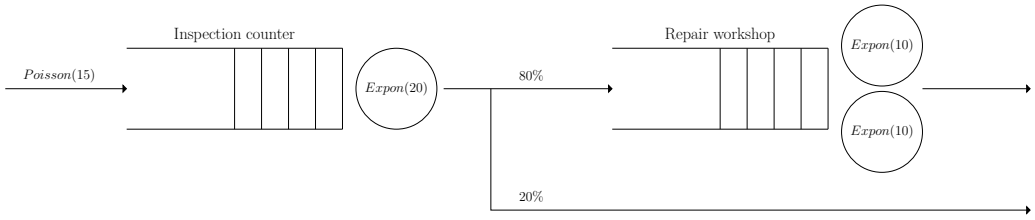

Figure 3.1 Diagrammatic representation of the bicycle repair shop as a queuing system.

3.2 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 can become 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, just like the weighted die, 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 D be the outcome of a roll of an unbiased die. Then D can be defined as:

$$D = \begin{cases} 1 & \text{if } 0 \leq X < \frac{1}{6} \\ 2 & \text{if } \frac{1}{6} \leq X < \frac{2}{6} \\ 3 & \text{if } \frac{2}{6} \leq X < \frac{3}{6} \\ 4 & \text{if } \frac{3}{6} \leq X < \frac{4}{6} \\ 5 & \text{if } \frac{4}{6} \leq X < \frac{5}{6} \\ 6 & \text{if } \frac{5}{6} \leq X < 1 \end{cases} \tag{3.1}$$

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 fundamental random events that need to be generated are:

- the 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 6.1. 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.

3.2.1 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, shown in Figure 3.1.

Then we 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.

3.2.2 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 → *seize inspection counter* → *delay* → *release inspection counter* → *seize repair shop* → *delay* → *release repair shop* → *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.

3.3 SOLVING WITH PYTHON

In this book we will use the Ciw library in order to conduct discrete event simulation in Python. 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 function below creates a Network object that defines the for a given set of parameters bicycle repair shop:

Python input

```python
import ciw


def build_network_object(
    num_inspectors=1, num_repairers=2,
):
    """Returns a Network object that defines the repair shop.

    Args:
        num_inspectors: a positive integer (default: 1)
        num_repairers: a positive integer (default: 2)

    Returns:
        a Ciw network object
    """
    arrival_rate = 15
    inspection_rate = 20
    repair_rate = 10
    prob_need_repair = 0.8
    N = ciw.create_network(
        arrival_distributions=[
            ciw.dists.Exponential(arrival_rate),
            ciw.dists.NoArrivals(),
        ],
        service_distributions=[
            ciw.dists.Exponential(inspection_rate),
            ciw.dists.Exponential(repair_rate),
        ],
        number_of_servers=[num_inspectors, num_repairers],
        routing=[[0.0, prob_need_repair], [0.0, 0.0]],
    )
    return N
```

A Network object is used by Ciw to access system parameters. For example one piece of information it holds is the number of nodes of the system:

Python input

```
N = build_network_object()
print(N.number_of_nodes)
```

which gives:

Python output

```
2
```

Now 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. Once this is built the simulation can be run, that is observe it for one virtual day. The following function does this:

Python input

```
def run_simulation(network, seed=0):
    """Builds a simulation object and runs it for 8 time units.

    Args:
        network: a Ciw network object
        seed: a float (default: 0)

    Returns:
        a Ciw simulation object after a run of the simulation
    """
    max_time = 8
    ciw.seed(seed)
    Q = ciw.Simulation(network)
    Q.simulate_until_max_time(max_time)
    return Q
```

Notice here a random seed is set. This is because there is some element of randomness when initialising this object, and much randomness in running the simulation, and in order to ensure reproducible results we force the pseudorandom number generator to produce the same sequence of pseudorandom numbers each time. Notice also 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 wish to count the number of bicycles that have finished service, and to count the number of those whose entire journey through the system lasted longer than 0.5 hours. In order to do so, we'll use the `pandas` library for efficient manipulation of data frames.

Python input

```
import pandas as pd


def get_proportion(Q):
    """Returns the proportion of bicycles spending over a given
    limit at the repair shop.

    Args:
        Q: a Ciw simulation object after a run of the
           simulation

    Returns:
        a real
    """
    limit = 0.5
    inds = Q.nodes[-1].all_individuals
    recs = pd.DataFrame(
        dr for ind in inds for dr in ind.data_records
    )
    recs["total_time"] = (
        recs["exit_date"] - recs["arrival_date"]
    )
    total_times = recs.groupby("id_number")["total_time"].sum()
    return (total_times > limit).mean()
```

Altogether these functions can define the system, run one day of our system, and then find the proportion of bicycles spending over half an hour in the shop:

Python input

```
N = build_network_object()
Q = run_simulation(N)
p = get_proportion(Q)
print(round(p, 6))
```

This piece of code gives

Python output

```
0.261261
```

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 over a number of trials, then finds an average proportion:

Python input

```
def get_average_proportion(num_inspectors=1, num_repairers=2):
    """Returns the average proportion of bicycles spending over
    a given limit at the repair shop.

    Args:
        num_inspectors: a positive integer (default: 1)
        num_repairers: a positive integer (default: 2)

    Returns:
        a real
    """
    num_trials = 100
    N = build_network_object(
        num_inspectors=num_inspectors,
        num_repairers=num_repairers,
    )
    proportions = []
    for trial in range(num_trials):
        Q = run_simulation(N, seed=trial)
        proportion = get_proportion(Q=Q)
        proportions.append(proportion)
    return sum(proportions) / num_trials
```

This can be used to find the average proportion over 100 trials for the current system of one inspector and two repair people:

Python input

```
p = get_average_proportion(num_inspectors=1, num_repairers=2)
print(round(p, 6))
```

which gives:

Python output

```
0.159354
```

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

```
366 p = get_average_proportion(num_inspectors=2, num_repairers=2)
367 print(round(p, 6))
```

which gives:

Python output

```
368 0.038477
```

that is 3.85% of bicycles.

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

Python input

```
369 p = get_average_proportion(num_inspectors=1, num_repairers=3)
370 print(round(p, 6))
```

which gives:

Python output

```
371 0.103591
```

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.

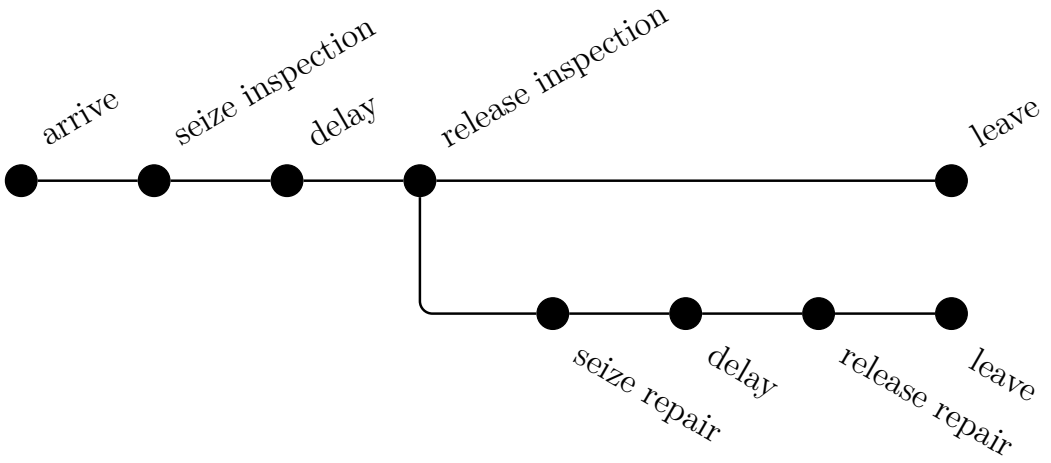

Figure 3.2 Diagrammatic representation of the forked trajectories a bicycle can take

3.4 SOLVING WITH R

In this book we will use the Simmer package in order to conduct discrete event simulation in R. 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 trajectories. The diagram in Figure 3.2 shows the branched trajectories than a bicycle would take at the repair shop:

The function below defines a simmer object that describes these trajectories:

R input

```r
library(simmer)

#' Returns a simmer trajectory object outlining the bicycles
#' path through the repair shop
#'
#' @return A simmer trajectory object
define_bicycle_trajectories <- function() {
  inspection_rate <- 20
  repair_rate <- 10
  prob_need_repair <- 0.8
  bicycle <-
    trajectory("Inspection") %>%
    seize("Inspector") %>%
    timeout(function() {
      rexp(1, inspection_rate)
    }) %>%
    release("Inspector") %>%
    branch(
      function() (runif(1) < prob_need_repair),
      continue = c(F),
      trajectory("Repair") %>%
        seize("Repairer") %>%
        timeout(function() {
          rexp(1, repair_rate)
        }) %>%
        release("Repairer"),
      trajectory("Out")
    )
  return(bicycle)
}
```

