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Title Page

LOC Page

Vince: to Riggins
Geraint: also, to Riggins



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Foreword

This is the foreword



Preface

This is the preface.



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I

Getting Started



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



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

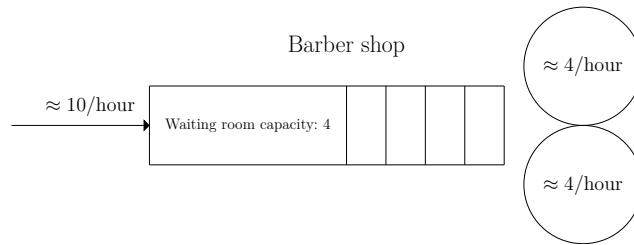


Figure 2.1 Diagrammatic representation of the barber shop as a queuing system.

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:

$$S = \{0, 1, 2, 3, 4, 5, 6\} \quad (2.1)$$

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

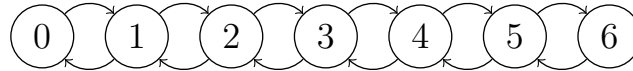


Figure 2.2 Diagrammatic representation of the state space

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:

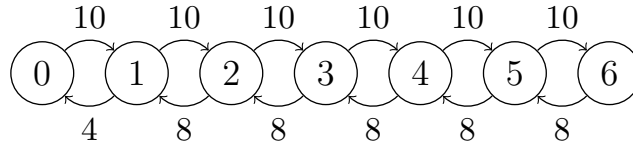


Figure 2.3 Diagrammatic representation of the state space and the transition rates

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

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 units. This 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:

$$P_t = e^{Qt} \quad (2.3)$$

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:

$$\pi Q = 0 \quad (2.4)$$

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

```

1 def get_transition_rate(
2     in_state,
3     out_state,
4     waiting_room=4,
5     num_barbers=2,
6 ):
7     """Return the transition rate for two given states.
8
9     Args:
10         in_state: an integer
11         out_state: an integer
12         waiting_room: an integer (default: 4)
13         num_barbers: an integer (default: 2)
14
15     Returns:
16         A real.
17     """
18     arrival_rate = 10
19     service_rate = 4
20
21     capacity = waiting_room + num_barbers
22     delta = out_state - in_state
23
24     if delta == 1 and in_state < capacity:
25         return arrival_rate
26
27     if delta == -1:
28         return min(in_state, num_barbers) * service_rate
29
30     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

```

31 import itertools
32 import numpy as np
33
34
35 def get_transition_rate_matrix(waiting_room=4, num_barbers=2):
36     """Return the transition matrix Q.
37
38     Args:
39         waiting_room: an integer (default: 4)
40         num_barbers: an integer (default: 2)
41
42     Returns:
43         A matrix.
44     """
45     capacity = waiting_room + num_barbers
46     state_pairs = itertools.product(
47         range(capacity + 1), repeat=2
48     )
49
50     flat_transition_rates = [
51         get_transition_rate(
52             in_state=in_state,
53             out_state=out_state,
54             waiting_room=waiting_room,
55             num_barbers=num_barbers,
56         )
57         for in_state, out_state in state_pairs
58     ]
59     transition_rates = np.reshape(
60         flat_transition_rates, (capacity + 1, capacity + 1)
61     )
62     np.fill_diagonal(
63         transition_rates, -transition_rates.sum(axis=1)
64     )
65
66     return transition_rates

```

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

Python input

```

67 Q = get_transition_rate_matrix()
68 print(Q)

```

which gives:

Python output

```

69 [[-10  10  0  0  0  0  0]
70 [  4 -14  10  0  0  0  0]
71 [  0  8 -18  10  0  0  0]
72 [  0  0  8 -18  10  0  0]
73 [  0  0  0  8 -18  10  0]
74 [  0  0  0  0  8 -18  10]
75 [  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

```

76 import scipy.linalg
77
78 print(scipy.linalg.expm(Q * 0.5).round(5))

```

which gives:

Python output

```

79 [[0.10492 0.21254 0.20377 0.17142 0.13021 0.09564 0.0815 ]
80 [0.08501 0.18292 0.18666 0.1708  0.14377 0.1189  0.11194]
81 [0.06521 0.14933 0.16338 0.16478 0.15633 0.14751 0.15346]
82 [0.04388 0.10931 0.13183 0.15181 0.16777 0.18398 0.21142]
83 [0.02667 0.07361 0.10005 0.13422 0.17393 0.2189  0.27262]
84 [0.01567 0.0487  0.07552 0.11775 0.17512 0.24484 0.32239]
85 [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

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

which gives:

Python output

```
87 [[0.03431 0.08577 0.10722 0.13402 0.16752 0.2094 0.26176]
88 [0.03431 0.08577 0.10722 0.13402 0.16752 0.2094 0.26176]
89 [0.03431 0.08577 0.10722 0.13402 0.16752 0.2094 0.26176]
90 [0.03431 0.08577 0.10722 0.13402 0.16752 0.2094 0.26176]
91 [0.03431 0.08577 0.10722 0.13402 0.16752 0.2094 0.26176]
92 [0.03431 0.08577 0.10722 0.13402 0.16752 0.2094 0.26176]
93 [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

```

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

```

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

Python input

```

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

```

we get:

Python output

```

110 [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

```

111 def get_probability_of_full_shop(
112     waiting_room=4, num_barbers=2
113 ):
114     """Return the probability of the barber shop being full.
115
116     Args:
117         waiting_room: an integer (default: 4)
118         num_barbers: an integer (default: 2)
119
120     Returns:
121         A real.
122     """
123     Q = get_transition_rate_matrix(
124         waiting_room=waiting_room,
125         num_barbers=num_barbers,
126     )
127     pi = get_steady_state_vector(Q)
128     return pi[-1]

```

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

Python input

```

129 print(round(get_probability_of_full_shop(), 6))

```

which gives:

Python output

```

130 0.261756

```

If we were too have 2 extra space in the waiting room:

Python input

```
131 print(round(get_probability_of_full_shop(waiting_room=6), 6))
```

which gives:

Python output

```
132 0.23557
```

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

Python input

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

Python output

```
134 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

```

135 #' Return the transition rate for two given states.
136 #'
137 #' @param in_state an integer
138 #' @param out_state an integer
139 #' @param waiting_room an integer (default: 4)
140 #' @param num_barbers an integer (default: 2)
141 #'
142 #' @return A real
143 get_transition_rate <- function(in_state,
144                                out_state,
145                                waiting_room = 4,
146                                num_barbers = 2){
147
148   arrival_rate <- 10
149   service_rate <- 4
150
151   capacity <- waiting_room + num_barbers
152   delta <- out_state - in_state
153
154   if (delta == 1) {
155     if (in_state < capacity) {
156       return(arrival_rate)
157     }
158   }
159
160   if (delta == -1) {
161     return(min(in_state, num_barbers) * service_rate)
162   }
163   return(0)
164 }

```

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

R input

```

164 vectorized_get_transition_rate <- Vectorize(
165   get_transition_rate,
166   vectorize.args = c("in_state", "out_state")
167 )

```

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

```

168  #' Return the transition rate matrix Q
169  #'
170  #' @param waiting_room an integer (default: 4)
171  #' @param num_barbers an integer (default: 2)
172  #'
173  #' @return A matrix
174  get_transition_rate_matrix <- function(waiting_room = 4,
175                                         num_barbers = 2){
176    max_state <- waiting_room + num_barbers
177
178    Q <- outer(0:max_state,
179              0:max_state,
180              vectorized_get_transition_rate,
181              waiting_room = waiting_room,
182              num_barbers = num_barbers
183            )
184    row_sums <- rowSums(Q)
185
186    diag(Q) <- -row_sums
187    Q
188  }

```

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

R input

```

189  Q <- get_transition_rate_matrix()
190  print(Q)

```

which gives:

R output

```

191      [,1] [,2] [,3] [,4] [,5] [,6] [,7]
192 [1,]  -10  10   0   0   0   0   0
193 [2,]   4 -14  10   0   0   0   0
194 [3,]   0  8 -18  10   0   0   0
195 [4,]   0  0  8 -18  10   0   0
196 [5,]   0  0  0  8 -18  10   0
197 [6,]   0  0  0  0  8 -18  10
198 [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

```

199 library(expm, warn.conflicts = FALSE, quietly = TRUE)
200 library(magrittr, warn.conflicts = FALSE, quietly = TRUE)
201
202 print( (Q * .5) %>% expm %>% round(5))

```

which gives:

R output

```

203      [,1] [,2] [,3] [,4] [,5] [,6] [,7]
204 [1,] 0.10492 0.21254 0.20377 0.17142 0.13021 0.09564 0.08150
205 [2,] 0.08501 0.18292 0.18666 0.17080 0.14377 0.11890 0.11194
206 [3,] 0.06521 0.14933 0.16338 0.16478 0.15633 0.14751 0.15346
207 [4,] 0.04388 0.10931 0.13183 0.15181 0.16777 0.18398 0.21142
208 [5,] 0.02667 0.07361 0.10005 0.13422 0.17393 0.21890 0.27262
209 [6,] 0.01567 0.04870 0.07552 0.11775 0.17512 0.24484 0.32239
210 [7,] 0.01068 0.03668 0.06286 0.10824 0.17448 0.25791 0.34914

```

After 500 time units we obtain:

R input

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

which gives:

R output

```
212      [,1] [,2] [,3] [,4] [,5] [,6] [,7]
213 [1,] 0.03431 0.08577 0.10722 0.13402 0.16752 0.2094 0.26176
214 [2,] 0.03431 0.08577 0.10722 0.13402 0.16752 0.2094 0.26176
215 [3,] 0.03431 0.08577 0.10722 0.13402 0.16752 0.2094 0.26176
216 [4,] 0.03431 0.08577 0.10722 0.13402 0.16752 0.2094 0.26176
217 [5,] 0.03431 0.08577 0.10722 0.13402 0.16752 0.2094 0.26176
218 [6,] 0.03431 0.08577 0.10722 0.13402 0.16752 0.2094 0.26176
219 [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

```

220 library(pracma, warn.conflicts = FALSE, quietly = TRUE)
221
222 #' Return the steady state vector of any given continuous time
223 #' transition rate matrix
224 #'
225 #' @param Q a transition rate matrix
226 #'
227 #' @return A vector
228 get_steady_state_vector <- function(Q){
229   state_space_size <- dim(Q)[1]
230   A <- rbind(t(Q), 1)
231   b <- c(integer(state_space_size), 1)
232   mldivide(A, b)
233 }

```

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

```

234 print(get_steady_state_vector(Q))

```

we get:

R output

```

235      [,1]
236 [1,] 0.03430888
237 [2,] 0.08577220
238 [3,] 0.10721525
239 [4,] 0.13401906
240 [5,] 0.16752383
241 [6,] 0.20940479
242 [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

