Dianne Cook and Ursula Laa

Interactively exploring high-dimensional data and models in R

Contents

Preface **9**

What's in this book? 9

Audience 10

How to use the book? 10

What should I know before reading this book? 11

Setting up your workflow 11

Suggestion, feedback or error? 12

1 Picturing high dimensions **13**

1.1 Getting familiar with tours 13

1.2 What's different about space beyond 2D? 15

1.3 What can you learn? 18

1.4 A little history 20

Exercises 21

2 Notation conventions and R objects **23**

Exercises 26

3 Dimension reduction overview **27**

Exercises 33

4 Principal component analysis **37**

4.1 Determining how many dimensions 38

4.2 Examining the PCA model in the data space 47

4.3 When relationships are not linear 52

Exercises 53

Project 57

5 Non-linear dimension reduction **59**

5.1 Explanation of NLDR methods 59

5.2 Assessing reliability of the NLDR representation 61

5.3 Example: `fake_trees` 64

Exercises 65

6 Introduction to clustering **67**

6.1 What are clusters? 67

6.2 The importance of defining similar 69

Exercises 72

7 Spin-and-brush approach **75**

Exercises 77

8 Hierarchical clustering **81**

8.1 Overview 81

8.2 Common patterns which confuse clustering algorithms 85

8.3 Dendrograms in high-dimensions 92

Exercises 101

9 k-means clustering **103**

9.1 Examining results in 2D 103

9.2 Examining results in high dimensions 105

Exercises 106

10 Model-based clustering **109**

10.1 Examining the model in 2D 110

10.2 Examining the model in high dimensions 112

Exercises 114

11 Self-organizing maps **115**

Exercises 118

12 Summarising and comparing clustering results 119

12.1 Summarising results 119

12.2 Comparing two clusterings 122

Exercises 123

Project 125

13 Introduction to supervised classification 127

14 Linear discriminant analysis 129

14.1 Extracting the key elements of the model 129

14.2 Checking assumptions 133

14.3 Examining results 136

Exercises 140

15 Trees and forests 141

15.1 Trees 141

15.2 Random forests 143

Exercises 152

16 Support vector machines 153

16.1 Components of the SVM model 153

16.2 Examining the model components in high-dimensions 156

Exercises 160

17 Neural networks and deep learning 161

17.1 Setting up the model 162

17.2 Checking the training/test split 163

17.3 Fit the model 164

17.4 Extracting model components 166

17.5 Examining predictive probabilities 169

17.6 Local explanations 170

17.7 Examining boundaries 171

17.8 Application to a large dataset 173

Exercises 178

18 Exploring misclassifications **179**

18.1 Errors for a single model 179

18.2 Comparison between LDA and CNN 181

18.3 Constructing data to diagnose your model 181

18.4 Explainability 181

Exercises 181

References **183**

A Toolbox **199**

A.1 Using tours in the `tourr` package 199

A.2 What not to do 203

A.3 Tours in other software 207

A.4 Supporting software 207

B Data **209**

B.1 Australian Football League Women 210

B.2 Bushfires 211

B.3 Australian election data 214

B.4 Palmer penguins 215

B.5 Program for International Student Assessment 217

B.6 Sketches 218

B.7 `multicluster` 219

B.8 `clusters`, `clusters_nonlin`, `simple_clusters` 220

B.9 `plane`, `plane_nonlin`, `box` 221

B.10 `c1` - `c7` 222

B.11 Fashion MNIST 223

C Links to Book Code and Additional Data **225**

C.1 Additional data 225

C.2 Code files 226

D Glossary **227**

Index **229**

Preface

It is important to visualise your data because you might discover things that you could never have anticipated. Although there are many resources available for data visualisation, there are few comprehensive resources on high-dimensional data visualisation. High-dimensional (or multivariate) data arises when many different things are measured for each observation. While we can learn many things from plotting with 1D and 2D or 3D methods there are likely more structures hidden in the higher dimensions. This book provides guidance on visualising high-dimensional data and models using linear projections, with R.

High-dimensional data spaces are fascinating places. You may think that there's a lot of ways to plot one or two variables, and a lot of types of patterns that can be found. You might use a density plot and see skewness or a dot plot to find outliers. A scatterplot of two variables might reveal a non-linear relationship or a barrier beyond which no observations exist. We don't as yet have so many different choices of plot types for high-dimensions, but these types of patterns are also what we seek in scatterplots of high-dimensional data. The additional dimensions can clarify these patterns, that clusters are likely to be more distinct. Observations that did not appear to be very different can be seen to be lonely anomalies in high-dimensions, that no other observations have quite the same combination of values.

What's in this book?

The book is divided into these parts:

- **Introduction**: Here we introduce you to high-dimensional spaces, how they can be visualised, and notation that is useful for describing methods in later chapters.

- **Dimension reduction**: This part covers linear and non-linear dimension reduction. It includes ways to help decide on the number of dimensions needed to summarise the high dimensional data, whether linear dimension

reduction is appropriate, detecting problems that might affect the dimension reduction, and examining how well or badly a non-linear dimension reduction is representing the data.
- **Cluster analysis**: This part described methods for finding groups in data. Although it includes an explanation of a purely graphical approach, it is mostly on using graphics in association with numerical clustering algorithms. There are explanations of assessing the suitability of different numerical techniques for extracting clusters, based on the data shapes, evaluating the clustering result, and showing the solutions in high dimensions.
- **Classification**: This part describes methods for exploring known groups in the data. You'll learn how to check model assumptions, to help decide if a method is suited to the data, examine classification boundaries and explore where errors arise.

In each of these parts an emphasis is also showing your model with your data in the high dimensional space.

Our hopes are that you will come away with understanding the importance of plotting your high dimensional data as a regular step in your statistical or machine learning analyses. There are many examples of what you might miss if you don't plot the data. Effective use of graphics goes hand-in-hand with analytical techniques. With high dimensions visualisation is a challenge but it is fascinating, and leads to many surprising moments.

Audience

High-dimensional data arises in many fields such as biology, social sciences, finance, and more. Anyone who is doing exploratory data analysis and model fitting for more than two variables will benefit from learning how to effectively visualise high-dimensions. This book will be useful for students and teachers of multivariate data analysis and machine learning, and researchers, data analysts, and industry professionals who work in these areas.

How to use the book?

The book is written with explanations accompanied by examples with R code. The chapters are organised by types of analysis and focus on how to use the high-dimensional visualisation to complement the commonly used analytical

methods. The toolbox chapter in the Appendix provides an overview of the primary high-dimensional visualisation methods discussed in the book and how to get started.

What should I know before reading this book?

The examples assume that you already use R, and have a working knowledge of base R and tidyverse way of thinking about data analysis. It also assumes that you have some knowledge of statistical methods, and some experience with machine learning methods.

If you feel like you need build up your skills in these areas in preparation for working through this book, these are our recommended resources:

- R for Data Science by Wickham and Grolemund for learning about data wrangling and visualisation.
- Introduction to Modern Statistics by Çetinkaya-Rundel and Hardin to learn about introductory statistics.
- Hands-On Machine Learning with R by Boehmke and Greenwell to learn about machine learning.

We will assume you know how to plot your data and models in 2D. Our material starts from 2D and beyond.

Setting up your workflow

To get started set up your computer with the current versions of R and ideally also with Rstudio Desktop.

In addition, we have made an R package to share the data and functions used in this book, called `mulgar`.[1][2]

[1] Mulga is a type of Australian habitat composed of woodland or open forest dominated by the mulga tree. Massive clearing of mulga led to the vast wheat fields of Western Australia. Here **mulgar** is an acronym for **MUL**tivariate **G**raphical **A**nalysis with **R**.

[2] Photo of mulga tree taken by L. G. Cook.

```
install.packages("mulgar", dependencies=TRUE)
# or the development version
devtools::install_github("dicook/mulgar")
```

To get a copy of the code and data used and an RStudio project to get started, you can download with this code:

```
book_url <- "https://dicook.github.io/mulgar_book/code_and_data.zip"
usethis::use_zip(url=book_url)
```

You will be able to click on the `mulgar_book.Rproj` to get started with the code.

Suggestion, feedback or error?

We welcome suggestions, feedback or details of errors. You can report them as an issue at the Github repo for this book.

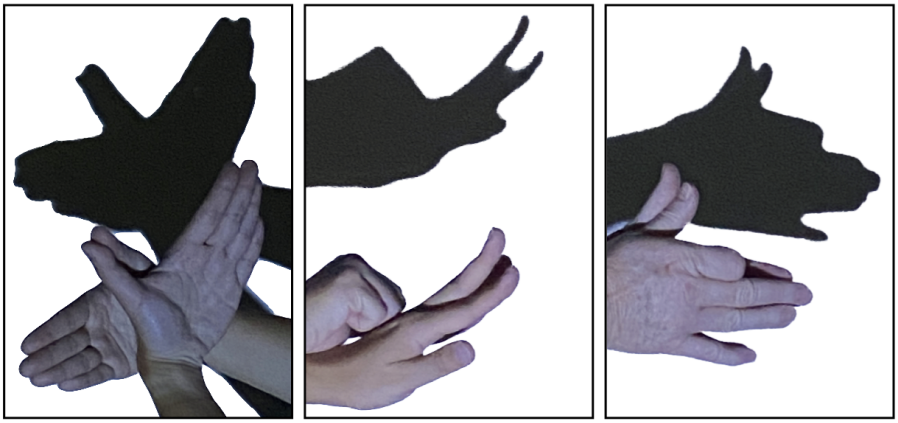
Please make a small reproducible example and report the error encountered. Reproducible examples have these components:

- a small amount of data
- small amount of code that generates the error
- copy of the error message that was generated

1

Picturing high dimensions

High-dimensional data means that we have a large number of numeric features or variables, which can be considered as dimensions in a mathematical space. The variables can be different types, such as categorical or temporal, but the handling of these variables involves different techniques.



1.1 Getting familiar with tours

Figure 1.1 illustrates a tour for 2D data and 1D projections. The (grand) tour will generate all possible 1D projections of the data, and display with a univariate plot like a histogram or density plot. For this data, the `simple_clusters` data, depending on the projection, the distribution might be clustered into two groups (bimodal), or there might be no clusters (unimodal). In this example, all projections are generated by rotating a line around the centre of the plot. Clustering can be seen in many of the projections, with the strongest being when the contribution of both variables is equal, and the projection is `(0.707, 0.707)` or `(-0.707, -0.707)`. (If you are curious about the number `0.707`, read the last section of this chapter.)

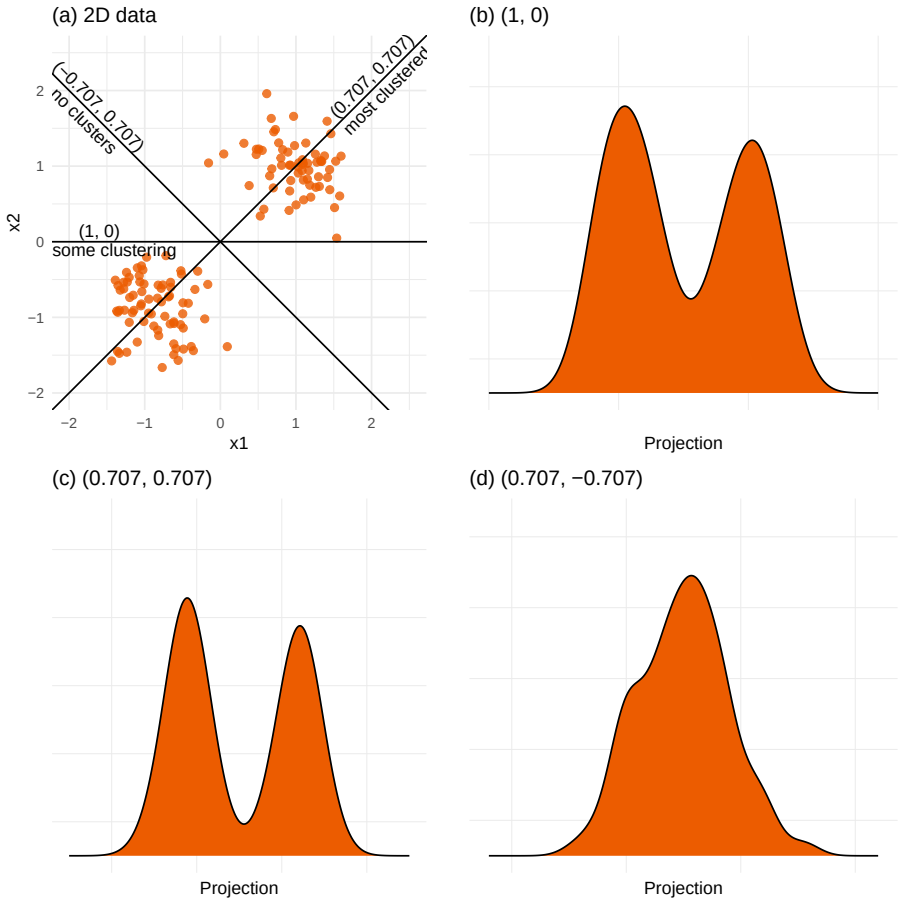


Figure 1.1: How a tour can be used to explore high-dimensional data illustrated using (a) 2D data with two clusters and (b,c,d) 1D projections from a tour shown as a density plot. Imagine spinning a line around the centre of the data plot, with points projected orthogonally onto the line. With this data, when the line is at `x1=x2 (0.707, 0.707)` or `(-0.707, -0.707)` the clustering is the strongest. When it is at `x1=-x2 (0.707, -0.707)` there is no clustering.

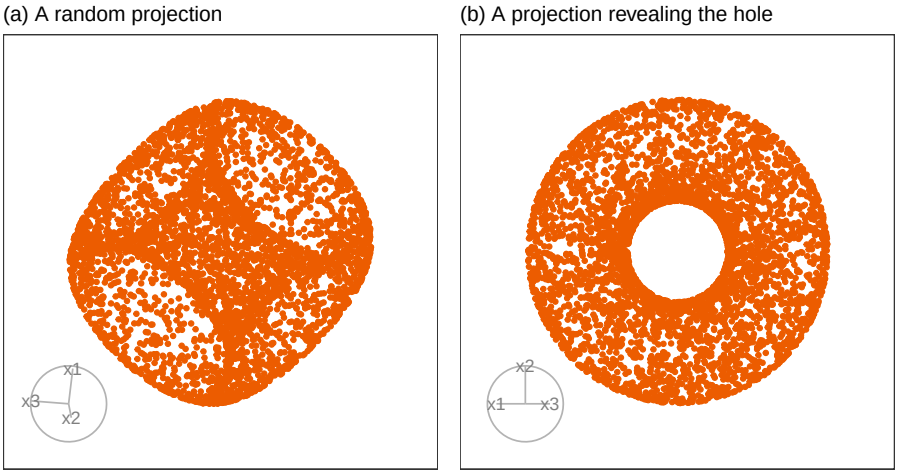


Figure 1.2: How a tour can be used to explore high-dimensional data illustrated by showing a sequence of random 2D projections of 3D data (a). The data has a donut shape with the hole revealed in a single 2D projection (b). Data usually arrives with a given number of observations, and when we plot it like this using a scatterplot, it is like shadows of a transparent object.

Figure 1.2 illustrates a tour for 3D data using 2D projections. The data are points on the surface of a donut shape. By showing the projections using a scatterplot the donut looks transparent and we can see through the data. The donut shape can be inferred from watching many 2D projections but some are more revealing that others. The projection shown in (b) is where the hole in the donut is clearly visible.

1.2 What's different about space beyond 2D?

The term "high-dimensional" in this book refers to the dimensionality of the Euclidean space. Figure 1.3 shows a way to imagine this. It shows a sequence of cube wireframes, ranging from one-dimensional (1D) through to five-dimensional (5D), where beyond 2D is a linear projection of the cube. As the dimension increases, a new orthogonal axis is added. For cubes, this is achieved by doubling the cube: a 2D cube consists of two 1D cubes, a 3D cube consists of two 2D cubes, and so forth. This is a great way to think about the space being examined by the visual methods, and also all of the machine learning methods mentioned, in this book.

Interestingly, the struggle with imagining high-dimensions this way is described

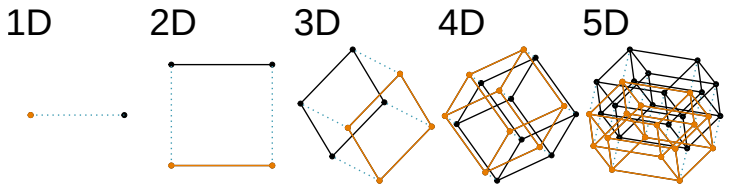


Figure 1.3: Space can be considered to be a high-dimensional cube. Here we have pictured a sequence of increasing dimension cubes, from 1D to 5D, as wireframes, it can be seen that as the dimension increase by one, the cube doubles.

in a novel published in 1884 (Abbott, 1884) [1]. Yes, more than 100 years ago! This is a story about characters living in a 2D world, being visited by an alien 3D character. It also is a social satire, serving the reader strong messages about gender inequity, although this provides the means to explain more intricacies in perceiving dimensions. There have been several movies made based on the book in recent decades (e.g. Martin (1965), D. Johnson & Travis (2007)). Although purchasing the movies may be prohibitive, watching the trailers available for free online is sufficient to gain enough geometric intuition on the nature of understanding high-dimensional spaces while living in a low-dimensional world.

When we look at high-dimensional spaces from a low-dimensional space, we meet the "curse of dimensionality", a term introduced by Bellman (1961) to express the difficulty of doing optimization in high dimensions because of the exponential growth in space as dimension increases. A way to imagine this is look at the cubes in Figure 1.3: As you go from 1D to 2D, 2D to 3D, the space expands a lot, and imagine how vast space might get as more dimensions are added[2]. The volume of the space grows exponentially with dimension, which makes it infeasible to sample enough points – any sample will be less densely covering the space as dimension increases. The effect is that most points will be far from the sample mean, on the edge of the sample space.

For visualisation, the curse manifests in an opposite manner. Projecting from high to low dimensions creates a crowding or piling of points near the center of the distribution. This was noted by Diaconis & Freedman (1984a). Figure 1.4 illustrates this phenomenon. As dimension increases, the points crowd the centre, even with as few as ten dimensions. This is something that we may need to correct for when exploring high dimensions with low-dimensional projections.

Figure 1.5 shows 2D tours of two different 5D data sets. One has clusters

[1] Thanks to Barret Schloerke for directing co-author Cook to this history when he was an undergraduate student and we were starting the geozoo project.

[2] "Space is big. Really big. You might think it's a long way to the pharmacy, but that's peanuts to space." from Douglas Adams' Hitchhiker's Guide to the Galaxy always springs to mind when thinking about high dimensions!

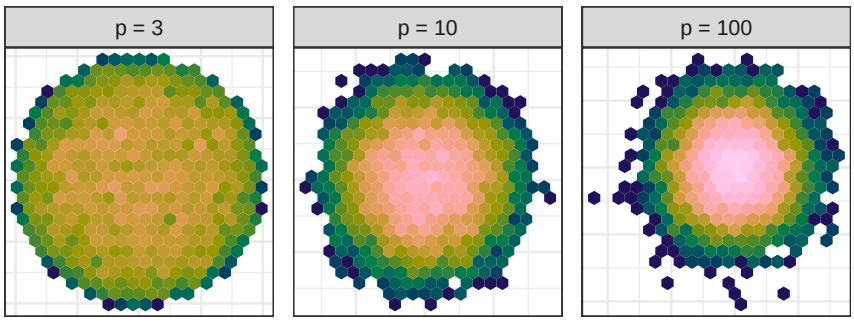
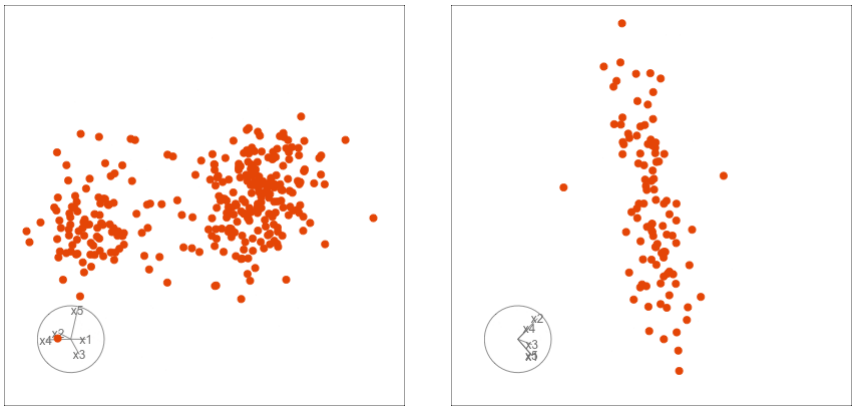


Figure 1.4: Illustration of data crowding in the low-dimensional projection as dimension increases, here from 3, 10, 100. Colour shows the number of points in each hexagon bin (pink is large, navy is small). As dimension increases the points concentrate near the centre.

(a) and the other has two outliers and a plane (b). Can you see these? One difference in the viewing of data with more than three dimensions with 2D projections is that the points seem to shrink towards the centre, and then expand out again. This the effect of dimensionality, with different variance or spread in some directions.



(a) Clusters (b) Outliers

Figure 1.5: Frames from 2D tours on two 5D datasets, with clusters of points in (a) and two outliers with a plane in (b). This figure is best viewed in the HTML version of the book.

1.3 What can you learn?

There are two ways of detecting structure in tours:

- patterns in a single low-dimensional projection
- movement patterns

with the latter being especially useful when displaying the projected data as a scatterplot. Figure 1.6 shows examples of patterns we typically look for when making a scatterplot of data. These include clustering, linear and non-linear association, outliers, barriers where there is a sharp edge beyond which no observations are seen. Not shown, but it also might be possible to observe multiple modes, or density of observations, L-shapes, discreteness or uneven spread of points. The tour is especially useful if these patterns are only visible in combinations of variables.

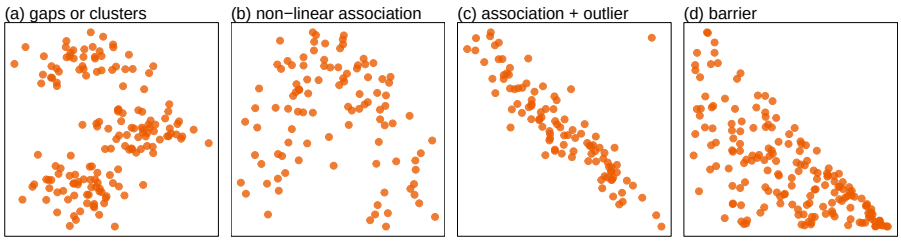
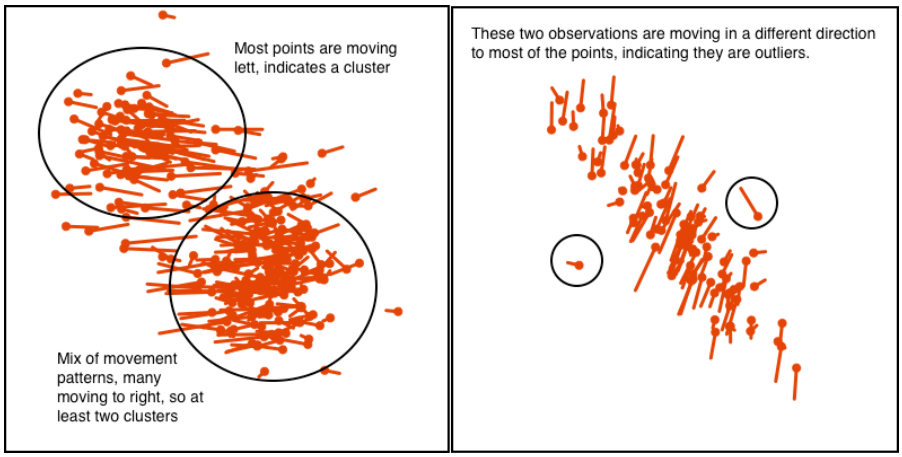


Figure 1.6: Example structures that might be visible in a 2D projection that imply presence of structure in high dimensions. These include clusters, linear and non-linear association, outliers and barriers.

Figure 1.7 illustrates how movement patterns of points when using scatterplots to display 2D projections indicate clustering (a, b) and outliers (c, d).

This type of visualisation is useful for many activities in dealing with high-dimensional data, including:

- exploring high-dimensional data.
- detecting if the data lives in a lower dimensional space than the number of variables.
- checking assumptions required for multivariate models to be applicable.
- check for potential problems in modeling such as multicollinearity among predictors.
- checking assumptions required for probabilities calculated for statistical hypothesis testing to be valid.



(a) Clustering (b) Outliers

Figure 1.7: The movement of points give further clues about the structure of the data in high-dimensions. In the data with clustering, often we can see a group of points moving differently from the others. Because there are three clusters, you should see three distinct movement patterns. It is similar with outliers, except these may be individual points moving alone, and different from all others. This can be seen in the static plot, one point (top left) has a movement pattern upwards whereas most of the other observations near it are moving down towards the right.

- diagnosing the fit of multivariate models.

With a tour we slowly rotate the viewing direction, this allows us to see many individual projections and to track movement patterns. Look for interesting structures such as clusters or outlying points.

1.4 A little history

Viewing high-dimensional data based on low-dimensional projections can probably be traced back to the early work on principal component analysis by Pearson (1901) and Hotelling (1933), which was extended to known classes as part of discriminant analysis by Fisher (1936a).

With computer graphics, the capability of animating plots to show more than a single best projection became possible. The video library (ASA Statistical Graphics Section, 2023) is the best place to experience the earliest work. Kruskal's 1962 animation of multidimensional scaling showed the process of finding a good 2D representation of high dimensional data, although the views are not projections. Chang's 1970 video shows her rotating a high dimensional point cloud along coordinate axes to find a special projection where all the numbers align. The classic video that must be watched is PRIM9 (Fisherkeller et al., 1973) where a variety of interactive and dynamic tools are used together to explore high dimensional physics data, documented in Fisherkeller et al. (1974).

The methods in this book primarily emerge from Asimov (1985)'s grand tour method. The algorithm provided the first smooth and continuous sequence of low dimensional projections, and guaranteed that all possible low dimensional projections were likely to be shown. The algorithm was refined in Buja & Asimov (1986) (and documented in detail in Buja et al. (2005)) to make it *efficiently* show all possible projections. Since then there have been numerous varieties of tour algorithms developed to focus on specific tasks in exploring high dimensional data, and these are documented in S. Lee et al. (2022).

This book is an evolution from Cook & Swayne (2007). One of the difficulties in working on interactive and dynamic graphics research has been the rapid change in technology. Programming languages have changed a little (FORTRAN to C to java to python) but graphics toolkits and display devices have changed a lot! The tour software used in this book evolved from XGobi, which was written in C and used the X Window System, which was then rewritten in

GGobi using gtk. The video library has engaging videos of these software systems There have been several other short-lived implementations, including orca (Sutherland et al., 2000a), written in java, and cranvas (Xie et al., 2014), written in R with a back-end provided by wrapper functions to qt libraries.

Although attempts were made with these ancestor systems to connect the data plots to a statistical analysis system, these were always limited. With the emergence of R, having graphics in the data analysis workflow has been much easier, albeit at the cost of the interactivity with graphics that matches the old systems. We are mostly using the R package, `tourr` (Wickham et al., 2011a) for examples in this book. It provides the machinery for running a tour, and has the flexibility that it can be ported, modified, and used as a regular element of data analysis.

Exercises

1. Randomly generate data points that are uniformly distributed in a hyper-cube of 3, 5 and 10 dimensions, with 500 points in each sample, using the `cube.solid.random` function of the `geozoo` package. What differences do we expect to see? Now visualise each set in a grand tour and describe how they differ, and whether this matched your expectations?
2. Use the `geozoo` package to generate samples from different shapes and use them to get a better understanding of how shapes appear in a grand tour. You can start with exploring the conic spiral in 3D, a torus in 4D and points along the wire frame of a cube in 5D.
3. For each of the challenge data sets, `c1`, ..., `c7` from the `mulgar` package, use the grand tour to view and try to identify structure (outliers, clusters, non-linear relationships).

2

Notation conventions and R objects

The data can be considered to be a matrix of numbers with the columns corresponding to variables, and the rows correspond to observations. It can be helpful to write this in mathematical notation, like:

$$X_{n\times p} = [X_1 \ X_2 \ \ldots \ X_p]_{n\times p} = \begin{bmatrix} X_{11} & X_{12} & \ldots & X_{1p} \\ X_{21} & X_{22} & \ldots & X_{2p} \\ \vdots & \vdots & & \vdots \\ X_{n1} & X_{n2} & \ldots & X_{np} \end{bmatrix}_{n\times p}$$

where X indicates the the $n\times p$ data matrix, X_j indicates variable $j, j = 1, \ldots, p$ and X_{ij} indicates the value j^{th} variable of the i^{th} observation. (It can be confusing to distinguish whether one is referring to the observation or a variable, because X_i is used to indicate observation also. When this is done it is usually accompanied by qualifying words such as **observation** X_3, or **variable** X_3.)

Having notation is helpful for concise explanations of different methods, to explain how data is scaled, processed and projected for various tasks, and how different quantities are calculated from the data.

When there is a response variable(s), it is common to consider X to be the predictors, and use Y to indicate the response variable(s). Y could be a matrix, also, and would be $n \times q$, where commonly $q = 1$. Y could be numeric or categorical, and this would change how it is handled with visualisation.

To make a low-dimensional projection (shadow) of the data, we need a projection matrix:

$$A_{p\times d} = \begin{bmatrix} A_{11} & A_{12} & \ldots & A_{1d} \\ A_{21} & A_{22} & \ldots & A_{2d} \\ \vdots & \vdots & & \vdots \\ A_{p1} & A_{p2} & \ldots & A_{pd} \end{bmatrix}_{p\times d}$$

A should be an orthonormal matrix, which means that the $\sum_{j=1}^{p} A_{jk}^2 = 1, k =$

$1, \ldots, d$ (columns represent vectors of length 1) and $\sum_{j=1}^{p} A_{jk}A_{jl} = 0, k, l = 1, \ldots, d; k \neq l$ (columns represent vectors that are orthogonal to each other). In matrix notation, this can be written as $A^\top A = I_d$.

Then the projected data is written as:

$$Y_{n\times d} = XA = \begin{bmatrix} y_{11} & y_{12} & \cdots & y_{1d} \\ y_{21} & y_{22} & \cdots & y_{2d} \\ \vdots & \vdots & & \vdots \\ y_{n1} & y_{n2} & \cdots & y_{nd} \end{bmatrix}_{n\times d}$$

where $y_{ij} = \sum_{k=1}^{p} X_{ik}A_{kj}$. Note that we are using Y as the projected data here, as well as it possibly being used for a response variable. Where necessary, this will be clarified with words in the text, when notation is used in explanations later.