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 function below, which begins by defining a `repair_shop` with one resource labelled "Inspector", and two resources labelled "Repairer". Once this is built the simulation can be run, that is observe it for one virtual day. The following function does all this:

R input

```r
#' Runs one trial of the simulation.
#'
#' @param bicycle a simmer trajectory object
#' @param num_inspectors positive integer (default: 1)
#' @param num_repairers positive integer (default: 2)
#' @param seed a float (default: 0)
#'
#' @return A simmer simulation object after one run of
#;         the simulation
run_simulation <- function(bicycle,
                           num_inspectors = 1,
                           num_repairers = 2,
                           seed = 0) {
  arrival_rate <- 15
  max_time <- 8
  repair_shop <-
    simmer("Repair Shop") %>%
    add_resource("Inspector", num_inspectors) %>%
    add_resource("Repairer", num_repairers) %>%
    add_generator("Bicycle", bicycle, function() {
      rexp(1, arrival_rate)
    })

  set.seed(seed)
  repair_shop %>% run(until = 8)
  return(repair_shop)
}
```

Notice here a random seed is set. This is because there are elements of randomness when running the simulation, and in order to ensure reproducible results we force the pseudorandom number generator to produce the same sequence of pseudorandom numbers each time. Notice also 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 wish to count the number of bicycles that have finished service, and to count the number of those whose entire journey through the system lasted longer than 0.5 hours. Using Simmer's `get_mon_arrivals()` function we can get a data frame of records to manipulate.

R input

```r
#' Returns the proportion of bicycles spending over 30
#' minutes in the repair shop
#'
#' @param repair_shop a simmer simulation object
#'
#' @return a float between 0 and 1
get_proportion <- function(repair_shop) {
  limit <- 0.5
  recs <- repair_shop %>% get_mon_arrivals()
  total_times <- recs$end_time - recs$start_time
  return(mean(total_times > 0.5))
}
```

Altogether these functions can define the system, run one day of our system, and then find the proportion of bicycles spending over half an hour in the shop:

R input

```r
bicycle <- define_bicycle_trajectories()
repair_shop <- run_simulation(bicycle = bicycle)
print(get_proportion(repair_shop = repair_shop))
```

This piece of code gives

R output

```
[1] 0.04032258
```

meaning 4.03% 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 over a number of trials, then finds an average proportion:

R input

```r
#' Returns the average proportion of bicycles spending over
#' a given limit at the repair shop.
#'
#' @param num_inspectors positive integer (default: 1)
#' @param num_repairers positive integer (default: 2)

#' @return a float between 0 and 1
get_average_proportion <- function(num_inspectors = 1,
                                   num_repairers = 2) {
  num_trials <- 100
  bicycle <- define_bicycle_trajectories()
  proportions <- c()
  for (trial in 1:num_trials) {
    repair_shop <- run_simulation(
      bicycle = bicycle,
      num_inspectors = num_inspectors,
      num_repairers = num_repairers,
      seed = trial
    )
    proportion <- get_proportion(
      repair_shop = repair_shop
    )
    proportions[trial] <- proportion
  }
  return(mean(proportions))
}
```

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

R input

```r
print(
  get_average_proportion(
    num_inspectors = 1,
    num_repairers = 2)
)
```

which gives:

R output

```
[1] 0.1551579
```

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:

R input

```
print(
  get_average_proportion(
    num_inspectors = 2,
    num_repairers = 2)
)
```

which gives:

R output

```
[1] 0.04115338
```

that is 4.12% of bicycles.

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

R input

```
print(
  get_average_proportion(
    num_inspectors = 1,
    num_repairers = 3)
)
```

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.

3.5 RESEARCH

TBA

III

Dynamical Systems

CHAPTER 4

Modelling with Differential Equations

Systems often change in a way that depends on their current state. For example, the speed at which a cup of coffee cools down depends on its current temperature. These types of systems are called dynamical systems and are modelled mathematically using differential equations. In this chapter we will consider a direct solution approach using symbolic mathematics.

4.1 PROBLEM

Consider the following situation: the entire population of a small rural town has caught a cold. All 100 individuals will recover at an average rate of 2 per day. The town leadership have noticed that being ill costs approximately £10 per day, this is due to general lack of productivity, poorer mood and other intangible aspects. They need to decide whether or not to order cold medicine which would **double** the recover rate. The cost of of the cold medicine is a one off cost of £5 per person.

4.2 THEORY

In the case of this town, the overall rate at which people get better is dependent on the number of people in how are ill. This can be represented mathematically using a differential equation which is a way of relating the rate of change of a system to the state of the system itself.

In general if we are interested in some variable x over time t the differential function equation will be of the form:

$$\frac{dx}{dt} = f(x) \tag{4.1}$$

For some function f. In our case, if we denote the number of infected individuals as I where we implicitly mean that I is a function of time: $I = I(t)$ and the rate at which individuals recover by α then the differential equation that describes the above situation is:

$$\frac{dI}{dt} = -\alpha I \tag{4.2}$$

Finding a solution to this differential equation means finding an expression for I that when differentiated gives $-alphaI$.

In this particular case, one such function is:

$$I(t) = e^{-\alpha t} \tag{4.3}$$

However, $I(0) = 1$ whereas for our problem we know that at time $t = 0$ there are 100 infected individuals. Indeed a differential equation defines a family of solutions and we need to know some sort of initial (also referred to as boundary) condition to have the exact solution. Which in this case would be:

$$I(t) = 100e^{-\alpha t} \tag{4.4}$$

To evaluate the cost we then need to know the sum of the values of that function over time. Integration gives us exactly this, so the cost would be:

$$K \int_0^\infty I(t)dt \tag{4.5}$$

where K is the cost per person per unit time.

In the upcoming sections we will confirm and use code to carry out the above efficiently so as to answer the original question.

4.3 SOLVING WITH PYTHON

The first step we will take is to write a function to obtain the differential equation. Note that here we will be using the Python library `sympy` which allows us to carry out symbolic calculations.

Python input

```
import sympy as sym

t = sym.Symbol("t")
alpha = sym.Symbol("alpha")
I_0 = sym.Symbol("I_0")
I = sym.Function("I")


def get_equation(alpha=alpha):
    """Return the differential equation.

    Args:
        alpha: a float (default: symbolic alpha)

    Returns:
        A symbolic equation
    """
    return sym.Eq(sym.Derivative(I(t), t), -alpha * I(t))
```

Using this we can get the equation that defines the population change over time:

Python input

```
eq = get_equation()
print(eq)
```

which gives:

Python output

```
Eq(Derivative(I(t), t), -alpha*I(t))
```

Note that if you are using Jupyter then your output will actually be a well rendered mathematical equation:

$$\frac{d}{dt}I(t) = -\alpha I(t)$$

Note that we can pass a value to α if we want to:

Python input

```
eq = get_equation(alpha=1)
print(eq)
```

Python output

```
Eq(Derivative(I(t), t), -I(t))
```

We will now write a function to obtain the solution to this differential

Python input

```
def get_solution(I_0=I_0, alpha=alpha):
    """Return the solution to the differential equation.

    Args:
        I_0: a float (default: symbolic I_0)
        alpha: a float (default: symbolic alpha)

    Returns:
        A symbolic equation
    """
    eq = get_equation(alpha=alpha)
    return sym.dsolve(eq, I(t), ics={I(0): I_0})
```

We can verify the solution discussed previously:

Python input

```
sol = get_solution()
print(sol)
```

which gives:

Python output

```
Eq(I(t), I_0*exp(-alpha*t))
```

$$I(t) = I_0 e^{-\alpha t}$$

We can use sympy itself to verify the result, by taking the derivative of the right hand side of our solution.

Python input

```
print(sym.diff(sol.rhs, t) == -alpha * sol.rhs)
```

which gives:

Python output

```
True
```

All of the above has given us the general solution in terms of $I(0) = I_0$ and α however we have written the code in such a way as we can pass the actual parameters:

Python input

```
sol = get_solution(alpha=2, I_0=100)
print(sol)
```

which gives:

Python output

```
Eq(I(t), 100*exp(-2*t))
```

Now, to calculate the cost we will write a function to integrate our result:

Python input

```
def get_cost(
    I_0=I_0, alpha=alpha, cost_per_person=10, cost_of_cure=0,
):
    """Return the cost.

    Args:
        I_0: a float (default: symbolic I_0)
        alpha: a float (default: symbolic alpha)
        cost_per_person: a float (default: 10)
        cost_of_cure: a float (default: 0)

    Returns:
        A symbolic expression
    """
    I_sol = get_solution(I_0=I_0, alpha=alpha)
    return (
        sym.integrate(I_sol.rhs, (t, 0, sym.oo))
        * cost_per_person
        + cost_of_cure * I_0
    )
```

We can now obtain the cost without purchasing the cure:

Python input

```
I_0 = 100
alpha = 2
cost_without_cure = get_cost(I_0=I_0, alpha=alpha)
print(cost_without_cure)
```

which gives:

Python output

```
500
```

The cost with cure can use the above with a modified α and a non zero cost of the cure itself:

Python input

```python
cost_of_cure = 5
cost_with_cure = get_cost(
    I_0=I_0, alpha=2 * alpha, cost_of_cure=cost_of_cure
)
print(cost_with_cure)
```

which gives:

Python output

```
750
```

So given the current parameters it is not worth purchasing the cure.