```

243 #' Return the probability of the barber shop being full
244 #'
245 #' @param waiting_room (default: 4)
246 #' @param num_barbers (default: 2)
247 #'
248 #' @return A real
249 get_probability_of_full_shop <- function(waiting_room = 4,
250                                         num_barbers = 2){
251     arrival_rate <- 10
252     service_rate <- 4
253     pi <- get_transition_rate_matrix(
254         waiting_room = waiting_room,
255         num_barbers = num_barbers
256     ) %>%
257         get_steady_state_vector()
258
259     capacity <- waiting_room + num_barbers
260     pi[capacity + 1]
261 }

```

Now we can run this code efficiently with both scenarios:

R input

```

262 print(get_probability_of_full_shop(waiting_room = 6))

```

which decreases the probability of a full shop to:

R output

```

263 [1] 0.2355699

```

but adding another barber and chair:

R input

264

```
print(get_probability_of_full_shop(num_barbers = 3))
```

gives:

R output

265

```
[1] 0.0786359
```

2.5 RESEARCH

TBA



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 it 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 an 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 if we roll the die a large number of times, we would expect $\frac{1}{6}$ 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 is 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 an 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:

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

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 8.1. 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

```

266 import ciw
267
268
269 def build_network_object(
270     num_inspectors=1,
271     num_repairers=2,
272 ):
273     """Returns a Network object that defines the repair shop.
274
275     Args:
276         num_inspectors: a positive integer (default: 1)
277         num_repairers: a positive integer (default: 2)
278
279     Returns:
280         a Ciw network object
281     """
282     arrival_rate = 15
283     inspection_rate = 20
284     repair_rate = 10
285     prob_need_repair = 0.8
286     N = ciw.create_network(
287         arrival_distributions=[
288             ciw.dists.Exponential(arrival_rate),
289             ciw.dists.NoArrivals(),
290         ],
291         service_distributions=[
292             ciw.dists.Exponential(inspection_rate),
293             ciw.dists.Exponential(repair_rate),
294         ],
295         number_of_servers=[num_inspectors, num_repairers],
296         routing=[[0.0, prob_need_repair], [0.0, 0.0]],
297     )
298     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

```

299 N = build_network_object()
300 print(N.number_of_nodes)

```

which gives:

Python output

```

301 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

```

302 def run_simulation(network, seed=0):
303     """Builds a simulation object and runs it for 8 time units.
304
305     Args:
306         network: a Ciw network object
307         seed: a float (default: 0)
308
309     Returns:
310         a Ciw simulation object after a run of the simulation
311     """
312     max_time = 8
313     ciw.seed(seed)
314     Q = ciw.Simulation(network)
315     Q.simulate_until_max_time(max_time)
316     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

```

317 import pandas as pd
318
319
320 def get_proportion(Q):
321     """Returns the proportion of bicycles spending over a given
322     limit at the repair shop.
323
324     Args:
325         Q: a Ciw simulation object after a run of the
326         simulation
327
328     Returns:
329         a real
330     """
331     limit = 0.5
332     inds = Q.nodes[-1].all_individuals
333     recs = pd.DataFrame(
334         dr for ind in inds for dr in ind.data_records
335     )
336     recs["total_time"] = (
337         recs["exit_date"] - recs["arrival_date"]
338     )
339     total_times = recs.groupby("id_number")["total_time"].sum()
340     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

```
341 N = build_network_object()
342 Q = run_simulation(N)
343 p = get_proportion(Q)
344 print(round(p, 6))
```

This piece of code gives

Python output

```
345 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

```

346 def get_average_proportion(num_inspectors=1, num_repairers=2):
347     """Returns the average proportion of bicycles spending over
348     a given limit at the repair shop.
349
350     Args:
351         num_inspectors: a positive integer (default: 1)
352         num_repairers: a positive integer (default: 2)
353
354     Returns:
355         a real
356     """
357     num_trials = 100
358     N = build_network_object(
359         num_inspectors=num_inspectors,
360         num_repairers=num_repairers,
361     )
362     proportions = []
363     for trial in range(num_trials):
364         Q = run_simulation(N, seed=trial)
365         proportion = get_proportion(Q=Q)
366         proportions.append(proportion)
367     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

```

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

```

which gives:

Python output

```

370 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 to 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

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

which gives:

Python output

```
373 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

```
374 p = get_average_proportion(num_inspectors=1, num_repairers=3)
375 print(round(p, 6))
```

which gives:

Python output

```
376 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

```

377 library(simmer)
378
379 #' Returns a simmer trajectory object outlining the bicycles
380 #' path through the repair shop
381 #'
382 #' @return A simmer trajectory object
383 define_bicycle_trajectories <- function() {
384   inspection_rate <- 20
385   repair_rate <- 10
386   prob_need_repair <- 0.8
387   bicycle <-
388     trajectory("Inspection") %>%
389     seize("Inspector") %>%
390     timeout(function() {
391       rexp(1, inspection_rate)
392     }) %>%
393     release("Inspector") %>%
394     branch(
395       function() (runif(1) < prob_need_repair),
396       continue = c(F),
397       trajectory("Repair") %>%
398         seize("Repairer") %>%
399         timeout(function() {
400           rexp(1, repair_rate)
401         }) %>%
402         release("Repairer"),
403       trajectory("Out")
404     )
405   return(bicycle)
406 }

```

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

```

407 #' Runs one trial of the simulation.
408 #'
409 #' @param bicycle a simmer trajectory object
410 #' @param num_inspectors positive integer (default: 1)
411 #' @param num_repairers positive integer (default: 2)
412 #' @param seed a float (default: 0)
413 #'
414 #' @return A simmer simulation object after one run of
415 #;         the simulation
416 run_simulation <- function(bicycle,
417                             num_inspectors = 1,
418                             num_repairers = 2,
419                             seed = 0) {
420   arrival_rate <- 15
421   max_time <- 8
422   repair_shop <-
423     simmer("Repair Shop") %>%
424     add_resource("Inspector", num_inspectors) %>%
425     add_resource("Repairer", num_repairers) %>%
426     add_generator("Bicycle", bicycle, function() {
427       rexp(1, arrival_rate)
428     })
429
430   set.seed(seed)
431   repair_shop %>% run(until = 8)
432   return(repair_shop)
433 }

```

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

```

434 #' Returns the proportion of bicycles spending over 30
435 #' minutes in the repair shop
436 #'
437 #' @param repair_shop a simmer simulation object
438 #'
439 #' @return a float between 0 and 1
440 get_proportion <- function(repair_shop) {
441   limit <- 0.5
442   recs <- repair_shop %>% get_mon_arrivals()
443   total_times <- recs$end_time - recs$start_time
444   return(mean(total_times > 0.5))
445 }

```

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

```

446 bicycle <- define_bicycle_trajectories()
447 repair_shop <- run_simulation(bicycle = bicycle)
448 print(get_proportion(repair_shop = repair_shop))

```

This piece of code gives

R output

```

449 [1] 0.1343284

```

meaning 13.43% 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

```

450  #' Returns the average proportion of bicycles spending over
451  #' a given limit at the repair shop.
452  #'
453  #' @param num_inspectors positive integer (default: 1)
454  #' @param num_repairers positive integer (default: 2)
455
456  #' @return a float between 0 and 1
457  get_average_proportion <- function(num_inspectors = 1,
458                                     num_repairers = 2) {
459
460    num_trials <- 100
461    bicycle <- define_bicycle_trajectories()
462    proportions <- c()
463    for (trial in 1:num_trials) {
464      repair_shop <- run_simulation(
465        bicycle = bicycle,
466        num_inspectors = num_inspectors,
467        num_repairers = num_repairers,
468        seed = trial
469      )
470      proportion <- get_proportion(
471        repair_shop = repair_shop
472      )
473      proportions[trial] <- proportion
474    }
475    return(mean(proportions))
476  }

```

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

R input

```

476  print(
477    get_average_proportion(
478      num_inspectors = 1,
479      num_repairers = 2)
480  )

```

which gives:

R output

```
481 [1] 0.1635779
```

that is, on average 16.36% of bicycles will spend longer than 30 minutes at the repair shop.

Now consider the two possible future scenarios we wish to 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

```
482 print(  
483   get_average_proportion(  
484     num_inspectors = 2,  
485     num_repairers = 2)  
486   )
```

which gives:

R output

```
487 [1] 0.04221602
```

that is 4.22% of bicycles.

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

R input

```
488 print(  
489   get_average_proportion(  
490     num_inspectors = 1,  
491     num_repairers = 3)  
492   )
```

which gives:

R output

```
493 [1] 0.1224761
```

that is 12.25% 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



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 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:

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

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:

$$\frac{dI}{dt} = -\alpha I \quad (4.2)$$

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

In this particular case, one such function is:

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

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:

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

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:

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

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

```

494 import sympy as sym
495
496 t = sym.Symbol("t")
497 alpha = sym.Symbol("alpha")
498 I_0 = sym.Symbol("I_0")
499 I = sym.Function("I")
500
501
502 def get_equation(alpha=alpha):
503     """Return the differential equation.
504
505     Args:
506         alpha: a float (default: symbolic alpha)
507
508     Returns:
509         A symbolic equation
510     """
511     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

```

512 eq = get_equation()
513 print(eq)

```

which gives:

Python output

```

514 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

```

515 eq = get_equation(alpha=1)
516 print(eq)

```

Python output

```

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

```

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

Python input

```

518 def get_solution(I_0=I_0, alpha=alpha):
519     """Return the solution to the differential equation.
520
521     Args:
522         I_0: a float (default: symbolic I_0)
523         alpha: a float (default: symbolic alpha)
524
525     Returns:
526         A symbolic equation
527     """
528     eq = get_equation(alpha=alpha)
529     return sym.dsolve(eq, I(t), ics={I(0): I_0})

```

We can verify the solution discussed previously:

Python input

```

530 sol = get_solution()
531 print(sol)

```

which gives:

Python output

```
532 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

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

which gives:

Python output

```
534 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

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

which gives:

Python output

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

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

Python input

```

538 def get_cost(
539     I_0=I_0,
540     alpha=alpha,
541     cost_per_person=10,
542     cost_of_cure=0,
543 ):
544     """Return the cost.
545
546     Args:
547         I_0: a float (default: symbolic I_0)
548         alpha: a float (default: symbolic alpha)
549         cost_per_person: a float (default: 10)
550         cost_of_cure: a float (default: 0)
551
552     Returns:
553         A symbolic expression
554     """
555     I_sol = get_solution(I_0=I_0, alpha=alpha)
556     return (
557         sym.integrate(I_sol.rhs, (t, 0, sym.oo))
558         * cost_per_person
559         + cost_of_cure * I_0
560     )

```

We can now obtain the cost without purchasing the cure:

Python input

```

561 I_0 = 100
562 alpha = 2
563 cost_without_cure = get_cost(I_0=I_0, alpha=alpha)
564 print(cost_without_cure)

```

which gives:

Python output

565 500

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

Python input

```
566 cost_of_cure = 5
567 cost_with_cure = get_cost(
568     I_0=I_0, alpha=2 * alpha, cost_of_cure=cost_of_cure
569 )
570 print(cost_with_cure)
```

which gives:

Python output

571 750

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

4.4 SOLVING WITH R

R has some capability for symbolic mathematics, however at the time of writing the options available are somewhat limited and/or not reliable. As such, we will actually solve the problem with R using a numerical integration approach. For an outline of the theory behind this approach see Chapter

First we write a function to give us the derivative for a given value of I .