When using R, if we only have the data corresponding to X it makes sense to use a `matrix` object. However, if the response variable is included and it is categorical, then we might use a `data.frame` or a `tibble` which can accommodate non-numerical values. Then to work with the data, we can use the base R methods:

```
X <- matrix(c(1.1, 1.3, 1.4, 1.2,
              2.7, 2.6, 2.4, 2.5,
              3.5, 3.4, 3.2, 3.6),
            ncol=4, byrow=TRUE)
X
```

```
     [,1] [,2] [,3] [,4]
[1,]  1.1  1.3  1.4  1.2
[2,]  2.7  2.6  2.4  2.5
[3,]  3.5  3.4  3.2  3.6
```

which is a data matrix with $n = 3, p = 4$ and to extract a column (variable):

```
X[,2]
```

```
[1] 1.3 2.6 3.4
```

or a row (observation):

```
X[2,]
```

```
[1] 2.7 2.6 2.4 2.5
```

or an individual cell (value):

```
X[3,2]
```

```
[1] 3.4
```

To make a projection we need an orthonormal matrix:

```
A <- matrix(c(0.707,0.707,0,0,0,0,0.707,0.707), ncol=2, byrow=FALSE)
A
```

```
      [,1]  [,2]
[1,] 0.707 0.000
[2,] 0.707 0.000
[3,] 0.000 0.707
[4,] 0.000 0.707
```

You can check that it is orthonormal by

```
sum(A[,1]^2)
```

```
[1] 0.999698
```

```
sum(A[,1]*A[,2])
```

```
[1] 0
```

and make a projection using matrix multiplication:

```
X %*% A
```

```
       [,1]   [,2]
[1,] 1.6968 1.8382
[2,] 3.7471 3.4643
[3,] 4.8783 4.8076
```

The seemingly magical number `0.707` used above and to create the projection in Figure 1.1 arises from normalising a vector with equal contributions from each variable, `(1, 1)`. Dividing by `sqrt(2)` gives `(0.707, 0.707)`.

The notation convention used throughout the book is:

`n` = number of observations `p` = number of variables, dimension of data `d` = dimension of the projection `g` = number of groups, in classification `X` = data matrix

Exercises

1. Generate a matrix A with $p = 5$ (rows) and $d = 2$ (columns), where each value is randomly drawn from a standard normal distribution. Extract the element at row 3 and column 1.
2. We will interpret A as a projection matrix and therefore it needs to be orthonormalised. Use the function `tourr::orthonormalise` to do this, and explicitly check that each column is normalised and that the two columns are orthogonal now. Which dimensions contribute most to the projection for your A?
3. Use matrix multiplication to calculate the projection of the `mulgar::clusters` data onto the 2D plane defined by A. Make a scatterplot of the projected data. Can you identify clustering in this view?

3

Dimension reduction overview

This chapter will focus on methods for reducing dimension, and how the tour[1] can be used to assist with the common methods such as principal component analysis (PCA), multidimensional scaling (MDS), t-stochastic neighbour embedding (t-SNE), and factor analysis.

Dimension is perceived in a tour using the spread of points. When the points are spread far apart, then the data is filling the space. Conversely when the points "collapse" into a sub-region then the data is only partially filling the space, and some dimension reduction to reduce to this smaller dimensional space may be worthwhile.

When points do not fill the plotting canvas fully, it means that it lives in a lower dimension. This low-dimensional space might be linear or non-linear, with the latter being much harder to define and capture.

Let's start with some 2D examples. You need at least two variables to be able to talk about association between variables. Figure 3.1 shows three plots of two variables. Plot (a) shows two variables that are strongly linearly associated[2], because when `x1` is low, `x2` is low also, and conversely when `x1` is high, `x2` is also high. This can also be seen by the reduction in spread of points (or "collapse") in one direction making the data fill less than the full square of the plot. *So from this we can conclude that the data is not fully 2D.* The second step is to infer which variables contribute to this reduction in dimension. The axes for `x1` and `x2` are drawn extending from $(0, 0)$ and because they both extend out of the cloud of points, in the direction away from the collapse of points we can say that they are jointly responsible for the dimension reduction.

Figure 3.1 (b) shows a pair of variables that are **not** linearly associated. Variable `x1` is more varied than `x3` but knowing the value on `x1` tells us nothing about possible values on `x3`. Before running a tour all variables are typically scaled

[1] Note that the animated tours from this chapter can be viewed at https://dicook.github.io/mulgar_book/3-intro-dimred.html.

[2] It is generally better to use *associated* than *correlated*. Correlation is a statistical quantity, measuring linear association. The term *associated* can be prefaced with the type of association, such as *linear* or *non-linear*.

to have equal spread. The purpose of the tour is to capture association and relationships between the variables, so any univariate differences should be removed ahead of time. Figure 3.1 (c) shows what this would look like when `x3` is scaled - the points are fully spread in the full square of the plot.

```
library(tibble)
set.seed(6045)
x1 <- runif(123)
x2 <- x1 + rnorm(123, sd=0.1)
x3 <- rnorm(123, sd=0.2)
df <- tibble(x1 = (x1-mean(x1))/sd(x1),
             x2 = (x2-mean(x2))/sd(x2),
             x3,
             x3scaled = (x3-mean(x3))/sd(x3))
```

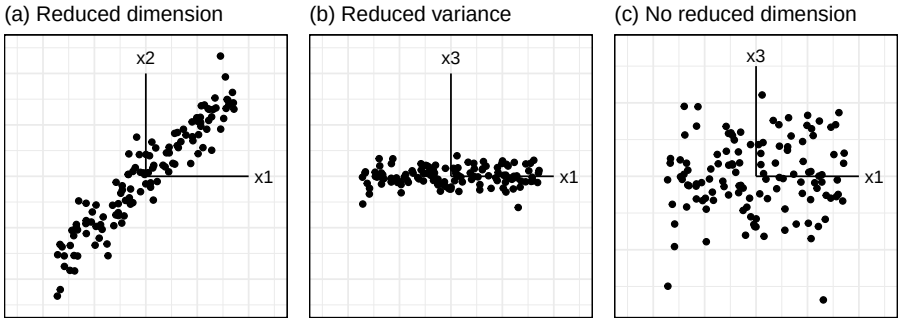
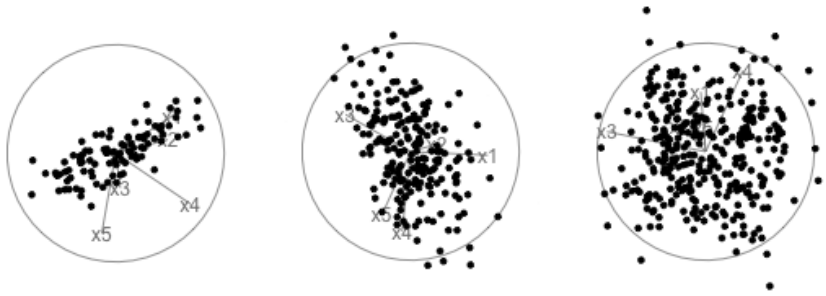


Figure 3.1: Explanation of how dimension reduction is perceived in 2D, relative to variables: (a) Two variables with strong linear association. Both variables contribute to the association, as indicated by their axes extending out from the 'collapsed' direction of the points; (b) Two variables with no linear association. But x3 has less variation, so points collapse in this direction; (c) The situation in plot (b) does not arise in a tour because all variables are (usually) scaled. When an axes extends out of a direction where the points are collapsed, it means that this variable is partially responsible for the reduced dimension.

Now let's think about what this looks like with five variables. Figure 3.2 shows a grand tour on five variables, with (a) data that is primarily 2D, (b) data that is primarily 3D and (c) fully 5D data. You can see that both (a) and (b) the spread of points collapse in some projections, with it happening more in (a). In (c) the data is always spread out in the square, although it does seem to concentrate or pile in the centre. This piling is typical when projecting from high dimensions to low dimensions. The sage tour (Laa et al., 2022) makes a correction for this.

The next step is to determine which variables contribute. In the examples just



(a) 2D plane in 5D (b) 3D plane in 5D (c) 5D plane in 5D

Figure 3.2: Single frames from different dimensional planes - 2D, 3D, 5D - displayed in a grand tour projecting into 2D. Notice that the 5D in 5D always fills out the box (although it does concentrate some in the middle which is typical when projecting from high to low dimensions). Also you can see that the 2D in 5D, concentrates into a line more than the 3D in 5D. This suggests that it is lower dimensional. (Animations can be viewed here.)

provided, all variables are linearly associated in the 2D and 3D data. You can check this by making a scatterplot matrix, Figure 3.3.

```
library(GGally)
library(mulgar)
data(plane)
ggscatmat(plane) +
  theme(panel.background =
          element_rect(colour="black", fill=NA),
    axis.text = element_blank(),
    axis.ticks = element_blank())
```

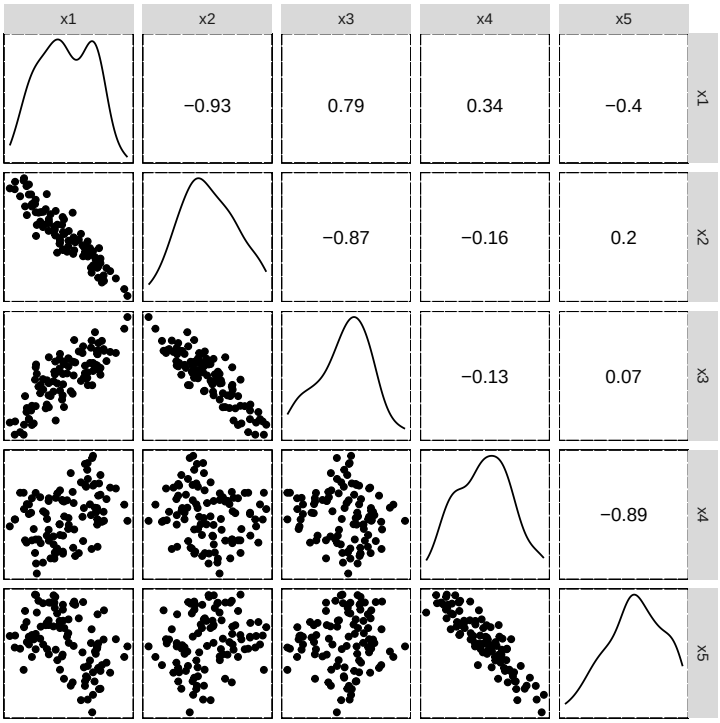


Figure 3.3: Scatterplot matrix of plane data. You can see that x1-x3 are strongly linearly associated, and also x4 and x5. When you watch the tour of this data, any time the data collapses into a line you should see only (x1, x2, x3) or (x4, x5). When combinations of x1 and x4 or x5 show, the data should be spread out.

To make an example where not all variables contribute, we have added two additional variables to the `plane` data set, which are purely noise.

```
# Add two pure noise dimensions to the plane
plane_noise <- plane
plane_noise$x6 <- rnorm(100)
plane_noise$x7 <- rnorm(100)
plane_noise <- data.frame(apply(plane_noise, 2,
    function(x) (x-mean(x))/sd(x)))
ggduo(plane_noise, columnsX = 1:5, columnsY = 6:7,
    types = list(continuous = "points")) +
  theme(aspect.ratio=1,
    panel.background =
          element_rect(colour="black", fill=NA),
```

```
    axis.text = element_blank(),
    axis.ticks = element_blank())
```

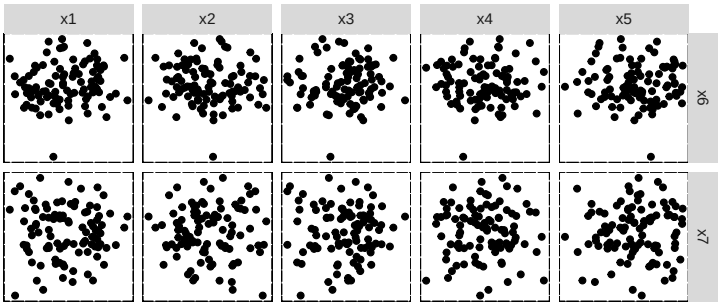


Figure 3.4: Scatterplots showing two additional noise variables that are not associated with any of the first five variables.

Now we have 2D structure in 7D, but only five of the variables contribute to the 2D structure, that is, five of the variables are linearly related with each other. The other two variables (x6, x7) are not linearly related to any of the others.

The data is viewed with a grand tour in Figure 3.5. We can still see the concentration of points along a line in some dimensions, which tells us that the data is not fully 7D. Then if you look closely at the variable axes you will see that the collapsing to a line only occurs when any of x1-x5 contribute strongly in the direction orthogonal to this. This does not happen when x6 or x7 contribute strongly to a projection - the data is always expanded to fill much of the space. That tells us that x6 and x7 don't substantially contribute to the dimension reduction, that is, they are not linearly related to the other variables.

To determine which variables are responsible for the reduced dimension look for the axes that extend out of the point cloud. These contribute to smaller variation in the observations, and thus indicate dimension reduction.

The simulated data here is very simple, and what we have learned from the tour could also be learned from principal component analysis. However, if there are small complications, such as outliers or nonlinear relationships, that might not be visible from principal component analysis, the tour can help you to see them.

Figure 3.6 and Figure 3.7(a) show example data with an outlier and Figure 3.7(b) shows data with non-linear relationships.

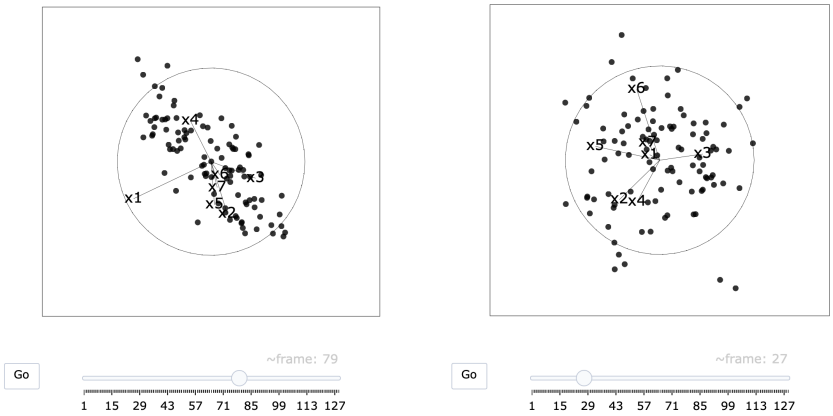


Figure 3.5: Two frames from a grand tour of the plane with two additional dimensions of pure noise. The collapsing of the points indicates that this is not fully 7D. This only happens when any of x1-x5 are contributing strongly (frame 49 x4, x5; frame 79 x1; frame 115 x2, x3). If x6 or x7 are contributing strongly the data is spread out fully (frames 27, 96). This tells us that x6 and x7 are not linearly associated, but other variables are.

```
# Add several outliers to the plane_noise data
plane_noise_outliers <- plane_noise
plane_noise_outliers[101,] <- c(2, 2, -2, 0, 0, 0, 0)
plane_noise_outliers[102,] <- c(0, 0, 0,-2, -2, 0, 0)

ggscatmat(plane_noise_outliers, columns = 1:5) +
  theme(aspect.ratio=1,
    panel.background =
          element_rect(colour="black", fill=NA),
    axis.text = element_blank(),
    axis.ticks = element_blank())
```

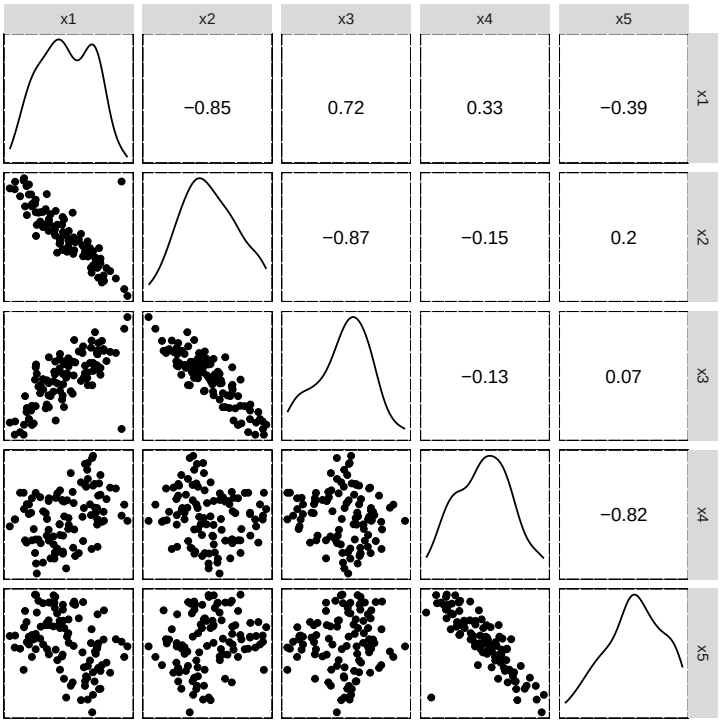
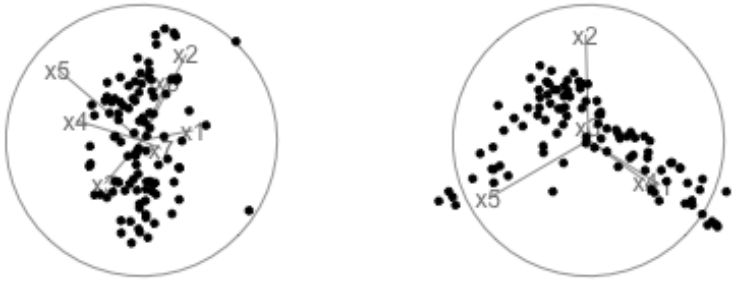


Figure 3.6: Scatterplot matrix of the plane with noise data, with two added outliers in variables with strong correlation.

Exercises

1. Multicollinearity is when the predictors for a model are strongly linearly associated. It can adversely affect the fitting of most models, because many possible models may be equally as good. Variable importance might be masked by correlated variables, and confidence intervals generated for linear models might be too wide. Check the for multicollinearity or other associations between the predictors in:
   a. 2001 Australian election data
   b. 2016 Australian election data
2. Examine 5D multivariate normal samples drawn from populations with a range of variance-covariance matrices. (You can use the `mvtnorm` package to do the sampling, for example.) Examine the data using a grand tour. What changes when you change the correlation



(a) Outliers (b) Non-linear relationship

Figure 3.7: Two frames from tours of examples of different types of dimensionality issues: outliers (a) and non-linearity (b). In (a) you can see two points far from the others in the projection. During a tour the two can be seen with different movement patterns – moving faster and in different directions than other points. Outliers will affect detection of reduced dimension, but they can be ignored when assessing dimensionality with the tour. In (b) there is a non-linear relationship between several variables, primarily with x3. Non-linear relationships may not be easily captured by other techniques but are often visible with the tour.

from close to zero to close to 1? Can you see a difference between strong positive correlation and strong negative correlation?

3. The following code shows how to hide a point in a four-dimensional space, so that it is not visible in any of the plots of two variables. Generate both `d` and `d_r` and confirm that the point is visible in a scatterplot matrix of `d`, but not in the scatterplot matrix of `d_r`. Also confirm that it is visible in both data sets when you use a tour.

```
library(tidyverse)
library(tourr)
library(GGally)
set.seed(946)
d <- tibble(x1=runif(200, -1, 1),
            x2=runif(200, -1, 1),
            x3=runif(200, -1, 1))
d <- d %>%
  mutate(x4 = x3 + runif(200, -0.1, 0.1))
# outlier is visible in d
d <- bind_rows(d, c(x1=0, x2=0, x3=-0.5, x4=0.5))

# Point is hiding in d_r
d_r <- d %>%
  mutate(x1 = cos(pi/6)*x1 + sin(pi/6)*x3,
         x3 = -sin(pi/6)*x1 + cos(pi/6)*x3,
         x2 = cos(pi/6)*x2 + sin(pi/6)*x4,
         x4 = -sin(pi/6)*x2 + cos(pi/6)*x4)
```

4

Principal component analysis

Reducing dimensionality using principal component analysis (PCA) dates back to Pearson (1901) and Hotelling (1933), and Jolliffe & Cadima (2016) provides a current overview. The goal is to find a smaller set of variables, $q(< p)$, that contain as much information as the original as possible. The new set of variables, known as principal components (PCs), are linear combinations of the original variables. The PCs can be used to represent the data in a lower-dimensional space.

The process is essentially an optimisation procedure, although PCA has an analytical solution. It solves the problem of

$$\max_{a_k} \text{Var}(Xa_k),$$

where X is the $n \times p$ data matrix, $a_k (k = 1, ..., p)$ is a 1D projection vector, called an eigenvector, and the $\text{Var}(Xa_k)$ is called an eigenvalue. So PCA is a sequential process, that will find the direction in the high-dimensional space (as given by the first eigenvector) where the data is most varied, and then find the second most varied direction, and so on. The eigenvectors define the combination of the original variables, and the eigenvalues define the amount of variance explained by the reduced number of variables.

PCA is very broadly useful for summarising linear association by using combinations of variables that are highly correlated. However, high correlation can also occur when there are outliers, or clustering. PCA is commonly used to detect these patterns also.

With visualisation we want to assess whether it is appropriate to use PCA to summarise any linear association by using combinations of variables that are highly correlated. It can help to detect other patterns that might affect the PCA results such as outliers, clustering or non-linear dependence.

PCA is not very effective when the distribution of the variables is highly skewed, so it can be helpful to transform variables to make them more symmetrically distributed before conducting PCA. It is also possible to summarise different

types of structure by generalising the optimisation criteria to any function of projected data, $f(XA)$, which is called *projection pursuit* (PP). PP has a long history (Kruskal (1964a), Friedman & Tukey (1974), Diaconis & Freedman (1984b), Jones & Sibson (1987), Huber (1985)), and there are regularly new developments (e.g. E.-K. Lee & Cook (2009), Perisic & Posse (2005), Y. D. Lee et al. (2013), Loperfido (2018), Bickel et al. (2018), C. Zhang et al. (2023)).

4.1 Determining how many dimensions

We would start by examining the data using a grand tour. The goal is to check whether there might be potential issues for PCA, such as skewness, outliers or clustering, or even non-linear dependencies.

We'll start be showing PCA on the simulated data from Chapter 3. The scree plots show that PCA supports that the data are 2D, 3D and 5D respectively.

```
# Conduct PCA and make the scree plot for
# the 2-, 3- and 5-D planar data
library(dplyr)
library(ggplot2)
library(mulgar)
data(plane)
data(box)
library(geozoo)
cube5d <- data.frame(cube.solid.random(p=5, n=300)$points)
colnames(cube5d) <- paste0("x", 1:5)
cube5d <- data.frame(apply(cube5d, 2,
                           function(x) (x-mean(x))/sd(x)))
p_pca <- prcomp(plane)
b_pca <- prcomp(box)
c_pca <- prcomp(cube5d)
p_scree <- ggscree(p_pca, q = 5) + theme_minimal()

b_scree <- ggscree(b_pca, q = 5) + theme_minimal()
c_scree <- ggscree(c_pca, q = 5) + theme_minimal()
```

The next step is to look at the coefficients for the selected number of PCs. Table 4.1 shows the coefficients for the first two PCs of the `plane` data. All five variables contribute, with `x1`, `x2`, `x3` contributing more to `PC1`, and `x4`, `x5` contributing more to `PC2`. Table 4.2 shows the coefficients for the first three PCs. Variables `x1`, `x2`, `x3` contribute strongly to `PC1`, `PC2` has contributions

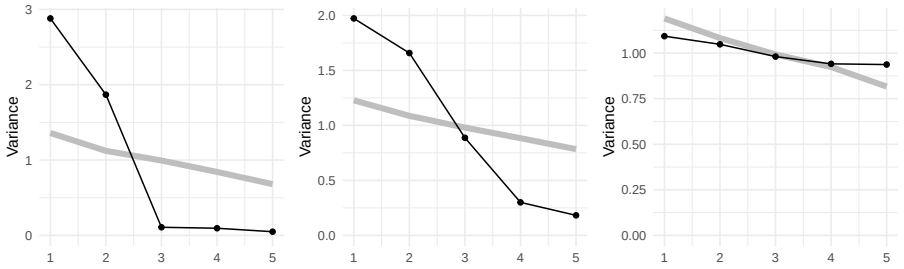


Figure 4.1: Scree plots for the three simulated data sets shown in Figure 3.2. The 2D in 5D is clearly recognised by PCA to be 2D because the variance drops substantially between 2-3 principal components. The 3D in 5D is possibly 3D because the variance drops from 3-4 principal components. The fully 5D data has no drop in variance, and all values are close to the typical value one would observe if the data was fully 5D.

from all variables except `x3` and variables `x4` and `x5` contribute strongly to `PC3`.

Table 4.1: Coefficients for the first two PCs for the plane data.

Variable	PC1	PC2
x1	0.58	−0.06
x2	−0.55	0.21
x3	0.47	−0.41
x4	0.25	0.64
x5	−0.29	−0.62

Table 4.2: Coefficients for the first three PCs for the box data.

Variable	PC1	PC2	PC3
x1	−0.51	0.46	0.11
x2	0.51	0.46	0.00
x3	−0.65	−0.09	0.23
x4	−0.22	0.36	−0.87
x5	0.02	0.66	0.43

In each of these simulated data sets, all five variables contributed to the dimension reduction. If we added two purely noise variables to the plane data, as done in Chapter 3, the scree plot would indicate that the data is now 4D, and we would get a different interpretation of the coefficients from the PCA. We see that `PC1` and `PC2` are approximately the same as before, with main

variables being (`x1`, `x2`, `x3`) and (`x4`, `x5`) respectively. `PC3` and `PC4` are both `x6` and `x7`.

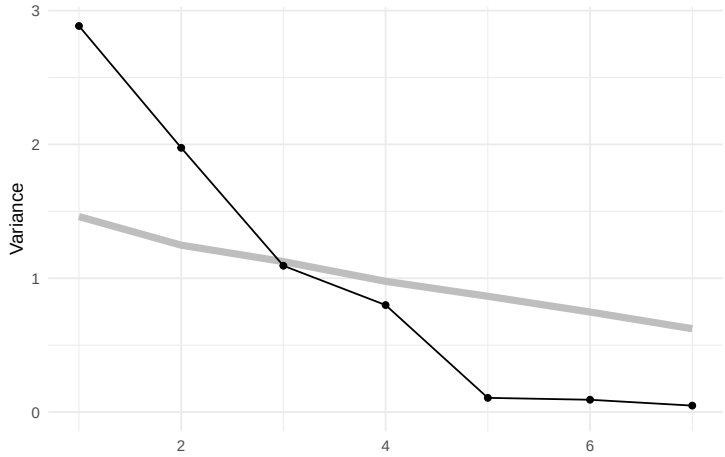


Figure 4.2: Additional noise variables expands the data to 4D.

Table 4.3: Coefficients for the first four PCs for the box data.

Variable	PC1	PC2	PC3	PC4
x1	0.58	0.04	0.01	0.00
x2	−0.55	−0.18	−0.03	0.07
x3	0.47	0.37	0.05	−0.20
x4	0.24	−0.62	−0.06	0.17
x5	−0.28	0.60	0.07	−0.14
x6	0.05	0.29	−0.58	0.76
x7	−0.02	−0.08	−0.81	−0.58

4.1.1 Example: pisa

The `pisa` data contains simulated data from math, reading and science scores, totalling 30 variables. PCA is used here to examine the association. We might expect that it is 3D, but what we see suggests it is primarily 1D. This means that a student that scores well in math, will also score well in reading and science.

```
data(pisa)
pisa_std <- pisa %>%
  filter(CNT == "Australia") %>%
  select(-CNT) %>%
```

```
  mutate_all(mulgar:::scale2)
pisa_pca <- prcomp(pisa_std)
pisa_scree <- ggscree(pisa_pca, q = 15) + theme_minimal()
```

The scree plot in Figure 4.3 shows a big drop from one to two PCs in the amount of variance explained. A grand tour on the 30 variables can be run using `animate_xy()`:

```
animate_xy(pisa_std, half_range=1)
```

or rendered as an animated gif using `render_gif()`:

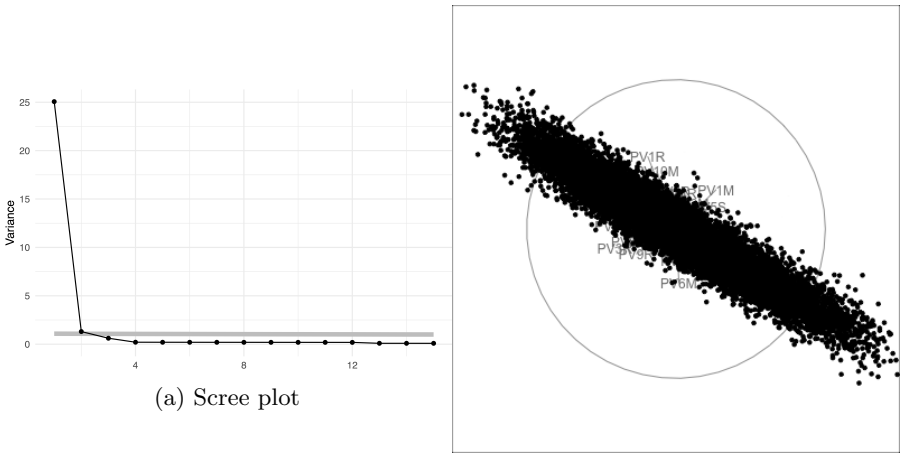
```
render_gif(pisa_std,
           grand_tour(),
           display_xy(half_range=0.9),
           gif_file="gifs/pisa_gt.gif",
           frames=500,
           width=400,
           height=400,
           loop=FALSE)
```

and we can see that the data is elliptical in most projections, sometimes shrinking to be a small circle. This pattern strongly indicates that there is one primary direction of variation in the data, with only small variation in any direction away from it. Shrinking to the small circle is analogous to to how *a pencil or cigar or water bottle in 3D looks from some angles.*

The coefficients of the first PC (first eigenvector) are roughly equal in magnitude (as shown below), which tells us that all variables roughly contribute. Interestingly, they are all negative, which is not actually meaningful. With different software these could easily have been all positive. The sign of the coefficients can be reversed, as long as all are reversed, which is the same as an arrow pointing one way, changing and pointing the other way.

```
round(pisa_pca$rotation[,1], 2)
```

```
 PV1MATH  PV2MATH  PV3MATH  PV4MATH  PV5MATH  PV6MATH
   -0.18    -0.18    -0.18    -0.18    -0.18    -0.18
 PV7MATH  PV8MATH  PV9MATH PV10MATH  PV1READ  PV2READ
   -0.18    -0.18    -0.18    -0.18    -0.19    -0.18
 PV3READ  PV4READ  PV5READ  PV6READ  PV7READ  PV8READ
   -0.19    -0.19    -0.19    -0.19    -0.19    -0.19
 PV9READ PV10READ  PV1SCIE  PV2SCIE  PV3SCIE  PV4SCIE
```



(a) Scree plot

(b) Grand tour frame

Figure 4.3: Scree plot and a frame from a tour of the `pisa` data, with 30 variables being the plausible scores for Australian students. In combination, these suggest that the data is effectively 1D.

```
  -0.19    -0.19    -0.18    -0.18    -0.19    -0.18
PV5SCIE  PV6SCIE  PV7SCIE  PV8SCIE  PV9SCIE PV10SCIE
  -0.19    -0.18    -0.19    -0.18    -0.19    -0.18
```

The tour verifies that the ‘pisa‘ data is primarily 1D, indicating that a student who scores well in math, probably scores well in reading and science, too. More interestingly, the regular shape of the data strongly indicates that it is "synthetic", simulated rather than observed.