4.4 SOLVING WITH R

R does not have a bespoke symbolic mathematics library however it has an interface to use Python's `sympy` called `rSymPy`. In general we would recommend to use Python directly when needing to carry out symbolic mathematical calculations however this is not always possible. Furthermore, the development of `rSymPy` seems to no longer be active and due to the dependency on Java could be problematic to use. One of other the difficulties of using `rSymPy` is that it works by passing string back and forth to Python's `sympy`. As such, we will need to have more of a manual approach and so we will not be able to write the modular code we have written throughout the book.

First let us setup and solve the differential equation:

R input

```r
library("rSymPy", warn.conflicts = FALSE, quietly = TRUE)

t <- Var("t")
alpha <- Var("alpha")
I <- Var("I")
sympy("dsolve(Derivative(I(t), t) - alpha *I(t), I(t))")
```

this will give us:

R output

```
570 [1] "C1*exp(alpha*t)"
```

We can then solve the equation directly to find the initial condition:

R input

```
571 sympy("solve(C1*exp(alpha*0) - I_0, C1)")
```

This gives:

R output

```
572 [1] "[I_0]"
```

Note here that this is in fact using a much older version of Sympy so we cannot take advantage of some of the newer commands.

So we now the form of our particular solution, thus we can now write a function that will give us the cost:

R input

```r
#' Return the cost
#'
#' @param I_0 a float (default: symbolic I_0)
#' @param alpha a float (default: symbolic alpha)
#' @param cost_per_person a float (default: 10)
#' @param cost_of_cure a float (default: 0)
#'
#' @return A symbolic expression
get_cost <- function(I_0 = Var("I_0"),
                     alpha = Var("alpha"),
                     cost_per_person = 10,
                     cost_of_cure = 0) {
  t <- Var("t")
  solution_cmd <- sprintf(
    "I_sol = %s * exp(-%s * t)",
    I_0,
    alpha
  )
  sympy(solution_cmd)
  cost_cmd <- sprintf(
    "integrate(I_sol, (t, 0, oo)) * %s + %s * %s",
    cost_per_person, cost_of_cure,
    I_0
  )
  return(sympy(cost_cmd))
}
```

Using this:

R input

```r
I_0 <- 100
alpha <- 2
cost_without_cure <- get_cost(I_0 = I_0, alpha = alpha)
print(cost_without_cure)
```

which gives:

R output

```
500
```

The cost with cure can use the above with a modified α and a non zero cost of the cure itself:

R input

```
cost_of_cure <- 5
cost_with_cure <- get_cost(
    I_0 = I_0, alpha = 2 * alpha, cost_of_cure = cost_of_cure
)
print(cost_with_cure)
```

which gives:

R output

```
750
```

So given the current parameters it is not worth purchasing the cure.

4.5 RESEARCH

TBA

CHAPTER 5

Systems Dynamics

In many situations systems are dynamical, in that the state or population of a number of entities or classes change according the current state or population of the system. For example population dynamics, chemical reactions, and systems of macroeconomics. It is often useful to be able to predict how these systems will behave over time, though the rules that govern these changes may be complex, and are not necessarily solvable analytically. In these cases numerical methods and visualisation may be used, which is the focus of this chapter.

5.1 PROBLEM

Consider the following scenario, where a population of 3000 people are susceptible to infection by some disease. This population can be described by the following parameters:

- They have a birth rate b of 0.01 per day;
- They have a death rate d of 0.01 per day;
- For every infectious individual, the infection rate α is 0.3 per day;
- Infectious people recover naturally (and thus gain an immunity from the disease), at a recovery rate r of 0.02 per day;
- For each day an individual is infected, they must take medication which costs a public healthcare system £10 per day.

A vaccine is produced, that allows new born individuals to gain an immunity. This vaccine costs the public health care system a one-off cost of £220 per vaccine. The healthcare providers would like to know if achieving a vaccination rate v of 85% would be beneficial financially.

5.2 THEORY

The above scenario is called a compartmental model of disease, and can be shown in the stock and flow diagram in Figure 5.1.

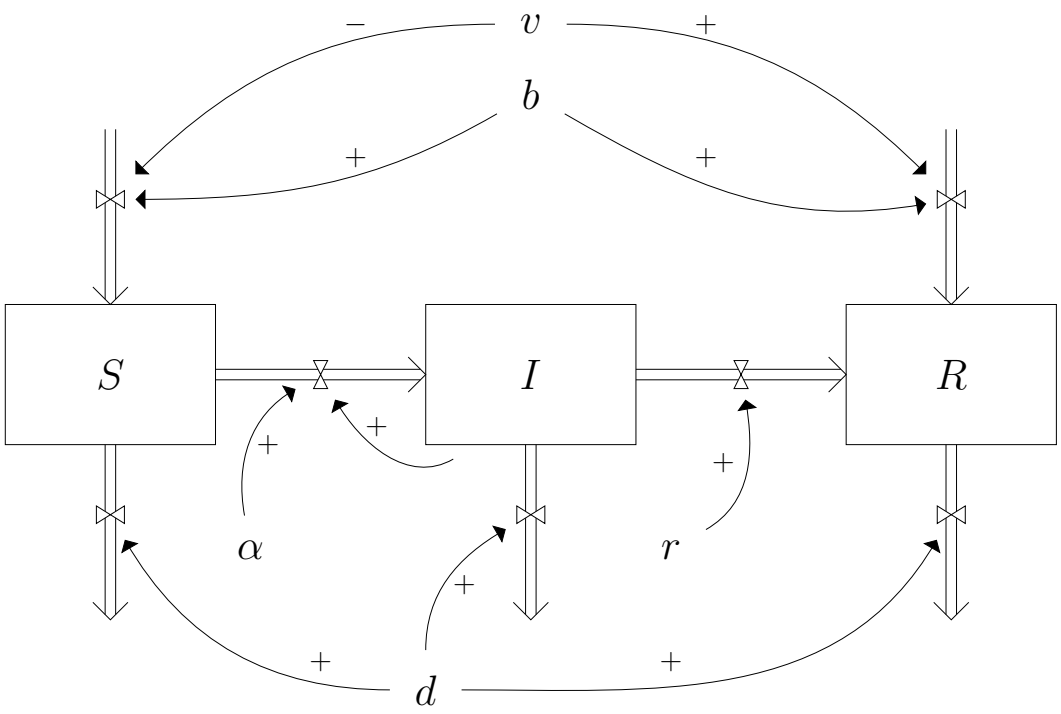

Figure 5.1 Diagrammatic representation of the epidemiology model

The system has three 'stocks' of different types of individuals, those susceptible to disease (S), those infected with the disease (I), and those who have recovered from the disease and so have gained immunity (R). The levels on these stocks change according to the flows in, out, and between them, controlled by 'taps'. The amount of flow the taps let through are influenced in a multiplicative way (either negatively or positively), by other factors, such as external parameters (e.g. birth rate, infection rate) and the stock levels.

In this system the following taps exist, influenced by the following parameters:

- *external* $\rightarrow S$*:* Influenced positively by the birth rate, and negatively by the vaccine rate.
- $S \rightarrow I$*:* Influenced positively by the infection rate, and the number of infected individuals.
- $S \rightarrow$ *external:* Influenced positively by the death rate.
- $I \rightarrow R$*:* Influenced positively by the recovery rate.
- $I \rightarrow$ *external:* Influenced positively by the death rate.
- $R \rightarrow$ *external:* Influenced positively by the birth rate and the vaccine rate.
- *external* $\rightarrow R$*:* Influenced positively by the death rate.

Mathematically the change in stock levels are written as the derivatives, for example the change in the number of susceptible individuals over time is denoted by $\frac{dS}{dt}$. This is equal to the sum of the taps in or out of that stock. Thus the system is described by the following system of differential equations:

$$\frac{dS}{dt} = -\frac{\alpha SI}{N} + (1-v)bN - dS \tag{5.1}$$

$$\frac{dI}{dt} = \frac{\alpha SI}{N} - (r+d)I \tag{5.2}$$

$$\frac{dR}{dt} = rI - dR + vbN \tag{5.3}$$

Where $N = S + I + R$ is the total number of individuals in the system.