R input

```
572 derivative <- function(t, y, parameters) {
573     with(as.list(c(y, parameters)), {
574         dIdt <- -alpha * I # nolint
575         list(dIdt) # nolint
576     })
577 }
```

For example, to see the value of the derivative when $I = 0$ we have:

R input

```
578 derivative(t = 0, y = c(I = 100), parameters = c(alpha = 2))
```

This gives:

R output

```
579 [[1]]
580 [1] -200
```

We will now make use of the `deSolve` library for solving differential equations numerically:

R input

```
581 library(deSolve) # nolint
582 integrate_ode <- function(times,
583                             y0 = c(I = 100),
584                             alpha = 2) {
585   params <- c(alpha = alpha)
586   ode(y = y0, times = times, func = derivative, parms = params)
587 }
```

This will return a sequence of time point and values of I at those time points. Using this we can compute the cost. Note that this function uses `stopifnot` to make sure our differential equation has been solved for a long enough time period.

R input

```

588 get_cost <- function(
589     I_0 = 100,
590     alpha = 2,
591     cost_per_person = 10,
592     cost_of_cure = 0,
593     step_size = 0.0001,
594     max_time = 10) {
595   times <- seq(0, max_time, by = step_size)
596   out <- integrate_ode(times,
597     y0 = c(I = I_0),
598     alpha = alpha
599   )
600   number_of_observations <- length(out[, "I"])
601
602   stopifnot(out[number_of_observations, "I"] < step_size)
603
604   time_between_steps <- diff(out[, "time"])
605   area_under_curve <- sum(
606     time_between_steps *
607     out[-number_of_observations, "I"]
608   )
609   area_under_curve *
610     cost_per_person + cost_of_cure *
611     I_0
612 }

```

Using this we can compute the costs:

R input

```

613 alpha <- 2
614 cost_without_cure <- get_cost(alpha = alpha)
615 print(round(cost_without_cure))

```

which gives:

R output

616

```
[1] 500
```

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

R input

617

```
cost_of_cure <- 5
```

618

```
cost_with_cure <- get_cost(
```

619

```
  alpha = 2 * alpha, cost_of_cure = cost_of_cure
```

620

```
)
```

621

```
print(round(cost_with_cure))
```

which gives:

R output

622

```
[1] 750
```

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

4.5 RESEARCH

TBA

Systems Dynamics

IN many situations systems are dynamical, in that the state or population of a number of entities or classes change according to 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.

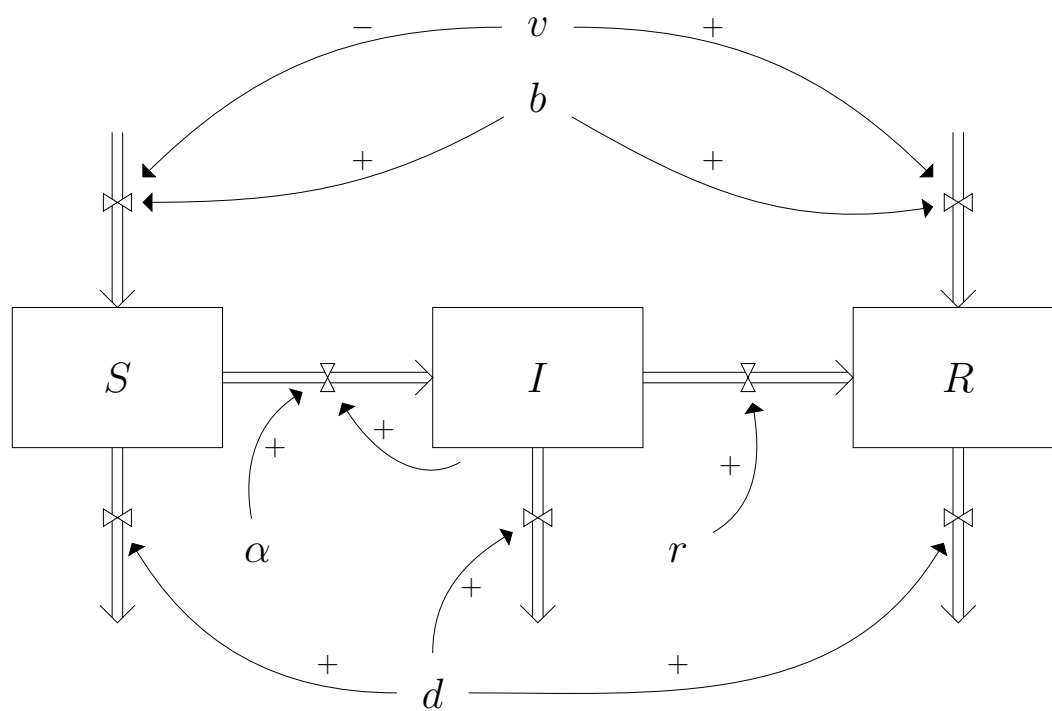


Figure 5.1 Diagrammatic representation of the epidemiology model

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:

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

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

$$\frac{dR}{dt} = rI - dR + vbN \quad (5.3)$$

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

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

This sequence approaches the true solution y as $h \rightarrow 0$. 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

```

623 def derivatives(y, t, vaccine_rate, birth_rate=0.01):
624     """Defines the system of differential equations that
625     describe the epidemiology model.
626
627     Args:
628         y: a tuple of three integers
629         t: a positive float
630         vaccine_rate: a positive float <= 1
631         birth_rate: a positive float <= 1
632
633     Returns:
634         A tuple containing dS, dI, and dR
635     """
636     infection_rate = 0.3
637     recovery_rate = 0.02
638     death_rate = 0.01
639     S, I, R = y
640     N = S + I + R
641     dSdt = (
642         -((infection_rate * S * I) / N)
643         + ((1 - vaccine_rate) * birth_rate * N)
644         - (death_rate * S)
645     )
646     dIdt = (
647         ((infection_rate * S * I) / N)
648         - (recovery_rate * I)
649         - (death_rate * I)
650     )
651     dRdt = (
652         (recovery_rate * I)
653         - (death_rate * R)
654         + (vaccine_rate * birth_rate * N)
655     )
656     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

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

Python output

```
658 (-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

```

659 from scipy.integrate import odeint
660
661
662 def integrate_ode(
663     derivative_function,
664     t,
665     y0=(2999, 1, 0),
666     vaccine_rate=0.85,
667     birth_rate=0.01,
668 ):
669     """Numerically solve the system of differential equations.
670
671     Args:
672         derivative_function: a function returning a tuple
673             of three floats
674         t: an array of increasing positive floats
675         y0: a tuple of three integers (default: (2999, 1, 0))
676         vaccine_rate: a positive float <= 1 (default: 0.85)
677         birth_rate: a positive float <= 1 (default: 0.01)
678
679     Returns:
680         A tuple of three arrays
681     """
682     results = odeint(
683         derivative_function,
684         y0,
685         t,
686         args=(vaccine_rate, birth_rate),
687     )
688     S, I, R = results.T
689     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%:

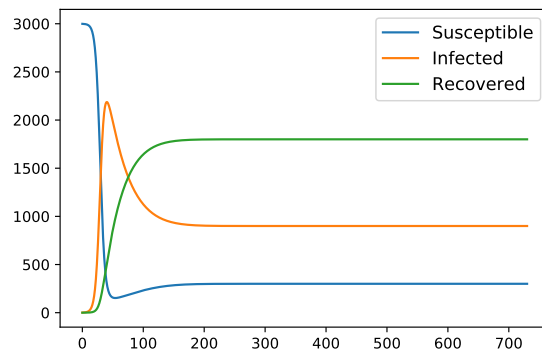


Figure 5.2 Output of code line 737-742

Python input

```

690 import numpy as np
691 from scipy.integrate import odeint
692
693 t = np.arange(0, 730.01, 0.01)
694 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

```

695 import matplotlib.pyplot as plt
696
697 fig, ax = plt.subplots(1)
698 ax.plot(t, S, label='Susceptible')
699 ax.plot(t, I, label='Infected')
700 ax.plot(t, R, label='Recovered')
701 ax.legend(fontsize=12)
702 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

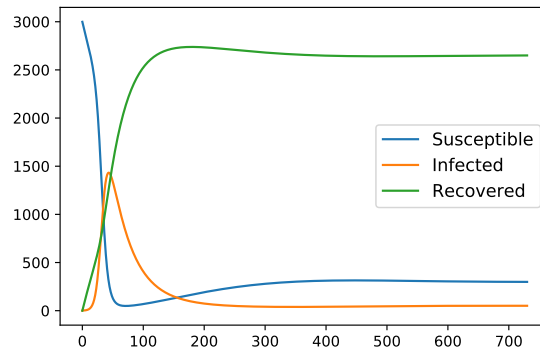


Figure 5.3 Output of code line 745-750

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

```
703 t = np.arange(0, 730.01, 0.01)
704 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

```
705 fig, ax = plt.subplots(1)
706 ax.plot(t, S, label='Susceptible')
707 ax.plot(t, I, label='Infected')
708 ax.plot(t, R, label='Recovered')
709 ax.legend(fontsize=12)
710 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

```

711 def daily_cost(
712     derivative_function=derivatives, vaccine_rate=0.85
713 ):
714     """Calculates the daily cost to the public health system
715     after 2 years.
716
717     Args:
718         derivative_function: a function returning a tuple
719             of three floats
720         vaccine_rate: a positive float <= 1 (default: 0.85)
721
722     Returns:
723         the daily cost
724     """
725     max_time = 730
726     time_step = 0.01
727     birth_rate = 0.01
728     vaccine_cost = 220
729     medication_cost = 10
730     t = np.arange(0, max_time + time_step, time_step)
731     S, I, R = integrate_ode(
732         derivatives,
733         t,
734         vaccine_rate=vaccine_rate,
735         birth_rate=birth_rate,
736     )
737     N = S[-1] + I[-1] + R[-1]
738     daily_vaccine_cost = (
739         N * birth_rate * vaccine_rate * vaccine_cost
740     ) / time_step
741     daily_meds_cost = (I[-1] * medication_cost) / time_step
742     return daily_vaccine_cost + daily_meds_cost

```

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

Python input

```

743 cost = daily_cost(vaccine_rate=0.0)
744 print(round(cost, 2))

```

which gives

Python output

```

745 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

```

746 cost = daily_cost(vaccine_rate=0.85)
747 print(round(cost, 2))