4.1.2 Example: aflw

This data has player statistics for all the matches in the 2021 season. We would be interested to know which variables contain similar information, and thus might be combined into single variables. We would expect that many statistics to group into a few small sets, such as offensive and defensive skills. We might also expect that some of the statistics are skewed, most players have low values and just a handful of players are stellar. It is also possible that there are some extreme values. These are interesting features, but they will distract from the main purpose of grouping the statistics. Thus the tour is used to check for potential problems with the data prior to conducting PCA.

```
library(tourr)
data(aflw)
aflw_std <- aflw %>%
  mutate_if(is.numeric, function(x) (x-
      mean(x, na.rm=TRUE))/
      sd(x, na.rm=TRUE))
```

To look at all of the 29 player statistics in a grand tour in Figure 4.4.

```
animate_xy(aflw_std[,7:35], half_range=0.9)
render_gif(aflw_std[,7:35],
           grand_tour(),
           display_xy(half_range=0.9),
           gif_file="gifs/aflw_gt.gif",
           frames=500,
           loop=FALSE)
```

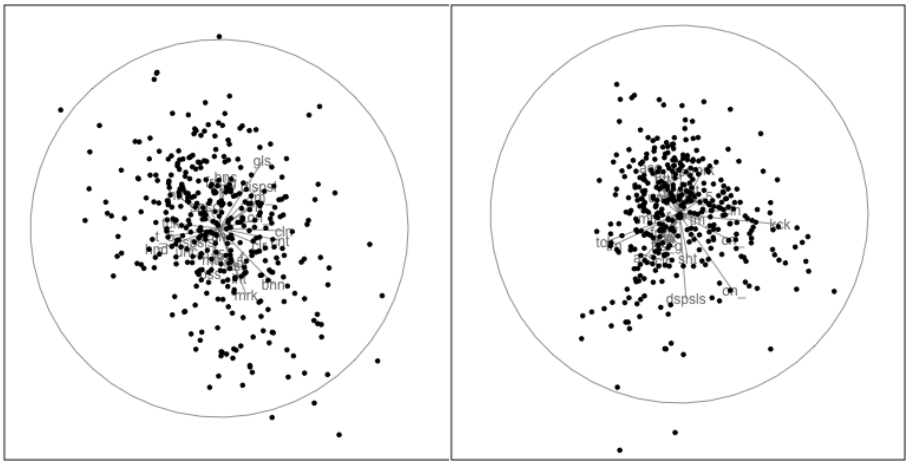


Figure 4.4: Two frames from a grand tour of the AFLW player statistics. Most player statistics concentrate near the centre, indicating most players are "average"! There are a few outliers appearing in different combinations of the skills, which one would expect to be the star players for particular skill sets.

No major surprises! There is a small amount of skewness, and there are no major outliers. Skewness indicates that most players have reasonably similar skills (bunching of points), except for some key players (the moderate outliers). The skewness could be reduced by applying a log or square root transformation to some variables prior to running the PCA. However, we elect not to do this because the moderate outliers are of interest. These correspond to talented players that we'd like to explore further with the analysis.

Below we have the conventional summary of the PCA, a scree plot showing the reduction in variance to be explained when each additional PC is considered. It is also conventional to look at a table summarising the proportions of variance explained by PCs, but with almost 30 variables it is easier to make some decision on the number of PCs needed based on the scree plot.

```
aflw_pca <- prcomp(aflw_std[,7:35],
                   scale = FALSE,
                   retx=TRUE)

ggscree(aflw_pca, q = 29) + theme_minimal()
```

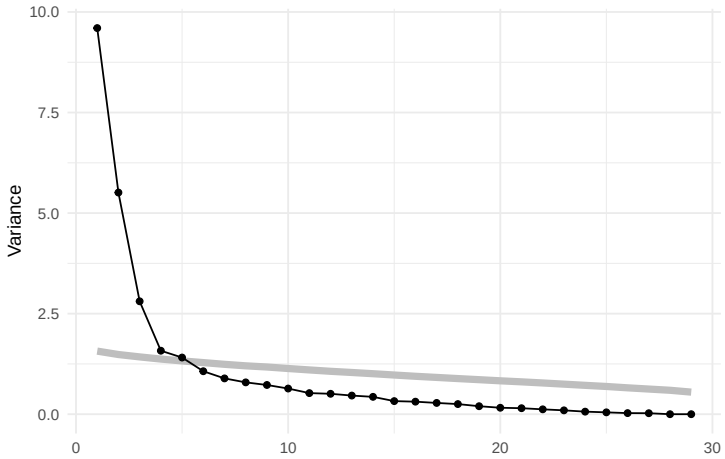


Figure 4.5: Scree plot showing decay in variance of PCs.

From the scree plot in Figure 4.5, we see a sharp drop from one to two, two to three and then smaller drops. After four PCs the variance drops again at six PCs and then gradually decays. We will choose four PCs to examine more closely. This explains 67.2% of the variance.

Table 4.4: Coefficients for the first four PCs.

Variable	PC1	PC2	PC3	PC4
disposals	0.31	−0.05	−0.03	0.07
possessions	0.31	−0.03	−0.07	0.09
kicks	0.29	−0.04	0.09	−0.12
metres	0.28	−0.03	0.10	−0.15
contested	0.28	0.01	−0.12	0.23
uncontested	0.28	−0.06	−0.01	−0.05

turnovers	0.27	−0.01	−0.01	−0.29
clearances	0.23	0.00	−0.29	0.19
clangers	0.23	−0.02	−0.06	−0.33
handballs	0.23	−0.04	−0.19	0.31
frees_for	0.21	0.02	−0.13	0.18
marks	0.21	0.03	0.32	0.02
tackles	0.20	0.01	−0.28	0.09
time_pct	0.16	−0.04	0.35	−0.02
intercepts	0.13	−0.28	0.24	0.03
rebounds_in50	0.13	−0.28	0.24	−0.06
frees_against	0.13	0.03	−0.16	−0.23
assists	0.09	0.23	0.00	0.05
bounces	0.09	0.03	0.02	−0.28
behinds	0.09	0.32	0.08	−0.02
shots	0.08	0.38	0.12	−0.03
tackles_in50	0.07	0.27	−0.18	0.03
marks_in50	0.06	0.34	0.18	0.04
contested_marks	0.05	0.16	0.34	0.15
goals	0.04	0.37	0.16	0.03
accuracy	0.04	0.34	0.10	0.06
one_pct	0.03	−0.21	0.33	0.08
disposal	0.02	−0.13	0.20	0.50
hitouts	−0.04	0.00	−0.03	0.32

When there are as many variables as this, it can be hard to digest the combinations of variables most contributing to each PC. Rearranging the table by sorting on a selected PC can help. Table 4.4 has been sorted according to the PC 1 coefficients.

PC 1 is primarily composed of `disposals`, `possessions`, `kicks`, `metres`, `uncontested`, `contested`, ... Actually almost all variables positively contribute, albeit in different amounts! It is quite common in PCA for the first PC to be a combination of all variables, although it might commonly be a closer to equal contribution, and it tells us that there is one main direction of variation in the data. For PC 1 in the `aflw` data, PCA is telling us that the primary variation is through a combination of skills, and this maps to basic football playing skills, where some skills (e.g. disposals, possessions, kicks, ...) are more important.

Thus the second PC might be the more interesting. PC 2 is primarily a combination of `shots`, `goals`, `marks_in50`, `accuracy`, and `behinds` contrasted against `rebounds_in50` and `intercepts`. The negative coefficients are primary offensive skills and the positive coefficients are defensive skills. This PC is reasonable measure of the offensive vs defensive skills of a player.

We would continue to interpret each PC by examining large coefficients to

help decide how many PCs are a suitable summary of the information in the data. Briefly, PC 3 is a measure of worth of the player because `time_pct` has a large coefficient, so players that are on the field longer will contribute strongly to this new variable. It also has large (and opposite) contributions from `clearances`, `tackles`, `contested_marks`. PC 4 appears to be related to aggressive play with `clangers`, `turnovers`, `bounces` and `frees_against` featuring. So all four PCs have useful information. (Note, if we had continued to examine large coefficients on PC 5 we would find that all variables already have had reasonably large coefficients on PC 1-4, which supports restricting attention to the first four.)

Ideally, when we tour the four PCs, we'd like to be able to stop and identify players. This involves creating a pre-computed animation, with additional mouse-over, made possible by `plotly`. This is only feasible with a small number of observations, like the `aflw` data, because all of the animation frames are constructed in a single object. This object gets large very quickly!

The code to make this animation, and the interactive plot is in the online version of the book.

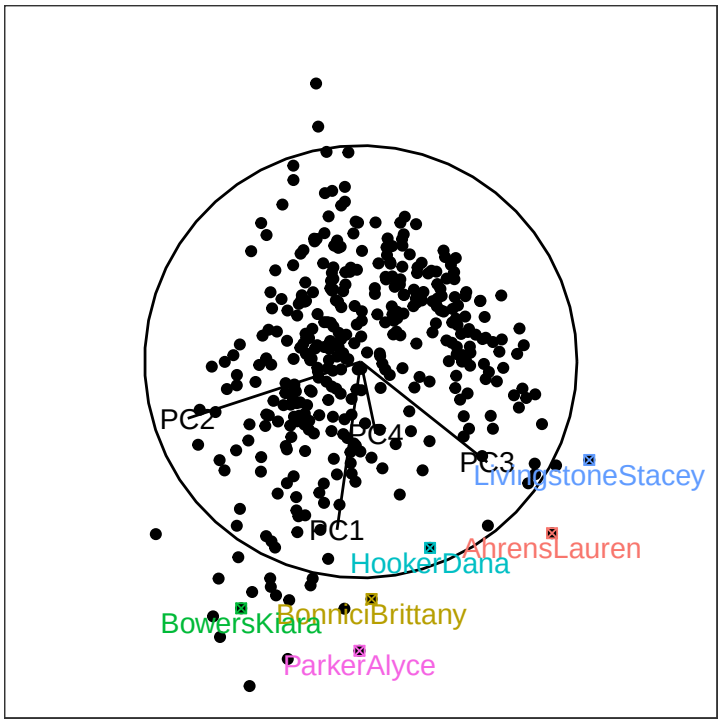


Figure 4.6: Frame 18 re-plotted so that players can be identified, ideally using on mouse-over. Here some points are labelled.

For any particular frame, like 18 re-plotted in Figure 4.6, we can investigate further. Here there is a branching pattern, where the branch points in the direction of PC 1. Mouse-over the players at the tip of this branch and we find players like Alyce Parker, Brittany Bonnici, Dana Hooker, Kiara Bowers. If you look up the bios of these players you'll find they all have generally good player descriptions like "elite disposals", "powerful left foot", "hard-running midfielder", "best and fairest".

In the direction of PC 2, you'll find players like Lauren Ahrens, Stacey Livingstone who are star defenders. Players in this end of PC 1, have high scores on `intercepts` and `rebounds_in50`.

Another interesting frame for inspecting PC 2 is 59. PC 2 at one end has players with high goal scoring skills, and the other good defending skills. So mousing over the other end of PC 2 finds players like Gemma Houghton and Katie Brennan who are known for their goal scoring. The branch pattern is an interesting one, because it tells us there is some combination of skills that are lacking among all players, primarily this appears to be there some distinction between defenders skills and general playing skills. It's not as simple as this because the branching is only visible when PC 1 and PC 2 are examined with PC 3.

PCA is useful for getting a sense of the variation in a high-dimensional data set. Interpreting the principal components is often useful, but it can be discombobulating. For the `aflw` data it would be good to think about it as a guide to the main directions of variation and to follow with a more direct engineering of variables into interesting player characteristics. For example, calculate offensive skill as an equal combination of goals, accuracy, shots, behinds. A set of new variables specifically computed to measure particular skills would make explaining an analysis easier.

The tour verifies that PCA on the 'aflw' data is complicated and doesn't capture all of the variation. However, it does provide useful insights. It detected outstanding players, and indicated the different skills sets of top goal scorers and top defensive players.

4.2 Examining the PCA model in the data space

When you choose a smaller number of PCs (k) than the number of original variables, this is essentially producing a model for the data. The model is the lower dimensional k-D space. It is analogous to a linear regression model, except that the residuals from the model are $(p-k)$-D.

It is common to show the model, that is the data projected into the k-D model space. When $k = 2$ this is called a "biplot". For the `plane` and `plane_noise` data the biplots are shown in Figure 4.7. This is useful for checking which variables contribute most to the new principal component variables, and also to check for any problems that might have affected the fit, such as outliers, clusters or non-linearity. Interestingly, biplots are typically only made in 2D, even if the data should be summarised by more than two PCs. Occasionally you will see the biplot made for PC j vs PC k also. With the `pca_tour()` function in the `tourr` package you can view a k-D biplot. This will display the k PCs with the axes displaying the original variables, and thus see their contribution to the PCs.

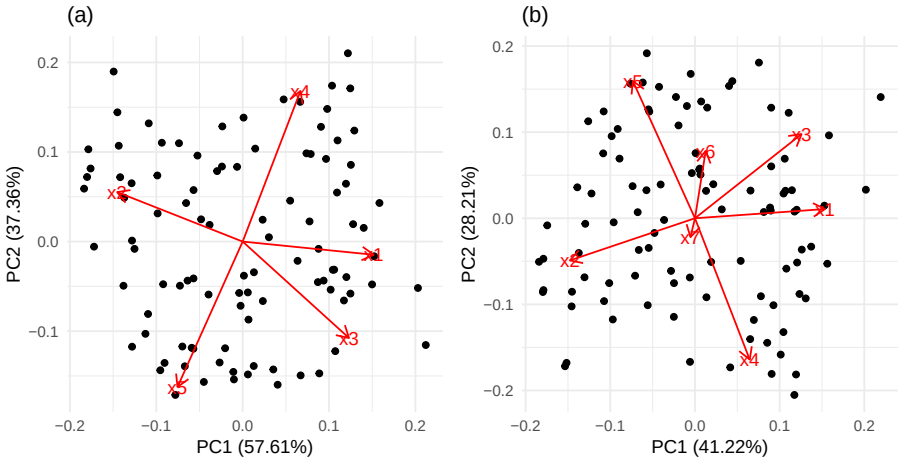
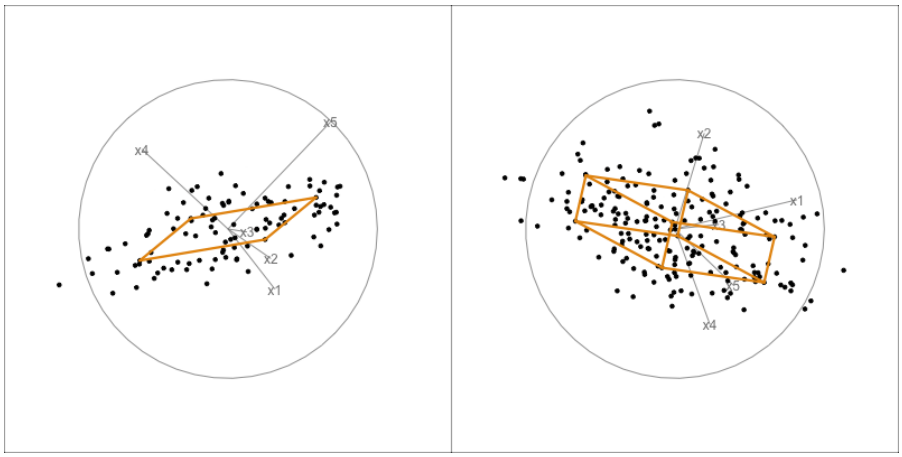


Figure 4.7: Biplots of the plane (a) and plane + noise (b) data. All five variables contribute strongly to the two principal components in (a): PC1 is primarily `x1`, `x2` and `x3` and PC2 is primarily `x4` and `x5`. In (b) the same four variables contribute in almost the same way, with variables `x6` and `x7` contributing very little. The data was constructed this way, that these two dimensions were purely noise.

It can be useful to examine this model using the tour. The model is simply a plane in high dimensions. This would be considered to be the model in the data space. The reason to do this is to check how well the model fits the data. The plane corresponding to the model should be oriented along the main direction of the points, and the spread of points around the plane should be small. We should also be able to see if there has been any strong non-linear relationship missed by the model, or outliers and clusters.

The function `pca_model()` from the `mulgar` package can be used to represent the model as a k-D wire-frame plane. Figure 4.8 shows the models for the `plane` and `box` data, 2D and 3D respectively.

We look at the model in the data space to check how well the model fits the data. If it fits well, the points will cluster tightly around the model representation, with little spread in other directions.



(a) Model for the 2D in 5D data. (b) Model for the 3D in 5D data.

Figure 4.8: PCA model overlaid on the data for the 2D in 5D, and 3D in 5D simulated data.

4.2.1 Example: pisa

The model for the `pisa` data is a 1D vector, shown in Figure 4.9.

4.2.2 Example: aflw

It is less useful to examine the PCA model for the `aflw` data, because the main patterns that were of interest were the exceptional players. However, we will do it anyway! Figure 4.10 shows the 4D PCA model overlain on the data. Even though the distribution of points is not as symmetric and balanced as the other examples, we can see that the cube structure mirrors the variation. We can see that the relationships between variables are not strictly linear, because the spread extends unevenly away from the box.

Figure 4.9: PCA model of the `pisa` data. The 1D model captures the primary variation in the data and there is a small amount of spread in all directions away from the model.

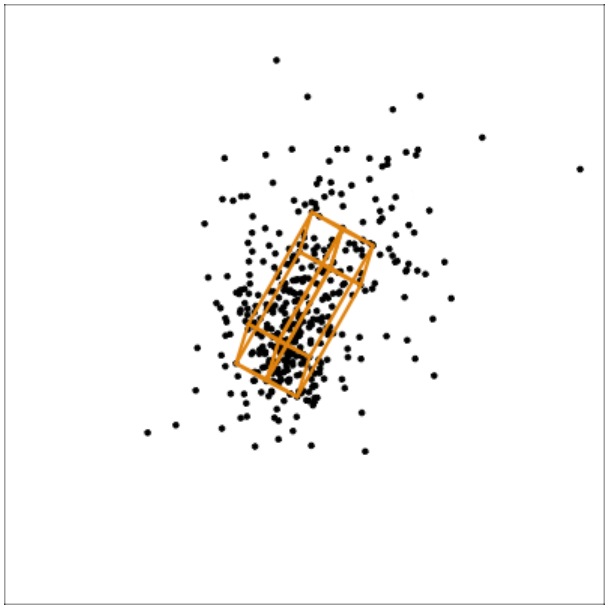


Figure 4.10: PCA model of the `aflw` data. The linear model is not ideal for this data, which has other patterns like outliers, and some branching. However, the model roughly captures the linear associations, and leaves unexplained variation in different directions.

From the tour we see that the 4D model leaves substantial variation unexplained. It is also not symmetric, and there is some larger variation away from the model in some combinations of variables than others.

4.3 When relationships are not linear

4.3.1 Example: outliers

Figure 4.11 shows the scree plot for the planar data with noise and outliers. It is very similar to the scree plot on the data without the outliers (Figure 4.2). However, what we see from Figure 4.12 is that PCA loses the outliers. The animation in (a) shows the full data, and the outliers marked by colour and labels 1, 2, are clearly unusual in some projections. When we examine the tour of the first four PCs (as suggested by the scree plot) the outliers are not unusual. They are almost contained in the point cloud. The reason is clear when all the PCs are plotted, and the outliers can be seen to be clearly detected only in PC5, PC6 and PC7.

```
plane_n_o_pca <- prcomp(plane_noise_outliers)
ggscree(plane_n_o_pca, q = 7) + theme_minimal()
```

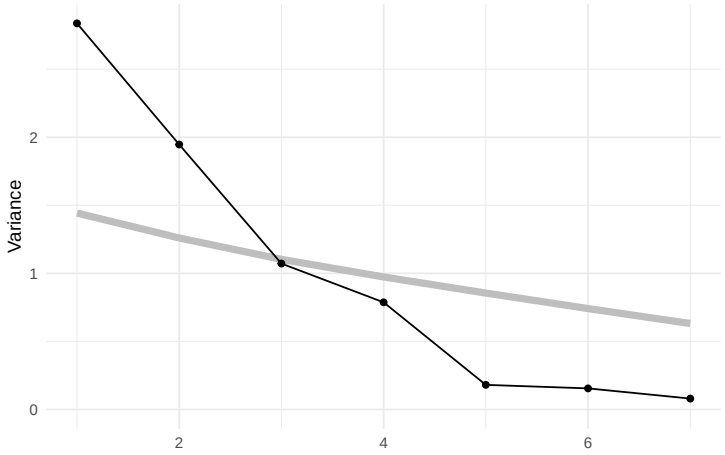
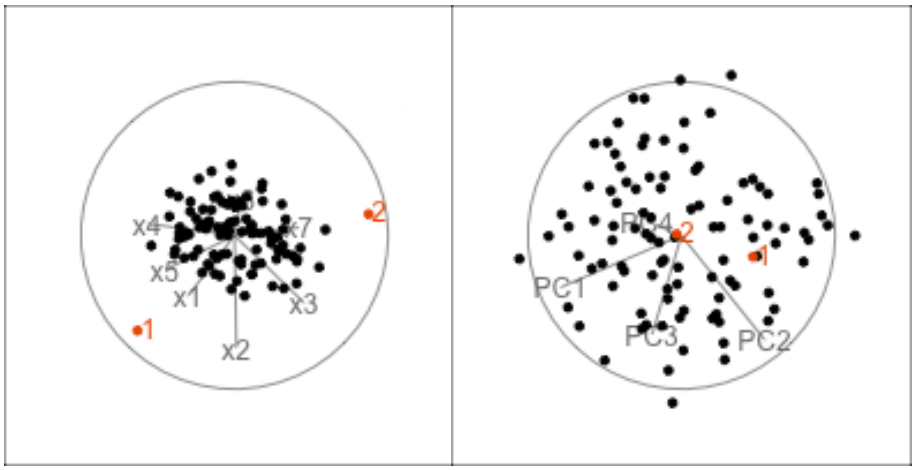


Figure 4.11: Scree plot of the planar data with noise and an outlier. It is almost the same as the data without the outliers.



(a) Outliers clearly visible (b) Outliers not clearly visible in PC1-4

Figure 4.12: Examining the handling of outliers in the PCA of the planar data with noise variables and two outliers. PCA has lost these two extreme values.

4.3.2 Example: Non-linear associations

Figure 4.15 shows the tour of the full 5D data containing non-linear relationships in comparison with a tour of the first three PCs, as recommended by the scree plot (Figure 4.14). The PCs capture some clear and very clean non-linear relationship, but it looks like it has missed some of the complexities of the relationships. The scatterplot matrix of all 5 PCs (Figure 4.16) shows that PC4 and PC5 contain interesting features: more non-linearity, and curiously an outlier.

One of the dangers of PCA is that interesting and curious details of the data only emerge in the lowest PCs, that are usually discarded. The tour, and examining the smaller PCs, can help to discover them.

Exercises

1. Make a scatterplot matrix of the first four PCs of the `aflw` data. Is the branch pattern visible in any pair?
2. Construct five new variables to measure these skills offense, defense,

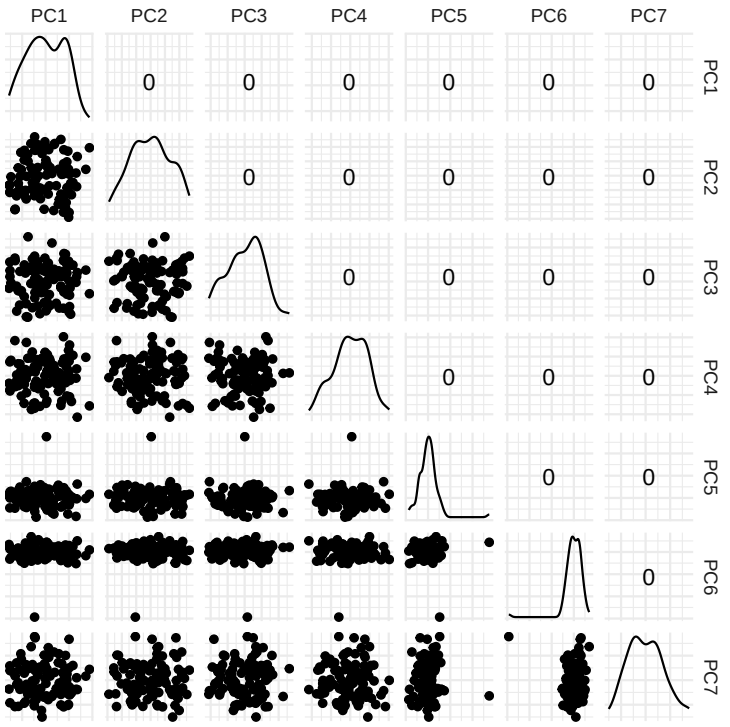


Figure 4.13: From the scatterplot matrix we can see that the outliers are present in PC5, PC6 and PC7. That means by reducing the dimensionality to the first four PCs the model has missed some important characteristics in the data.

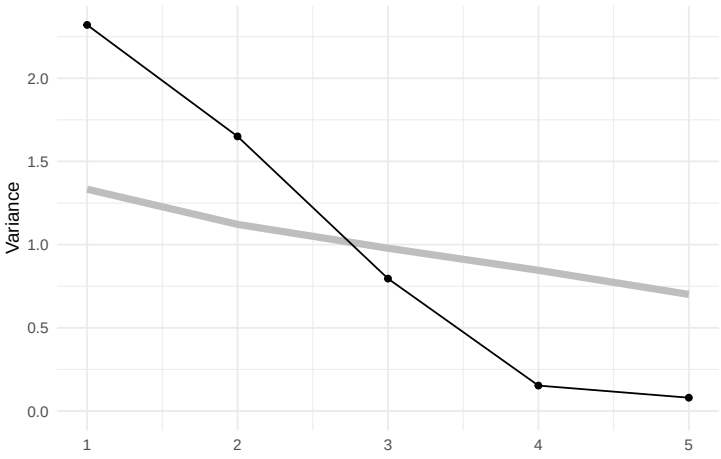
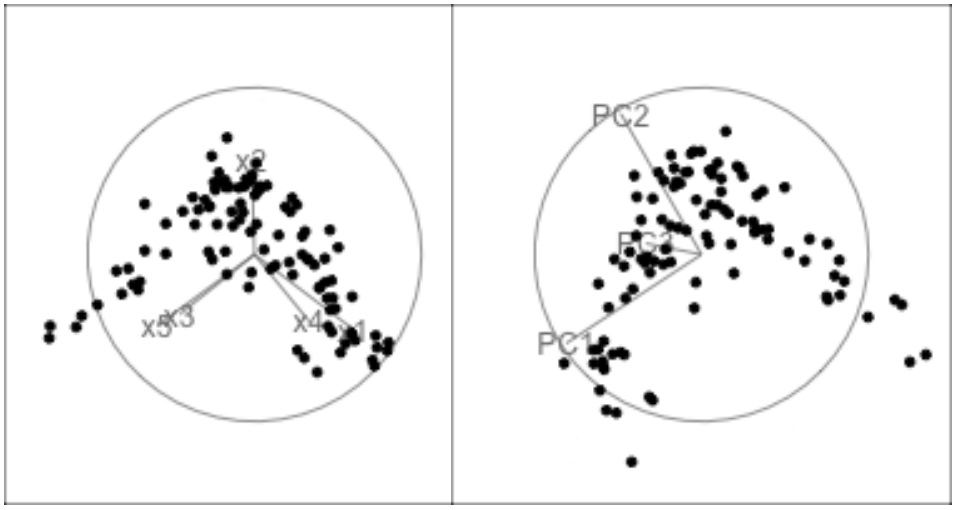


Figure 4.14: Scree plot of the non-linear data suggests three PCs.



(a) All five variables (b) First three PCs

Figure 4.15: Comparison of the full data and first three principal components. Non-linear relationships between several variables can be seen in a tour on all five variables. The first three principal components reveal a strong non-linear relationship. Some of the non-linearity is clearly visible in the reduced dimension space, but the full data has more complexities.

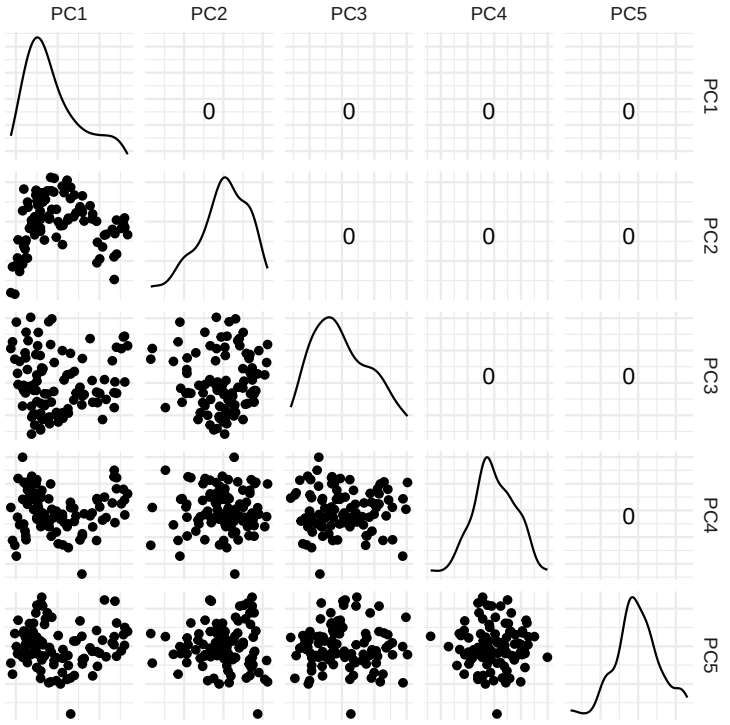


Figure 4.16: From the scatterplot matrix we can see that the there is a non-linear relationship visible in PC1 and PC2, with perhaps a small contribution from PC3. However, we can see that when the data is reduced to three PCs, it misses catching all on the non-linear relationships and also interestingly it seems that there is an unusual observation also.

playing time, ball movement, errors. Using the tour, examine the relationship between these variables. Map out how a few players could be characterised based on these directions of skills.