We would like to understand the behaviour of the functions S, I and R under these rules, that is we would like to solve this system of differential equations. This system contains some non-linear terms, implying that this may be difficult to solve analytically, so we will use a numerical method instead.

There are a number of numerical methods, and the solvers we will use in Python and R cleverly choose the most appropriate for the problem at hand. In general methods for this kind of problems use the principle that the derivative denotes the rate of instantaneous change. Thus for a differential equation $\frac{dy}{dt} = f(t, y)$, consider the function y as a discrete sequence of points $\{y_0, y_1, y_2, y_3, \dots\}$ on $\{t_0, t_0 + h, t_0 + 2h, t_0 + 3h, \dots\}$ then

$$y_{n+1} = h \times f(t_0 + nh, y_n). \tag{5.4}$$

This sequence approaches the true solution y as $h \to 0$. Thus numerical methods, including the Runge-Kutta methods and the Euler method, step through this sequence $\{y_n\}$, choosing appropriate values of h and employing other methods of error reduction.

5.3 SOLVING WITH PYTHON

In this book we will use the `odeint` method of the SciPy library to numerically solve the above epidemiology models.

We first define the system of differential equations described in Equations 5.1, 5.2 and 5.3. This is a regular Python function, where the first two arguments are the system state and the current time respectively.

Python input

```python
def derivatives(y, t, vaccine_rate, birth_rate=0.01):
    """Defines the system of differential equations that
    describe the epidemiology model.

    Args:
        y: a tuple of three integers
        t: a positive float
        vaccine_rate: a positive float <= 1
        birth_rate: a positive float <= 1

    Returns:
        A tuple containing dS, dI, and dR
    """
    infection_rate = 0.3
    recovery_rate = 0.02
    death_rate = 0.01
    S, I, R = y
    N = S + I + R
    dSdt = (
        -((infection_rate * S * I) / N)
        + ((1 - vaccine_rate) * birth_rate * N)
        - (death_rate * S)
    )
    dIdt = (
        ((infection_rate * S * I) / N)
        - (recovery_rate * I)
        - (death_rate * I)
    )
    dRdt = (
        (recovery_rate * I)
        - (death_rate * R)
        + (vaccine_rate * birth_rate * N)
    )
    return dSdt, dIdt, dRdt
```

Using this function returns the instantaneous rate of change for each of the three stocks, S, I and R. If we begin at time 0.0, with 4 susceptible individuals, 1 infected individual, 0 recovered individuals, and a vaccine rate of 50%, then:

Python input

```
644 print(derivatives(y=(4, 1, 0), t=0.0, vaccine_rate=0.5))
```

Python output

```
645 (-0.255, 0.21, 0.045)
```

we would expect the number of susceptible individuals to reduce by around 0.255 per time unit, the number of infected individuals to increase by 0.21 per time unit, and the number of recovered individuals to increase by 0.045 per time unit. Now of course, after a tiny fraction of a time unit the stock levels will change, and thus the rates of change will change. So we will require something more sophisticated in order to determine the true behaviour of the system.

The following function observes the system's behaviour over some time period, using SciPy's `odeint` to numerically solve the system of differential equations:

Python input

```python
from scipy.integrate import odeint


def integrate_ode(
    derivative_function,
    t,
    y0=(2999, 1, 0),
    vaccine_rate=0.85,
    birth_rate=0.01,
):
    """Numerically solve the system of differential equations.

    Args:
        derivative_function: a function returning a tuple
                             of three floats
        t: an array of increasing positive floats
        y0: a tuple of three integers (default: (2999, 1, 0))
        vaccine_rate: a positive float <= 1 (default: 0.85)
        birth_rate: a positive float <= 1 (default: 0.01)

    Returns:
        A tuple of three arrays
    """
    results = odeint(
        derivative_function,
        y0,
        t,
        args=(vaccine_rate, birth_rate),
    )
    S, I, R = results.T
    return S, I, R
```

Now we can use this function to investigate the difference in behaviour between a vaccination rate of 0% and a vaccination rate of 85%. Let's observe the system for two years, that is 730 days, in time steps of 0.01 days.

Begin with a vaccine rate of 0%:

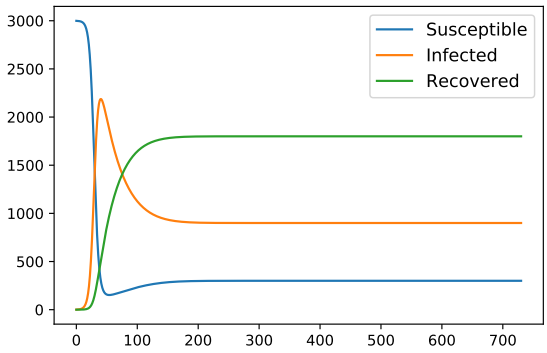

Figure 5.2 Output of code line 737-742

Python input

```
677 import numpy as np
678 from scipy.integrate import odeint
679
680 t = np.arange(0, 730.01, 0.01)
681 S, I, R = integrate_ode(derivatives, t, vaccine_rate=0.0)
```

Now `S`, `I` and `R` are arrays of values of the stock levels of S, I and R over the time steps `t`. Using `matplotlib` we can plot these to visualise their behaviour. The following code gives the plot shown in Figure 5.2.

Python input

```
682 import matplotlib.pyplot as plt
683
684 fig, ax = plt.subplots(1)
685 ax.plot(t, S, label='Susceptible')
686 ax.plot(t, I, label='Infected')
687 ax.plot(t, R, label='Recovered')
688 ax.legend(fontsize=12)
689 fig.savefig("plot_no_vaccine_python.pdf")
```

We observe that the number of infected individuals increases quickly, and in fact the rate of change increases as more individuals are infected. However this growth

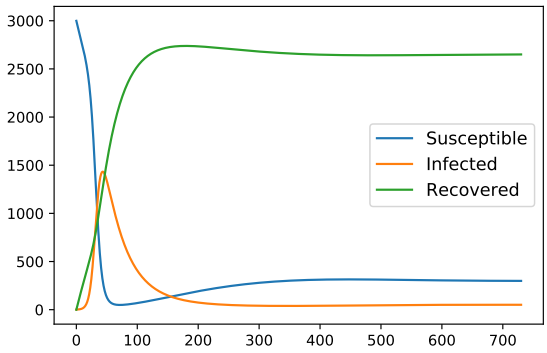

Figure 5.3 Output of code line 745-750

slows down as there are fewer susceptible individuals to infect. Due to the equal birth and death rates the overall population size remains constant; but we also see after some time period (around 300 time units) the levels of susceptible, infected, and recovered individuals becomes seemingly steady, and the disease becomes endemic. We can estimate once this steadiness occurs, around 10% of the population remain susceptible to the disease, 30% are infected, and 60% are recovered and immune.

Now with a vaccine rate of 85%:

Python input

```
690 t = np.arange(0, 730.01, 0.01)
691 S, I, R = integrate_ode(derivatives, t, vaccine_rate=0.85)
```

And again we can plot these to visualise their behaviour. The following code gives the plot shown in Figure 5.3.

Python input

```
692 fig, ax = plt.subplots(1)
693 ax.plot(t, S, label='Susceptible')
694 ax.plot(t, I, label='Infected')
695 ax.plot(t, R, label='Recovered')
696 ax.legend(fontsize=12)
697 fig.savefig("plot_with_vaccine_python.pdf")
```

With vaccination the disease remains endemic, however now we estimate that

once, steadiness occurs, around 10% of the population remain susceptible to the disease, 1.7% are infected, and 88.3% are immune or recovered and immune.

We've seen that vaccination lowers the percentage of the population living with the infection, which will lower the public healthcare system's medication costs. Let's now investigate if this saving is comparable to the cost of providing the vaccination to the newborns.

The following function calculates the total cost to the public healthcare system, that is the sum of the medication costs for those living with the infection and the vaccination costs:

Python input

```
def daily_cost(
    derivative_function=derivatives, vaccine_rate=0.85
):
    """Calculates the daily cost to the public health system
    after 2 years.

    Args:
        derivative_function: a function returning a tuple
                             of three floats
        vaccine_rate: a positive float <= 1 (default: 0.85)

    Returns:
        the daily cost
    """
    max_time = 730
    time_step = 0.01
    birth_rate = 0.01
    vaccine_cost = 220
    medication_cost = 10
    t = np.arange(0, max_time + time_step, time_step)
    S, I, R = integrate_ode(
        derivatives,
        t,
        vaccine_rate=vaccine_rate,
        birth_rate=birth_rate,
    )
    N = S[-1] + I[-1] + R[-1]
    daily_vaccine_cost = (
        N * birth_rate * vaccine_rate * vaccine_cost
    ) / time_step
    daily_meds_cost = (I[-1] * medication_cost) / time_step
    return daily_vaccine_cost + daily_meds_cost
```

Now let's compare the total daily cost with and without vaccination. Without vaccinations:

Python input

```
730 cost = daily_cost(vaccine_rate=0.0)
731 print(round(cost, 2))
```

which gives

Python output

```
732 900000.0
```

Therefore without vaccinations, once the infection is endemic, the public health care system would expect to spend £900,000 a day.