```

which gives

Python output

```

748 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

```

749 #' Defines the system of differential equations that describe
750 #' the epidemiology model.
751 #'
752 #' @param t a positive float
753 #' @param y a tuple of three integers
754 #' @param vaccine_rate a positive float <= 1
755 #' @param birth_rate a positive float <= 1
756 #'
757 #' @return a list containing dS, dI, and dR
758 derivatives <- function(t, y, parameters){
759   infection_rate <- 0.3
760   recovery_rate <- 0.02
761   death_rate <- 0.01
762   with(as.list(c(y, parameters)), {
763     N <- S + I + R
764     dSdt <- ( - ( (infection_rate * S * I) / N) # nolint
765               + ( (1 - vaccine_rate) * birth_rate * N)
766               - (death_rate * S))
767     dIdt <- ( ( (infection_rate * S * I) / N) # nolint
768               - (recovery_rate * I)
769               - (death_rate * I))
770     dRdt <- ( (recovery_rate * I) # nolint
771               - (death_rate * R)
772               + (vaccine_rate * birth_rate * N))
773     list(c(dSdt, dIdt, dRdt)) # nolint
774   })
775 }

```

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

```
776 derivatives(t = 0,  
777           y = c(S = 4, I = 1, R = 0),  
778           parameters = c(vaccine_rate = 0.5,  
779                         birth_rate = 0.01)  
780 )
```

R output

```
781 [[1]]  
782 [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

```

783 library(deSolve) # nolint
784
785 #' Numerically solve the system of differential equations
786 #'
787 #' @param t an array of increasing positive floats
788 #' @param y0 list of integers (default: c(S=2999, I=1, R=0))
789 #' @param birth_rate a positive float <= 1 (default: 0.01)
790 #' @param vaccine_rate a positive float <= 1 (default: 0.85)
791 #'
792 #' @return a matrix of times, S, I and R values
793 integrate_ode <- function(times,
794                             y0 = c(S = 2999, I = 1, R = 0),
795                             birth_rate = 0.01,
796                             vaccine_rate = 0.84){
797   params <- c(birth_rate = birth_rate,
798               vaccine_rate = vaccine_rate)
799   ode(y = y0,
800       times = times,
801       func = derivatives,
802       parms = params)
803 }

```

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

```

804 times <- seq(0, 730, by = 0.01)
805 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.

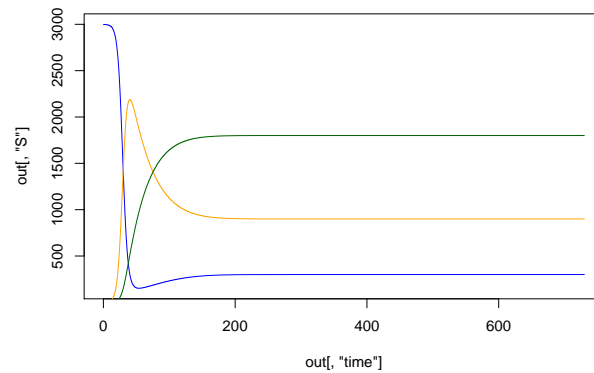


Figure 5.4 Output of code line 846-850

R input

```

806 pdf("plot_no_vaccine_R.pdf", width = 7, height = 5)
807 plot(out[, "time"], out[, "S"], type = "l", col = "blue")
808 lines(out[, "time"], out[, "I"], type = "l", col = "orange")
809 lines(out[, "time"], out[, "R"], type = "l", col = "darkgreen")
810 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

```

811 times <- seq(0, 730, by = 0.01)
812 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.

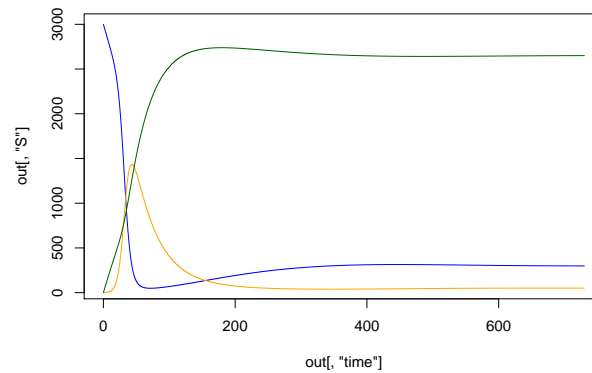


Figure 5.5 Output of code line 853-857

R input

```

813 pdf("plot_with_vaccine_R.pdf", width = 7, height = 5)
814 plot(out[, "time"], out[, "S"], type = "l", col = "blue")
815 lines(out[, "time"], out[, "I"], type = "l", col = "orange")
816 lines(out[, "time"], out[, "R"], type = "l", col = "darkgreen")
817 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

```

818 #' Calculates the daily cost to the public health
819 #' system after 2 years
820 #'
821 #' @param derivative_function: a function returning a
822 #'                               list of three floats
823 #' @param vaccine_rate: a positive float <= 1 (default: 0.85)
824 #'
825 #' @return the daily cost
826 daily_cost <- function(derivative_function = derivatives,
827                        vaccine_rate = 0.85){
828   max_time <- 730
829   time_step <- 0.01
830   birth_rate <- 0.01
831   vaccine_cost <- 220
832   medication_cost <- 10
833   times <- seq(0, max_time, by = time_step)
834   out <- integrate_ode(times, vaccine_rate = vaccine_rate)
835   N <- sum(tail(out[, c("S", "I", "R")], n = 1))
836   daily_vaccine_cost <- (N
837                         * birth_rate
838                         * vaccine_rate
839                         * vaccine_cost) / time_step
840   daily_medication_cost <- ( (tail(out[, "I"], n = 1)
841                             * medication_cost)) / time_step
842   daily_vaccine_cost + daily_medication_cost
843 }

```

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

R input

```

844 cost <- daily_cost(vaccine_rate = 0.0)
845 print(cost)

```

which gives

R output

```
846 [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

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

which gives

R output

```
849 [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

Emergent Behaviour



Game Theory

MOST when modelling certain situations two approaches are valid: to make assumptions about the overall behaviour or to make assumptions about the detailed behaviour. The latter falls is akin to measuring emergent behaviour. One tool used to do this is the study of interactive decision making: Game Theory.

6.1 PROBLEM

Consider a city council. Two electric taxi companies are going to move in to the city and the city wants to ensure that the customers are best served by this new duopoly. The two taxi firms will be deciding how many vehicles to deploy: one, two or three. The city wants to encourage them to both use three as this ensures the highest level of availability to the population.

Some exploratory data analysis gives the following insights:

- If both companies use the same number of taxis then they make the same profit which will go down slightly as the number of taxis goes up.
- If one company uses more taxis than the other then they make more profit.

The expected profits are given in Table 6.1.

Taxi numbers	Other company taxi numbers		
	1	2	3
1	$\frac{1}{3}$	$\frac{1}{2}$	$\frac{1}{3}$
2	$\frac{3}{2}$	$\frac{19}{20}$	$\frac{1}{2}$
3	$\frac{5}{3}$	$\frac{4}{5}$	$\frac{17}{20}$

Table 6.1 Profits (in GBP per hour) of a given company based on their vehicle numbers and the other companies vehicle numbers.

Given these expected profits, the council wants to understand what is likely to happen and potentially give a financial incentive to each company to ensure their behaviour is in the population's interest.

The mathematical tool used to find the expected behaviour is Game Theory.

6.2 THEORY

In the case of this City, the interaction can be modelled using a mathematical object called a game which in the field of game theory is defined as follows. There are a number of games, the ones we will consider here require:

1. A given collection of actors that make decisions (players).
2. Options available to each player (actions).
3. A numerical value associated to each player for every possible choice of action made by all the players. This is the utility or reward.

There are called normal form games and are formally defined by:

1. A finite set of N players;
2. Action spaces for each player: $\{A_1, A_2, A_3, \dots, A_N\}$;
3. Utility functions that for each player $u_1, u_2, u_3, \dots, u_N$ where $u_i : A_1 \times A_2 \times A_3 \dots A_N \rightarrow \mathbb{R}$.

When $N = 2$ the utility function is often represented by a pair of matrices (1 for each player) of with the same number of rows and columns. The rows correspond to the actions available to the first player and the columns to the actions available to the second player.

Given a pair of actions (a row and column) we can read the utilities to both player by looking at the corresponding entry of the corresponding matrix.

A strategy corresponds to an way of choosing actions, this is represented by a probability vector. For the i th player, this vector v would be of size $|A_i|$ (the size of the action space) and v_i corresponds to the probability of choosing the i th action.

For the example of our City, the two matrices would be:

$$M = \begin{pmatrix} 1 & 1/2 & 1/3 \\ 3/2 & 19/20 & 1/2 \\ 5/3 & 4/5 & 17/20 \end{pmatrix} \quad N = M^T = \begin{pmatrix} 1 & 3/2 & 5/3 \\ 1/2 & 19/20 & 1/2 \\ 1/3 & 4/5 & 17/20 \end{pmatrix}$$

A diagram of the system is shown in Figure 6.1

Both taxis always choosing to use 2 taxis (the second row/column) would correspond to the strategy: $(0, 1, 0)$. If the both companies use this strategy and the row player (who controls the rows) wants to improve their outcome it's evident by inspecting the second column that the highest number is $19/20$: thus the row player has no reason to change what they are doing.

This is in fact called a Nash equilibrium: when both players are playing a strategy that is the best response against the other.

Whilst a Nash equilibria is not necessarily a set of strategies that players will converge towards, once they are there they have no reason to move away from it. It is the particular concept we will use to understand the emergent behaviour in our city.

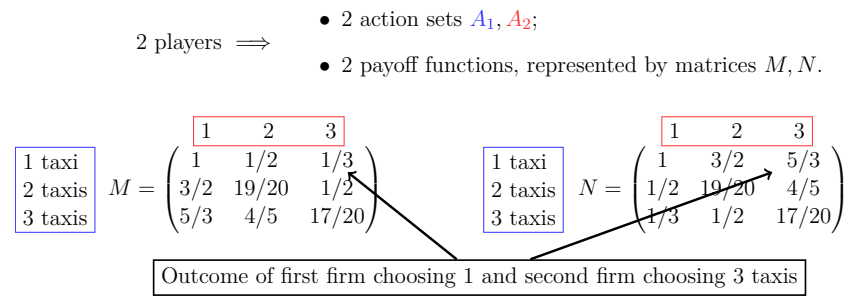


Figure 6.1 Diagrammatic representation of the action sets and payoff matrices for the game.

6.3 SOLVING WITH PYTHON

The first step we will take is to write a function to create a game using the matrix expected profits. We will use the `nashpy` library for this.

Python input

```

850 import nashpy as nash
851
852
853 def get_game(profits):
854     """Return the game object.
855
856     Args:
857         profits: a matrix with expected profits
858
859     Returns:
860         A nashpy game object
861     """
862     return nash.Game(profits, profits.T)

```

Using this we can obtain the game for the our problem:

Python input

```

863 import numpy as np
864
865 profits = np.array(
866     (
867         (1, 1 / 2, 1 / 3),
868         (3 / 2, 19 / 20, 1 / 2),
869         (5 / 3, 4 / 5, 17 / 20),
870     )
871 )
872 game = get_game(profits=profits)
873 print(game)

```

which gives:

Python output

```

874 Bi matrix game with payoff matrices:
875
876 Row player:
877 [[1.          0.5          0.33333333]
878  [1.5         0.95         0.5        ]
879  [1.66666667 0.8          0.85        ]]
880
881 Column player:
882 [[1.          1.5          1.66666667]
883  [0.5         0.95         0.8         ]
884  [0.33333333 0.5          0.85        ]]

```

We can now use this to investigate what stable behaviours might emerge:

Python input

```

885 for eq in game.support_enumeration():
886     print(eq)

```

which gives:

Python output

```

887 (array([0., 1., 0.]), array([0., 1., 0.]))
888 (array([0., 0., 1.]), array([0., 0., 1.]))
889 (array([0. , 0.7, 0.3]), array([0. , 0.7, 0.3]))

```

We see that there are 3 Nash equilibria: 3 possible pairs of behaviour that the two companies might converge to.