3. Symmetrise any `aflw` variables that have skewed distributions using a log or square root transformation. Then re-do the PCA. What do we learn that is different about associations between the skill variables?
4. Examine the `bushfires` data using a grand tour on the numeric variables, ignoring the `cause` (class) variable. Note any issues such as outliers, or skewness that might affect PCA. How many principal components would be recommended by the scree plot? Examine this PCA model with the data, and explain how well it does or doesn't fit.
5. Use the `pca_tour` to examine the first five PCs of the `bushfires` data. How do all of the variables contribute to this reduced space?
6. Reduce the dimension of the `sketches` data to 12 PCs. How much variation does this explain? Is there any obvious clustering in this lower dimensional space?

Project

Linear dimension reduction can optimise for other criteria, and here we will explore one example: the algorithm implemented in the `dobin` package finds a basis in which the first few directions are optimized for the detection of outliers in the data. We will examine how it performs for the `plane_noise_outliers` data (the example where outliers were hidden in the first four principal components.)

1. Start by looking up the documentation of `dobin::dobin`. How many parameters does the method depend on?
2. We first apply the function to the `plane_noise_outliers` data using default values for all parameters.
3. Recall that the outliers were added in rows 101 and 102 of the data. Make a scatter plots showing the projection onto the first, second and third component, using color to highlight the outliers. Are they visible as outliers with three components?
4. Adjust the `frac` parameter of the `dobin` function to `frac = 0.99` and repeat the graphical evaluation from point 3. How does it compare to the previous solution?

5

Non-linear dimension reduction

5.1 Explanation of NLDR methods

Non-linear dimension reduction (NLDR) aims to find a low-dimensional representation of the high-dimensional data that shows the main features of the data. In statistics, it dates back to Kruskal (1964a)'s work on multidimensional scaling (MDS). Some techniques only require an interpoint similarity or distance matrix as the main ingredient, rather than the full data. We'll focus on when the full data is available here, so we can also compare structure perceived using the tour on the high-dimensional space, relative to structure revealed in the low-dimensional embedding.

There are many methods available for generating non-linear low dimensional representations of the data. MDS is a classical technique that minimises the difference between two interpoint distance matrices, the distance between points in the high-dimensions, and in the low-dimensional representations. A good resource for learning about MDS is Borg & Groenen (2005).

```
library(mulgar)
library(Rtsne)
library(uwot)
library(ggplot2)
library(patchwork)
set.seed(42)
cnl_tsne <- Rtsne(clusters_nonlin)
cnl_umap <- umap(clusters_nonlin)
n1 <- ggplot(as.data.frame(cnl_tsne$Y), aes(x=V1, y=V2)) +
  geom_point() +
  ggtitle("(a) t-SNE") +
  theme_minimal() +
  theme(aspect.ratio=1)
n2 <- ggplot(as.data.frame(cnl_umap), aes(x=V1, y=V2)) +
  geom_point() +
  ggtitle("(b) UMAP") +
  theme_minimal() +
```

```
  theme(aspect.ratio=1)
n1 + n2
```

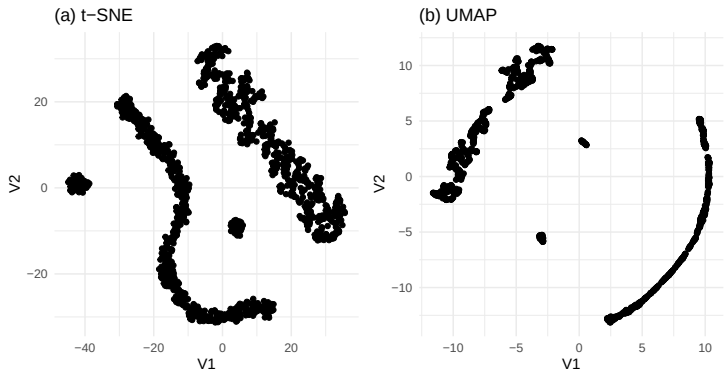


Figure 5.1: Two non-linear embeddings of the non-linear clusters data: (a) t-SNE, (b) UMAP. Both suggest four clusters, with two being non-linear in some form.

Figure 5.1 show two NLDR views of the `clusters_nonlin` data set from the `mulgar` package. Both suggest that there are four clusters, and that some clusters are non-linearly shaped. They disagree on the type of non-linear pattern, where t-SNE represents one cluster as a wavy-shape and UMAP both have a simple parabolic shape. Popular methods in current use include t-SNE (Maaten & Hinton, 2008), UMAP (McInnes et al., 2018) and PHATE (Moon et al., 2019).

```
library(tourr)
render_gif(clusters_nonlin,
           grand_tour(),
           display_xy(),
           gif_file = "gifs/clusters_nonlin.gif",
           frames = 500,
           width = 300,
           height = 300)
```

The full 4D data is shown with a grand tour in Figure 5.2 @. The four clusters suggested by the NLDR methods can be seen. We also get a better sense of the relative size and proximity of the clusters. There are two small spherical clusters, one quite close to the end of the large sine wave cluster. The fourth cluster is relatively small, and has a slight curve, like a bent rod. The t-SNE representation is slightly more accurate than the UMAP representation. We would expect that the wavy cluster is the sine wave seen in the tour.

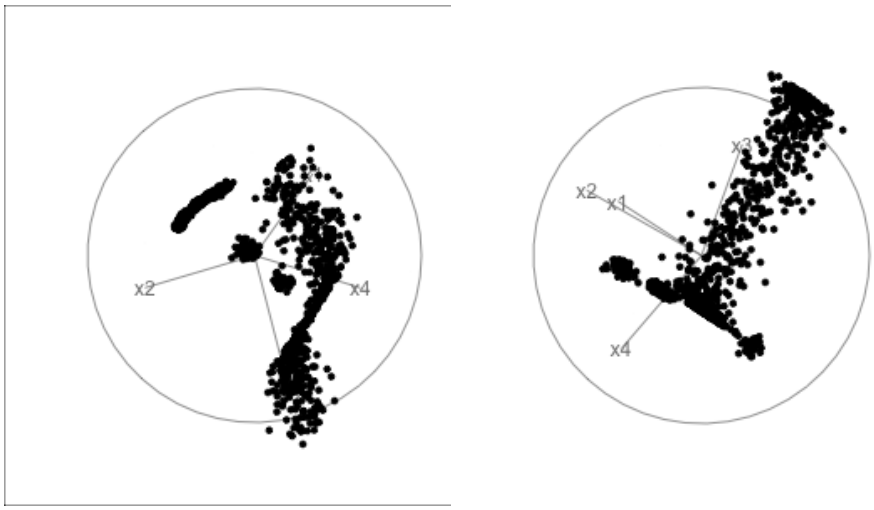


Figure 5.2: Two frames from a grand tour of the nonlinear clusters data set, shows four clusters. Two are very small and spherical in shape. One is large, and has a sine wave shape, and the other is fairly small with a bent rod shape.

NLDR can provide useful low-dimensional summaries of high-dimensional structure but you need to check whether it is a sensible and accurate representation by comparing with what is perceived from a tour.

5.2 Assessing reliability of the NLDR representation

NLDR can produce useful low-dimensional summaries of structure in high-dimensional data, like those shown in Figure 5.1. However, there are numerous pitfalls. The fitting procedure can produce very different representations depending on the parameter choices, and even the random number seeding the fit. (You can check this by changing the `set.seed` in the code above, and by changing from the default parameters.) Also, it may not be possible to represent the high-dimensional structures faithfully low dimensions. For these reasons, one needs to connect the NLDR view with a tour of the data, to help assess its usefulness and accuracy. For example, with this data, we would want to know which of the two curved clusters in the UMAP representation correspond to the sine wave cluster.

5.2.1 Using `liminal`

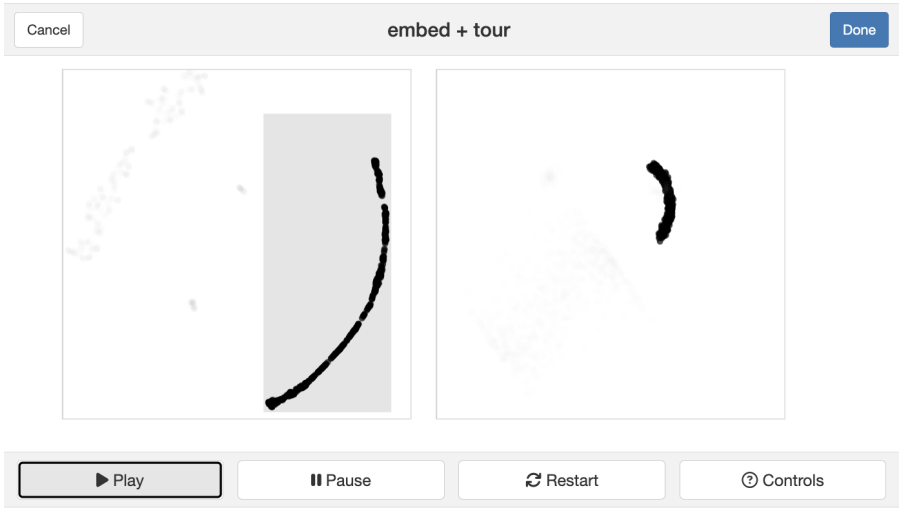
Figure 5.3 shows how the NLDR plot can be linked to a tour view, using the `liminal` package, to better understand how well the structure of the data is represented. Here we see learn that the smile in the UMAP embedding is the small bent rod cluster, and that the unibrow is the sine wave.

```
library(liminal)
umap_df <- data.frame(umapX = cnl_umap[, 1],
                      umapY = cnl_umap[, 2])
limn_tour_link(
  umap_df,
  clusters_nonlin,
  cols = x1:x4
)
```

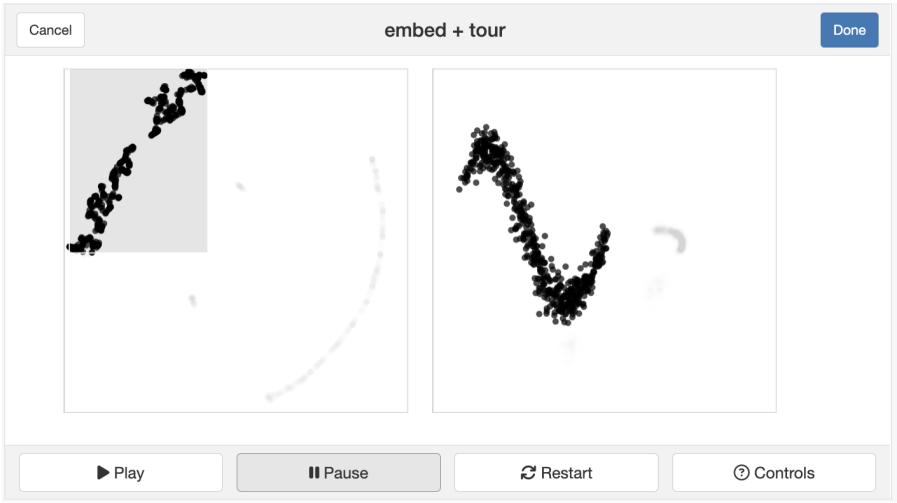
5.2.2 Using `detourr`

Figure 5.4 shows how the linking is achieved using `detourr`. It uses a shared data object, as made possible by the `crosstalk` package, and the UMAP view is made interactive using `plotly`.

```
library(detourr)
library(dplyr)
library(crosstalk)
library(plotly)
umap_df <- data.frame(umapX = cnl_umap[, 1],
                      umapY = cnl_umap[, 2])
cnl_df <- bind_cols(clusters_nonlin, umap_df)
shared_cnl <- SharedData$new(cnl_df)

detour_plot <- detour(shared_cnl, tour_aes(
  projection = starts_with("x"))) |>
    tour_path(grand_tour(2),
                    max_bases=50, fps = 60) |>
       show_scatter(alpha = 0.7, axes = FALSE,
                    width = "100%", height = "450px")

umap_plot <- plot_ly(shared_cnl,
                    x = ~umapX,
                    y = ~umapY,
                    color = I("black"),
                    height = 450) %>%
```



(a) Smile matches bent rod.



(b) Unibrow matches sine wave.

Figure 5.3: Two screenshots from liminal showing which clusters match between the UMAP representation and the tour animation. The smile corresponds to the small bent rod cluster. The unibrow matches to the sine wave cluster.

```
    highlight(on = "plotly_selected",
              off = "plotly_doubleclick") %>%
    add_trace(type = "scatter",
              mode = "markers")

bscols(
     detour_plot, umap_plot,
     widths = c(5, 6)
 )
```

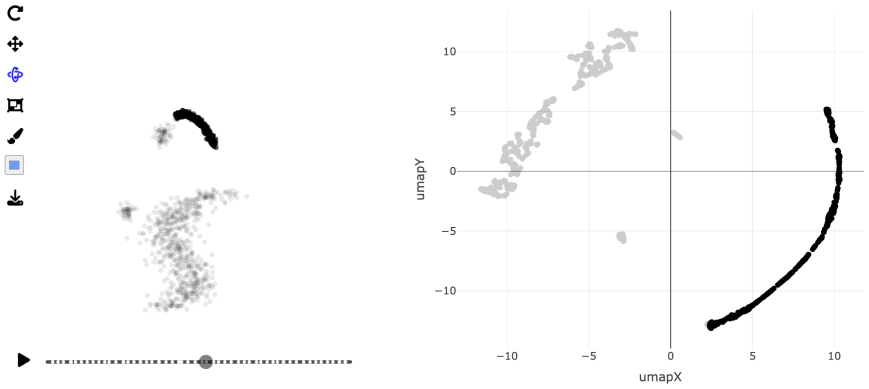


Figure 5.4: Screenshot from detourr showing which clusters match between the UMAP representation and the tour animation. The smile corresponds to the small bent rod cluster.

5.3 Example: `fake_trees`

Figure 5.5 shows a more complex example, using the `fake_trees` data. We know that the 10D data has a main branch, and 9 branches (clusters) attached to it, based on our explorations in the earlier chapters. The t-SNE view, where points are coloured by the known branch ids, is very helpful for seeing the linear branch structure.

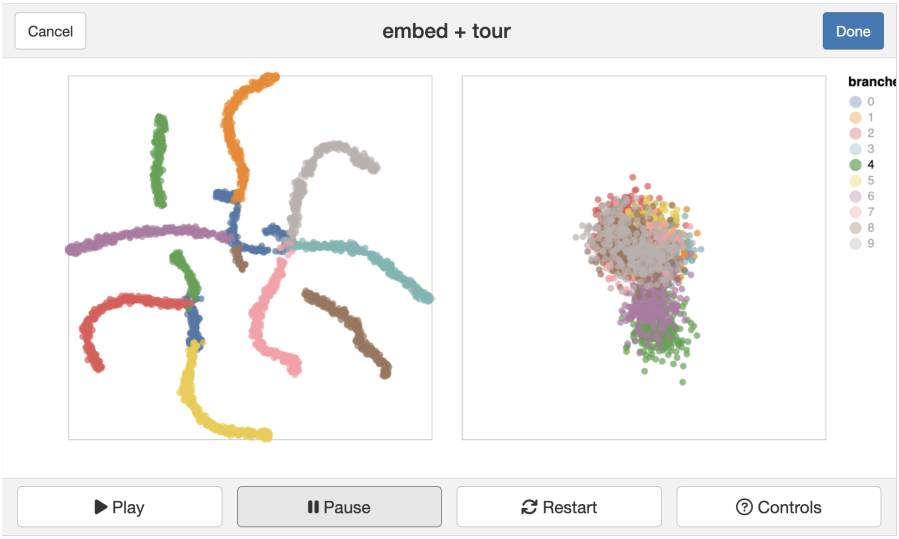
What we can't tell is that there is a main branch from which all of the others extend. We also can't tell which of the clusters corresponds to this branch. Linking the plot with a tour helps with this. Although, not shown in the sequence of snapshots in Figure 5.5, the main branch is actually the dark blue cluster, which is separated into three pieces by t-SNE.

```
library(liminal)
library(Rtsne)
data(fake_trees)
set.seed(2020)
tsne <- Rtsne::Rtsne(
  dplyr::select(fake_trees,
                dplyr::starts_with("dim")))
tsne_df <- data.frame(tsneX = tsne$Y[, 1],
                      tsneY = tsne$Y[, 2])
limn_tour_link(
  tsne_df,
  fake_trees,
  cols = dim1:dim10,
  color = branches
)
```

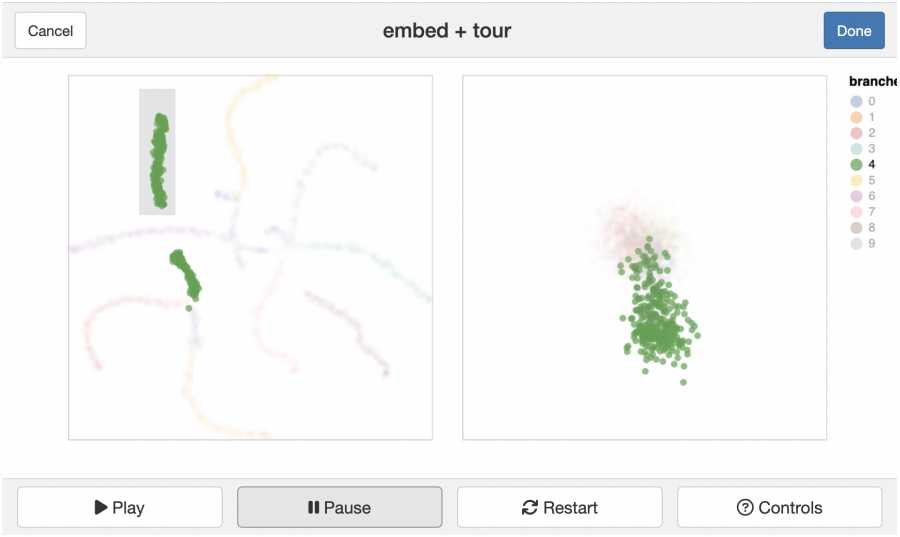
The t-SNE representation clearly shows the linear structures of the data, but viewing this 10D data with the tour shows that t-SNE makes several inaccurate breaks of some of the branches.

Exercises

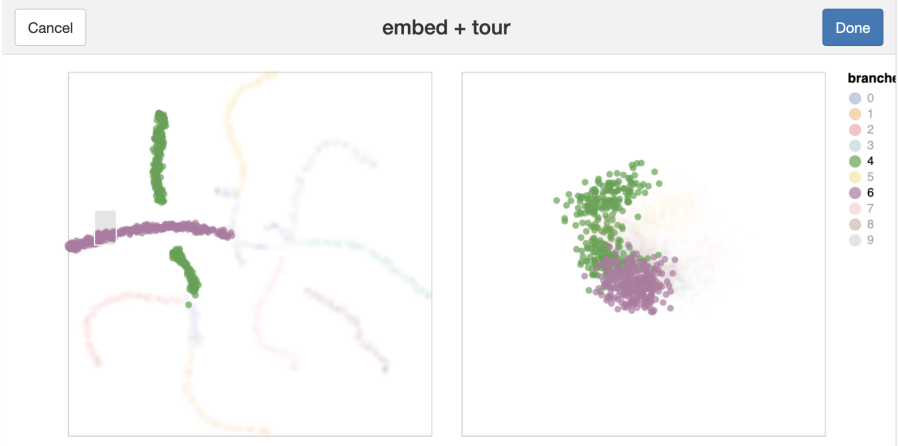
1. Using the `penguins_sub` data generate a 2D representation using t-SNE. Plot the points mapping the colour to species. What is most surprising? (Hint: Are the three species represented by three distinct clusters?)
2. Re-do the t-SNE representation with different parameter choices. Are the results different each time, or could they be considered to be equivalent?
3. Use `liminal` or `detourr` to link the t-SNE representation to a tour of the penguins. Highlight the points that have been placed in an awkward position by t-SNE from others in their species. Watch them relative to the others in their species in the tour view, and think about whether there is any rationale for the awkward placement.
4. Use UMAP to make the 2D representation, and use `liminal` or `detourr` to link with a tour to explore the result.
5. Conduct your best t-SNE and UMAP representations of the `aflw` data. Compare and contrast what is learned relative to a tour on the principal component analysis.



(a) Linked views of t-SNE dimension reduction with a tour of the fake trees data. The t-SNE view clearly shows ten 1D non-linear clusters, while the tour of the full 100 variables suggests a lot more variation in the data, and less difference between clusters.



(b) Focus on the green cluster which is split by t-SNE. The shape as viewed in many linear projections shown by the tour shows that it is a single curved cluster. The split is an artifact of the t-SNE mapping.



6

Introduction to clustering

Unsupervised classification, or cluster analysis, organizes observations into similar groups. Cluster analysis is a commonly used, appealing, and conceptually intuitive statistical method. Some of its uses include market segmentation, where customers are grouped into clusters with similar attributes for targeted marketing; gene expression analysis, where genes with similar expression patterns are grouped together; and the creation of taxonomies for animals, insects, or plants. Clustering can be used as a way of reducing a massive amount of data because observations within a cluster can be summarized by its centre. Also, clustering effectively subsets the data thus simplifying analysis because observations in each cluster can be analyzed separately.

6.1 What are clusters?

Organizing objects into groups is a common task to help make sense of the world around us. Perhaps this is why it is an appealing method of data analysis. However, cluster analysis is more complex than it initially appears. Many people imagine that it will produce neatly separated clusters like those in Figure 6.1(a), but it almost never does. Such ideal clusters are rarely encountered in real data, so we often need to modify our objective from *find the natural clusters in this data*. Instead, we need to organize the *cases into groups that are similar in some way*. Even though this may seem disappointing when compared with the ideal, it is still often an effective means of simplifying and understanding a dataset.

Knowing what shapes are in your data helps to decide on the best method and to diagnose the result. For example, if the clusters are elliptical model-based clustering is recommended.

At the heart of the clustering process is the work of discovering which variables are most important for defining the groups. It is often true that we only require a subset of the variables for finding clusters, whereas another subset (called

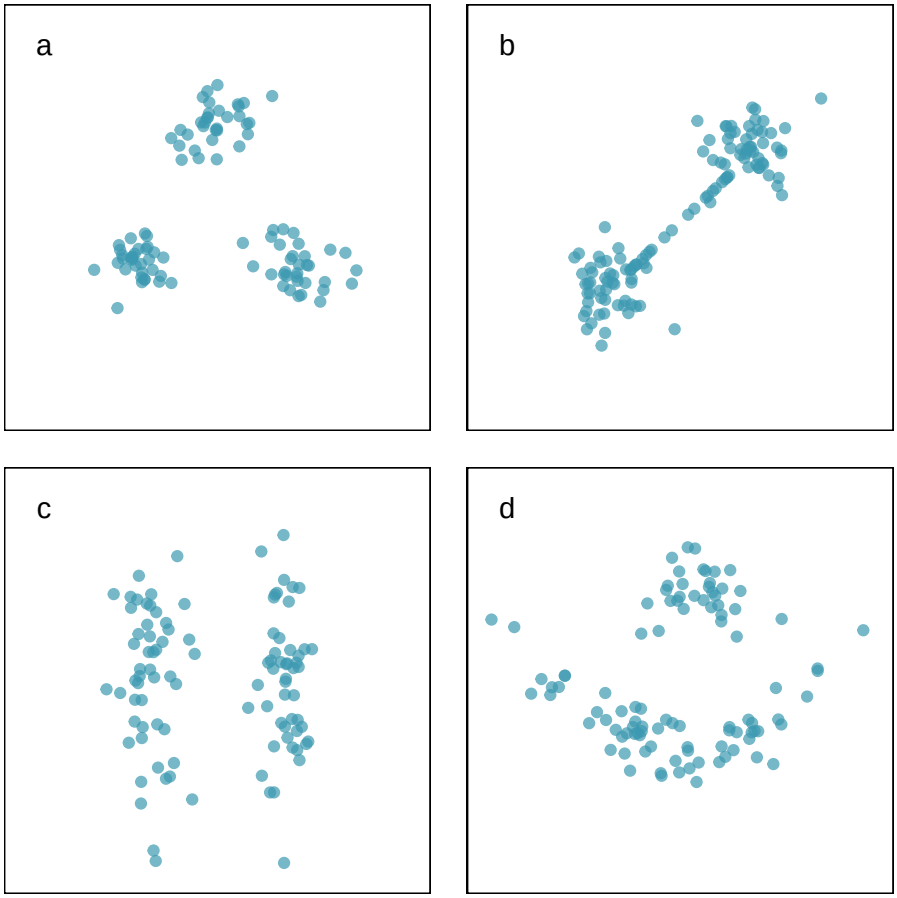


Figure 6.1: Different structures in data impact cluster analysis. When there are well-separated groups (a), it is simple to group similar observations. Even when there are not, partitioning observations into groups may still be useful. There may be nuisance observations (b) or nuisance variables (c) that affect the interpoint distance calculations and distract the clustering algorithm, and there may oddly shaped clusters (d) which are hard to numerically describe.

nuisance variables) has no impact. In the bottom left plot of Figure 6.1, it is clear that the variable plotted horizontally is important for splitting this data into two clusters, whereas the variable plotted vertically is a nuisance variable. Nuisance is an apt term for these variables, because they can radically change the interpoint distances and impair the clustering process.

Dynamic graphical methods help us to find and understand the cluster structure in high dimensions. With the tools in our toolbox, primarily tours, along with linked scatterplots and parallel coordinate plots, we can see clusters in high-dimensional spaces. We can detect gaps between clusters, the shape and relative positions of clusters, and the presence of nuisance variables. We can even find unusually shaped clusters, like those in the bottom right plot in Figure 6.1. In simple situations we can use graphics alone to group observations into clusters, using a "spin and brush" method. In more difficult data problems, we can assess and refine numerical solutions using graphics.

This part of the book discusses the use of interactive and dynamic graphics in the clustering of data. Section 6.2 introduces cluster analysis, focusing on interpoint distance measures. Chapter 7 describes an example of a purely graphical approach to cluster analysis, the spin and brush method. In the example shown in that section, we were able to find simplifications of the data that had not been found using numerical clustering methods, and to find a variety of structures in high-dimensional space. Chapter 8 describes methods for reducing the interpoint distance matrix to an intercluster distance matrix using hierarchical algorithms, Chapter 10 covers model-based clustering, and Chapter 11 described clustering with self-organising maps. Each of these chapters shows how graphical tools can be used to assess the results of numerical methods. Chapter 12 summarizes the chapter and revisits the data analysis strategies used in the examples. Additional references that provide good companions to the material presented in these chapters are Venables & Ripley (2002a), Boehmke & Greenwell (2019), Hennig et al. (2015), Giordani et al. (2020), Kassambara (2017), and the CRAN Task View (Leisch & Gruen, 2023). Chapter 12 summarizes the chapter and revisits the data analysis strategies used in the examples.

6.2 The importance of defining similar

Before we can begin finding groups of cases that are similar[1], we need to decide how to define or measure whether they are close together or far apart. Consider a

[1]Both *similarity* and *dissimilarity* measures are used for defining how similar cases are. It can be confusing! They measure similar in opposite directions. With a dissimilarity measure, a smaller number means the cases are closer, as in a distance metric. A similarity measure

dataset with three cases (a_1, a_2, a_3) and four variables (V_1, V_2, V_3, V_4), described in matrix format as

$$X = \begin{array}{c|cccc} & V_1 & V_2 & V_3 & V_4 \\ \hline a_1 & x_{11} & x_{12} & x_{13} & x_{14} \\ a_2 & x_{21} & x_{22} & x_{23} & x_{24} \\ a_3 & x_{31} & x_{32} & x_{33} & x_{34} \end{array} = \begin{array}{c|cccc} & V_1 & V_2 & V_3 & V_4 \\ \hline a_1 & 7.3 & 7.6 & 7.7 & 8.0 \\ a_2 & 7.4 & 7.2 & 7.3 & 7.2 \\ a_3 & 4.1 & 4.6 & 4.6 & 4.8 \end{array}$$

which is plotted in Figure 6.2. The Euclidean distance between two cases (rows of the matrix) with p elements is defined as

$$d_{\text{Euc}}(a_i, a_j) = \qquad ||a_i - a_j|| \qquad i, j = 1, \ldots, n,$$

where $||x_i|| = \sqrt{x_{i1}^2 + x_{i2}^2 + \cdots + x_{ip}^2}$. For example, the Euclidean distance between cases 1 and 2 in the above data, is

$$\begin{aligned} d_{\text{Euc}}(a_1, a_2) &= \sqrt{(7.3 - 7.4)^2 + (7.6 - 7.2)^2 + (7.7 - 7.3)^2 + (8.0 - 7.2)^2} \\ &= 1.0 \end{aligned}$$

For the three cases, the interpoint Euclidean distance matrix is

$$d_{\text{Euc}} = \begin{array}{c|ccc} & a_1 & a_2 & a_3 \\ \hline a_1 & 0.0 & 1.0 & 6.3 \\ a_2 & 1.0 & 0.0 & 5.5 \\ a_3 & 6.3 & 5.5 & 0.0 \end{array}$$

Cases a_1 and a_2 are more similar to each other than they are to case a_3, because the Euclidean distance between cases a_1 and a_2 is much smaller than the distance between cases a_1 and a_3 and between cases a_2 and a_3.

There are many different ways to calculate similarity. Similarity measures based on correlation distance can be useful. It is typically used where similarity of structure or shape is more important than similarity in magnitude.

As an example, see the parallel coordinate plot of the sample data at the right of Figure 6.2. Cases a_1 and a_3 are widely separated, but their shapes are similar (low, medium, medium, high). Case a_2, although overlapping with

usually ranges between 0 and 1, with 1 indicating that the cases are closer, for example, correlation.