With a vaccine rate of 85%:

Python input

```
733 cost = daily_cost(vaccine_rate=0.85)
734 print(round(cost, 2))
```

which gives

Python output

```
735 611903.36
```

So vaccinating 85% of newborns would cost the public health care system, once the infection is endemic £611,903.36 a day. That is a saving of around 32%.

5.4 SOLVING WITH R

In this book we will use the `deSolve` library to numerically solve the above epidemiology models.

We first define the system of differential equations described in Equations 5.1, 5.2 and 5.3. This is an R function where the arguments are the current time, the system state, and a list of other parameters, respectively.

R input

```r
#' Defines the system of differential equations that describe
#' the epidemiology model.
#'
#' @param t a positive float
#' @param y a tuple of three integers
#' @param vaccine_rate a positive float <= 1
#' @param birth_rate a positive float <= 1
#'
#' @return a list containing dS, dI, and dR
derivatives <- function(t, y, parameters){
  infection_rate <- 0.3
  recovery_rate <- 0.02
  death_rate <- 0.01
  with(as.list(c(y, parameters)), {
    N <- S + I + R
    dSdt <- ( - ( (infection_rate * S * I) / N)  # nolint
              + ( (1 - vaccine_rate) * birth_rate * N)
              - (death_rate * S))
    dIdt <- ( ( (infection_rate * S * I) / N)  # nolint
             - (recovery_rate * I)
             - (death_rate * I))
    dRdt <- ( (recovery_rate * I)  # nolint
              - (death_rate * R)
              + (vaccine_rate * birth_rate * N))
    list(c(dSdt, dIdt, dRdt))  # nolint
  })
}
```

Using this function returns the instantaneous rate of change for each of the three stocks, S, I and R. If we begin at time 0.0, with 4 susceptible individuals, 1 infected individual, 0 recovered individuals, a vaccine rate of 50% and a birth rate of 0.01, then:

R input

```
derivatives(t = 0,
            y = c(S = 4, I = 1, R = 0),
            parameters = c(vaccine_rate = 0.5,
                           birth_rate = 0.01)
)
```

R output

```
[[1]]
[1] -0.255  0.210  0.045
```

we would expect the number of susceptible individuals to reduce by around 0.255 per time unit, the number of infected individuals to increase by 0.21 per time unit, and the number of recovered individuals to increase by 0.045 per time unit. Now of course, after a tiny fraction of a time unit the stock levels will change, and thus the rates of change will change. So we will require something more sophisticated in order to determine the true behaviour of the system.

The following function observes the system's behaviour over some time period, using the `deSolve` library to numerically solve the system of differential equations:

R input

```
library(deSolve)  # nolint

#' Numerically solve the system of differential equations
#'
#' @param t an array of increasing positive floats
#' @param y0 list of integers (default: c(S=2999, I=1, R=0))
#' @param birth_rate a positive float <= 1 (default: 0.01)
#' @param vaccine_rate a positive float <= 1 (default: 0.85)
#'
#' @return a matrix of times, S, I and R values
integrate_ode <- function(times,
                          y0 = c(S = 2999, I = 1, R = 0),
                          birth_rate = 0.01,
                          vaccine_rate = 0.84){
  params <- c(birth_rate = birth_rate,
                  vaccine_rate = vaccine_rate)
  ode(y = y0,
      times = times,
      func = derivatives,
      parms = params)
}
```

Now we can use this function to investigate the difference in behaviour between a vaccination rate of 0% and a vaccination rate of 85%. Let's observe the system for two years, that is 730 days, in time steps of 0.01 days.

Begin with a vaccine rate of 0%:

R input

```
times <- seq(0, 730, by = 0.01)
out <- integrate_ode(times, vaccine_rate = 0.0)
```

Now `out`, is a matrix with four columns, `time`, `S`, `I` and `R`, which are arrays of values of the time points, and the stock levels of S, I and R over the time respectively. We can plot these to visualise their behaviour. The following code gives the plot shown in Figure 5.4.

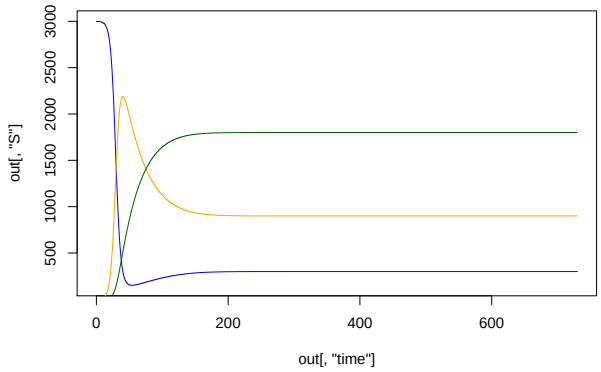

Figure 5.4 Output of code line 846-850

R input

```
pdf("plot_no_vaccine_R.pdf", width = 7, height = 5)
plot(out[, "time"], out[, "S"], type = "l", col = "blue")
lines(out[, "time"], out[, "I"], type = "l", col = "orange")
lines(out[, "time"], out[, "R"], type = "l", col = "darkgreen")
dev.off()
```

We observe that the number of infected individuals increases quickly, and in fact the rate of change increases as more individuals are infected. However this growth slows down as there are fewer susceptible individuals to infect. Due to the equal birth and death rates the overall population size remains constant; but we also see after some time period (around 300 time units) the levels of susceptible, infected, and recovered individuals becomes seemingly steady, and the disease becomes endemic. We can estimate once this steadiness occurs, around 10% of the population remain susceptible to the disease, 30% are infected, and 60% are recovered and immune.

Now with a vaccine rate of 85%:

R input

```
times <- seq(0, 730, by = 0.01)
out <- integrate_ode(times, vaccine_rate = 0.85)
```

And again we can plot these to visualise their behaviour. The following code gives the plot shown in Figure 5.5.

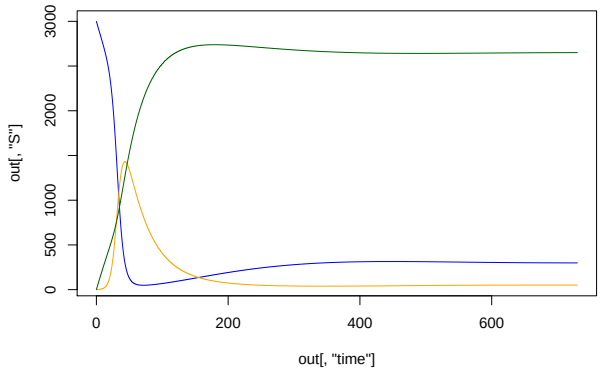

Figure 5.5 Output of code line 853-857

R input

```
800 pdf("plot_with_vaccine_R.pdf", width = 7, height = 5)
801 plot(out[, "time"], out[, "S"], type = "l", col = "blue")
802 lines(out[, "time"], out[, "I"], type = "l", col = "orange")
803 lines(out[, "time"], out[, "R"], type = "l", col = "darkgreen")
804 dev.off()
```

With vaccination the disease remains endemic, however now we estimate that once, steadiness occurs, around 10% of the population remain susceptible to the disease, 1.7% are infected, and 88.3% are immune or recovered and immune.

We've seen that vaccination lowers the percentage of the population living with the infection, which will lower the public healthcare system's medication costs. Let's now investigate if this saving is comparable to the cost of providing the vaccination to the newborns.

The following function calculates the total cost to the public healthcare system, that is the sum of the medication costs for those living with the infection and the vaccination costs:

R input

```
#' Calculates the daily cost to the public health
#' system after 2 years
#'
#' @param derivative_function: a function returning a
#'                             list of three floats
#' @param vaccine_rate: a positive float <= 1 (default: 0.85)
#'
#' @return the daily cost
daily_cost <- function(derivative_function = derivatives,
                       vaccine_rate = 0.85){
  max_time <- 730
  time_step <- 0.01
  birth_rate <- 0.01
  vaccine_cost <- 220
  medication_cost <- 10
  times <- seq(0, max_time, by = time_step)
  out <- integrate_ode(times, vaccine_rate = vaccine_rate)
  N <- sum(tail(out[, c("S", "I", "R")], n = 1))
  daily_vaccine_cost <- (N
                         * birth_rate
                         * vaccine_rate
                         * vaccine_cost) / time_step
  daily_medication_cost <- ( (tail(out[, "I"], n = 1)
                              * medication_cost)) / time_step
  daily_vaccine_cost + daily_medication_cost
}
```

Now let's compare the total daily cost with and without vaccination. Without vaccinations:

R input

```
cost <- daily_cost(vaccine_rate = 0.0)
print(cost)
```

which gives

R output

```
[1] 9e+05
```

Therefore without vaccinations, once the infection is endemic, the public health care system would expect to spend £900,000 a day.