- The first equilibria $((0, 1, 0), (0, 1, 0))$ corresponds to both firms always using 2 taxis.
- The second equilibria $((0, 0, 1), (0, 0, 1))$ corresponds to both firms always using 3 taxis.
- The third equilibria $((0, 0.7, 0.3), (0, 0.7, 0.3))$ corresponds to both firms using 2 taxis 70% of the time and 3 taxis otherwise.

A good thing to note is that the two taxi companies will never only provide a single taxi (which would be harmful to the customers).

However, the Council would like to offset the cost of 3 taxis so as to encourage the taxi company to provide a better service. This involves modifying the `get_game` function as follows:

Python input

```

890 def get_game(profits, offset):
891     """Return the game object with a given offset when 3 taxis
892     are provided.
893
894     Args:
895         profits: a matrix with expected profits
896         offset: a float
897
898     Returns:
899         A nashpy game object
900     """
901     new_profits = np.array(profits)
902     new_profits[2] += offset
903     return nash.Game(new_profits, new_profits.T)

```

we will write a function `get_equilibria` which will directly compute the equilibria:

Python input

```

904 def get_equilibria(profits, offset):
905     """Return the equilibria for a given offset when 3 taxis
906     are provided.
907
908     Args:
909         profits: a matrix with expected profits
910         offset: a float
911
912     Returns:
913         A nashpy game object
914     """
915     game = get_game(profits=profits, offset=offset)
916     return tuple(game.support_enumeration())

```

Using this we can obtain the number of equilibria for a given offset and stop when there is a single equilibria:

Python input

```

917 offset = 0
918 while len(get_equilibria(profits=profits, offset=offset)) > 1:
919     offset += 0.01

```

This gives a final offset value of:

Python input

```

920 print(round(offset, 2))

```

Python output

```

921 0.15

```

and we can confirm that the Nash equilibria is where both taxi firms provide three vehicles:

Python input

```
922 print(tuple(get_equilibria(profits=profits, offset=offset)))
```

giving:

Python output

```
923 ((array([0., 0., 1.]), array([0., 0., 1.])),)
```

6.4 SOLVING WITH R

R does not have a single appropriate library for the game considered here, we will choose to use **Recon** which has functionality for finding the Nash equilibria for two player games when only considering pure strategies (where the players only choose to use a single action at a time).

R input

```
924 library(Recon)
925
926 #' Returns the equilibria in pure strategies
927 #' 
928 #' @param profits: a matrix with expected profits
929 #' 
930 #' @return a list of equilibria
931 get_equilibria <- function(profits){
932     sim_nasheq(profits, t(profits))
933 }
```

Using this we can obtain the pure Nash equilibria:

R input

```

934 profits <- rbind(
935     c(1, 1 / 2, 1 / 3),
936     c(3 / 2, 19 / 20, 1 / 2),
937     c(5 / 3, 4 / 5, 17 / 20)
938 )
939 eqs <- get_equilibria(profits = profits)
940 print(eqs)

```

which gives:

R output

```

941 $`Equilibrium 1`
942 [1] "2" "2"
943
944 $`Equilibrium 2`
945 [1] "3" "3"

```

We see that there are 2 pure Nash equilibria: 2 possible pairs of behaviour that the two companies might converge to.

- The first equilibria $((0, 1, 0), (0, 1, 0))$ corresponds to both firms always using 2 taxis.
- The second equilibria $((0, 0, 1), (0, 0, 1))$ corresponds to both firms always using 3 taxis.

There is in fact a third Nash equilibria where both taxi firms use 2 taxis 70% of the time and 3 taxis the rest of the time but **Recon** is unable to find Nash equilibria with mixed behaviour for games with more than two strategies.

As an aside, if we remove the option of using a single taxi then **Recon** can give us all three equilibria by passing the `type = "mixed"` argument to `sim_nasheq`.

A good thing to note is that the two taxi companies will not only provide a single taxi (which would be harmful to the customers).

As discussed, the Council would like to offset the cost of 3 taxis so as to encourage the taxi company to provide a better service. This involves modifying the `get_equilibria` function as follows:

R input

```

946 #' Returns the equilibria in pure strategies
947 #' for a given offset
948 #'
949 #' @param profits: a matrix with expected profits
950 #' @param offset: a float
951 #'
952 #' @return a list of equilibria
953 get_equilibria <- function(profits, offset){
954   new_profits <- rbind(
955     profits[c(1, 2), ],
956     profits[3, ] + offset)
957   sim_nasheq(new_profits, t(new_profits))
958 }

```

Using this we can obtain the number of equilibria for a given offset and stop when there is a single equilibria:

R input

```

959 offset <- 0
960 while (length(
961   get_equilibria(profits = profits, offset = offset)
962 ) > 1){
963   offset <- offset + 0.01
964 }

```

This gives a final offset value of:

R input

```

965 print(round(offset, 2))

```

R output

```

966 [1] 0.15

```

and we can confirm that the Nash equilibria is where both taxi firms provide three vehicles:

R input

```
967 print(get_equilibria(profits = profits, offset = offset))
```

giving:

R output

```
968 $`Equilibrium 1`  
969 [1] "3" "3"
```

6.5 RESEARCH

TBA

V

Optimisation



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.

7.1 PROBLEM

A university runs 14 modules over three subjects: Art, Biology, and Chemistry. Each subject runs core modules and optional modules. Table 7.1 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,

Art Core	Biology Core	Chemistry Core
M00	M05	M09
M01	M06	M10
Art Optional	Biology Optional	Chemistry Optional
M02	M07	M11
M03	M08	M12
M04		M13

Table 7.1 List of modules on offer at the university.

- All chemistry modules share students,
- 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.

How can every exam be scheduled with no clashes, that using the least amount of time slots?

7.2 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 constraints) lie within that region, and all infeasible solutions (those that break at least one constraint) lie outside that region.

We are interested in optimising, that is either minimising or maximising, some linear function, called the objective function. Therefore 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, stopping at the optimum. Therefore to solve such a problem, we 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 are 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, representing total profit, that is to be maximised; and two linear constraints, representing the availability of ingredients X and Y. They are written as:

$$\text{Maximise: } 50A + 60B \quad (7.1)$$

Subject to:

$$4A + 6B \leq 24 \quad (7.2)$$

$$5A + 4B \leq 20 \quad (7.3)$$

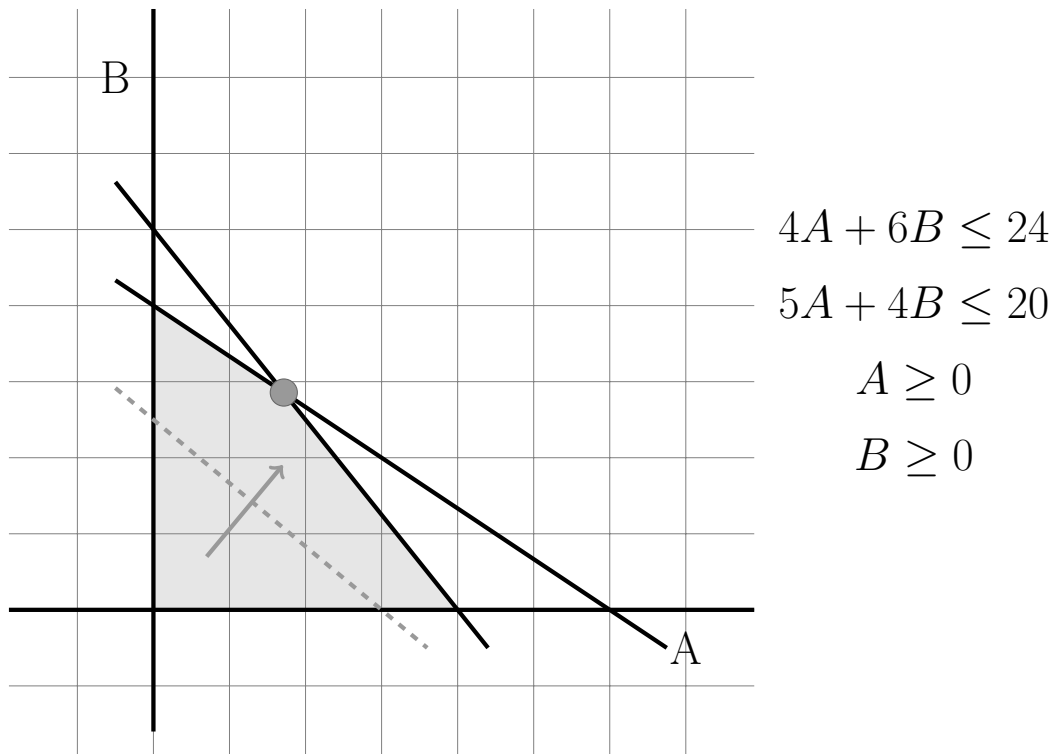


Figure 7.1 Visual representation of the paint linear program. The feasible convex region is shaded in grey; the objective function with arbitrary value is shown in a dashed line.

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 function given by expression 7.1. Inequalities 7.2 and 7.3 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 7.1.

Expression 7.1 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 within the feasible region, demonstrated in Figure 7.1. 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 8.1, and let's formulate this as a linear program. Define M as the set of all modules to be scheduled, and define T as the set of possible time slots. At worst each exam is scheduled for a different day, thus $|T| = |M| = 14$ in this case. Let $\{X_{mt}$ for $m \in M$ and $t \in T\}$ be a set of binary decision variables, that is $X_{mt} = 1$ if module m is scheduled for time t , and 0 otherwise.

There are six 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; and C_c, C_o representing core and optional chemistry modules respectively. Therefore $M = A_c \cup A_o \cup B_c \cup B_o \cup C_c \cup C_o$.

Additionally there are further clashes between these sets:

- No modules in $A_c \cup A_o$ can be scheduled together as they may share students, this is given by the constraint in inequality 7.7.
- No modules in $B_c \cup B_o \cup A_c$, can be scheduled together as they may share students, given by inequality 7.8.
- No modules in $B_c \cup B_o \cup C_o$, can be scheduled together as they may share students, given by inequality 7.9.
- No modules in $B_o \cup C_c \cup C_o$, can be scheduled together as they may share students, given by inequality 7.10.

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 7.5.