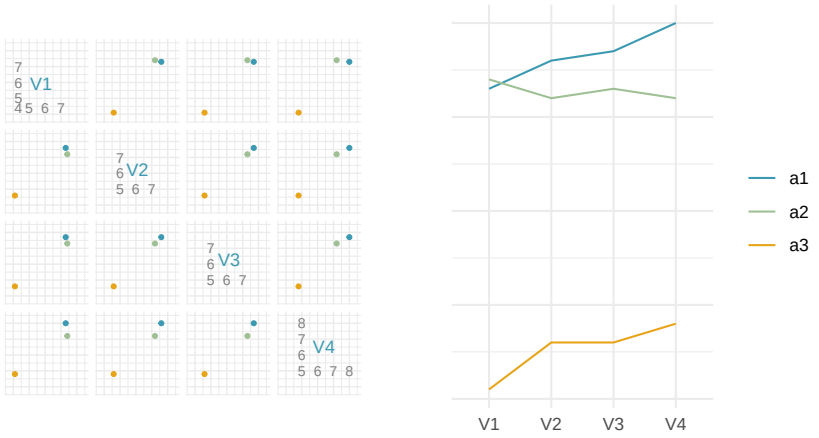


Figure 6.2: The scatterplot matrix (left) shows that cases a_1 and a_2 have similar values. The parallel coordinate plot (right) allows a comparison of other structure, which shows the similarity in the trend of the profiles on cases a_1 and a_3.

case a_1, has a very different shape (high, medium, medium, low). The Pearson correlation between two cases, $\rho(a_i, a_j)$, is defined as

$$\rho(a_i, a_j) = \frac{(a_i - c_i)^\top (a_j - c_j)}{\sqrt{(a_i - c_i)^\top (a_i - c_i)}\sqrt{(a_j - c_j)^\top (a_j - c_j)}}$$

Typically, c_i, c_j are the sample means of each case, $\bar{a}_i, \bar{a}_j$. For these three observations, $c_1 = \bar{a}_1 = 7.650, c_2 = \bar{a}_2 = 7.275, c_3 = \bar{a}_3 = 4.525$. An interesting geometric fact, is that if c_i, c_j are set to be 0, as is commonly done, ρ is a generalized correlation that describes the angle between the two data vectors. The correlation is then converted to a distance metric, with one possibility being as follows:

$$d_{\text{Cor}}(a_i, a_j) = \sqrt{2(1 - \rho(a_i, a_j))}$$

This distance metric will treat cases that are strongly negatively correlated as the most distant. If you want to consider strong negative correlation as close, then you could take the absolute value of $\rho(a_i, a_j)$ in the above equation, and remove the multiplication by 2.

The interpoint distance matrix for the sample data using d_{Cor} and the Pearson correlation coefficient is

$$d_{\text{Cor}} = \begin{array}{c|ccc} & a_1 & a_2 & a_3 \\ \hline a_1 & 0.0 & 3.6 & 0.1 \\ a_2 & 3.6 & 0.0 & 3.8 \\ a_3 & 0.1 & 3.8 & 0.0 \end{array}$$

By this metric, cases a_1 and a_3 are the most similar, because the correlation distance is smaller between these two cases than the other pairs of cases.

Note that these interpoint distances differ dramatically from those for Euclidean distance. As a consequence, the way the cases would be clustered is also very different. Choosing the appropriate distance measure is an important part of a cluster analysis.

After a distance metric has been chosen and a cluster analysis has been performed, the analyst must evaluate the results, and this is actually a difficult task. A cluster analysis does not generate p-values or other numerical criteria, and the process tends to produce hypotheses rather than testing them. Even the most determined attempts to produce the "best" results using modeling and validation techniques may result in clusters that, although seemingly significant, are useless for practical purposes. As a result, cluster analysis is best thought of as an exploratory technique, and it can be quite useful despite the lack of formal validation because of its power in data simplification.

Defining an appropriate distance metric from the context of the problem is a most important decision. For example, if your variables are all numeric, and on the same scale then Euclidean distance might be best. If your variables are categorical, you might need to use something like Hamming distance.

The context in which the data arises is the key to assessing the results. If the clusters can be characterized in a sensible manner, and they increase our knowledge of the data, then we are on the right track. To use an even more pragmatic criterion, if a company can gain an economic advantage by using a particular clustering method to carve up their customer database, then that is the method they should use.

Exercises

Use the following data to answer these questions:

```
     x1   x2   x3
a1 0.13 0.21 0.09
a2 0.91 0.95 0.85
a3 0.62 0.73 0.65
a4 0.21 0.92 0.43
```

1. Compute the Euclidean distance between cases `a1`, `a2`, `a3`, `a4`.
2. Compute the correlation distance (as defined above) between cases `a1`, `a2`, `a3`, `a4`.
3. Which two points have the (a) biggest (b) smallest Mahalanobis (statistical) distance, assuming that the covariance matrix is:

```
    x1  x2  x3
x1 1.0 0.8 0.8
x2 0.8 1.0 0.8
x3 0.8 0.8 1.0
```

(The function `mahalanobis` will calculate this in R. Technically this gives distance between each case and the mean vector.)

4. Is the ordering of distance between cases the same if Manhattan distance is used instead of Euclidean?
5. Compute the Chebychev distance between cases `a1`, `a2`, `a3`, `a4`.
6. Compute Bray-Curtis distance between cases `a1`, `a2`, `a3`, `a4`.
7. Make a plot of the data, and write a paragraph describing how the different distance metrics agree and disagree on how close or far the cases are from each other.

7

Spin-and-brush approach

Several examples of the spin-and-brush approach are documented in the literature, such as Cook et al. (1995a) and Wilhelm et al. (1999). The steps are:

1. Run the (grand) tour.
2. Stop when you see a separated cluster of points.
3. Paint the cluster a chosen colour.
4. Repeat 1-2 until the data is grouped, and when no other separated cluster is visible in any projection. You may need to re-paint some points if they appear to be grouped incorrectly in a different projection, or paint more points that after spinning most likely belong to an existing group.

Spin-and-brush is useful for exploring clustering when the data is numeric, and contains well-separated clusters. Patterns that adversely affect numerical techniques, such as nuisance variables or cases, differences in variances or shapes between clusters, don't pose any problems for spin-and-brush. It is also effective if the data has connected low-dimensional (1D or 2D) clusters in high dimensions.

It will not work very well when there are no distinct clusters and the purpose of clustering is to partition the data into subsets. Here, you could begin with a solution provided by some numerical clustering algorithm, and to use visual tools to evaluate it, with goal of refining the results.

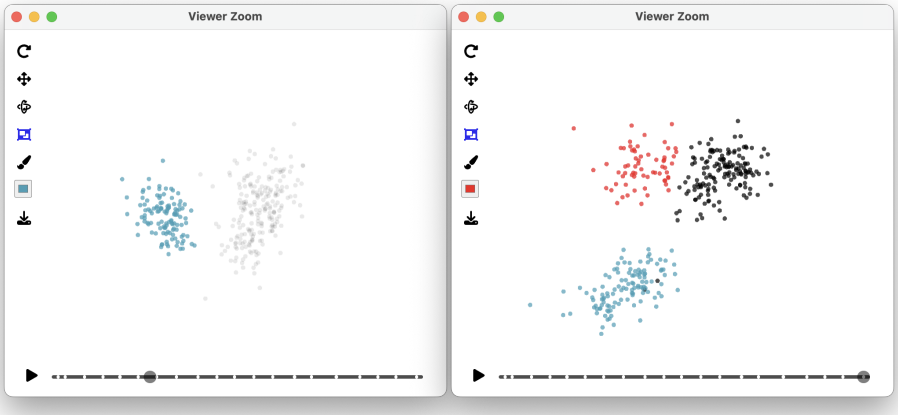
With a complex problem where there are many clusters, one can work sequentially, and remove each cluster after it is brushed, to de-clutter the display, in order to find more clusters.

Spin-and-brush is best achieved using a fully interactive graphics system like in the `detourr` package, where the results can be saved for further analysis. The code is very easy, and then all the controls are interactive.

```
library(detourr)
grDevices::hcl.colors(3, palette="Zissou 1")
detour(penguins_sub[,1:4],
       tour_aes(projection = bl:bm)) |>
```

```
        tour_path(grand_tour(2), fps = 60,
                  max_bases=20) |>
        show_scatter(alpha = 0.7,
                     axes = FALSE)
```

- `tour_aes(projection = bl:bm))` is `ggplot`-style syntax for specifying the variables `bl:bm` to include in the tour.
- `tour_path(grand_tour(2), fps = 60, max_bases=20)` specifies 2D grand tour path, with a longer than default path set by `max_bases=20` and the `fps` argument sets the smoothness.
- Brush interaction is set by choosing the square icon (4th from top), so when the cursor is moved over the window points are selected.
- You can choose specific colours to brush, from the colour palette by using hexcolours to match your favourite palette. Here we've used colours from the Zissou palette.
- The paintbrush icon sets the selected points to the current colour.
- Save the final colour labels using the download icon.



(a) One cluster painted (b) Another cluster painted

Figure 7.1: Screenshots of the spin-and-brush approach using `detourr` on the penguins data.

Figure 7.1 shows the stages of spin-and-brush on the penguins data using detourr. The final results can be examined and used for later analysis. Because this data came with a class variable, the penguin species, it is interesting to see how close the spin-and-brush clustering approach came to recovering these:

```
library(readr)
load("data/penguins_sub.rda")
detourr_penguins <- read_csv("data/detourr_penguins.csv")
table(penguins_sub$species, detourr_penguins$colour)
```

```
           000000 3e9eb6 f5191c
  Adelie      143      0      3
  Chinstrap     6      0     62
  Gentoo        2    117      0
```

It's quite close! All but two of the 119 Gentoo penguins were identified as a cluster (labelled as "3e9eb6" from the chosen light blue hex colour), and all but three of the 146 Adelie penguins were identified as a cluster, (labelled as "000000" which is the unbrushed black group). Most of the Chinstrap species were recovered also (labelled as "f5191c" for the red hex colour).

Exercises

1. Use the spin-and-brush approach to identify the three clusters in the `mulgar::clusters` data set.
2. Use the spin-and-brush approach to identify the six clusters in the `mulgar::multicluster` data set. (The code below using detourr could be useful.)
3. Use spin-and-brush on the challenge data sets, `c1`-`c7` from the `mulgar` package. How many clusters do you detect in each?

```
library(detourr)

# Use a random starting basis because the first two variables make it too easy
strt <- tourr::basis_random(10, 2)
detour(multicluster,
       tour_aes(projection = -group)) |>
       tour_path(grand_tour(2), start=strt, fps = 60) |>
       show_scatter(alpha = 0.7, axes = FALSE)
```

3. Use the spin-and-brush technique to identify the branches of the `fake_trees` data. The result should look something like this:

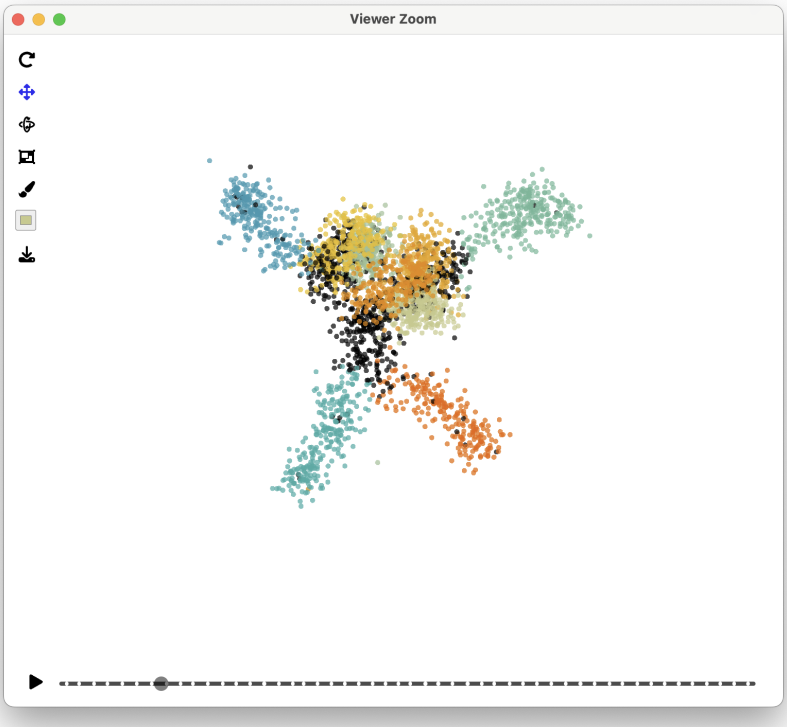


Figure 7.2: Example solution after spin-and-brush on fake trees data.

You can use the download button to save the data with the colours. Tabulate the `branches` id variable in the original data with the `colour` groups created from brushing, to see how closely you have recovered the original classes.

8

Hierarchical clustering

8.1 Overview

Hierarchical cluster algorithms sequentially fuse neighboring points to form ever-larger clusters, starting from a full interpoint distance matrix. *Distance between clusters* is described by a "linkage method", of which there are many. For example, single linkage measures the distance between clusters by the smallest interpoint distance between the members of the two clusters, complete linkage uses the maximum interpoint distance, and average linkage uses the average of the interpoint distances. Wards linkage, which usually produces the best clustering solutions, defines the distance as the reduction in the within-group variance. A good discussion on cluster analysis and linkage can be found in Boehmke & Greenwell (2019), on Wikipedia or any multivariate textbook.

Hierarchical clustering is summarised by a dendrogram, which sequentially shows points being joined to form a cluster, with the corresponding distances. Breaking the data into clusters is done by cutting the dendrogram at the long edges.

Here we will take a look at hierarchical clustering, using Wards linkage, on the `simple_clusters` data. The steps taken are to:

1. Plot the data to check for presence of clusters and their shape.
2. Compute the hierarchical clustering.
3. Plot the dendrogram to help decide on an appropriate number of clusters, using the `dendro_data` function from the `ggdendro` package.
4. Show the dendrogram overlaid on the data, calculated by the `hierfly` function in `mulgar`.
5. Plot the clustering result, by colouring points in the plot of the data.

```
library(ggplot2)
library(mulgar)
library(ggdendro)
library(dplyr)
library(patchwork)
library(tourr)
library(plotly)
library(htmlwidgets)
library(colorspace)
library(GGally)
```

```
data(simple_clusters)

# Compute hierarchical clustering with Ward's linkage
cl_hw <- hclust(dist(simple_clusters[,1:2]),
                method="ward.D2")
cl_ggd <- dendro_data(cl_hw, type = "triangle")

# Compute dendrogram in the data
cl_hfly <- hierfly(simple_clusters, cl_hw, scale=FALSE)

# Show result
simple_clusters <- simple_clusters %>%
  mutate(clw = factor(cutree(cl_hw, 2)))
```

Figure 8.1 illustrates the hierarchical clustering approach for a simple simulated data set (a) with two well-separated clusters in 2D. The dendrogram (b) is a representation of the order that points are joined into clusters. The dendrogram strongly indicates two clusters because the two branches representing the last join are much longer than all of the other branches.

Although, the dendrogram is usually a good summary of the steps taken by the algorithm, it can be misleading. The dendrogram might indicate a clear clustering (big differences in heights of branches) but the result may be awful. You need to check this by examining the result on the data, called model-in-the-data space by Wickham et al. (2015).

Plot (c) shows the dendrogram in 2D, overlaid on the data. The segments show how the points are joined to make clusters. In order to represent the dendrogram this way, new points (represented by a "+" here) need to be added corresponding to the centroid of groups of points that have been joined. These are used to draw the segments between other points and other clusters. We can see that the longest (two) edges stretches across the gap between the two clusters. This corresponds to the top of the dendrogram, the two long branches where we would cut it to make the two-cluster solution. This two-cluster solution is shown in plot (d).

```
# Plot the data
pd <- ggplot(simple_clusters, aes(x=x1, y=x2)) +
  geom_point(colour="#3B99B1", size=2, alpha=0.8) +
  ggtitle("(a)") +
  theme_minimal() +
  theme(aspect.ratio=1)

# Plot the dendrogram
ph <- ggplot() +
  geom_segment(data=cl_ggd$segments,
               aes(x = x, y = y,
                   xend = xend, yend = yend)) +
  geom_point(data=cl_ggd$labels, aes(x=x, y=y),
             colour="#3B99B1", alpha=0.8) +
  ggtitle("(b)") +
  theme_minimal() +
  theme_dendro()

# Plot the dendrogram on the data
pdh <- ggplot() +
  geom_segment(data=cl_hfly$segments,
                aes(x=x, xend=xend,
                    y=y, yend=yend)) +
  geom_point(data=cl_hfly$data,
             aes(x=x1, y=x2,
                 shape=factor(node),
                 colour=factor(node),
                 size=1-node), alpha=0.8) +
  xlab("x1") + ylab("x2") +
  scale_shape_manual(values = c(16, 3)) +
  scale_colour_manual(values = c("#3B99B1", "black")) +
  scale_size(limits=c(0,17)) +
  ggtitle("(c)") +
  theme_minimal() +
  theme(aspect.ratio=1, legend.position="none")

# Plot the resulting clusters
pc <- ggplot(simple_clusters) +
  geom_point(aes(x=x1, y=x2, colour=clw),
             size=2, alpha=0.8) +
  scale_colour_discrete_divergingx(palette = "Zissou 1",
                                   nmax=5, rev=TRUE) +
  ggtitle("(d)") +
  theme_minimal() +
```

```
  theme(aspect.ratio=1, legend.position="none")

pd + ph + pdh + pc + plot_layout(ncol=2)
```

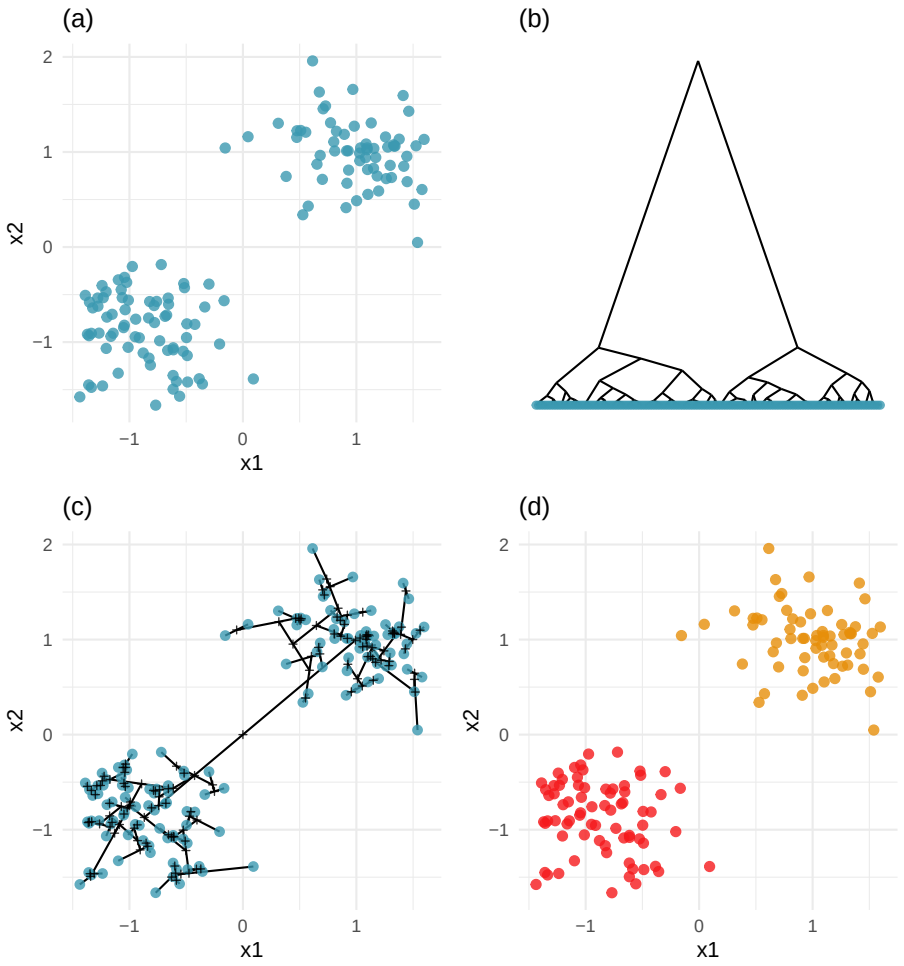


Figure 8.1: Hierarchical clustering on simulated data: (a) data, (b) dendrogram, (c) dendrogram on the data, and (d) two cluster solution. The extra points corresponding to nodes of the dendrogram are indicated by + in (c). The last join in the dendrogram (b), can be seen to correspond to the edges connecting the gap, when displayed with the data (c). The other joins can be seen to be pulling together points within each clump.

Plotting the dendrogram in the data space can help you understand how the hierarchical clustering has collected the points together into clusters. You can learn if the algorithm has been confused by nuisance patterns in the data, and how different choices of linkage method affects the result.

8.2 Common patterns which confuse clustering algorithms

Figure 8.2 shows two examples of structure in data that will confuse hierarchical clustering: nuisance variables and nuisance cases. We usually do not know that these problems exist prior to clustering the data. Discovering these iteratively as you conduct a clustering analysis is important for generating useful results.

```
# Nuisance observations
set.seed(20190514)
x <- (runif(20)-0.5)*4
y <- x
d1 <- data.frame(x1 = c(rnorm(50, -3),
                        rnorm(50, 3), x),
                 x2 = c(rnorm(50, -3),
                        rnorm(50, 3), y),
                 cl = factor(c(rep("A", 50),
                               rep("B", 70))))
d1 <- d1 %>%
  mutate_if(is.numeric, function(x) (x-mean(x))/sd(x))
pd1 <- ggplot(data=d1, aes(x=x1, y=x2)) +
  geom_point() +
    ggtitle("Nuisance observations") +
  theme_minimal() +
    theme(aspect.ratio=1)

# Nuisance variables
set.seed(20190512)
d2 <- data.frame(x1=c(rnorm(50, -4),
                        rnorm(50, 4)),
                 x2=c(rnorm(100)),
                 cl = factor(c(rep("A", 50),
                               rep("B", 50))))
```

```
d2 <- d2 %>%
  mutate_if(is.numeric, function(x) (x-mean(x))/sd(x))
pd2 <- ggplot(data=d2, aes(x=x1, y=x2)) +
  geom_point() +
    ggtitle("Nuisance variables") +
  theme_minimal() +
    theme(aspect.ratio=1)

pd1 + pd2 + plot_layout(ncol=2)
```

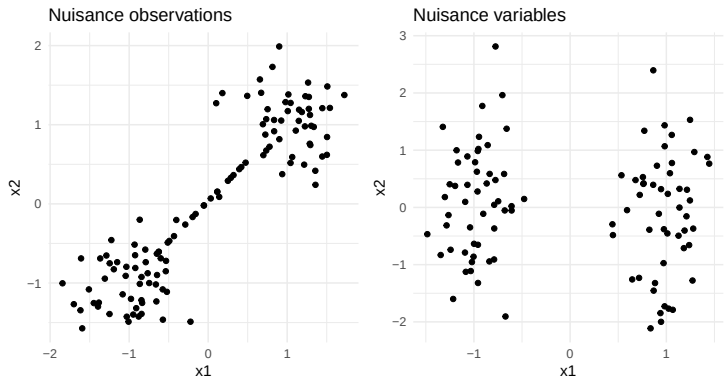


Figure 8.2: Two examples of data structure that causes problems for hierarchical clustering. Nuisance observations can cause problems because the close observations between the two clusters can cause some chaining in the hierarchical joining of observations. Nuisance variables can cause problems because observations across the gap can seem closer than observations at the end of each cluster.

If an outlier is a point that is extreme relative to other observations, an "inlier" is a point that is extreme relative to a cluster, but inside the domain of all of the observations. Nuisance observations are inliers, cases that occur between larger groups of points. If they were excluded there might be a gap between clusters. These can cause problems for clustering when distances between clusters are measured, and can be very problematic when single linkage hierarchical clustering is used. Figure 8.3 shows how nuisance observations affect single linkage but not Wards linkage hierarchical clustering.

```
# Compute single linkage
d1_hs <- hclust(dist(d1[,1:2]),
                method="single")
d1_ggds <- dendro_data(d1_hs, type = "triangle")
pd1s <- ggplot() +
```

```
  geom_segment(data=d1_ggds$segments,
               aes(x = x, y = y,
                   xend = xend, yend = yend)) +
  geom_point(data=d1_ggds$labels, aes(x=x, y=y),
             colour="#3B99B1", alpha=0.8) +
  theme_minimal() +
  ggtitle("(a) Single linkage dendrogram") +
  theme_dendro()

# Compute dendrogram in data
d1_hflys <- hierfly(d1, d1_hs, scale=FALSE)

pd1hs <- ggplot() +
  geom_segment(data=d1_hflys$segments,
                aes(x=x, xend=xend,
                    y=y, yend=yend)) +
  geom_point(data=d1_hflys$data,
             aes(x=x1, y=x2,
                 shape=factor(node),
                 colour=factor(node),
                 size=1-node), alpha=0.8) +
  scale_shape_manual(values = c(16, 3)) +
  scale_colour_manual(values = c("#3B99B1", "black")) +
  scale_size(limits=c(0,17)) +
  ggtitle("(b) Dendrogram in data space") +
  theme_minimal() +
  theme(aspect.ratio=1, legend.position="none")

# Show result
d1 <- d1 %>%
  mutate(cls = factor(cutree(d1_hs, 2)))
pc_d1s <- ggplot(d1) +
  geom_point(aes(x=x1, y=x2, colour=cls),
             size=2, alpha=0.8) +
  scale_colour_discrete_divergingx(palette = "Zissou 1",
                                   nmax=4, rev=TRUE) +
  ggtitle("(c) Two-cluster solution") +
  theme_minimal() +
  theme(aspect.ratio=1, legend.position="none")

# Compute Wards linkage
d1_hw <- hclust(dist(d1[,1:2]),
                method="ward.D2")
d1_ggdw <- dendro_data(d1_hw, type = "triangle")
```

```
pd1w <- ggplot() +
  geom_segment(data=d1_ggdw$segments,
               aes(x = x, y = y,
                   xend = xend, yend = yend)) +
  geom_point(data=d1_ggdw$labels, aes(x=x, y=y),
             colour="#3B99B1", alpha=0.8) +
  ggtitle("(d) Ward's linkage dendrogram") +
  theme_minimal() +
  theme_dendro()

# Compute dendrogram in data
d1_hflyw <- hierfly(d1, d1_hw, scale=FALSE)

pd1hw <- ggplot() +
  geom_segment(data=d1_hflyw$segments,
                aes(x=x, xend=xend,
                    y=y, yend=yend)) +
  geom_point(data=d1_hflyw$data,
             aes(x=x1, y=x2,
                 shape=factor(node),
                 colour=factor(node),
                 size=1-node), alpha=0.8) +
  scale_shape_manual(values = c(16, 3)) +
  scale_colour_manual(values = c("#3B99B1", "black")) +
  scale_size(limits=c(0,17)) +
  ggtitle("(e) Dendrogram in data space") +
  theme_minimal() +
  theme(aspect.ratio=1, legend.position="none")

# Show result
d1 <- d1 %>%
  mutate(clw = factor(cutree(d1_hw, 2)))
pc_d1w <- ggplot(d1) +
  geom_point(aes(x=x1, y=x2, colour=clw),
             size=2, alpha=0.8) +
  scale_colour_discrete_divergingx(palette = "Zissou 1",
                                   nmax=4, rev=TRUE) +
  ggtitle("(f) Two-cluster solution") +
  theme_minimal() +
  theme(aspect.ratio=1, legend.position="none")

pd1s + pd1hs + pc_d1s +
  pd1w + pd1hw + pc_d1w +
  plot_layout(ncol=3)
```

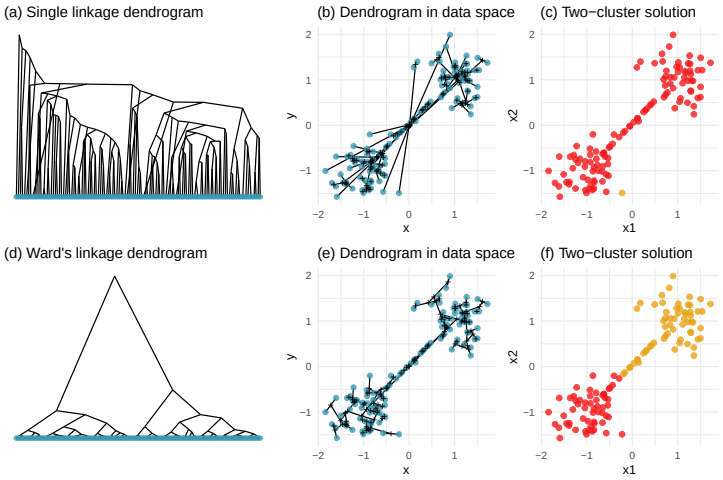


Figure 8.3: The effect of nuisance observations on single linkage (a, b, c) and Ward's linkage hierarchical clustering (d, e, f). The single linkage dendrogram is very different to the Wards linkage dendrogram. When plotted with the data (b) we can see a pin cushion or asterisk pattern, where points are joined to others through a place in the middle of the line of nuisance observations. This results in the bad two cluster solution of a singleton cluster, and all the rest. Conversely, Ward's dendrogram (d) strongly suggests two clusters, although the final join corresponds to just a small gap when shown on the data (e) but results in two sensible clusters.