With a vaccine rate of 85%:

R input

```
cost <- daily_cost(vaccine_rate = 0.85)
print(cost)
```

which gives

R output

```
[1] 611903.4
```

So vaccinating 85% of newborns would cost the public health care system, once the infection is endemic £611,903.40 a day. That is a saving of around 32%.

5.5 RESEARCH

IV

Optimisation

CHAPTER 6

Linear Programming

FINDING the best configuration of some system can be challenging, especially when there is a seemingly endless amount of possible solutions. Optimisation techniques are a way to mathematically derive solutions that maximise or minimise some objective function, subject to a number of feasibility constraints. When all components of the problem can be written in a linear way, then linear programming is one technique that can be used to find the solution.

6.1 PROBLEM

A university runs 26 modules over four subjects: Art, Biology, Chemistry, and Dutch. Each subject runs core modules and optional modules. Table 6.1 gives the module numbers for each of these.

The university is required to schedule examinations for each of these modules. The university would like the exams to be scheduled using the least amount of time slots possible. However not all modules can be scheduled at the same time as they share some students:

- All art modules share students,
- All biology modules share students,
- All chemistry modules share students,
- All Dutch modules share students,
- Art students have the option of taking the core Dutch modules, and so all art modules may share students with core Dutch modules,
- Biology students have the option of taking optional modules from chemistry, so all biology modules may share students with optional chemistry modules,
- Chemistry students have the option of taking optional modules from biology, so all chemistry modules may share students with optional biology modules,
- Biology students have the option of taking core art modules, and so all biology modules may share students with core art modules.

Art Core	Biology Core	Chemistry Core	Dutch Core
M00	M08	M16	M22
M01	M09	M17	M23
M02	M10	M18	
	M11	M19	
	M12		
Art Optional	**Biology Optional**	**Chemistry Optional**	**Dutch Optional**
M03	M13	M20	M24
M04	M14	M21	M25
M05	M15		
M06			
M07			

Table 6.1 List of modules on offer at the university.

What is the least number of exam time slots required to hold all 26 exams with no clashes?

6.2 THEORY

Linear programming is a method that solves an optimisation problem of n variables by defining all constraints as planes in n-dimensional space. These planes combine to create a convex region where all feasible solutions (those that satisfy the constrains) lie within the convex region, and all infeasible solutions (those that break at least one constraint) lie outside this convex region.

As we are interested in optimising some linear function, that is either minimising or maximising some function, the solution must lie at the very edge of the feasible convex region. That is we have improved so much that if we were to improve any further we would lie outside the feasible region - hence the optimum lies on the edge.

Linear programming employs algorithms such as the Simplex method to mathematically traverse the edges of the feasible convex region, and stops at the optimum. Therefore we only need to define out objective function and constraints in a linear fashion, and then apply appropriate algorithms.

Consider a 2-dimensional example: I am able to make £50 profit on each tonne of paint A I produce, and £60 profit on each tonne of paint B I produce. A tonne of paint A needs 4 tonnes of ingredient X and 5 tonnes of ingredient Y. A tonne of paint B needs 6 tonnes of ingredient X and 4 tonnes of ingredient Y. Only 24 tonnes of X and 20 tonnes of Y available per day. How much of paint A and paint B should I produce daily to maximise profit?

This is formulated as a linear objective function (total profit) to maximise, and two linear constraints (availability of ingredients X and Y). They are written as:

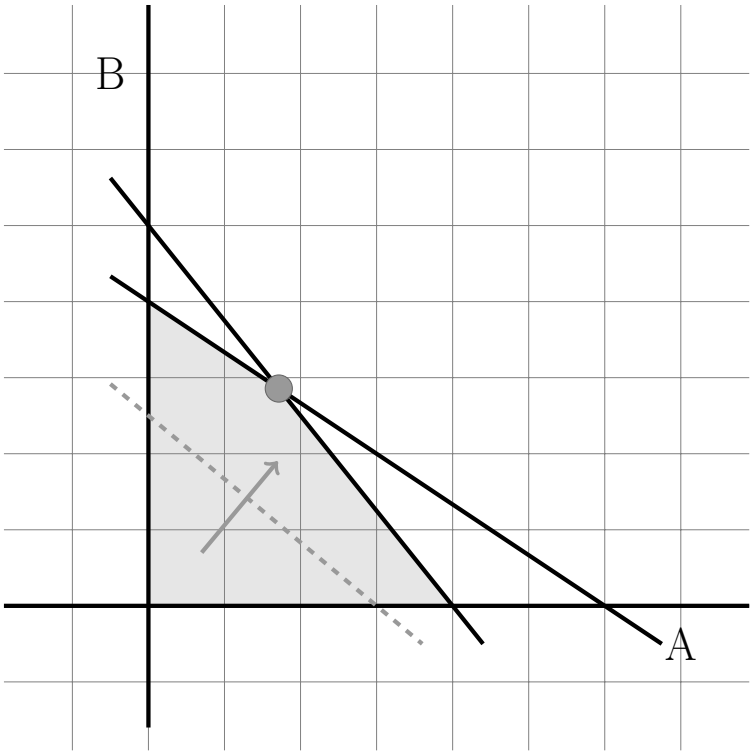

Figure 6.1 Visual representation of the paint linear program. The feasible convex region is shaded in grey; the objective function with arbitrary value is shown in a dashed line.

$$\text{Maximise: } 50A + 60B \tag{6.1}$$

$$\text{Subject to:}$$

$$4A + 6B \leq 24 \tag{6.2}$$

$$5A + 4B \leq 20 \tag{6.3}$$

Now we have a linear system in 2-dimensional space with coordinates A and B. These are called the decision variables, whose values we wish to find that optimises the objective given by expression 6.5. Inequalities **??** and 6.3 correspond to the amount of ingredient X and Y available per day. These, along with the additional constraints that we cannot produce a negative amount of paint ($A \geq 0$ and $B \geq 0$), form the convex feasible region shown in Figure 6.1.

Expression 6.5 corresponds to the total profit, which is the expression we are trying to maximise. As a line in the 2-dimensional space, this expression fixes its gradient, but its value determines the size of the y-intercept. Therefore optimising this function corresponds to pushing a line with that gradient to its furthest extreme

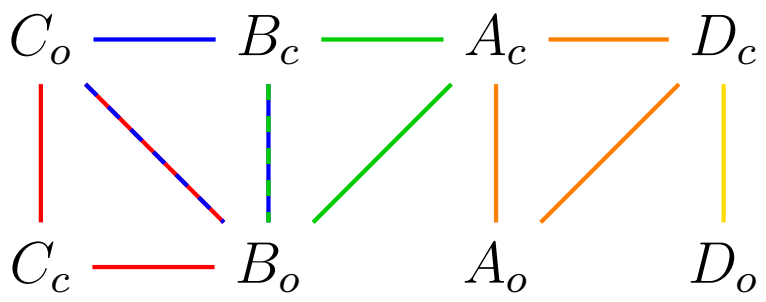

Figure 6.2 Visualisation of sets of modules with shared students.

within the feasible region, demonstrated in Figure **??**. Therefore for this problem the optimum occurs in a particular vertex of the feasible region, at $A = \frac{12}{7}$ and $B = \frac{20}{7}$.

This works well as A and B can take any real value in the feasible region. It is common however to formulate Integer Linear Programmes where the decision variables are restricted to integers. There are a number of methods that can help us adapt a real solution to an integer solution. These include cutting planes, which introduce new constraints around the real solution to force an integer value; and branch and bound methods, where we iteratively convert decision variables to their closest two integers and remove any infeasible solutions.

Both Python and R have libraries that carry out the linear and integer programming algorithms for us. When solving these kinds of problems, formulating them as linear systems is the most important challenge.

Consider again the exam scheduling problem from Section 6.1. There are eight distinct sets of modules in which exams cannot be scheduled simultaneously: A_c, A_o representing core and optional art modules respectively; B_c, B_o representing core and optional biology modules respectively; C_c, C_o representing core and optional chemistry modules respectively; and D_c, D_o representing core and optional Dutch modules respectively.

Additionally there are further clashes between these sets, this can be visualised as a graph, shown in Figure 6.2 where edges between sets represent shared students. This shows there are five cliques (shown in red, blue, green, orange and yellow), that is five larger sets of modules that may share students: $C_o \cup C_c \cup B_o$, $C_o \cup B_o \cup B_c$, $B_c \cup B_o \cup A_c$, $A_c \cup A_o \cup D_c$, and $D_c \cup D_o$. These sets of modules will form the basis for out constraints, Inequalities 6.8 to 6.12.