Finally we have one final constraint, Equation 7.6, which ensures all modules are scheduled once and once only. Thus altogether our integer program becomes:

$$\text{Minimise: } \sum_{t \in T} Y_j \quad (7.4)$$

Subject to:

$$\frac{1}{|M|} \sum_{m \in M} X_{mt} \leq Y_j \text{ for all } j \in T \quad (7.5)$$

$$\sum_{t \in T} X_{mt} = 1 \text{ for all } m \in M \quad (7.6)$$

$$\sum_{m \in A_c \cup A_o} X_{mt} \leq 1 \text{ for all } t \in T \quad (7.7)$$

$$\sum_{m \in B_c \cup B_o \cup A_c} X_{mt} \leq 1 \text{ for all } t \in T \quad (7.8)$$

$$\sum_{m \in B_c \cup B_o \cup C_o} X_{mt} \leq 1 \text{ for all } t \in T \quad (7.9)$$

$$\sum_{m \in B_o \cup C_c \cup C_o} X_{mt} \leq 1 \text{ for all } t \in T \quad (7.10)$$

Another common way to define this linear program is by representing the coefficients of the constraints as a matrix. That is:

$$\text{Minimise: } c^T Z \quad (7.11)$$

Subject to:

$$AZ \star b \quad (7.12)$$

where Z is a vector representing the decision variables, c is the coefficients of the Z in the objective function, A is the matrix of the coefficients of Z in the constraints, b is the vector of the right hand side of the constraints, and \star represents either \leq , $=$ or \geq as required.

As Z is a one-dimensional vector of decisions variables, we ‘flatten’ the matrix X and the vector Y together to form this new variable. We can do this by first ordering by X then Y , within that ordering by time slot, then within that ordering by module number. Therefore:

$$Z_{|M|t+m} = X_{mt} \quad (7.13)$$

$$Z_{|M|^2+m} = Y_m \quad (7.14)$$

where t and m are indices starting at 0. For example Z_{17} would correspond to $X_{3,2}$, the decision variable representing whether module number 4 is scheduled on day 3; Z_{208} would correspond to Y_{12} , the decision variable representing whether there’s an exam scheduled for day 12.

Parameters c , A , and b can be determined by using this same conversion from the model in Equations 7.4 to 7.10. The vector c would be $|M|^2$ zeroes followed by $|M|$ ones. The vector b would be zeroes for all the rows representing Equation 7.5, and ones for all other constraints.

7.3 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

```

970 Ac = [0, 1]
971 Ao = [2, 3, 4]
972 Bc = [5, 6]
973 Bo = [7, 8]
974 Cc = [9, 10]
975 Co = [11, 12, 13]
976 modules = Ac + Ao + Bc + Bo + Cc + Co
977 times = range(14)

```

Now let's begin by defining an empty problem:

Python input

```

978 import pulp
979
980 prob = pulp.LpProblem("ExamScheduling", pulp.LpMinimize)

```

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

Python input

```

981 xshape = (modules, times)
982 x = pulp.LpVariable.dicts("X", xshape, cat=pulp.LpBinary)
983 y = pulp.LpVariable.dicts("Y", times, cat=pulp.LpBinary)

```

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

Python input

```

984 print(y[3])

```


Python output

985 Y_3

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

Python input

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

Python output

987 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, Equation 7.4:

Python input

988 `objective_function = sum([y[day] for day in times])`
 989 `prob += objective_function`

Now the constraints, Inequalities 7.5-7.10:

Python input

```

990 M = 1 / len(modules)
991 for day in times:
992     prob += M * sum(x[m][day] for m in modules) <= y[day]
993     prob += sum([x[mod][day] for mod in Ac + Ao]) <= 1
994     prob += sum([x[mod][day] for mod in Bc + Bo + Co]) <= 1
995     prob += sum([x[mod][day] for mod in Bc + Bo + Ac]) <= 1
996     prob += sum([x[mod][day] for mod in Cc + Co + Bo]) <= 1
997
998 for mod in modules:
999     prob += sum(x[mod][day] for day in times) == 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 if the need arises.

Now we can go ahead and solve the problem:

Python input

```

1000 prob.solve(pulp.apis.PULP_CBC_CMD(msg=False))

```

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

Python input

```

1001 print(x[2][5].value())

```

Python output

```

1002 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 9:

Python input

```
1003 print(x[2][9].value())
```

Python output

```
1004 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

```
1005 for day in times:
1006     if y[day].value() == 1:
1007         schedule = f"Day {day}: "
1008         for mod in modules:
1009             if x[mod][day].value() == 1:
1010                 schedule += f"{mod}, "
1011         print(schedule)
```

giving:

Python output

```
1012 Day 0: 1, 12,
1013 Day 3: 5, 9,
1014 Day 5: 0, 13,
1015 Day 6: 3, 11,
1016 Day 7: 6, 10,
1017 Day 9: 2, 7,
1018 Day 13: 4, 8,
```

Now the order of the days do not matter here, but we can see that 7 days are required in order to schedule all exams with no clashes, with two exams scheduled each day.

7.4 SOLVING WITH R

In R we will use the R package R0I, 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 the `rcbc` package.

The R0I package requires that the linear programme is represented in its matrix form, with a one-dimensional array of decision variables. Therefore we will use the form of the model described at the end of Section 8.2. We will write functions that define the objective function c , the coefficient matrix A , the vector of the right hand side of the constraints b , and the vector of equality or inequalities directions \star .

First we consider the objective function:

R input

```

1019  #' Writes the row of coefficients for the objective function
1020  #'
1021  #' @param n_modules: the number of modules to schedule
1022  #' @param n_days: the maximum number of days to schedule
1023  #'
1024  #' @return the objective function row to minimise
1025  write_objective <- function(n_modules, n_days){
1026    all_days <- rep(0, n_modules * n_days)
1027    Ys <- rep(1, n_days)
1028    append(all_days, Ys)
1029  }

```

For 3 modules and 3 days:

R input

```

1030  write_objective(3, 3)

```

Which gives the following array, corresponding the the coefficients of the array Z for Equation 7.4.

R output

```

1031  [1] 0 0 0 0 0 0 0 0 0 1 1 1

```

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 7.7 to 7.10:

R input

```

1032 #' Writes the constraint row dealing with clashes
1033 #'
1034 #' @param clashes: a vector of module indices that all cannot
1035 #'                  be scheduled at the same time
1036 #' @param day: an integer representing the day
1037 #'
1038 #' @return the constraint row corresponding to that set of
1039 #'         clashes on that day
1040 write_X_clashes <- function(clashes, day, n_days, n_modules){
1041   today <- rep(0, n_modules)
1042   today[clashes] = 1
1043   before_today <- rep(0, n_modules * (day - 1))
1044   after_today <- rep(0, n_modules * (n_days - day))
1045   all_days <- c(before_today, today, after_today)
1046   full_coeffs <- c(all_days, rep(0, n_days))
1047   full_coeffs
1048 }

```

where `clashes` is 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 7.6:

R input

```

1049 #' Writes the constraint row to ensure that every module is
1050 #' scheduled once and only one
1051 #'
1052 #' @param module: an integer representing the module
1053 #'
1054 #' @return the constraint row corresponding to scheduling a
1055 #'         module on only one day
1056 write_X_requirements <- function(module, n_days, n_modules){
1057   today <- rep(0, n_modules)
1058   today[module] = 1
1059   all_days <- rep(today, n_days)
1060   full_coeffs <- c(all_days, rep(0, n_days))
1061   full_coeffs
1062 }

```

The following function is used to write one row of the coefficients matrix corresponding to the auxiliary constraints of Inequality 7.5:

R input

```

1063 #' Writes the constraint row representing the Y variable,
1064 #' whether at least one exam is scheduled on that day
1065 #'
1066 #' @param day: an integer representing the day
1067 #'
1068 #' @return the constraint row corresponding to creating Y
1069 write_Y_constraints <- function(day, n_days, n_modules){
1070   today <- rep(1, n_modules)
1071   before_today <- rep(0, n_modules * (day - 1))
1072   after_today <- rep(0, n_modules * (n_days - day))
1073   all_days <- c(before_today, today, after_today)
1074   all_Ys <- rep(0, n_days)
1075   all_Ys[day] = -n_modules
1076   full_coeffs <- append(all_days, all_Ys)
1077   full_coeffs
1078 }

```

Finally the following function uses them all to assemble a coefficients matrix. It loops through 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

```

1079 #' Writes all the constraints as a matrix, column of
1080 #' inequalities, and right hand side column.
1081 #'
1082 #' @param list_clashes: a list of vectors with sets of modules
1083 #' that cannot be scheduled at the same time
1084 #'
1085 #' @return f.con the LHS of the constraints as a matrix
1086 #' @return f.dir the directions of the inequalities
1087 #' @return f.rhs the values of the RHS of the inequalities
1088 write_constraints <- function(list_clashes, n_days, n_modules){
1089   all_rows <- c()
1090   all_dirs <- c()
1091   all_rhss <- c()
1092   n_rows <- 0
1093
1094   for (clash in list_clashes){
1095     for (day in 1:n_days){
1096       clashes <- write_X_clashes(clash, day, n_days, n_modules)
1097       all_rows <- append(all_rows, clashes)
1098       all_dirs <- append(all_dirs, "<=")
1099       all_rhss <- append(all_rhss, 1)
1100       n_rows <- n_rows + 1
1101     }
1102   }
1103
1104   for (module in 1:n_modules){
1105     reqs <- write_X_requirements(module, n_days, n_modules)
1106     all_rows <- append(all_rows, reqs)
1107     all_dirs <- append(all_dirs, "==")
1108     all_rhss <- append(all_rhss, 1)
1109     n_rows <- n_rows + 1
1110   }
1111
1112   for (day in 1:n_days){
1113     Yconstraints <- write_Y_constraints(day, n_days, n_modules)
1114     all_rows <- append(all_rows, Yconstraints)
1115     all_dirs <- append(all_dirs, "<=")
1116     all_rhss <- append(all_rhss, 0)
1117     n_rows <- n_rows + 1
1118   }
1119
1120   f.con <- matrix(all_rows, nrow = n_rows, byrow = TRUE)
1121   f.dir <- all_dirs
1122   f.rhs <- all_rhss
1123   list(f.con, f.dir, f.rhs)
1124 }

```


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

```
1125 write_constraints(list_clashes = list(c(1, 2)),
1126                   n_days = 2,
1127                   n_modules = 2)
```

This would give three components:

- a coefficient matrix of the left hand side of the constraints, A , (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 6 defining the decision variables Y),
- an array of direction of the constraint inequalities, \star ,
- and an array of the right hand side values of the constraints, b .

R output

```
1128 [[1]]
1129      [,1] [,2] [,3] [,4] [,5] [,6]
1130 [1,]    1    1    0    0    0    0
1131 [2,]    0    0    1    1    0    0
1132 [3,]    1    0    1    0    0    0
1133 [4,]    0    1    0    1    0    0
1134 [5,]    1    1    0    0   -2    0
1135 [6,]    0    0    1    1    0   -2
1136
1137 [[2]]
1138 [1] "<=" "<=" "==" "==" "<=" "<="
1139
1140 [[3]]
1141 [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

```

1142 n_modules = 14
1143 n_days = 14
1144
1145 Ac <- c(0, 1)
1146 Ao <- c(2, 3, 4)
1147 Bc <- c(5, 6)
1148 Bo <- c(7, 8)
1149 Cc <- c(9, 10)
1150 Co <- c(11, 12, 13)
1151
1152 list_clashes <- list(
1153   c(Ac, Ao),
1154   c(Bc, Bo, Co),
1155   c(Bc, Bo, Ac),
1156   c(Bo, Cc, Co)
1157 )