Nuisance variables are ones that do not contribute to the clustering, such as `x2` here. When we look at this data we see a gap between two elliptically shape clusters, with the gap being only in the horizontal direction, `x1`. When we compute the distances between points, in order to start clustering, without knowing that `x2` is a nuisance variable, points across the gap might be considered to be closer than points within the same cluster. Figure 8.4 shows how nuisance variables affects complete linkage but not Wards linkage hierarchical clustering. (Wards linkage can be affected but it isn't for this data.) Interestingly, the dendrogram for complete linkage looks ideal, that it suggests two clusters. It is not until you examine the resulting clusters in the data that you can see the error, that it has clustered across the gap.

```
# Compute complete linkage
d2_hc <- hclust(dist(d2[,1:2]),
                method="complete")
d2_ggdc <- dendro_data(d2_hc, type = "triangle")
pd2c <- ggplot() +
  geom_segment(data=d2_ggdc$segments,
               aes(x = x, y = y,
```

```
                    xend = xend, yend = yend)) +
  geom_point(data=d2_ggdc$labels, aes(x=x, y=y),
             colour="#3B99B1", alpha=0.8) +
  ggtitle("(a) Complete linkage dendrogram") +
  theme_minimal() +
  theme_dendro()

# Compute dendrogram in data
d2_hflyc <- hierfly(d2, d2_hc, scale=FALSE)

pd2hc <- ggplot() +
  geom_segment(data=d2_hflyc$segments,
               aes(x=x, xend=xend,
                   y=y, yend=yend)) +
  geom_point(data=d2_hflyc$data,
             aes(x=x1, y=x2,
                 shape=factor(node),
                 colour=factor(node),
                 size=1-node), alpha=0.8) +
  scale_shape_manual(values = c(16, 3)) +
  scale_colour_manual(values = c("#3B99B1", "black")) +
  scale_size(limits=c(0,17)) +
  ggtitle("(b) Dendrogram in data space") +
  theme_minimal() +
  theme(aspect.ratio=1, legend.position="none")

# Show result
d2 <- d2 %>%
  mutate(clc = factor(cutree(d2_hc, 2)))
pc_d2c <- ggplot(d2) +
  geom_point(aes(x=x1, y=x2, colour=clc),
             size=2, alpha=0.8) +
  scale_colour_discrete_divergingx(palette = "Zissou 1",
                                   nmax=4, rev=TRUE) +
  ggtitle("(c) Two-cluster solution") +
  theme_minimal() +
  theme(aspect.ratio=1, legend.position="none")

# Compute Wards linkage
d2_hw <- hclust(dist(d2[,1:2]),
                method="ward.D2")
d2_ggdw <- dendro_data(d2_hw, type = "triangle")
pd2w <- ggplot() +
  geom_segment(data=d2_ggdw$segments,
```

```
                aes(x = x, y = y,
                    xend = xend, yend = yend)) +
  geom_point(data=d2_ggdw$labels, aes(x=x, y=y),
             colour="#3B99B1", alpha=0.8) +
  ggtitle("(d) Ward's linkage dendrogram") +
  theme_minimal() +
  theme_dendro()

# Compute dendrogram in data
d2_hflyw <- hierfly(d2, d2_hw, scale=FALSE)

pd2hw <- ggplot() +
  geom_segment(data=d2_hflyw$segments,
                aes(x=x, xend=xend,
                    y=y, yend=yend)) +
  geom_point(data=d2_hflyw$data,
             aes(x=x1, y=x2,
                 shape=factor(node),
                 colour=factor(node),
                 size=1-node), alpha=0.8) +
  scale_shape_manual(values = c(16, 3)) +
  scale_colour_manual(values = c("#3B99B1", "black")) +
  scale_size(limits=c(0,17)) +
  ggtitle("(e) Dendrogram in data space") +
  theme_minimal() +
  theme(aspect.ratio=1, legend.position="none")

# Show result
d2 <- d2 %>%
  mutate(clw = factor(cutree(d2_hw, 2)))
pc_d2w <- ggplot(d2) +
  geom_point(aes(x=x1, y=x2, colour=clw),
             size=2, alpha=0.8) +
  scale_colour_discrete_divergingx(palette = "Zissou 1",
                                   nmax=4, rev=TRUE) +
  ggtitle("(f) Two-cluster solution") +
  theme_minimal() +
  theme(aspect.ratio=1, legend.position="none")

pd2c + pd2hc + pc_d2c +
  pd2w + pd2hw + pc_d2w +
  plot_layout(ncol=3)
```

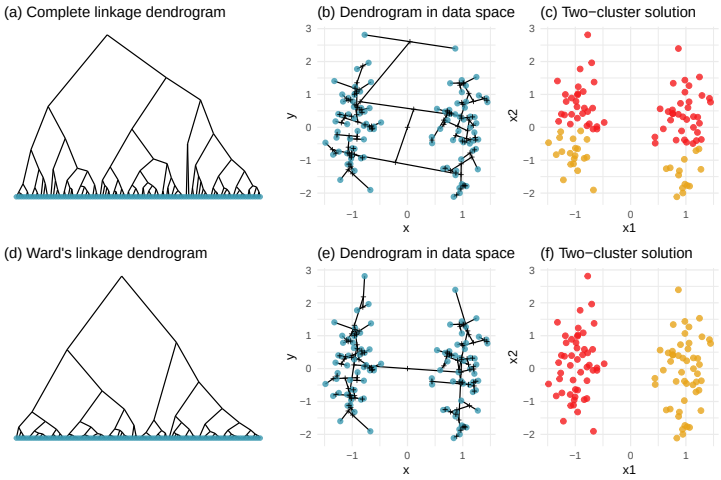


Figure 8.4: Complete linkage clustering (a, b, c) on nuisance variables in comparison to Ward's linkage (d, e, f). The two dendrograms (a, d) look similar but when plotted on the data (b, e) we can see they are very different solutions. The complete linkage result breaks the data into clusters across the gap (c), which is a bad solution. It has been distract by the nuisance variables. Conversely, the Wards linkage two-cluster solution does as hoped, divided the data into two clusters separated by the gap (f).

Two dendrograms might look similar but the resulting clustering can be very different. They can also look very different but correspond to very similar clusterings. Plotting the dendrogram in the data space is important for understanding how the algorithm operated when grouping observations, even more so for high dimensions.

8.3 Dendrograms in high-dimensions

The first step with any clustering with high dimensional data is also to check the data. You typically don't know whether there are clusters, or what shape they might be, or if there are nuisance observations or variables. A pairs plot like in Figure 8.5 is a nice complement to using the tour (Figure 8.6) for this. Here you can see three elliptical clusters, with one is further from the others.

```
load("data/penguins_sub.rda")
ggscatmat(penguins_sub[,1:4]) +
  theme_minimal() +
  xlab("") + ylab("")
```

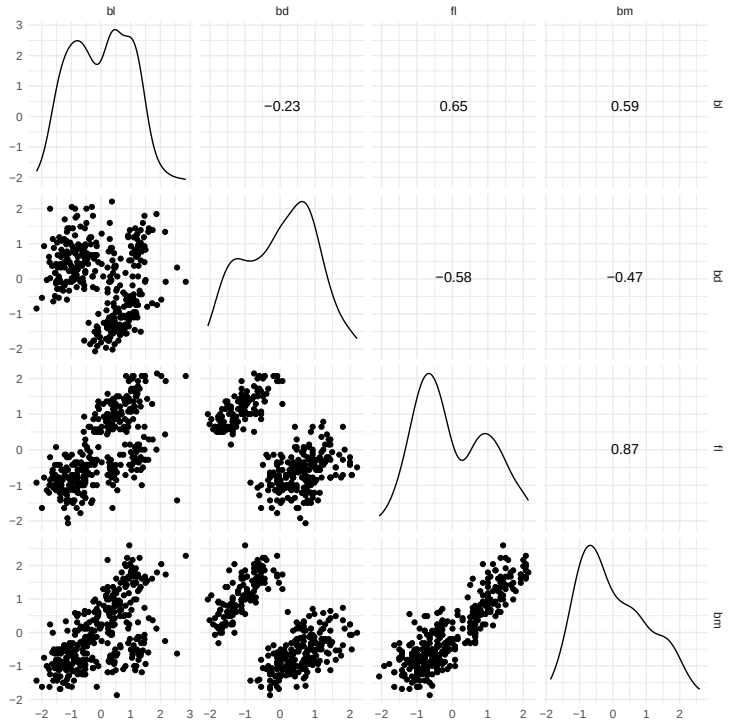


Figure 8.5: Make a scatterplot matrix to check for the presence of clustering, shape of clusters and presence of nuisance observations and variables. In the penguins it appears that there might be three elliptically shaped clusters, with some nuisance observations.

```
set.seed(20230329)
b <- basis_random(4,2)
pt1 <- save_history(penguins_sub[,1:4],
                    max_bases = 500,
                    start = b)
save(pt1, file="data/penguins_tour_path.rda")

# To re-create the gifs
load("data/penguins_tour_path.rda")
animate_xy(penguins_sub[,1:4],
```

```
            tour_path = planned_tour(pt1),
            axes="off", rescale=FALSE,
            half_range = 3.5)

render_gif(penguins_sub[,1:4],
            planned_tour(pt1),
            display_xy(half_range=0.9, axes="off"),
            gif_file="gifs/penguins_gt.gif",
            frames=500,
            loop=FALSE)
```

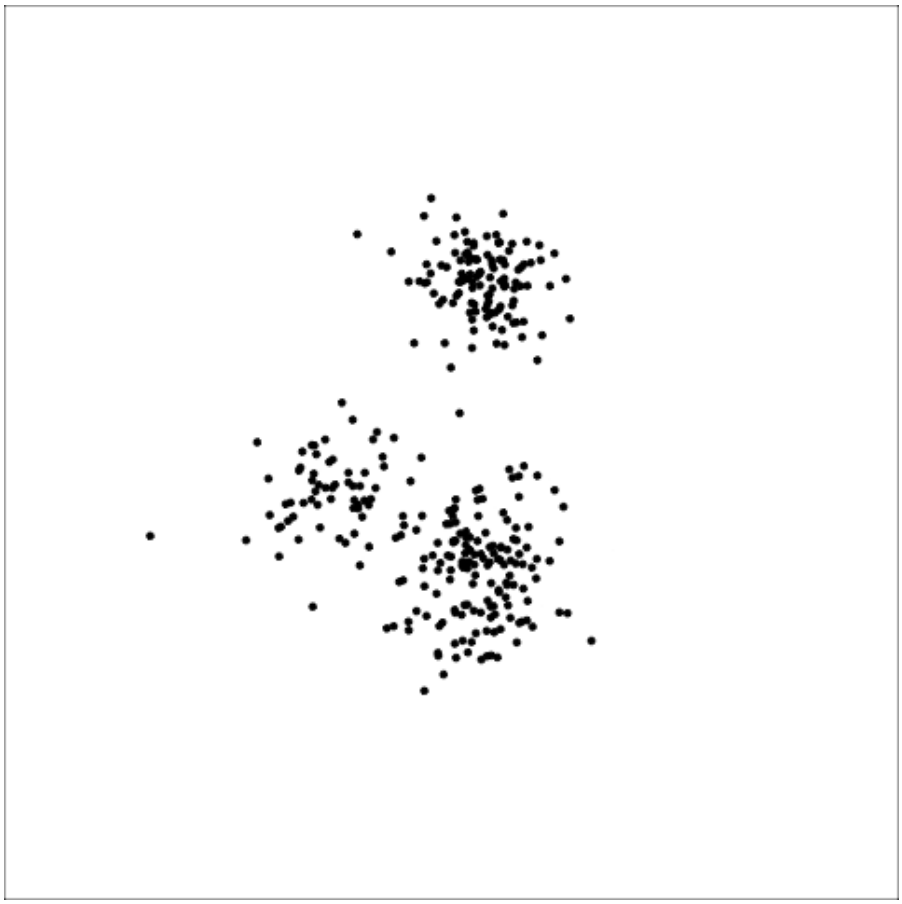


Figure 8.6: One frame from a grand tour being used to check for clusters, the shape of clusters and for nuisance observations and variables. Here the penguins data looks like it has possibly three elliptical clusters, one more separated than the other two, with some nuisance observations.

The process is the same as for the simpler example. We compute and draw the dendrogram in 2D, compute it in p-D and view with a tour. Here we have also chosen to examine the three cluster solution for single linkage and wards linkage clustering.

```
p_dist <- dist(penguins_sub[,1:4])
p_hcw <- hclust(p_dist, method="ward.D2")
p_hcs <- hclust(p_dist, method="single")

p_clw <- penguins_sub %>%
  mutate(cl = factor(cutree(p_hcw, 3))) %>%
  as.data.frame()
p_cls <- penguins_sub %>%
  mutate(cl = factor(cutree(p_hcs, 3))) %>%
  as.data.frame()

p_w_hfly <- hierfly(p_clw, p_hcw, scale=FALSE)
p_s_hfly <- hierfly(p_cls, p_hcs, scale=FALSE)
```

```
# Generate the dendrograms in 2D
p_hcw_dd <- dendro_data(p_hcw)
pw_dd <- ggplot() +
  geom_segment(data=p_hcw_dd$segments,
               aes(x = x, y = y,
                   xend = xend, yend = yend)) +
  geom_point(data=p_hcw_dd$labels, aes(x=x, y=y),
             alpha=0.8) +
  theme_dendro()

p_hcs_dd <- dendro_data(p_hcs)
ps_dd <- ggplot() +
  geom_segment(data=p_hcs_dd$segments,
               aes(x = x, y = y,
                   xend = xend, yend = yend)) +
  geom_point(data=p_hcs_dd$labels, aes(x=x, y=y),
             alpha=0.8) +
  theme_dendro()
```

```
load("data/penguins_tour_path.rda")
glyphs <- c(16, 46)
pchw <- glyphs[p_w_hfly$data$node+1]
pchs <- glyphs[p_s_hfly$data$node+1]

animate_xy(p_w_hfly$data[,1:4],
           #col=colw,
```

```
            tour_path = planned_tour(pt1),
            pch = pchw,
            edges=p_w_hfly$edges,
            axes="bottomleft")

animate_xy(p_s_hfly$data[,1:4],
            #col=colw,
            tour_path = planned_tour(pt1),
            pch = pchs,
            edges=p_s_hfly$edges,
            axes="bottomleft")

render_gif(p_w_hfly$data[,1:4],
            planned_tour(pt1),
            display_xy(half_range=0.9,
                       pch = pchw,
                       edges = p_w_hfly$edges,
                       axes = "off"),
            gif_file="gifs/penguins_hflyw.gif",
            frames=500,
            loop=FALSE)

render_gif(p_s_hfly$data[,1:4],
            planned_tour(pt1),
            display_xy(half_range=0.9,
                       pch = pchs,
                       edges = p_s_hfly$edges,
                       axes = "off"),
            gif_file="gifs/penguins_hflys.gif",
            frames=500,
            loop=FALSE)

# Show three cluster solutions
clrs <- hcl.colors(3, "Zissou 1")
w3_col <- clrs[p_w_hfly$data$cl[p_w_hfly$data$node == 0]]
render_gif(p_w_hfly$data[p_w_hfly$data$node == 0, 1:4],
            planned_tour(pt1),
            display_xy(half_range=0.9,
                       col=w3_col,
                       axes = "off"),
            gif_file="gifs/penguins_w3.gif",
            frames=500,
            loop=FALSE)
```

```
s3_col <- clrs[p_s_hfly$data$cl[p_w_hfly$data$node == 0]]
render_gif(p_s_hfly$data[p_w_hfly$data$node == 0,1:4],
           planned_tour(pt1),
           display_xy(half_range=0.9,
                      col=s3_col,
                      axes = "off"),
           gif_file="gifs/penguins_s3.gif",
           frames=500,
           loop=FALSE)
```

Figure 8.7 and Figure 8.8 show results for single linkage and wards linkage clustering of the penguins data. The 2D dendrograms are very different. Wards linkage produces a clearer indication of clusters, with a suggestion of three, or possibly four or five clusters. The dendrogram for single linkage suggests two clusters, and has the classical waterfall appearance that is often seen with this type of linkage. (If you look carefully, though, you will see it is actually a three cluster solution. At the very top of the dendrogram there is another branch connecting one observation to the other two clusters.)

Figure 8.8 (a) and (b) show the dendrograms in 4D overlaid on the data. The two are starkly different. The single linkage clustering is like pins pointing to (three) centres, with some long extra edges.

Plots (c) and (d) show the three cluster solutions, with Wards linkage almost recovering the clusters of the three species. Single linkage has two big clusters, and the singleton cluster. Although the Wards linkage produces the best result, single linkage does provide some interesting and useful information about the data. That singleton cluster is an outlier, an unusually-sized penguin. We can see it as an outlier just from the tour in Figure 8.6 but single linkage emphasizes it, bringing it more strongly to our attention.

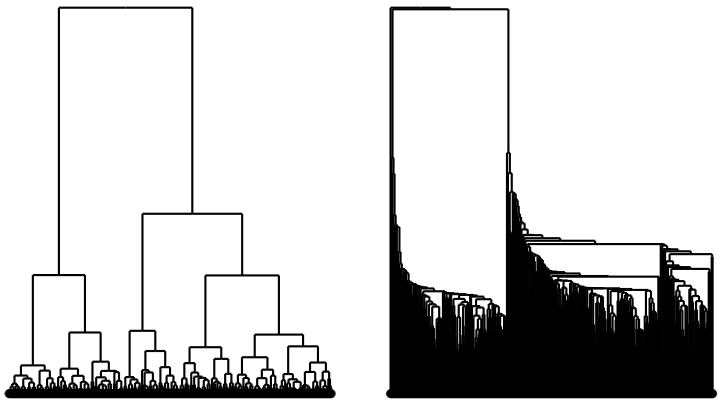
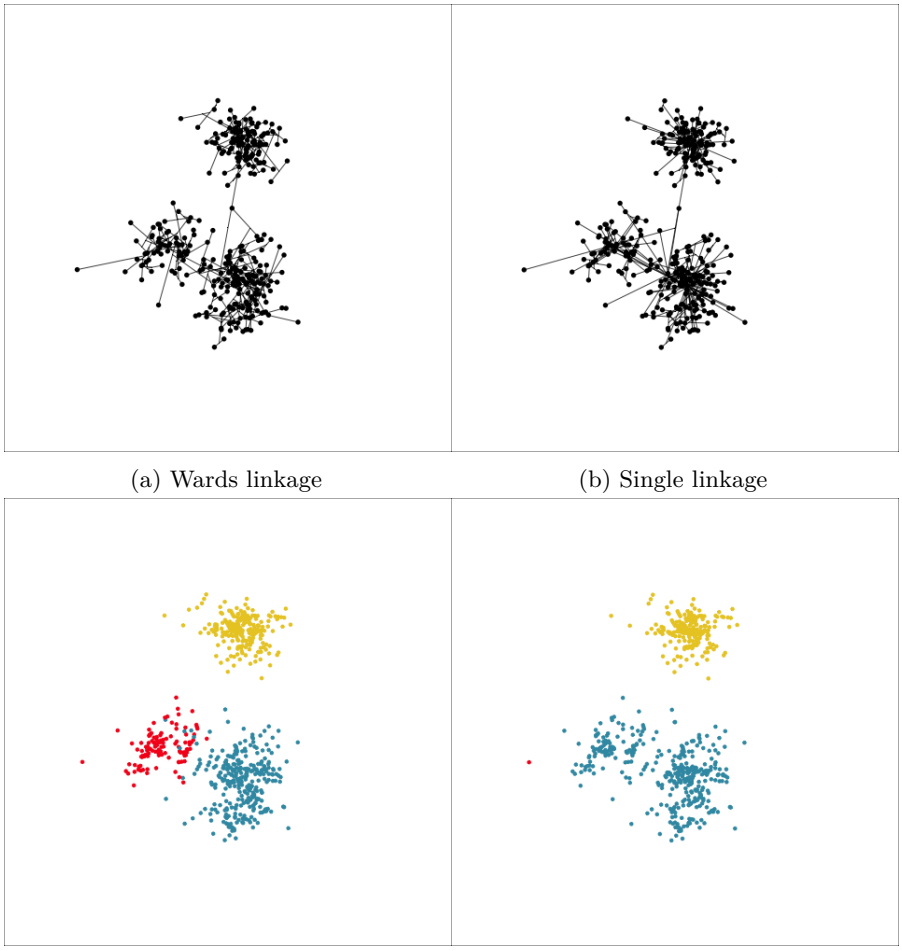


Figure 8.7: Wards linkage (left) and single linkage (right).



(a) Wards linkage (b) Single linkage

(c) Wards linkage (d) Single linkage

Figure 8.8: Dendrograms for Wards and single linkage of the penguins data, shown in 2D (top) and in 4D (middle), and the three-cluster solution of each.

Single linkage on the penguins has a very different joining pattern to Wards! While Wards provides the better result, single linkage provides useful information about the data, such as emphasizing the outlier.

```
load("data/penguins_tour_path.rda")
# Create a smaller one, for space concerns
pt1i <- interpolate(pt1[,,1:5], 0.1)
pw_anim <- render_anim(p_w_hfly$data,
                       vars=1:4,
                       frames=pt1i,
                       edges = p_w_hfly$edges,
             obs_labels=paste0(1:nrow(p_w_hfly$data),
                               p_w_hfly$data$cl))

pw_gp <- ggplot() +
     geom_segment(data=pw_anim$edges,
                    aes(x=x, xend=xend,
                        y=y, yend=yend,
                        frame=frame)) +
     geom_point(data=pw_anim$frames,
                aes(x=P1, y=P2,
                    frame=frame,
                    shape=factor(node),
                    label=obs_labels),
                alpha=0.8, size=1) +
     xlim(-1,1) + ylim(-1,1) +
     scale_shape_manual(values=c(16, 46)) +
     coord_equal() +
     theme_bw() +
     theme(legend.position="none",
           axis.text=element_blank(),
           axis.title=element_blank(),
           axis.ticks=element_blank(),
           panel.grid=element_blank())

pwg <- ggplotly(pw_gp, width=450, height=500,
                tooltip="label") %>%
       animation_button(label="Go") %>%
       animation_slider(len=0.8, x=0.5,
                        xanchor="center") %>%
       animation_opts(easing="linear", transition = 0)
htmlwidgets::saveWidget(pwg,
```

```
          file="html/penguins_cl_ward.html",
          selfcontained = TRUE)

# Single
ps_anim <- render_anim(p_s_hfly$data, vars=1:4,
                         frames=pt1i,
                       edges = p_s_hfly$edges,
             obs_labels=paste0(1:nrow(p_s_hfly$data),
                               p_s_hfly$data$cl))

ps_gp <- ggplot() +
     geom_segment(data=ps_anim$edges,
                    aes(x=x, xend=xend,
                        y=y, yend=yend,
                        frame=frame)) +
     geom_point(data=ps_anim$frames,
                aes(x=P1, y=P2,
                    frame=frame,
                    shape=factor(node),
                    label=obs_labels),
                alpha=0.8, size=1) +
     xlim(-1,1) + ylim(-1,1) +
     scale_shape_manual(values=c(16, 46)) +
     coord_equal() +
     theme_bw() +
     theme(legend.position="none",
           axis.text=element_blank(),
           axis.title=element_blank(),
           axis.ticks=element_blank(),
           panel.grid=element_blank())

psg <- ggplotly(ps_gp, width=450, height=500,
                tooltip="label") %>%
       animation_button(label="Go") %>%
       animation_slider(len=0.8, x=0.5,
                        xanchor="center") %>%
       animation_opts(easing="linear", transition = 0)
htmlwidgets::saveWidget(psg,
          file="html/penguins_cl_single.html",
          selfcontained = TRUE)
```

Viewing the dendrograms in high-dimensions provides insight into how the observations have joined points to clusters. For example, single linkage often has edges leading to a single focal point, which might not be yield a useful clustering but might help to identify outliers. If the edges point to multiple focal points, with long edges bridging gaps in the data, the result is more likely yielding a useful clustering.

Exercises

1. Compute complete linkage clustering for the **nuisance observations** data set. Does it perform more similarly to single linkage or Wards linkage?
2. Compute single linkage clustering for the **nuisance variables** data. Does it perform more similarly to complete linkage or Wards linkage?
3. Use hierarchical clustering with Euclidean distance and Wards linkage to split the `clusters_nonlin` data into four clusters. Look at the dendrogram in 2D and 4D. In 4D you can also include the cluster assignment as color. Does this look like a good solution?
4. Repeat the same exercise using single linkage instead of Wards linkage. How does this solution compare to what we have found with Wards linkage? Does the solution match how you would cluster the data in a spin-and-brush approach?
5. Argue why single linkage might not perform well for the `fake_trees` data. Which method do you think will work best with this data? Conduct hierarchical clustering with your choice of linkage method. Does the 2D dendrogram suggest 10 clusters for the 10 branches? Take a look at the high-dimensional representation of the dendrogram. Has your chosen method captured the branches well, or not, explaining what you think worked well or poorly?
6. What would a useful clustering of the first four PCs of the `aflw` data be? What linkage method would you expect works best to cluster it this way? Conduct the clustering. Examine the 2D dendrogram and decide on how many clusters should be used. Examine the cluster solution using a tour with points coloured by cluster.

7. Based on your assessment of the cluster structure in the challenge data sets, `c1-c7`, from the `mulgar` package, which linkage method would you recommend. Use your suggested linkage method to cluster

each data set, and summarise how well it performed in detecting the clusters that you have seen.

9

k-means clustering

One of the simplest and efficient techniques for clustering data is the k-means algorithm. The algorithm begins with a choice for k, the number of clusters to divide the data into. It is seeded with k initial means, and sequentially iterates through the observations, assigning them to the nearest mean, and re-calculating the k means. It stops at a given number of iterations or when points no longer change clusters. The algorithm will tend to segment the data into roughly equal sized, or spherical clusters, and thus will work well if the clusters are separated and equally spherical in shape.

A good place to learn ore about the k-means algorithm is Chapter 20 of Boehmke & Greenwell (2019). The algorithm has been in use for a long time! It was named k-means by MacQueen (1967), but developed by Lloyd in 1957 (as described in Lloyd (1982)) and separately by Forgy (1965), and perhaps others as it is a very simple procedure.

The key elements to examine in a k-means clustering algorithm result are:

- means
- boundaries

9.1 Examining results in 2D

Figure 9.1 shows the results of k-means clustering on the 2D `simple_clusters` data and two variables of the penguins data. We can see that it works well when the clusters are spherical, but for the penguins data it fails because the shape of the clusters is elliptical. It actually makes a mistake that would not be made if we simply visually clustered: cluster 3 has grouped points across a gap, a divide that visually we would all agree should form a separation.

```
library(mulgar)
library(ggplot2)
library(dplyr)
library(colorspace)
library(patchwork)
data("simple_clusters")
load("data/penguins_sub.rda")

set.seed(202305)
sc_bl_bd_km <- kmeans(simple_clusters[,1:2], centers=2,
                      iter.max = 50, nstart = 5)
sc_bl_bd_km_means <- data.frame(sc_bl_bd_km$centers) %>%
  mutate(cl = factor(rownames(sc_bl_bd_km$centers)))
sc_bl_bd_km_d <- simple_clusters[,1:2] %>%
  mutate(cl = factor(sc_bl_bd_km$cluster))
```

```
sc_bl_bd_km_p <- ggplot() +
  geom_point(data=sc_bl_bd_km_d,
             aes(x=x1, y=x2, colour=cl),
             shape=16, alpha=0.4) +
  geom_point(data=sc_bl_bd_km_means,
             aes(x=x1, y=x2, colour=cl),
             shape=3, size=5) +
    scale_color_discrete_divergingx("Zissou 1") +
  ggtitle("(a)") +
  theme_minimal() +
  theme(aspect.ratio = 1,
        legend.position = "bottom",
        legend.title = element_blank())

p_bl_bd_km <- kmeans(penguins_sub[,1:2], centers=3,
                     iter.max = 50, nstart = 5)
p_bl_bd_km_means <- data.frame(p_bl_bd_km$centers) %>%
  mutate(cl = factor(rownames(p_bl_bd_km$centers)))
p_bl_bd_km_d <- penguins_sub[,1:2] %>%
  mutate(cl = factor(p_bl_bd_km$cluster))

p_bl_bd_km_p <- ggplot() +
  geom_point(data=p_bl_bd_km_d,
             aes(x=bl, y=bd, colour=cl),
             shape=16, alpha=0.4) +
  geom_point(data=p_bl_bd_km_means,
             aes(x=bl, y=bd, colour=cl),
             shape=3, size=5) +
```

```
    scale_color_discrete_divergingx("Zissou 1") +
  ggtitle("(b)") +
  theme_minimal() +
  theme(aspect.ratio = 1,
        legend.position = "bottom",
        legend.title = element_blank())

sc_bl_bd_km_p + p_bl_bd_km_p + plot_layout(ncol=2)
```

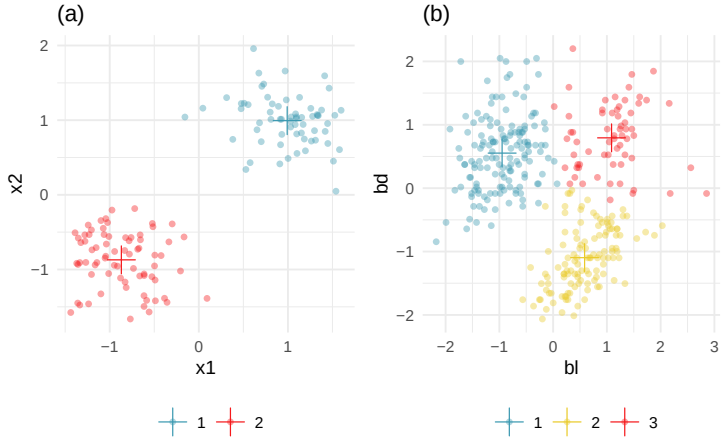


Figure 9.1: Examining k-means clustering results for simple clusters (a) and two variables of the penguins data (b). The means are indicated by a +. The results are perfect for the simple clusters but not for the penguins data. The penguin clusters are elliptically shaped which is not captured by k-means. Cluster 3 has observations grouped across a gap in the data.

9.2 Examining results in high dimensions

This approach extends to high-dimensions. One colours observations by the cluster label, and overlays the final cluster means. If we see gaps in points in a single cluster it would mean that k-means fails to see important cluster structure. This is what happens with the 4D penguins data as shown in Figure 9.2.

```
p_km <- kmeans(penguins_sub[,1:4], centers=3,
                       iter.max = 50, nstart = 5)
```

```
p_km_means <- data.frame(p_km$centers) %>%
  mutate(cl = factor(rownames(p_km$centers)))
p_km_d <- penguins_sub[,1:4] %>%
  mutate(cl = factor(p_km$cluster))
```

```
library(tourr)
p_km_means <- p_km_means %>%
  mutate(type = "mean")
p_km_d <- p_km_d %>%
  mutate(type = "data")
p_km_all <- bind_rows(p_km_means, p_km_d)
p_km_all$type <- factor(p_km_all$type, levels=c("mean", "data"))
p_pch <- c(3, 20)[as.numeric(p_km_all$type)]
p_cex <- c(3, 1)[as.numeric(p_km_all$type)]
animate_xy(p_km_all[,1:4], col=p_km_all$cl,
           pch=p_pch, cex=p_cex, axes="bottomleft")
render_gif(p_km_all[,1:4],
           grand_tour(),
           display_xy(col=p_km_all$cl,
                      pch=p_pch,
                      cex=p_cex,
                      axes="bottomleft"),
           gif_file="gifs/p_km.gif",
           width=400,
           height=400,
           frames=500)
```

Generally, there is no need to choose k ahead of time. One would re-fit k-means with various choices of k, and compare the `tot.withinss` and examine the clusters visually, to decide on the optimal final value of k. This can be assessed in a similar way to the scree plot for PCA.