Define M as the set of all modules to be scheduled, that is $M = A_c \cup A_o \cup B_c \cup B_o \cup C_c \cup C_o \cup D_c \cup D_o$. Define also T as the set of possible time slots. At worst each exam is scheduled for a different day, thus $|T| = |M| = 26$ in this case. Let $\{X_{mt}$ for $m \in M$ and $t \in T\}$ be a set of binary decision variables, that is X_{mt} is 1 if module m is scheduled for time t, and 0 otherwise. Let's also define $\{Y_t$ for $t \in T\}$ as a set of auxiliary binary decision variables, where Y_t is 1 if time slot t is being used. This is enforced by Inequality 6.6.

Finally we have one final constraint, Inequality 6.7, which ensures all modules are scheduled once and once only. Thus altogether our integer program becomes:

$$\text{Minimise: } \sum_{t \in T} Y_j \tag{6.4}$$

Subject to:

$$\frac{1}{|M|} \sum_{m \in M} X_{mt} \leq Y_j \text{ for all } j \in T \tag{6.5}$$

$$\sum_{t \in T} X_{mt} = 1 \text{ for all } m \in M \tag{6.6}$$

$$\sum_{m \in C_o \cup C_c \cup B_o} X_{mt} \leq 1 \text{ for all } t \in T \tag{6.7}$$

$$\sum_{m \in C_o \cup B_o \cup B_c} X_{mt} \leq 1 \text{ for all } t \in T \tag{6.8}$$

$$\sum_{m \in B_c \cup B_o \cup A_c} X_{mt} \leq 1 \text{ for all } t \in T \tag{6.9}$$

$$\sum_{m \in A_c \cup A_o \cup D_c} X_{mt} \leq 1 \text{ for all } t \in T \tag{6.10}$$

$$\sum_{m \in D_c \cup D_o} X_{mt} \leq 1 \text{ for all } t \in T \tag{6.11}$$

$$\tag{6.12}$$

6.3 SOLVING WITH PYTHON

In this book we will use the Python library `PuLP` to formulate and solve the integer program. First let's define all the sets we will use to formulate the problem.

Python input

```
Ac = [0, 1, 2]
Ao = [3, 4, 5, 6, 7]
Bc = [8, 9, 10, 11, 12]
Bo = [13, 14, 15]
Cc = [16, 17, 18, 19]
Co = [20, 21]
Dc = [22, 23]
Do = [24, 25]
modules = Ac + Ao + Bc + Bo + Cc + Co + Dc + Do
time_slots = range(26)
```

Now let's begin by defining an empty problem:

Python input

```
847 import pulp
848 prob = pulp.LpProblem("ExamScheduling", pulp.LpMinimize)
```

We also need to define our sets of binary decision variables:

Python input

```
849 x = pulp.LpVariable.dicts("X", (modules, time_slots), cat=pulp.LpBinary)
850 y = pulp.LpVariable.dicts('Y', time_slots, cat=pulp.LpBinary)
```

Now `y` is a dictionary of binary decision variables, with keys as elements of the list `time_slots`. Let's look at Y_3 corresponding to the third day:

Python input

```
851 print(y[3])
```

Python output

```
852 Y_3
```

While `x` is a dictionary of dictionaries of binary decision variables, with keys as elements of the lists `modules` and `time_slots`. Let's look at $X_{2,5}$, the variable corresponing to module 2 being scheduled on day 5:

Python input

```
853 print(x[2][5])
```

Python output

```
854 X_2_5
```

Now we have an empty problem, all relevant sets, and all decision variables defined, we can go ahead and add the objective function and constraints to the problem.

For the objective function:

Python input

```
objective_function = sum([y[day] for day in time_slots])
prob += objective_function
```

Now the constraints:

Python input

```
for day in time_slots:
    prob += (1/len(modules)) * sum([x[module][day] for module in modules]) <= y[day]
    prob += sum([x[module][day] for module in Ac+Ao+Dc]) <= 1
    prob += sum([x[module][day] for module in Bc+Bo+Co]) <= 1
    prob += sum([x[module][day] for module in Bc+Bo+Ac]) <= 1
    prob += sum([x[module][day] for module in Cc+Co+Bo]) <= 1
    prob += sum([x[module][day] for module in Dc+Do]) <= 1

for module in modules:
    prob += sum([x[module][day] for day in time_slots]) == 1
```

At this stage we could print the `prob` object, which would explicitly give all constraints written out fully. This can be used to error check is the need arises.

Now we can go ahead and solve the problem:

Python input

```
prob.solve()
```

This returns a status code: 1 for ‘optimal’, 0 for ‘not solved’, -1 for ‘infeasible’, -2 for ‘unbounded’, or -3 for ‘undefined’. A problem is successfully solved is this methods returns 1:

Python output

```
1
```

This method has also assigned values to our decision variables. These can be inspected, lets check if module 2 was scheduled for day 5:

Python input

```
869 print(x[2][5])
```

Python output

```
870 0.0
```

This was assigned the value 0, and so module 2 was not scheduled for that day. Let's check if module 2 was scheduled for day 14:

Python input

```
871 print(x[2][14])
```

Python output

```
872 1.0
```

This was assigned a value of 1, and so module 2 was scheduled for that day.

We can iterate through all decision variables and make a print solutions in order to read off the schedule easier:

Python input

```
873 for day in time_slots:
874     if y[day].value() == 1:
875         schedule = f"Day {day}: "
876         for module in modules:
877             if x[module][day].value() == 1:
878                 schedule += f"{module}, "
879         print(schedule)
```

giving:

Python output

```
Day 0: 7, 9, 25,
Day 1: 6, 12, 17, 24,
Day 3: 3, 14,
Day 4: 10, 19,
Day 10: 4, 8, 16,
Day 11: 13, 22,
Day 12: 11, 23,
Day 13: 5, 15,
Day 14: 2, 20,
Day 17: 0, 18,
Day 18: 1, 21,
```

Now the order of the days do not matter here, but we can see that 11 days are required in order to schedule all exams with no clashes. Most days (8) have two exams scheduled, 2 days have 3 exams scheduled, and it was possible on 1 day to have 4 exams scheduled simultaneously.

6.4 SOLVING WITH R

In R we will use the R package `ROI`, the R Optimization Infrastructure. This is a library of code that acts as a front end to a number of other solvers that need to be installed externally, allowing a range of optimisation problems to be solved with a number of different solvers, using similar problem structures and syntax. The solver that we will use here is called the CBC MILP Solver, which needs to be installed as well as `rcbc` package.

In Section 6.2 the exam scheduling problem was formulated with two arrays of decision variables, a one-dimensional array Y and a two dimensional array X. In `ROI` we need our decision variables to be a one-dimensional array, so we 'flatten' these by first ordering by X then Y, within that ordering by time slot, then within that ordering by module number. Call these variables Z_i for $i \in 1, 2, ...702$. For example Z_{29} would correspond to $X_{3,2}$, the decision variable representing whether module number 3 is scheduled on day 2; Z_{700} would correspond to Y_{24}, the decision variable representing whether there's an exam scheduled for day 24.

Once this array is defined, then the objective function is an ordered array of the coefficients of each of these variables:

R input

```
#' Writes the row of coefficients for the objective function
#'
#' @param n_modules: the number of modules to schedule
#' @param n_days: the maximum number of days to schedule
#'
#' @return the objective function row to minimise
write_objective <- function(n_modules, n_days){
  all_days <- rep(0, n_modules * n_days)
  Ys <- rep(1, n_days)
  append(all_days, Ys)
}
```

For 3 modules and 3 days:

R input

```
write_objective(3, 3)
```

Which gives the following array, corresponding the the coefficients of the array Z for Equation 6.5.