```

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

R input

```

1158 constraints <- write_constraints(list_clashes = list_clashes,
1159                                n_days = n_days,
1160                                n_modules = n_modules)
1161 f.con <- constraints[[1]]
1162 f.dir <- constraints[[2]]
1163 f.rhs <- constraints[[3]]
1164 f.obj <- write_objective(n_modules = n_modules, n_days = n_days)

```

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

R input

```

1165 library(ROI)
1166
1167 milp <- OP(objective = L_objective(f.obj),
1168           constraints = L_constraint(L = f.con,
1169                                     dir = f.dir,
1170                                     rhs = f.rhs),
1171           types = rep("B", length(f.obj)),
1172           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 of `"B"` for each decision variable), and we want to minimise the objective function so we set `maximum = FALSE`.

Now to solve:

R input

```
1173 sol <- ROI_solve(milp)
```

The solver will output information about the solve process and runtime. We can now print the solution:

R input

```
1174 | print(sol$solution)
```

R output

[illegible]

This gives the values of each of the Z decision variables. We know the structure of this, that is the first 14 variables are the modules scheduled for day 1, and so on. The following code prints a readable schedule:

R input

```

1183 for (day in 1:n_days){
1184   if (sol$solution[(n_days * n_modules) + day] == 1){
1185     schedule <- paste("Day", day, ":")
1186     for (module in 1:n_modules){
1187       var <- ((day - 1) * n_modules) + module
1188       if (sol$solution[var] == 1){
1189         schedule <- paste(schedule, module)
1190       }
1191     }
1192     print(schedule)
1193   }
1194 }

```

R output

```

1195 [1] "Day 2 : 4 11"
1196 [1] "Day 6 : 1 12"
1197 [1] "Day 8 : 7"
1198 [1] "Day 10 : 8"
1199 [1] "Day 11 : 3 13"
1200 [1] "Day 12 : 2 6 9 14"
1201 [1] "Day 14 : 5 10"

```

This gives that 7 days are the minimum required to schedule the 14 exams without clashes, with either 1, 2 or 4 exams scheduled on each day.

7.5 RESEARCH

Heuristics

IT is often necessary to find the most desirable choice from a large, or indeed, infinite set of options. Sometimes this can be done using exact techniques but often this is not possible and finding an almost perfect choice quickly is just as good. This is where the field of heuristics comes in to play.

8.1 PROBLEM

Consider a delivery company that needs to find itineraries for a driver. In the past, the management team has noticed that drivers will often drive to whichever next stop is closest but this often makes for longer deliveries.

The stops are represented in Figure 8.2.

The distance matrix is given in equation (8.1).

$$d = \begin{bmatrix} 0 & 35 & 35 & 29 & 70 & 35 & 42 & 27 & 24 & 44 & 58 & 71 & 69 \\ 35 & 0 & 67 & 32 & 72 & 40 & 71 & 56 & 36 & 11 & 66 & 70 & 37 \\ 35 & 67 & 0 & 63 & 64 & 68 & 11 & 12 & 56 & 77 & 48 & 67 & 94 \\ 29 & 32 & 63 & 0 & 93 & 8 & 71 & 56 & 8 & 33 & 84 & 93 & 69 \\ 70 & 72 & 64 & 93 & 0 & 101 & 56 & 56 & 92 & 81 & 16 & 5 & 69 \\ 35 & 40 & 68 & 8 & 101 & 0 & 76 & 62 & 11 & 39 & 91 & 101 & 76 \\ 42 & 71 & 11 & 71 & 56 & 76 & 0 & 15 & 65 & 81 & 40 & 60 & 94 \\ 27 & 56 & 12 & 56 & 56 & 62 & 15 & 0 & 50 & 66 & 41 & 58 & 82 \\ 24 & 36 & 56 & 8 & 92 & 11 & 65 & 50 & 0 & 39 & 81 & 91 & 74 \\ 44 & 11 & 77 & 33 & 81 & 39 & 81 & 66 & 39 & 0 & 77 & 79 & 37 \\ 58 & 66 & 48 & 84 & 16 & 91 & 40 & 41 & 81 & 77 & 0 & 20 & 73 \\ 71 & 70 & 67 & 93 & 5 & 101 & 60 & 58 & 91 & 79 & 20 & 0 & 65 \\ 69 & 37 & 94 & 69 & 69 & 76 & 94 & 82 & 74 & 37 & 73 & 65 & 0 \end{bmatrix} \quad (8.1)$$

The value d gives the travel distance between stops i and j . For example, $d_{23} = 89$ indicates that the distance between the 2nd and 3rd stop in the third itinerary is given 89.

Given these parameters, we aim to find a *sufficiently good* set of itineraries that gives a low total amount of travel.

The emphasis on needing a good solution, but not necessarily the best one, prioritising computational efficiency is where the field of heuristics comes in to its own.

8.2 THEORY

The heuristic approach take here will be to use a neighborhood search algorithm. This algorithm works by considering a given potential solution, evaluating it and then trying another potential solution *close* to it. What *close* means depends on

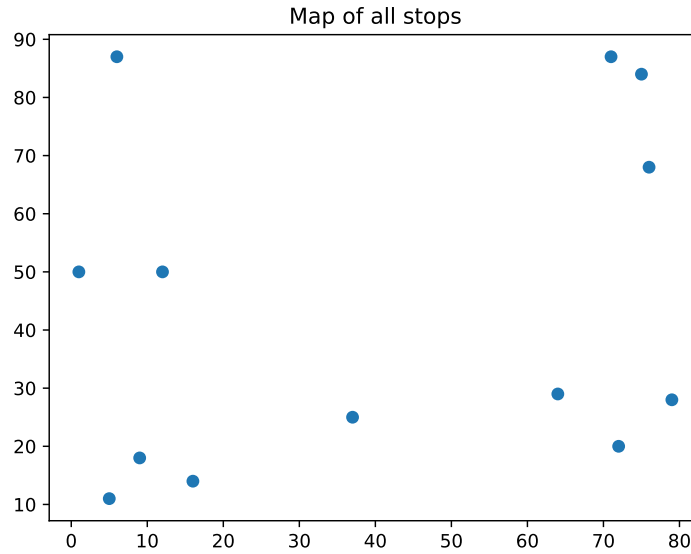


Figure 8.1 Diagrammatic representation of the action sets and payoff matrices for the game.

different approaches and problems: it is referred to as the neighbourhood. As a new solution is evaluated if it is *good* (this is again a term that depends on the approach and problem) then the search continues from the neighbourhood of this new solution.

For our problem, the first aspect of this is to represent a given trajectory between all the potential stops as a *tour*. If we have 3 total stops and require that the tour starts and stops at the first one then there are two possible tours:

$$t \in \{(1, 2, 3, 1), (1, 3, 2, 1)\}$$

Given a distance matrix d such that d_{ij} is the distance between stop i and j the total cost of a tour is given by:

$$C(t) = \sum_{i=1}^n d_{t_i, t_{i+1}}$$

Thus, with:

$$d = \begin{pmatrix} 0 & 1 & 3 \\ 1 & 0 & 15 \\ 3 & 3 & 7 \end{pmatrix}$$

We have:

$$c((1, 2, 3, 1)) = d_{12} + d_{23} + d_{31} = 1 + 15 + 3 = 19$$

$$c((1, 3, 2, 1)) = d_{13} + d_{32} + d_{21} = 3 + 3 + 1 = 7$$

Using this framework, the neighbourhood search can be written down as:

1. Start with a given tour: t .
2. Evaluate $C(t)$.
3. Identify a new \tilde{t} from t and accept it as a replacement for t if $C(\tilde{t}) < C(t)$.
4. Repeat the 3rd step until some stopping condition is met.

This is shown diagrammatically in Figure 8.2.

A number of stopping conditions can be used including some specific overall cost or a number of total iterations of the algorithm.

The neighbourhood of a tour t is taken as some set of tours that can be obtained from t using a specific and computationally efficient **neighbourhood operator**.

To illustrate two such neighbourhoods operators, consider the following tour on 7 stops:

$$t = (0, 1, 2, 3, 4, 5, 6, 0)$$

One possible neighbourhood is to choose 2 stops at random and swap. For example, the tour $t^{(1)} \in N(t)$ is obtained by swapping the 3rd and 5th stops.

$$t^{(1)} = (0, 1, 5, 3, 4, 2, 6, 0)$$

Another possible neighbourhood is to choose 2 stops at random and reversing the order of all stops between (including) those two stops. For example, the tour $t^{(2)} \in N(t)$ is obtained by reversing the order of all stops between the 3rd and the 5th stop.

$$t^{(2)} = (0, 1, 5, 4, 3, 2, 6, 0)$$

Examples of these tours are shown in Figure 8.3.

8.3 SOLVING WITH PYTHON

To solve this problem using Python we will write functionality that matches the first three steps in the Section 8.2.

The first step is to write the `get_initial_candidate` function that creates an initial tour:

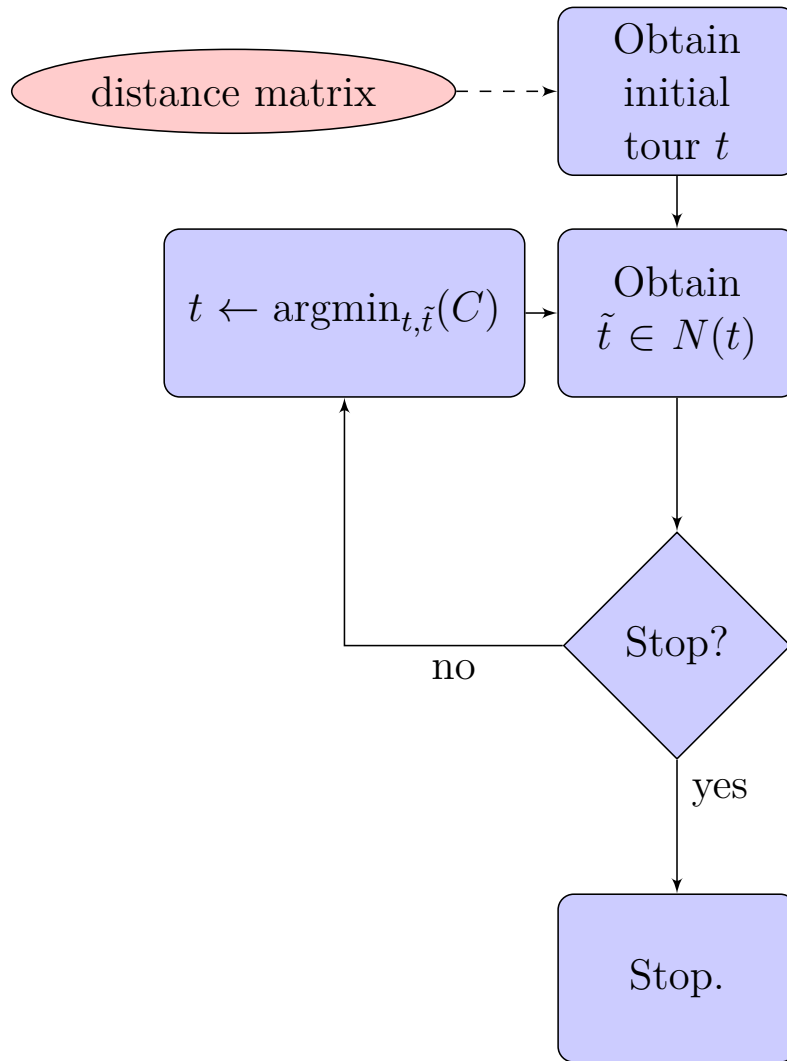


Figure 8.2 The general neighbourhood search algorithm. $N(t)$ refers to some neighbourhood of t .

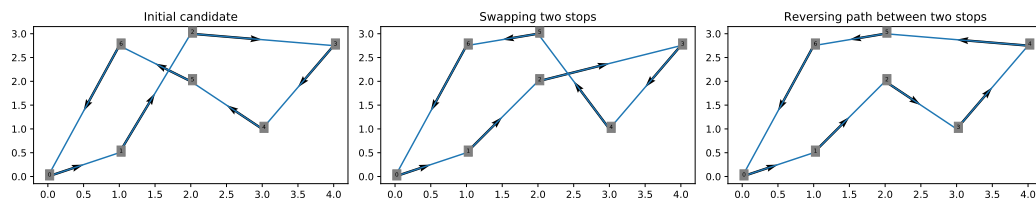


Figure 8.3 The effect of two neighborhood operators on t . $t^{(1)}$ is obtained by swapping stops 3 and 5. $t^{(2)}$ is obtained by reversing the path between stops 3 and 5.

Python input