Exercises

1. Compute a k-means clustering for the `fake_trees` data, varying k to about 20. Choose your best k, and examine the solution using the first 10 PCs on the data. It should capture the data quite nicely, although it will break up each branch into multiple clusters.
2. Compute a k-means clustering of the first four PCs of the `aflw` data. Examine the best solution (you choose which k), and describe

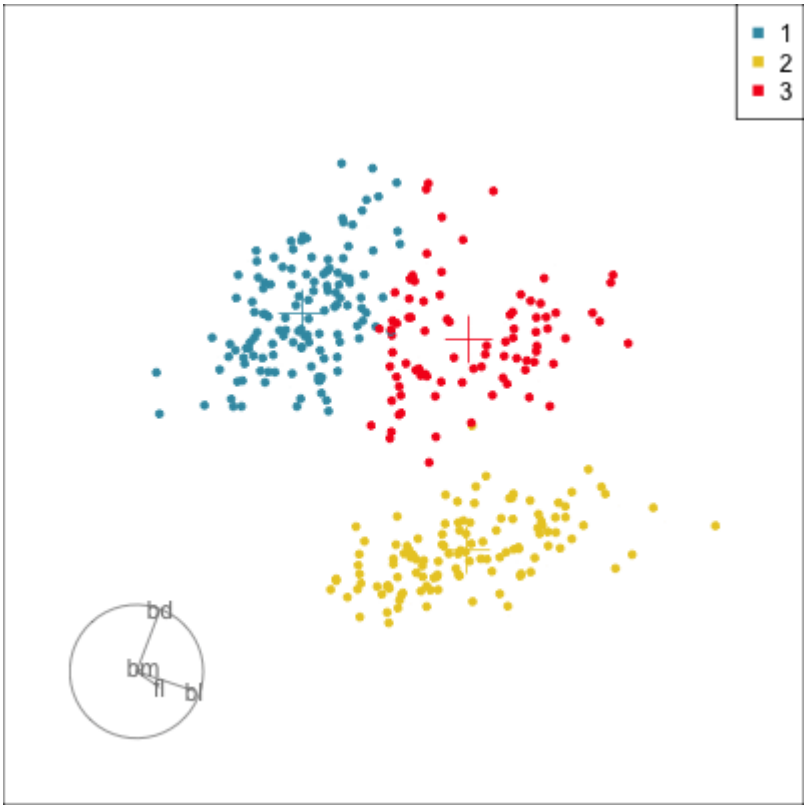


Figure 9.2: Exploring the k-means clustering result for the 4D penguins data. You can see cluster 2 clearly separated from the other observations. Cluster 3, like in the 2D example, is a mix of observations across a gap. Even the mean of the cluster is almost in the gap.

how it divides the data. By examining the means, can you tell if it extracts clusters of offensive vs defensive vs midfield players? Or does it break the data into high skills vs low skills?

3. Use k-means clustering on the challenge data sets, `c1-c7` from the `mulgar` package. Explain what choice of k is best for each data set, and why or why not the cluster structure, as you have described it from earlier chapters, is detected or not.

10

Model-based clustering

Model-based clustering Fraley & Raftery (2002) fits a multivariate normal mixture model to the data. It uses the EM algorithm to fit the parameters for the mean, variance–covariance of each population, and the mixing proportion. The variance-covariance matrix is re-parameterised using an eigen-decomposition

$$\Sigma_k = \lambda_k D_k A_k D_k^\top, \quad k = 1, \ldots, g \ \text{ (number of clusters)}$$

resulting in several model choices, ranging from simple to complex, as shown in Table 10.1.

Table 10.1: Parameterizations of the covariance matrix.

Model	Sigma	Family	Volume	Shape	Orientation
EII	λI	Spherical	Equal	Equal	NA
VII	$\lambda_k I$	Spherical	Variable	Equal	NA
EEI	λA	Diagonal	Equal	Equal	Coordinate axes
VEI	$\lambda_k A$	Diagonal	Variable	Equal	Coordinate axes
EVI	λA_k	Diagonal	Equal	Variable	Coordinate axes
VVI	$\lambda_k A_k$	Diagonal	Variable	Variable	Coordinate axes
EEE	$\lambda D A D^\top$	Diagonal	Equal	Equal	Equal
EVE	$\lambda D A_k D^\top$	Ellipsoidal	Equal	Variable	Equal
VEE	$\lambda_k D A D^\top$	Ellipsoidal	Variable	Equal	Equal
VVE	$\lambda_k D A_k D^\top$	Ellipsoidal	Variable	Equal	Equal
EEV	$\lambda D_k A D_k^\top$	Ellipsoidal	Equal	Variable	Variable
VEV	$\lambda_k D_k A D_k^\top$	Ellipsoidal	Variable	Variable	Variable
EVV	$\lambda D_k A_k D_k^\top$	Ellipsoidal	Equal	Variable	Variable
VVV	$\lambda_k D_k A_k D_k^\top$	Ellipsoidal	Variable	Variable	Variable

Note the distribution descriptions “spherical” and “ellipsoidal”. These are descriptions of the shape of the variance-covariance for a multivariate normal distribution. A standard multivariate normal distribution has a variance-covariance matrix with zeros in the off-diagonal elements, which corresponds to spherically shaped data. When the variances (diagonals) are different or the

variables are correlated, then the shape of data from a multivariate normal is ellipsoidal.

The models are typically scored using the Bayes Information Criterion (BIC), which is based on the log likelihood, number of variables, and number of mixture components. They should also be assessed using graphical methods, as we demonstrate using the penguins data.

10.1 Examining the model in 2D

We start with two of the four real-valued variables (`bl`, `fl`) and the three `species`. The goal is to determine whether model-based methods can discover clusters that closely correspond to the three species. Based on the scatterplot in Figure 10.1 we would expect it to do well, and suggest an elliptical variance-covariance of roughly equal sizes as the model.

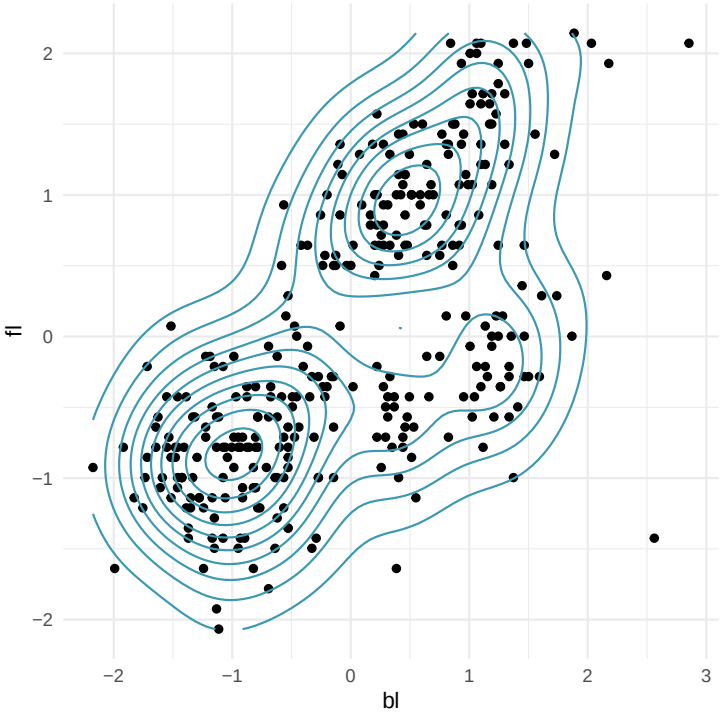


Figure 10.1: Scatterplot of flipper length by bill length of the penguins data.

```
penguins_BIC <- mclustBIC(penguins_sub[,c(1,3)])
ggmc <- ggmcbic(penguins_BIC, cl=2:9, top=4) +
  scale_color_discrete_divergingx(palette = "Roma") +
  ggtitle("(a)") +
  theme_minimal()
penguins_mc <- Mclust(penguins_sub[,c(1,3)],
                      G=3,
                      modelNames = "EVE")
penguins_mce <- mc_ellipse(penguins_mc)
penguins_cl <- penguins_sub[,c(1,3)]
penguins_cl$cl <- factor(penguins_mc$classification)
ggell <- ggplot() +
   geom_point(data=penguins_cl, aes(x=bl, y=fl,
                                    colour=cl),
              alpha=0.3) +
   geom_point(data=penguins_mce$ell, aes(x=bl, y=fl,
                                         colour=cl),
              shape=16) +
   geom_point(data=penguins_mce$mn, aes(x=bl, y=fl,
                                        colour=cl),
              shape=3, size=2) +
  scale_color_discrete_divergingx(palette = "Zissou 1")  +
  theme_minimal() +
  theme(aspect.ratio=1, legend.position="none") +
  ggtitle("(b)")
ggmc + ggell + plot_layout(ncol=2)
```

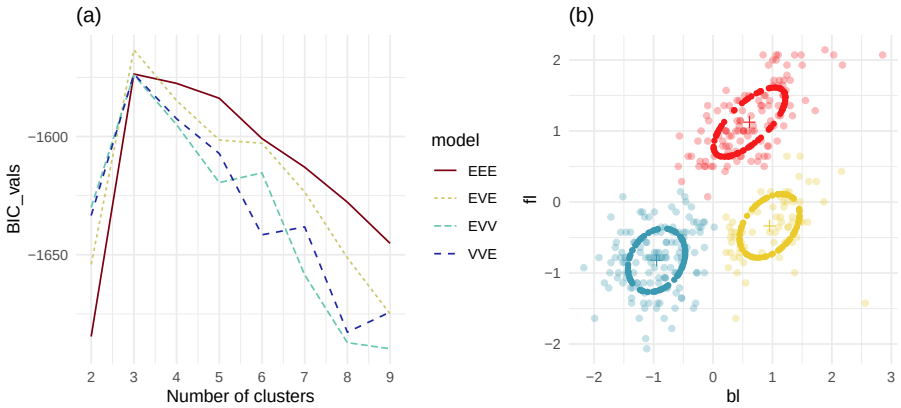


Figure 10.2: Summary plots from model-based clustering: (a) BIC values for clusters 2-9 of top four models, (b) variance-covariance ellipses and cluster means (+) corresponding to the best model. The best model is three-cluster EVE, which has differently shaped variance-covariances albeit the same volume and orientation.

Figure 10.2 summarises the results. All models agree that three clusters is the best. The different variance-covariance models for three clusters have similar BIC values with EVE (different shape, same volume and orientation) being slightly higher. These plots are made from the `mclust` package output using the `ggmcbic` and `mc_ellipse` functions fro the `mulgar` package.

10.2 Examining the model in high dimensions

Now we will examine how model-based clustering will group the penguins data using all four variables. Figure 10.3 shows the summary of different models, of which we would choose the four-cluster VEE, if we strictly followed the BIC choice. Figure 10.4 shows this model in a tour, and the best three-cluster model. You can see that the four-cluster result is inadequate, in various ways. One of the species (Chinstrap) does have a bimodal density, due to the two species, and we would expect that a four cluster solution might detect this. The tour shows that the three-cluster solution is the best match to the data shape.

```
penguins_BIC <- mclustBIC(penguins_sub[,1:4])
ggmc <- ggmcbic(penguins_BIC, cl=2:9, top=7) +
  scale_color_discrete_divergingx(palette = "Roma") +
```

```
  theme_minimal()
ggmc
```

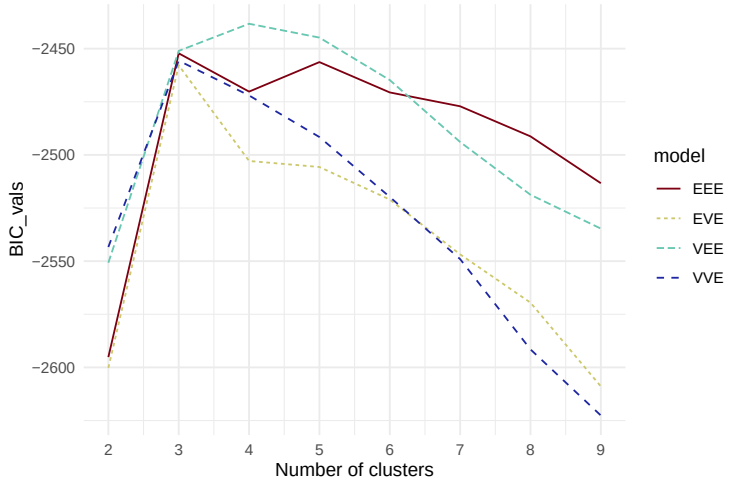
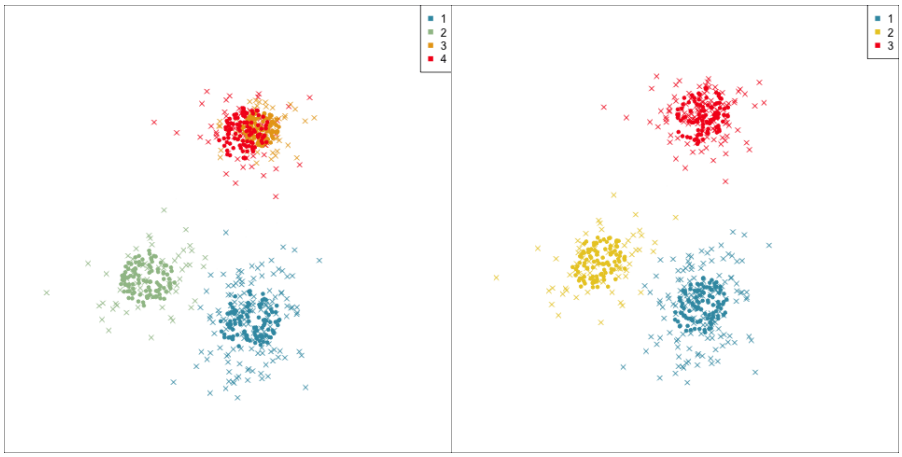


Figure 10.3: BIC values for the top models for 2-9 clusters on the penguins data. The interpretation is mixed: if one were to choose three clusters any of the variance-covariance models would be equally as good, but the very best model is the four-cluster VEE.

```
penguins_mc <- Mclust(penguins_sub[,1:4],
                      G=4,
                      modelNames = "VEE")
penguins_mce <- mc_ellipse(penguins_mc)
penguins_cl <- penguins_sub
penguins_cl$cl <- factor(penguins_mc$classification)

penguins_mc_data <- penguins_cl %>%
  select(bl:bm, cl) %>%
  mutate(type = "data") %>%
  bind_rows(bind_cols(penguins_mce$ell,
                      type=rep("ellipse",
                               nrow(penguins_mce$ell)))) %>%
  mutate(type = factor(type))
```

Using the tour to visualise the final choices of models with similarly high BIC values helps to choose which best fits the data. It may not be the one with the highest BIC value.



(a) Four-cluster VEE (b) Three-cluster EEE

Figure 10.4: Examining the model-based clustering results for the penguins data: (a) best model according to BIC value, (b) simpler three-cluster model. Dots are ellipse points, and "x" are data points. It is important to note that the three cluster solution fits the data better, even though it has a lower BIC.

Exercises

1. Examine the three cluster EVE, VVE and VEE models with the tour, and explain whether these are distinguishably different from the EEE three cluster model.
2. Fit model-based clustering to the the `clusters`. Does it suggest the data has three clusters? Using the tour examine the best model model. How well does this fit the data?
3. Fit model-based clustering to the the `multicluster`. Does it suggest the data has six clusters? Using the tour examine the best model model. How well does this fit the data?
4. Fit model-based clustering to the `fake_trees` data. Does it suggest that the data has 10 clusters? If not, why do you think this is? Using the tour examine the best model model. How well does this fit the branching structure?
5. Try fitting model-based clustering to the `aflw` data? What is the best model? Is the solution related to offensive vs defensive vs mid-fielder skills?
6. Use model-based clustering on the challenge data sets, `c1-c7` from the `mulgar` package. Explain why or why not the best model fits the cluster structure or not.

11

Self-organizing maps

A self-organizing map (SOM) Kohonen (2001) is constructed using a constrained k-means algorithm. A 1D or 2D net is stretched through the data. The knots, in the net, form the cluster means, and the points closest to the knot are considered to belong to that cluster. The similarity of nodes (and their corresponding clusters) is defined as proportional to their distance from one another on the net. Unlike k-means one would normally choose a largish net, with more nodes than expected clusters. A well-separated cluster in the data would likely be split across multiple nodes in the net. Examining the net where nodes are empty of points we would interpret this as a gap in the original data.

A self-organising map is like a fisherwoman's net, as the net is pulled in it catches the fish near knots in the net. We would examine the net in

- 2D to extract the fish.
- high-dimensions to see how it was woven through the space to catch fish.

Figure **??** illustrates how the SOM fits the penguins data. SOM is not ideal for clustered data where there are gaps. It is better suited for data that lies on a non-linear low-dimensional manifold. To model data like the penguins the first step is to set up a net that will cover more than the three clusters. Here we have chosen to use a 5×5 rectangular grid. (The option allows for a hexagonal grid, which would make for a better tiled 2D map, but this is not useful for viewing the model in high dimensions.) Like k-means clustering the fitted model can change substantially depending on the initialisation, so setting a seed will ensure a consistent result. We have also initialised the positions of the knots using PCA, which stretches the net in the main two directions of variance of the data, generally giving better results.

```
library(kohonen)
library(aweSOM)
library(mulgar)
library(dplyr)
```

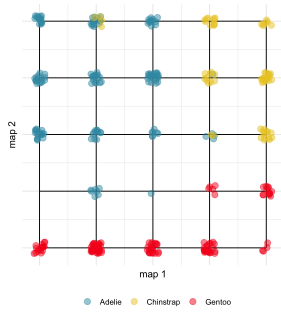
```
library(ggplot2)
library(colorspace)
load("data/penguins_sub.rda")

set.seed(947)
p_grid <- kohonen::somgrid(xdim = 5, ydim = 5,
                           topo = 'rectangular')
p_init <- somInit(as.matrix(penguins_sub[,1:4]), 5, 5)
p_som <- som(as.matrix(penguins_sub[,1:4]),
             rlen=2000,
             grid = p_grid,
             init = p_init)
```

The resulting model object is used to construct an object containing the original data, the 2D map, the map in p-D, with edges, and segments to connect points to represent the next using the `som_model()` function from `mulgar`. The 2D map shows a configuration of the data in 2D which best displays the clusters, much like how a PCA or LDA plot would eb used.

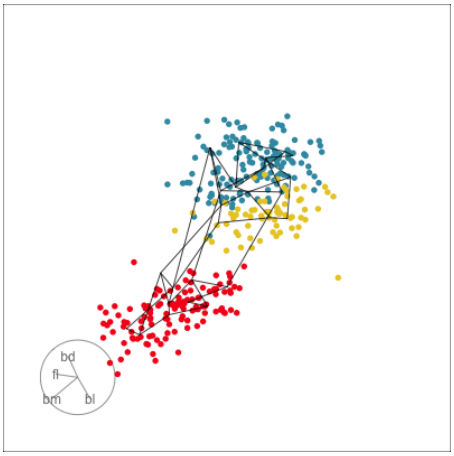
```
p_som_df_net <- som_model(p_som)
p_som_data <- p_som_df_net$data %>%
  mutate(species = penguins_sub$species)
p_som_map_p <- ggplot() +
  geom_segment(data=p_som_df_net$edges_s,
               aes(x=x, xend=xend, y=y,
                   yend=yend)) +
  geom_point(data=p_som_data,
             aes(x=map1, y=map2,
                 colour=species),
             size=3, alpha=0.5) +
  xlab("map 1") + ylab("map 2") +
  scale_color_discrete_divergingx(
    palette="Zissou 1") +
  theme_minimal() +
  theme(aspect.ratio = 1,
        legend.position = "bottom",
        legend.title = element_blank(),
        axis.text = element_blank())
```

The object can also be modified into the pieces needed to show the net in p-D. You need the data, points marking the net, and edges indicating which points to connect to draw the net.

```
library(tourr)

# Set up data
p_som_map <- p_som_df_net$net %>%
  mutate(species = "0", type="net")
p_som_data <- p_som_data %>%
  select(bl:bm, species) %>%
  mutate(type="data",
         species = as.character(species))
p_som_map_data <- bind_rows(p_som_map, p_som_data)
p_som_map_data$type <- factor(p_som_map_data$type,
  levels=c("net", "data"))
p_som_map_data$species <- factor(p_som_map_data$species,
  levels=c("0","Adelie","Chinstrap","Gentoo"))
p_pch <- c(46, 16)[as.numeric(p_som_map_data$type)]
p_col <- c("black", hcl.colors(3, "Zissou 1"))[as.numeric(p_som_map_data$species)]
animate_xy(p_som_map_data[,1:4],
           col=p_col,
           pch=p_pch,
           edges=as.matrix(p_som_df_net$edges),
           edges.col = "black",
           axes="bottomleft")
```



(a) 2D map



(b) Map in 4D

Examining the SOM map views in 2D and with the data in 4D. Points are coloured by species, which was not used for the modeling. The 2D map shows that the `map 2` direction is primarily distinguishing the Gentoo from the others, and `map 1` is imperfectly distinguishing the Chinstrap from Adelie. The map in the data space shows how it is woven into the shape of the data.

The SOM fit, with a 5×5 grid, for the penguins has the data clustered into 25 groups. This doesn't work as a clustering technique on its own, if we remember that the data has three clusters corresponding to three species of penguins. Using species to colour the points helps to see what SOM has done. It has used about seven nodes to capture the separated Gentoo group. These are mostly in the `map 2` direction, which means that this direction (like a direction in PCA) is useful for distinguishing the Gentoo penguins from the others. The other two species are mixed on the map, but roughly spread out on the direction of `map 1`.

Exercises

1. Fit an SOM to the first four PCs of the `aflw` data. Examine the best solution (you choose the size of the net), and describe how the map lays out the data. Does it show offensive vs defensive vs midfield players? Or does it tend to show high skills vs low skills?
2. Fit an SOM to the first 10 PCs of the `fake_trees` data, using your choice of net size. How well does the map show the branching structure?
3. Examine a range of SOM nets fitted to the first 10 PCs of the `fake_trees` data in the 10D space using a tour. Set the values of `rlen` to be 5, 50, 500. How does the net change on this parameter?
4. Plot the distances output for the SOM fit to the penguins data. Mark the observations that have the 5 biggest distances, and show these in a tour. These are the observations where the net has fitted least well, and may be outliers.
5. Use SOM on the challenge data sets, `c1-c7` from the `mulgar` package. What is the best choice of number of knots for each? Explain why or why not the model fits the cluster structure of each or not.

12

Summarising and comparing clustering results

12.1 Summarising results

The key elements for summarising cluster results are the centres of the clusters and the within-cluster variability of the observations. Adding cluster means to any plot, including tour plots, is easy. You add the additional rows, or a new data set, and set the point shape to be distinct.

Summarising the variability is difficult. For model-based clustering, the shape of the clusters is assumed to be elliptical, so p-dimensional ellipses can be used to show the solution, as done in Chapter 10. Generally, it is common to plot a convex hull of the clusters, as in Figure 12.1. This can also be done in high-dimensions, using the R package `cxhull` to compute the p-D convex hull.

```
library(mclust)
library(tidyr)
library(dplyr)
library(gt)
library(cxhull)
library(ggplot2)
library(colorspace)
```

```
library(mclust)
library(tidyr)
library(dplyr)
library(gt)
library(cxhull)
library(ggplot2)
library(colorspace)
load("data/penguins_sub.rda")
p_dist <- dist(penguins_sub[,1:4])
p_hcw <- hclust(p_dist, method="ward.D2")

p_cl <- data.frame(cl_w = cutree(p_hcw, 3))
```

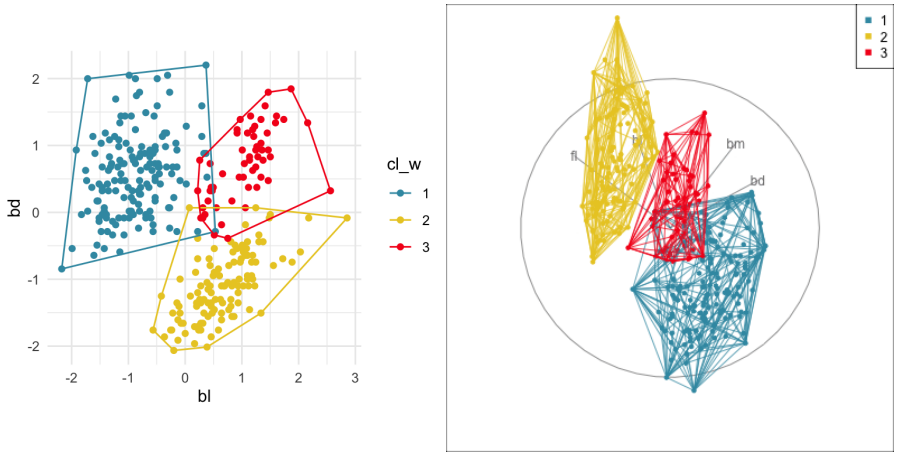
```
penguins_mc <- Mclust(penguins_sub[,1:4],
                      G=3,
                      modelNames = "EEE")
p_cl <- p_cl %>%
  mutate(cl_mc = penguins_mc$classification)

p_cl <- p_cl %>%
  mutate(cl_w_j = jitter(cl_w),
         cl_mc_j = jitter(cl_mc))

# Arranging by cluster id is important to define edges
penguins_cl <- penguins_sub %>%
  mutate(cl_w = p_cl$cl_w,
         cl_mc = p_cl$cl_mc) %>%
  arrange(cl_w)
```

```
# Penguins in 2D
# Duplicate observations need to be removed fo convex hull calculation
psub <- penguins_cl %>%
  select(bl, bd)
dup <- duplicated(psub)
psub <- penguins_cl %>%
  select(bl, bd, cl_w) %>%
  filter(!dup) %>%
  arrange(cl_w)

ncl <- psub %>%
  count(cl_w) %>%
  arrange(cl_w) %>%
  mutate(cumn = cumsum(n))
phull <- NULL
for (i in unique(psub$cl_w)) {
  x <- psub %>%
    dplyr::filter(cl_w == i) %>%
    select(bl, bd)
  ph <- cxhull(as.matrix(x))$edges
  if (i > 1) {
    ph <- ph + ncl$cumn[i-1]
  }
  ph <- cbind(ph, rep(i, nrow(ph)))
  phull <- rbind(phull, ph)
}
phull <- as.data.frame(phull)
colnames(phull) <- c("from", "to", "cl_w")
```

```
phull_segs <- data.frame(x = psub$bl[phull$from],
                         y = psub$bd[phull$from],
                         xend = psub$bl[phull$to],
                         yend = psub$bd[phull$to],
                         cl_w = phull$cl_w)
phull_segs$cl_w <- factor(phull$cl_w)
psub$cl_w <- factor(psub$cl_w)
p_chull2D <- ggplot() +
  geom_point(data=psub, aes(x=bl, y=bd,
                            colour=cl_w)) +
  geom_segment(data=phull_segs, aes(x=x, xend=xend,
                                    y=y, yend=yend,
                                    colour=cl_w)) +
  scale_colour_discrete_divergingx(palette = "Zissou 1") +
  theme_minimal() +
  theme(aspect.ratio = 1)
```

```
ncl <- penguins_cl %>%
  count(cl_w) %>%
  arrange(cl_w) %>%
  mutate(cumn = cumsum(n))
phull <- NULL
for (i in unique(penguins_cl$cl_w)) {
  x <- penguins_cl %>%
    dplyr::filter(cl_w == i)
  ph <- cxhull(as.matrix(x[,1:4]))$edges
  if (i > 1) {
    ph <- ph + ncl$cumn[i-1]
  }
  ph <- cbind(ph, rep(i, nrow(ph)))
  phull <- rbind(phull, ph)
}
phull <- as.data.frame(phull)
colnames(phull) <- c("from", "to", "cl_w")
phull$cl_w <- factor(phull$cl_w)
penguins_cl$cl_w <- factor(penguins_cl$cl_w)

animate_xy(penguins_cl[,1:4], col=penguins_cl$cl_w,
           edges=as.matrix(phull[,1:2]), edges.col=phull$cl_w)
render_gif(penguins_cl[,1:4],
           tour_path = grand_tour(),
           display = display_xy(col=penguins_cl$cl_w,
                                edges=as.matrix(phull[,1:2]),
                                edges.col=phull$cl_w),
```

```
          gif_file = "gifs/penguins_chull.gif",
          frames = 500,
          width = 400,
          height = 400)
```



(a) 2D (b) 4D

Figure 12.1: Convex hulls summarising the extent of Wards linkage clustering in 2D and 4D.

12.2 Comparing two clusterings

Each cluster analysis will result in a vector of class labels for the data. To compare two results we would tabulate and plot the pair of integer variables. The labels given to each cluster will likely differ. If the two methods agree, there will be just a few cells with large counts among mostly empty cells.

Below is a comparison between the three cluster results of Wards linkage hierarchical clustering (rows) and model-based clustering (columns). The two methods mostly agree, as seen from the three cells with large counts, and most cells with zeros. They disagree only on eight penguins. These eight penguins would be considered to be part of cluster 1 by Wards, but model-based considers them to be members of cluster 2.

The two methods label them clusters differently: what Wards labels as cluster 3, model-based labels as cluster 2. The labels given by any algorithm are arbitrary, and can easily be changed to coordinate between methods.

```
p_cl %>%
  count(cl_w, cl_mc) %>%
  pivot_wider(names_from = cl_mc,
              values_from = n,
              values_fill = 0) %>%
  gt() %>%
  tab_spanner(label = "cl_mc", columns=c(`2`, `3`, `1`)) %>%
  cols_width(everything() ~ px(60))
```

	cl_mc		
cl_w	2	3	1
1	8	0	149
2	0	119	0
3	57	0	0

We can examine the disagreement by linking a plot of the table, with a tour plot. Here is how to do this with `liminal`. Figure 12.2 and Figure 12.3 show screenshots of the exploration of the eight penguins on which the methods disagree. It makes sense that there is some confusion. These penguins are part of the large clump of observations that don't separate cleanly into two clusters. The eight penguins are in the middle of this clump. Realistically, both methods result in a plausible clustering, and it is not clear how these penguins should be grouped.

```
library(liminal)
limn_tour_link(
  p_cl[,3:4],
  penguins_cl,
  cols = bl:bm,
  color = cl_w
)
```

Exercises

1. Compare the results of the four cluster model-based clustering with that of the four cluster Wards linkage clustering of the penguins data.

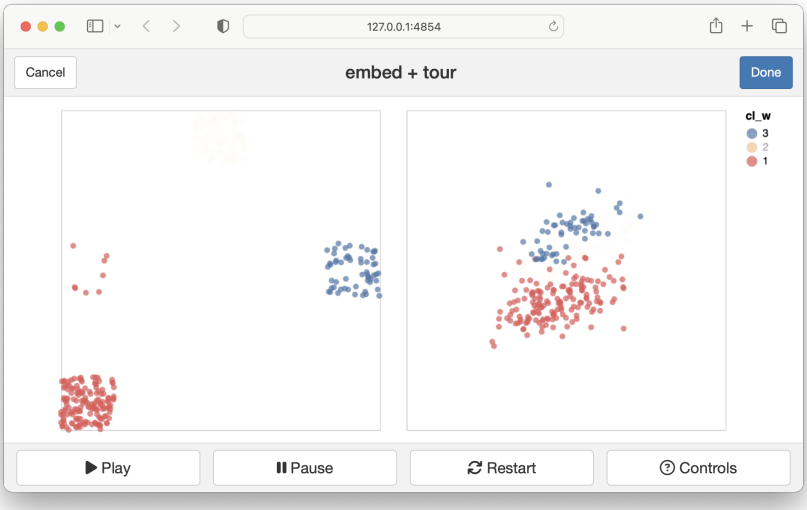


Figure 12.2: Linking the confusion table with a tour using liminal. Points are coloured according to Wards linkage. The disagreement on eight penguins is with cluster 1 from Wards and cluster 2 from model-based.