R output

```
[1] 0 0 0 0 0 0 0 0 0 1 1 1
```

Now the constraints have three components: the coefficients matrix, the right hand side array, and the array of directions. The coefficients matrix is a matrix of the coefficients of the left hand side of inequalities, where again columns represent the coefficients of the array Z, and rows represent each separate constraint. The following function is used to write one row of that coefficients matrix, for a given day, for a given set of clashes, corresponding to Inequalities 6.8 to 6.12:

R input

```r
#' Writes the constraint row dealing with clashes
#'
#' @param clashes: a vector of module indices that all cannot
#'                 be scheduled at the same time
#' @param day: an integer representing the day
#'
#' @return the constraint row corresponding to that set of
#'         clashes on that day
write_X_clashes <- function(clashes, day, n_days, n_modules){
  today <- rep(0, n_modules)
  today[clashes] = 1
  before_today <- rep(0, n_modules * (day - 1))
  after_today <- rep(0, n_modules * (n_days - day))
  all_days <- c(before_today, today, after_today)
  full_coeffs <- c(all_days, rep(0, n_days))
  full_coeffs
}
```

where an array containing the module numbers of a set of modules that may all share students. The following function is used to write one row of the coefficients matrix, for each module, ensuring that each module is scheduled on one day and one day only, corresponding to Equation 6.7:

R input

```r
#' Writes the constraint row to ensure that every module is
#' scheduled once and only one
#'
#' @param module: an integer representing the module
#'
#' @return the constraint row corresponding to scheduling a
#'         module on only one day
write_X_requirements <- function(module, n_days, n_modules){
  today <- rep(0, n_modules)
  today[module] = 1
  all_days <- rep(today, n_days)
  full_coeffs <- c(all_days, rep(0, n_days))
  full_coeffs
}
```

The following function is used to write one row of the coefficients matrix corresponding to the auxiliary constraints of Inequalities ??:

R input

```r
#' Writes the constraint row representing the Y variable,
#' whether at least one exam is scheduled on that day
#'
#' @param day: an integer representing the day
#'
#' @return the constraint row corresponding to creating Y
write_Y_constraints <- function(day, n_days, n_modules){
  today <- rep(1, n_modules)
  before_today <- rep(0, n_modules * (day - 1))
  after_today <- rep(0, n_modules * (n_days - day))
  all_days <- c(before_today, today, after_today)
  all_Ys <- rep(0, n_days)
  all_Ys[day] = -n_modules
  full_coeffs <- append(all_days, all_Ys)
  full_coeffs
}
```

Finally the following function uses them all to assemble a coefficients matrix. It loops though the parameters for each constraint row required, uses the appropriate function to create the row of the coefficients matrix, sets the appropriate inequality direction ($\leq$, $=$, $\geq$), and the value of the right hand side. It returns all three components:

R input

```r
#' Writes all the constraints as a matrix, column of
#' inequalities, and right hand side column.
#'
#' @param list_clashes: a list of vectors with sets of modules
#'         that cannot be scheduled at the same time
#'
#' @return f.con the LHS of the constraints as a matrix
#' @return f.dir a vector of directions of the inequalities
#' @return f.rhs a vector of the values of the RHS of the inequalities
write_constraints <- function(list_clashes, n_days, n_modules){
  all_rows <- c()
  all_dirs <- c()
  all_rhss <- c()
  n_rows <- 0

  for (clash in list_clashes){
    for (day in 1:n_days){
      clashes <- write_X_clashes(clash, day, n_days, n_modules)
      all_rows <- append(all_rows, clashes)
      all_dirs <- append(all_dirs, "<=")
      all_rhss <- append(all_rhss, 1)
      n_rows <- n_rows + 1
    }
  }

  for (module in 1:n_modules){
    reqs <- write_X_requirements(module, n_days, n_modules)
    all_rows <- append(all_rows, reqs)
    all_dirs <- append(all_dirs, "==")
    all_rhss <- append(all_rhss, 1)
    n_rows <- n_rows + 1
  }

  for (day in 1:n_days){
    Yconstraints <- write_Y_constraints(day, n_days, n_modules)
    all_rows <- append(all_rows, Yconstraints)
    all_dirs <- append(all_dirs, "<=")
    all_rhss <- append(all_rhss, 0)
    n_rows <- n_rows + 1
  }

  f.con <- matrix(all_rows, nrow = n_rows, byrow = TRUE)
  f.dir <- all_dirs
  f.rhs <- all_rhss
  list(f.con, f.dir, f.rhs)
}
```

For demonstration, if we had two modules and two possible days, with the single constraint that both modules cannot be scheduled at the same time, then:

R input

```
write_constraints(list_clashes = list(c(1, 2)),
                  n_days = 2,
                  n_modules = 2)
```

This would give three components, a coefficient matrix of the left hand side of the constraints (rows 1 and 2 corresponding to the clash on days 1 and 2, row 3 ensuring module 1 is scheduled on one day only, row 4 ensuring module 2 is scheduled on one day only, and rows 5 and 5 defining the Y decision variables), an array of direction of the constraint inequalities, and an array of the right hand side values of the constraints.

R output

```
[[1]]
     [,1] [,2] [,3] [,4] [,5] [,6]
[1,]    1    1    0    0    0    0
[2,]    0    0    1    1    0    0
[3,]    1    0    1    0    0    0
[4,]    0    1    0    1    0    0
[5,]    1    1    0    0   -2    0
[6,]    0    0    1    1    0   -2

[[2]]
[1] "<=" "<=" "==" "==" "<=" "<="

[[3]]
[1] 1 1 1 1 0 0
```

Now we are ready to use these to solve the exam scheduling problem. First we define some parameters, including the sets of modules that all share students, that is the list of clashes:

R input

```
n_modules = 26
n_days = 26

Ac <- c(1, 2, 3)
Ao <- c(4, 5, 6, 7, 8)
Bc <- c(9, 10, 11, 12, 13)
Bo <- c(14, 15, 16)
Cc <- c(17, 18, 19, 20)
Co <- c(21, 22)
Dc <- c(23, 24)
Do <- c(25, 26)

list_clashes <- list(
  c(Ac, Ao, Dc),
  c(Bc, Bo, Co),
  c(Bc, Bo, Ac),
  c(Cc, Co, Bo),
  c(Dc, Do)
)
```

Then we can use the functions defined above to create the objective function and the three elements of the constraints:

R input

```
constraints <- write_constraints(list_clashes = list_clashes,
                                 n_days = n_days,
                                 n_modules = n_modules)
f.con <- constraints[[1]]
f.dir <- constraints[[2]]
f.rhs <- constraints[[3]]
f.obj <- write_objective(n_modules = n_modules, n_days = n_days)
```

Finally, once these objects are in place, we can use the to construct an optimisation problem object:

R input

```
library(ROI)

milp <- OP(objective = L_objective(f.obj),
           constraints = L_constraint(L = f.con,
                                      dir = f.dir,
                                      rhs = f.rhs),
           types = rep("B", length(f.obj)),
           maximum = FALSE)
```

This creates an `OP` object from our objective row `f.obj`, and our constraints which are made up from the three components `f.con`, `f.dir` and `f.rhs`. When creating this object we also denote the `types` as binary variables (an array o `"B"` for each decision variable), and we want to minimise out objective function so we set `maximum = FALSE`.

Now to solve:

R input

```
sol <- ROI_solve(milp)
```

The solver will not output information about the solve process and runtime. We can now print the solution:

R input

```
print(sol$solution)
```

R output

```
  [1] 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 [30] 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 [59] 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
 [88] 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
[117] 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0
[146] 0 0 0 0 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
[175] 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1 1 0 0 0 0 0 0 0 0 1 0 0
[204] 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
[233] 0 0 0 0 0 0 1 0 0 0 0 0 0 0 1 0 0 0 0 0 0 1 0 0 0 0 0 0 0 0
[262] 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1 0 0 0 0 1 0 0 0 0 0
[291] 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
[320] 0 0 0 0 0 0 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1 0 0 0 0 0
[349] 0 0 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
[378] 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
[407] 0 0 0 0 0 0 0 0 0 0 0 0 0 1 0 0 0 0 0 0 0 0 0 1 0 0 0 0 0 0
[436] 0 0 0 0 0 1 0 0 0 0 0 0 0 1 0 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0
[465] 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
[494] 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
[523] 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
[552] 0 0 0 0 0 0 1 0 0 0 0 1 0 0 0 0 0 0 1 0 0 0 0 0 0 0 0 0 0 0
[581] 0 1 0 0 0 0 0 0 0 0 0 0 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
[610] 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0
[639] 0 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
[668] 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1 0 1 0 1 1 0 1 1 0 0 1 1 0 0
[697] 0 1 1 0 1 0
```

This gives the values of each of the Z decision variables. We know the structure of this, that is the first 26 variables are the modules scheduled for day 1, and so on. The following code prints a readable schedule:

R input

```r
for (day in 1:n_days){
  if (sol$solution[(n_days*n_modules) + day] == 1){
    schedule <- paste("Day", day, ":")
    for (module in 1:n_modules){
      var <- ((day - 1) * n_modules) + module
      if (sol$solution[var] == 1){
        schedule <- paste(schedule, module)
      }
    }
    print(schedule)
  }
}
```

R output

```
[1] "Day 6 : 2 22"
[1] "Day 8 : 8 9 19"
[1] "Day 10 : 5 13 20"
[1] "Day 11 : 3 21 26"
[1] "Day 13 : 16"
[1] "Day 14 : 6 15"
[1] "Day 17 : 4 14 25"
[1] "Day 18 : 7 11"
[1] "Day 22 : 12 17 24"
[1] "Day 23 : 10 23"
[1] "Day 25 : 1 18"
```

Giving that 11 days are the minimum required to schedule the 26 exams without clashes.

6.5 RESEARCH

Bibliography