```

1202 import numpy as np
1203
1204
1205 def get_initial_candidate(number_of_stops, seed=None):
1206     """Return an initial tour.
1207
1208     Args:
1209         number_of_stops: The number of stops
1210         seed: An integer seed. If an integer value is
1211             passed it will create a random tour.
1212
1213     Returns:
1214         A tour starting and ending at stop with index 0.
1215     """
1216     internal_stops = list(range(1, number_of_stops))
1217     if seed is not None:
1218         np.random.seed(seed)
1219         np.random.shuffle(internal_stops)
1220     return [0] + internal_stops + [0]

```

Using this we can get a random tour on 13 stops:

Python input

```

1221 number_of_stops = 13
1222 seed = 0
1223 initial_candidate = get_initial_candidate(
1224     number_of_stops=number_of_stops,
1225     seed=seed,
1226 )
1227 print(initial_candidate)

```

Python output

```

1228 [0, 7, 12, 5, 11, 3, 9, 2, 8, 10, 4, 1, 6, 0]

```

To be able to evaluate any given tour we see that we must also be able to evaluate its cost. Here we define `get_cost` to do this:

Python input

```
1229 def get_cost(tour, distance_matrix):
1230     """Return the cost of a tour
1231
1232     Args:
1233         tour: A given tuple of successive stops.
1234         distance_matrix: The distance matrix of the problem.
1235
1236     Returns:
1237         The cost
1238     """
1239     return sum(
1240         distance_matrix[current_stop, next_stop]
1241         for current_stop, next_stop in
1242         zip(tour[:-1], tour[1:])
1243     )
```

Python input

```

1244 distance_matrix = np.array(
1245     (
1246         (0, 35, 35, 29, 70, 35, 42, 27, 24, 44, 58, 71, 69),
1247         (35, 0, 67, 32, 72, 40, 71, 56, 36, 11, 66, 70, 37),
1248         (35, 67, 0, 63, 64, 68, 11, 12, 56, 77, 48, 67, 94),
1249         (29, 32, 63, 0, 93, 8, 71, 56, 8, 33, 84, 93, 69),
1250         (70, 72, 64, 93, 0, 101, 56, 56, 92, 81, 16, 5, 69),
1251         (35, 40, 68, 8, 101, 0, 76, 62, 11, 39, 91, 101, 76),
1252         (42, 71, 11, 71, 56, 76, 0, 15, 65, 81, 40, 60, 94),
1253         (27, 56, 12, 56, 56, 62, 15, 0, 50, 66, 41, 58, 82),
1254         (24, 36, 56, 8, 92, 11, 65, 50, 0, 39, 81, 91, 74),
1255         (44, 11, 77, 33, 81, 39, 81, 66, 39, 0, 77, 79, 37),
1256         (58, 66, 48, 84, 16, 91, 40, 41, 81, 77, 0, 20, 73),
1257         (71, 70, 67, 93, 5, 101, 60, 58, 91, 79, 20, 0, 65),
1258         (69, 37, 94, 69, 69, 76, 94, 82, 74, 37, 73, 65, 0),
1259     )
1260 )
1261 cost = get_cost(
1262     tour=initial_candidate,
1263     distance_matrix=distance_matrix,
1264 )
1265 print(cost)

```

Python output

```

1266 827

```

We will now define two different neighbourhood operators:

- `swap_stops`: this swaps two stops in a given tour.
- `reverse_path`: this swaps two stops and reverts the stops in between them.

Python input

```

1267 def swap_stops(tour):
1268     """
1269     Return a new tour by swapping two stops
1270
1271     Args:
1272         tour: A given tuple of successive stops.
1273
1274     Returns:
1275         A tour
1276     """
1277     number_of_stops = len(tour) - 1
1278     i, j = sorted(
1279         np.random.choice(range(1, number_of_stops), 2)
1280     )
1281     new_tour = list(tour)
1282     new_tour[i], new_tour[j] = tour[j], tour[i]
1283     return new_tour
1284
1285 def reverse_path(tour):
1286     """
1287     Return a new tour by reversing the path between two stops
1288
1289     Args:
1290         tour: A given tuple of successive stops.
1291
1292     Returns:
1293         A tour
1294     """
1295     number_of_stops = len(tour) - 1
1296     i, j = sorted(
1297         np.random.choice(range(1, number_of_stops), 2)
1298     )
1299     new_tour = tour[:i] + tour[i:j + 1][::-1] + tour[j + 1:]
1300     return new_tour

```

If we apply these two neighbourhood operators to our initial candidate we can see the effects:

Python input

```
1301 print(swap_stops(initial_candidate))
```

which swaps the 3rd and 8th stops:

Python output

```
1302 [0, 7, 12, 5, 11, 3, 9, 2, 8, 1, 4, 10, 6, 0]
```

Python input

```
1303 print(reverse_path(initial_candidate))
```

which reverses the order between the 3rd and the 8th stop:

Python output

```
1304 [0, 7, 2, 9, 3, 11, 5, 12, 8, 10, 4, 1, 6, 0]
```

Now we have all the tools in place to build a tool to carry out the neighbourhood search `run_neighbourhood_search`.

Python input

```

1305 def run_neighbourhood_search(
1306     distance_matrix,
1307     number_of_stops,
1308     iterations,
1309     seed=None,
1310     get_cost=get_cost,
1311     get_initial_candidate=get_initial_candidate,
1312     neighbourhood_operator=reverse_path,
1313 ):
1314     """Returns a tour by carrying out a neighbourhood search.
1315
1316     Args:
1317         distance_matrix: the distance matrix
1318         number_of_stops: the number of stops
1319         iterations: the number of iterations for which to
1320             run the algorithm
1321         seed: a random seed (default: None)
1322         neighbourhood_operator: the neighbourhood operator
1323             (default: swap_paths)
1324
1325     Returns:
1326         A tour
1327     """
1328     np.random.seed(seed)
1329
1330     candidate = get_initial_candidate(
1331         number_of_stops=number_of_stops,
1332     )
1333
1334     best_cost = get_cost(
1335         tour=candidate,
1336         distance_matrix=distance_matrix,
1337     )
1338
1339     for _ in range(iterations):
1340         new_candidate = neighbourhood_operator(candidate)
1341         if (cost:=get_cost(
1342             tour=new_candidate,
1343             distance_matrix=distance_matrix,
1344         )
1345             ) <= best_cost:
1346             best_cost = cost
1347             candidate = new_candidate
1348
1349     return candidate

```

Using this we can see the effect of running 1000 iterations using different neighbourhood functions:

Python input

```
1350 number_of_iterations = 1000
1351
1352 solution_with_swap_stops = run_neighbourhood_search(
1353     distance_matrix=distance_matrix,
1354     number_of_stops=number_of_stops,
1355     iterations=number_of_iterations,
1356     seed=seed,
1357     neighbourhood_operator=swap_stops,
1358 )
1359 print(solution_with_swap_stops)
```

giving:

Python output

```
1360 [0, 7, 6, 2, 8, 5, 3, 1, 9, 12, 11, 4, 10, 0]
```

Python input

```
1361 solution_with_swap_paths = run_neighbourhood_search(
1362     distance_matrix=distance_matrix,
1363     number_of_stops=number_of_stops,
1364     iterations=number_of_iterations,
1365     seed=seed,
1366     neighbourhood_operator=reverse_path,
1367 )
1368 print(solution_with_swap_paths)
```

giving:

Python output

```
1369 [0, 7, 2, 6, 10, 4, 11, 12, 9, 1, 3, 5, 8, 0]
```

Importantly the costs differ substantially:

Python input

```
1370 cost = get_cost(  
1371     tour=solution_with_swap_stops,  
1372     distance_matrix=distance_matrix,  
1373 )  
1374 print(cost)
```

which gives:

Python output

```
1375 352
```

Whereas using the entire swapping of paths

Python input

```
1376 cost = get_cost(  
1377     tour=solution_with_swap_paths,  
1378     distance_matrix=distance_matrix,  
1379 )  
1380 print(cost)
```

which gives:

Python output

```
1381 299
```

8.4 SOLVING WITH R

8.5 RESEARCH

TBA

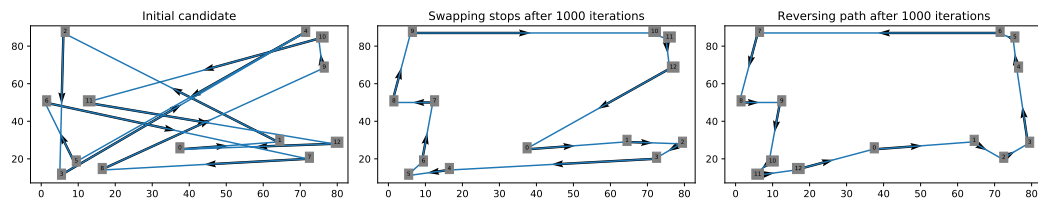


Figure 8.4 The final tours obtained by using the neighbourhood search.



Bibliography