Figure 12.3: Highlighting the penguins where the methods disagree so we can see where these observations are located relative to the two clusters.

2. Compare the results from clustering of the `fake_trees` data for two different choices of k. (This follows from the exercise in Chapter 9.) Which choice of k is best? And what choice of k best captures the 10 known branches?
3. Compare and contrast the cluster solutions for the first four PCs of the `aflw` data, conducted in Chapter 8 and Chapter 9. Which provides the most useful clustering of this data?
4. Pick your two clusterings on one of the challenge data sets, `c1-c7` from the `mulgar` package, that give very different results. Compare and contrast the two solutions, and decide which is the better solution.

Project

Most of the time your data will not neatly separate into clusters, but partitioning it into groups of similar observations can still be useful. In this case our toolbox will be useful in comparing and contrasting different methods, understanding to what extend a cluster mean can describe the observations in the cluster, and also how the boundaries between clusters have been drawn. To explore this we will use survey data that examines the risk taking behavior of tourists. The data was collected in Australia in 2015 (Hajibaba et al., 2016) and includes six types of risks (recreational, health, career, financial, safety and social) with responses on a scale from 1 (never) to 5 (very often). The data is available in `risk_MSA.rds` from the book web site.

1. We first examine the data in a grand tour. Do you notice that each variable was measured on a discrete scale?
2. Next we explore different solutions from hierarchical clustering of the data. For comparison we will keep the number of clusters fixed to 6 and we will perform the hierarchical clustering with different combinations of distance functions (Manhattan distance and Euclidean distance) and linkage (single, complete and Ward linkage). Which combinations make sense based on what we know about the method and the data?
3. For each of the hierarchical clustering solutions draw the dendrogram in 2D and also in the data space. You can also map the grouping into 6 clusters to different colors. How would you describe the different solutions?
4. Using the method introduced in this chapter, compare the solution using Manhattan distance and complete linkage to one using Euclidean distance and Ward linkage. First compute a confusion

table and then use `liminal` to explore some of the differences. For example, you should be able to see how small subsets where the two clustering solutions disagree can be outlying and are grouped differently depending on the choices we make.

5. Selecting your preferred solution from hierarchical clustering, we will now compare it to what is found using k-means clustering with $k = 6$. Use a tour to show the cluster means together with the data points (make sure to pick an appropriate symbol for the data points to avoid too much overplotting). What can you say about the variation within the clusters? Can you match some of the clusters with the most relevant variables from following the movement of the cluster means during the tour?
6. Use a projection pursuit guided tour to best separate the clusters identified with k-means clustering. How are the clusters related to the different types of risk?
7. Use the approaches from this chapter to summarize and compare the k-means solution to your selected hierarchical clustering results. Are the groupings mostly similar? You can also use convex hulls to better compare what part of the space is occupied. Either look at subsets (selected from the liminal display) or you could facet the display using `tourr::animate_groupxy`.
8. Some other possible activities include examining how model-based methods would cluster the data. We expect it should be similar to Wards hierarchical or k-means, that it will partition into roughly equal chunks with an EII variance-covariance model being optimal. Also examining an SOM fit. SOM is not ideal for this data because the data fills the space. If the SOM model is fitted properly it should be a tangled net where the nodes (cluster means) are fairly evenly spread out. Thus the result should again be similar to Wards hierarchical or k-means. A common problem with fitting an SOM is that optimisation stops early, before fully capturing the data set. This is the reasons to use the tour for SOM. If the net is bunched in one part of the data space, it means that the optimisation wasn't successful.

13

Introduction to supervised classification

Methods for supervised classification originated in the field of Statistics in the early nineteenth century, under the moniker *discriminant analysis* (see, for example, Fisher (1936b)). An increase in the collection of data, and storage in databases, in the late twentieth century has inspired a growing desire to extract knowledge from data, particularly to be able accurately predict the class labels. This has contributed to an explosion of research on new methods, especially on algorithms that focus on accurate prediction of new data based on training samples.

In contrast to unsupervised classification, the class label (categorical response variable) is known, in the training sample. The training sample is used to build the prediction model, and also to estimate the accuracy, or inversely error, of the model for future data. It is also important to understand the model and to interpret it, so that we can know how predictions are made. High-dimensional visualisation can help with this, and helps to tackle questions like:

- Are the classes well separated in the data space, so that they correspond to distinct clusters? If so, what are the shapes of the clusters? Is each cluster sufficiently ellipsoidal so that we can assume that the data arises from a mixture of multivariate normal distributions? Do the clusters exhibit characteristics that suggest one algorithm in preference to others?
- Where does the boundary between classes fall? Are the classes linearly separable, or does the difference between classes suggest a non-linear boundary? How do changes in the input parameters affect these boundaries? How do the boundaries generated by different methods vary?
- What cases are misclassified, or have more uncertain predictions? Are there places in the data space where predictions are especially good or bad?
- Which predictors most contribute to the model predictions? Is it possible to reduce the set of explanatory variables?

Addressing these types of queries also motivate the emerging field called explainable artificial intelligence (XAI), which goes beyond predictive accuracy to more completely satisfy the *desire to extract knowledge from data.*

Although we focus on categorical response, some of the techniques here can be modified or adapted for problems with a numeric, or continuous, response

variable. With a categorical response, and numerical predictors, we map colour to the response variable and use the tour to examine the relationship between predictors, and the different classes.

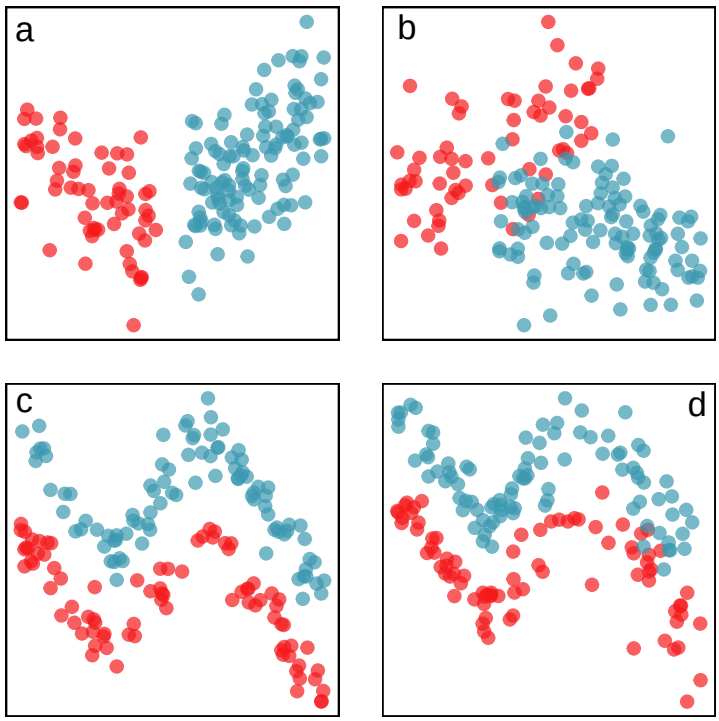


Figure 13.1: Examples of supervised classification patterns: (a) linearly separable, (b) linear but not completely separable, (c) non-linearly separable, (d) non-linear, but not completely separable.

Figure 13.1 shows some 2D examples where the two classes are (a) linearly separable, (b) not completely separable but linearly different, (c) non-linearly separable and (d) not completely separable but with a non-linear difference. We can also see that in (a) only the horizontal variable would be important for the model because the two classes are completely separable in this direction. Although the pattern in (c) is separable classes, most models would have difficulty capturing the separation. It is for this reason that it is important to understand the boundary between classes produced by a fitted model. In each of b, c, d it is likely that some observations would be misclassified. Identifying these cases, and inspecting where they are in the data space is important for understanding the model's future performance.

14

Linear discriminant analysis

Linear discriminant analysis (LDA) dates to the early 1900s. It's one of the most elegant and simple techniques for both modeling separation between groups, and as an added bonus, producing a low-dimensional representation of the differences between groups. LDA has two strong assumptions: the groups are samples from multivariate normal distributions, and each have the same variance-covariance. If the latter assumption is relaxed, a slightly less elegant solution results from quadratic discriminant analysis.

Useful explanations can be found in Venables & Ripley (2002a) and Ripley (1996). A good general treatment of parametric methods for supervised classification can be found in R. A. Johnson & Wichern (2002) or another similar multivariate analysis textbook. It's also useful to know that hypothesis testing for the difference in multivariate means using multivariate analysis of variance (MANOVA) has similar assumptions to LDA. Also model-based clustering assumes that each cluster arises from a multivariate normal distribution, and is related to LDA. The methods described here can be used to check these assumptions when applying these methods, too.

Because LDA is a parametric model it is important to check that these assumptions are reasonably satisfied:

- shape of clusters are elliptical.
- spread of the observations are the same.

14.1 Extracting the key elements of the model

LDA builds the model on the between-group sum-of-square matrix

$$B = \sum_{k=1}^{g} n_k (\bar{X}_k - \bar{X})(\bar{X}_k - \bar{X})^\top$$

which measures the differences between the class means, compared with the overall data mean $\bar{X}$ and the within-group sum-of-squares matrix,

$$W = \sum_{k=1}^{g} \sum_{i=1}^{n_k} (X_{ki} - \bar{X}_k)(X_{ki} - \bar{X}_k)^\top$$

which measures the variation of values around each class mean. The linear discriminant space is generated by computing the eigenvectors (canonical coordinates) of $W^{-1}B$, and this is the $(g-1)$-D space where the group means are most separated with respect to the pooled variance-covariance. For each class we compute

$$\delta_k(x) = (x - \mu_k)^\top W^{-1} \mu_k + \log \pi_k$$

where π_k is a prior probability for class k that might be based on unequal sample sizes, or cost of misclassification. The LDA classifier rule is to *assign a new observation to the class with the largest value* of $\delta_k(x)$.

We can fit an LDA model using the `lda()` function from the `MASS` package. Here we have used the `penguins` data, assuming equal prior probability, to illustrate.

```
# Code to fit the model
library(dplyr)
library(mulgar)
library(MASS)
load("data/penguins_sub.rda")

p_lda <- lda(species~bl+bd+fl+bm,
             data=penguins_sub,
             prior=c(1/3, 1/3, 1/3))
options(digits=2)
# p_lda
```

Because there are three classes the dimension of the discriminant space is 2D. We can easily extract the group means from the model.

```
# Extract the sample means
p_lda$means
```

```
             bl    bd    fl    bm
Adelie    -0.95  0.60 -0.78 -0.62
Chinstrap  0.89  0.64 -0.37 -0.59
Gentoo     0.65 -1.10  1.16  1.10
```

The coefficients to project the data into the discriminant space, that is the eigenvectors of $W^{-1}B$ are:

```
# Extract the discriminant space
p_lda$scaling
```

```
     LD1   LD2
bl -0.24 -2.31
bd  2.04  0.19
fl -1.20  0.08
bm -1.22  1.24
```

and the predicted values, which include class predictions, and coordinates in the discriminant space are generated as:

```
# Extract the fitted values
p_lda_pred <- predict(p_lda, penguins_sub)
```

The best separation between classes can be viewed from this object, which can be shown to match the original data projected using the `scaling` component of the model object (see Figure 14.1).

```
# Check calculations from the fitted model, and equations
library(colorspace)
library(ggplot2)
library(ggpubr)
# Using the predicted values from the model object
p_lda_pred_x1 <- data.frame(p_lda_pred$x)
p_lda_pred_x1$species <- penguins_sub$species
p_lda1 <- ggplot(p_lda_pred_x1,
                 aes(x=LD1, y=LD2,
                     colour=species)) +
  geom_point() +
  xlim(-6, 8) + ylim(-6.5, 5.5) +
  scale_color_discrete_divergingx("Zissou 1") +
  ggtitle("(a)") +
  theme_minimal() +
  theme(aspect.ratio = 1, legend.title = element_blank())

# matches the calculations done manually
p_lda_pred_x2 <- data.frame(as.matrix(penguins_sub[,1:4]) %*%
                              p_lda$scaling)
p_lda_pred_x2$species <- penguins_sub$species
p_lda2 <- ggplot(p_lda_pred_x2,
```

```
                  aes(x=LD1, y=LD2,
                      colour=species)) +
  geom_point() +
  xlim(-6, 8) + ylim(-7, 5.5) +
  scale_color_discrete_divergingx("Zissou 1") +
  ggtitle("(b)") +
  theme_minimal() +
  theme(aspect.ratio = 1, legend.title = element_blank())
ggarrange(p_lda1, p_lda2, ncol=2,
          common.legend = TRUE, legend = "bottom")
```

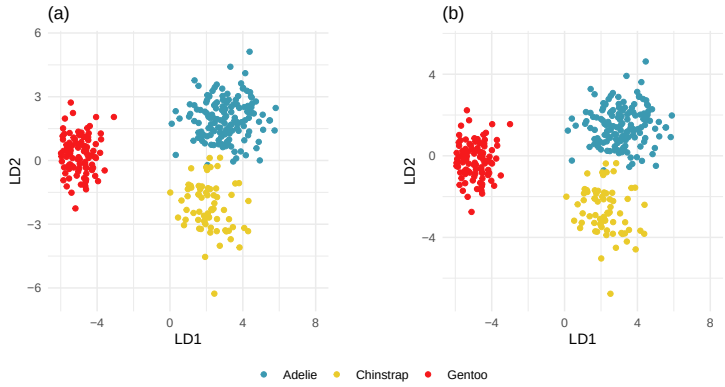


Figure 14.1: Penguins projected into the 2D discriminant space, done two ways: (a) using the predicted values, (b) directly projecting using the model component. The scale is not quite the same but the projected data is identical in shape.

The W and B matrices cannot be extracted from the model object, so we need to compute these separately. We only need W actually. It is useful to think of this as the pooled variance-covariance matrix. Because the assumption for LDA is that the population group variance-covariances are identical, we estimate this by computing them for each class and then averaging them to get the pooled variance-covariance matrix. It's laborious, but easy.

```
# Compute pooled variance-covariance
p_vc_pool <- mulgar::pooled_vc(penguins_sub[,1:4],
                               penguins_sub$species)
p_vc_pool
```

```
     bl   bd   fl   bm
bl 0.31 0.18 0.13 0.18
```

```
bd 0.18 0.32 0.14 0.20
fl 0.13 0.14 0.23 0.16
bm 0.18 0.20 0.16 0.31
```

This can be used to draw an ellipse corresponding to the pooled variance-covariance that is used by the LDA model.

14.2 Checking assumptions

This LDA approach is widely applicable, but it is useful to check the underlying assumptions on which it depends: (1) that the cluster structure corresponding to each class forms an ellipse, showing that the class is consistent with a sample from a multivariate normal distribution, and (2) that the variance of values around each mean is nearly the same. Figure 14.2 and Figure 14.3 illustrates two datasets, of which only one is consistent with these assumptions. Other parametric models, such as quadratic discriminant analysis or logistic regression, also depend on assumptions about the data which should be validated.

To check the equal and elliptical variance-covariance assumption, generate points on the surface of an ellipse corresponding to the variance-covariance for each group. When watching these ellipses in a tour, they should similar in all projections.

```
# Generate ellipses for each group's variance-covariance
p_ell <- NULL
for (i in unique(penguins_sub$species)) {
  x <- penguins_sub %>% dplyr::filter(species == i)
  e <- gen_xvar_ellipse(x[,1:2], n=150, nstd=1.5)
  e$species <- i
  p_ell <- bind_rows(p_ell, e)
}
```

The equal and elliptical variance-covariance assumption is reasonable for the penguins data because the ellipse shapes roughly match the spread of the data. It is not a suitable assumption for the bushfires data, because the spread is not elliptically-shaped and varies in size between groups.

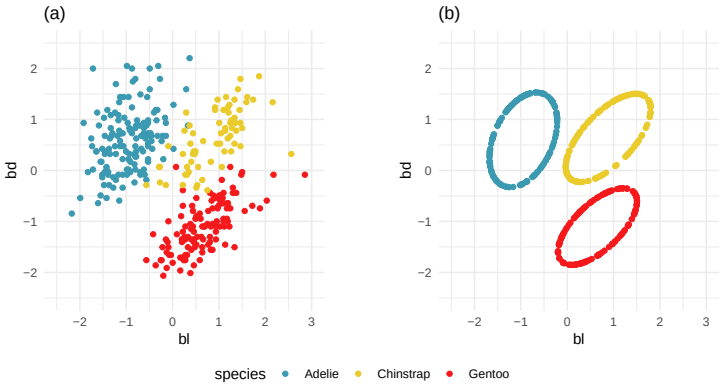


Figure 14.2: Scatterplot of flipper length by bill length of the penguins data, and corresponding variance-covariance ellipses. There is a small amount of difference between the ellipses, but they are similar enough to be confident in assuming the population variance-covariances are equal.

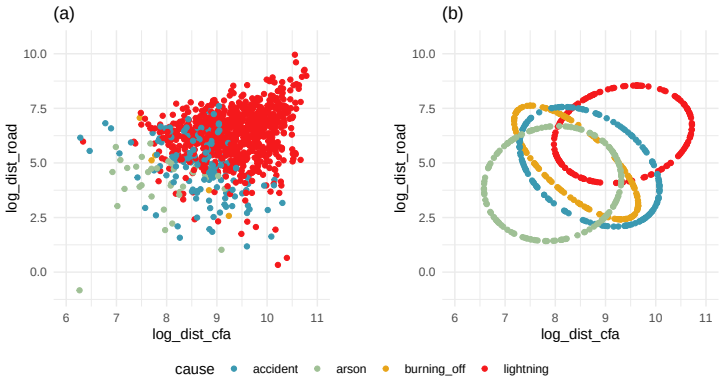
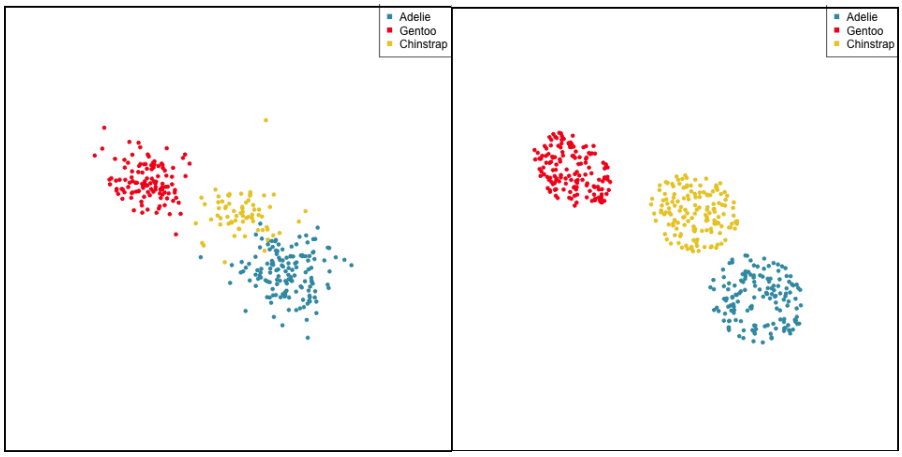


Figure 14.3: Scatterplot of distance to cfa and road for the bushfires data, and corresponding variance-covariance ellipses. There is a lot of difference between the ellipses, so it cannot be assumed that the population variance-covariances are equal.

This approach extends to any dimension. We would use the same projection sequence to view both the data and the variance-covariance ellipses, as in Figure 14.4. It can be seen that there is some difference in the shape and size of the ellipses between species, in some projections, and also with the spread of points in the projected data. However, it is the differences are small, so it would be safe to assume that the population variance-covariances are equal.



(a) Data (b) Variance-covariance ellipses

Figure 14.4: Checking the assumption of equal variance-covariance matrices for the 4D penguins data. Each ellipse corresponds to the sample variance-covariance for each species.

As a further check, we could generate three ellipses corresponding to the pooled variance-covariance matrix, as would be used in the model, centered at each of the means. Overlay this with the data, as done in Figure 14.5. Now you will compare the spread of the observations in the data, with the elliptical shape of the pooled variance-covariance. If it matches reasonably we can safely use LDA. This can also be done group by group when multiple groups make it difficult to view all together.

To check the fit of the equal variance-covariance assumption, simulate points on the ellipse corresponding to the *pooled sample variance-covariance matrix*. Generate one for each group centered at the group mean, and compare with the data.

```
# Create an ellipse corresponding to pooled vc
pool_ell <- gen_vc_ellipse(p_vc_pool,
                           xm=rep(0, ncol(p_vc_pool)))
```

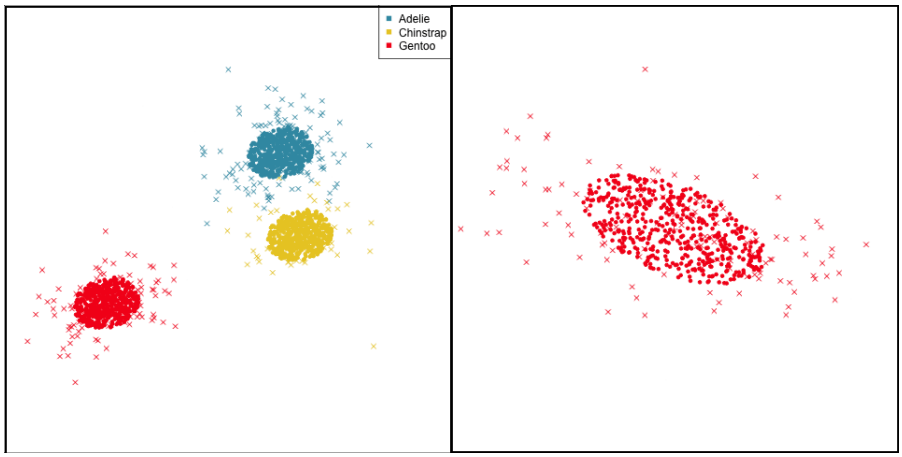
```
# Add means to produce ellipses for each species
p_lda_pool <- data.frame(rbind(
  pool_ell +
    matrix(rep(p_lda$means[1,],
      each=nrow(pool_ell)), ncol=4),
  pool_ell +
    matrix(rep(p_lda$means[2,],
      each=nrow(pool_ell)), ncol=4),
  pool_ell +
    matrix(rep(p_lda$means[3,],
      each=nrow(pool_ell)), ncol=4)))
# Create one data set with means, data, ellipses
p_lda_pool$species <- factor(rep(levels(penguins_sub$species),
                           rep(nrow(pool_ell), 3)))
p_lda_pool$type <- "ellipse"
p_lda_means <- data.frame(
  p_lda$means,
  species=factor(rownames(p_lda$means)),
                           type="mean")
p_data <- data.frame(penguins_sub[,1:5],
                     type="data")
p_lda_all <- bind_rows(p_lda_means,
                       p_data,
                       p_lda_pool)
p_lda_all$type <- factor(p_lda_all$type,
   levels=c("mean", "data", "ellipse"))
shapes <- c(3, 4, 20)
p_pch <- shapes[p_lda_all$type]
```

From the tour, we can see that the assumption of equal elliptical variance-covariance is a reasonable assumption for the penguins data. In all projections the ellipse is reasonably matching the spread of the observations.

14.3 Examining results

The boundaries for a classification model can be examined by:

1. generating a large number of test points in the domain of the data



(a) All species (b) Gentoo

Figure 14.5: Checking how the pooled variance-covariance matches the spread of points in each group.

2. predicting the class for each test point

We'll look at this for 2D using the LDA model fitted to `bl`, and `bd` of the `penguins` data.

```
p_bl_bd_lda <- lda(species~bl+bd, data=penguins_sub,
                                  prior = c(1/3, 1/3, 1/3))
```

The fitted model means $\bar{x}_{Adelie} =$ (-0.95, 0.6)$^\top$, $\bar{x}_{Chinstrap} =$ (0.89, 0.64)$^\top$, and $\bar{x}_{Gentoo} =$ (0.65, -1.1)$^\top$ can be added to the plots.

The boundaries can be examined using the `explore()` function from the `classifly` package, which generates observations in the range of all values of`bl` and `bd` and predicts their class. Figure 14.6 shows the resulting prediction regions, with the observed data and the sample means overlaid.

```
# Compute points in domain of data and predict
library(classifly)

p_bl_bd_lda_boundaries <- explore(p_bl_bd_lda, penguins_sub)
p_bl_bd_lda_m1 <- ggplot(p_bl_bd_lda_boundaries) +
  geom_point(aes(x=bl, y=bd,
                 colour=species,
                 shape=.TYPE), alpha=0.8) +
  scale_color_discrete_divergingx("Zissou 1") +
```

```
  scale_shape_manual(values=c(46, 16)) +
  theme_minimal() +
  theme(aspect.ratio = 1, legend.position = "none")

p_bl_bd_lda_means <- data.frame(p_bl_bd_lda$means,
                        species=rownames(p_bl_bd_lda$means))
p_bl_bd_lda_m1 +
  geom_point(data=p_bl_bd_lda_means,
             aes(x=bl, y=bd),
             colour="black",
             shape=3,
             size=3)
```

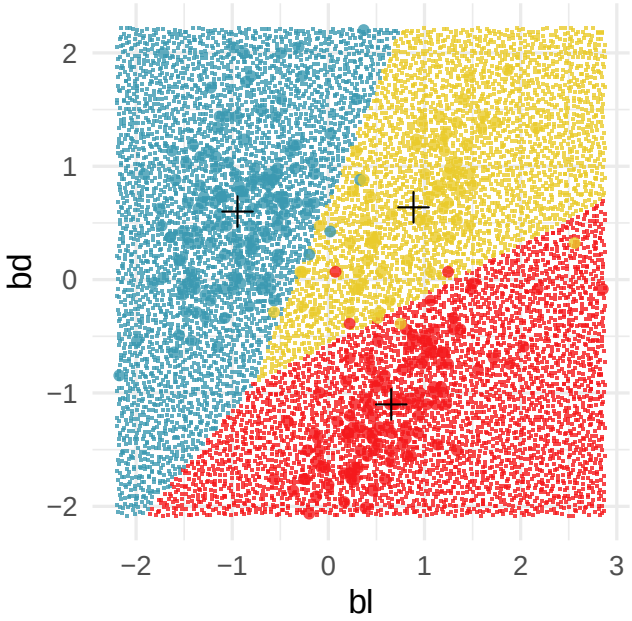
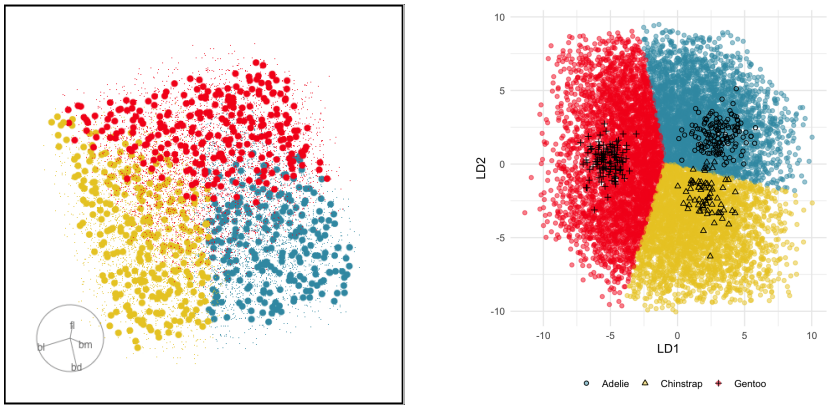


Figure 14.6: Prediction regions of the LDA model for two variables of the three species of penguins indicated by the small points. Large points are the observations, and the sample mean of each species is represented by the plus. The boundaries between groups can be seen to be roughly half-way between the means, taking the elliptical spread into account, and mostly distinguishes the three species.

This approach can be readily extended to higher dimensions. One first fits the model with all four variables, and uses the `explore()` to generate points in the 4D space with predictions, generating a representation of the prediction

regions. Figure 14.7(a) shows the results using a slice tour (Laa et al., 2020a). Points inside the slice are shown in larger size. The slice is made in the centre of the data, to show the boundaries in this neighbourhood. As the tour progresses we see a thin slice through the centre of the data, parallel with the projection plane. In most projections there is some small overlap of points between groups, which happens because we are examining a 4D object with 2D. The slice helps to alleviate this, allowing a focus on the boundaries in the centre of the cube. In all projections the boundaries between groups is linear, as would be expected when using LDA. We can also see that the model roughly divides the cube into three relatively equally-sized regions.

Figure 14.7(b) shows the three prediction regions, represented by points in 4D, projected into the discriminant space. Linear boundaries neatly divide the full space, which is to be expected because the LDA model computes it's classification rules in this 2D space.



(a) 4D (b) Discriminant space

Figure 14.7: Examining the boundaries produced by the LDA model in the full 4D with a slice tour (left shows a single frame) and in the discriminant space (right). Large points indicate observations within the slice, and dots are observations outside the slice. Focusing on the within-slice points, there is some overlap of points between regions in most views which represents the occlusion of 4D shapes when examining projections with thin slices. The linear boundaries are seen exactly in the discriminant space, that is they are orthogonal to these two dimensions.

From the tour, we can see that the LDA boundaries divide the classes only in the discriminant space. It is not using the space orthogonal to the 2D discriminant space. You can see this because the boundary is sharp in just one 2D projection, while most of the projections show some overlap of regions.

Exercises

1. For the `simple_clusters` compute the LDA model, and make a plot of the data, with points coloured by the class. Overlay variance-covariance ellipses, and a + indicating the sample mean for each class. Is it reasonable to assume that the two classes are sampled from populations with the same variance-covariance?
2. Examine the clusters corresponding to the classes in the `clusters` data set, using a tour. Based on the shape of the data is the assumption of equal variance-covariance reasonable?
3. Examine the pooled variance-covariance for the `clusters` data, overlaid on the data in a tour on the 5D. Does it fit the variance of each cluster nicely?
4. Fit an LDA model to the `simple_clusters` data. Examine the boundaries produced by the model, in 2D.
5. Fit an LDA model to the `clusters` data. Examine the boundaries produced by the model in 5D.
6. Assess the LDA assumptions for the `multicluster` data. Is LDA an appropriate model?
7. Compute the first 12 PCs of the `sketches` data. Check the assumption of equal, elliptical variance-covariance of the 6 groups. Regardless of whether you decide that the assumption is satisfied or not, fit an LDA to the 12 PCs. Extract the discriminant space (the `x` component of the `predict` object), and examine the separation (or not) of the 6 groups in this 5D space. Is LDA providing a good classification model for this data?
8. Even though the `bushfires` data does not satisfy the assumptions for LDA, fit LDA to the first five PCs. Examine the class differences in the 3D discriminant space.
9. Compute the boundary between classes, for the LDA model where the prior probability reflects the sample size, and the LDA model where the priors are equal for all groups. How does the boundary between lightning caused fires and the other groups change?

15

Trees and forests

15.1 Trees

The tree algorithm (Breiman et al., 1984) is a simple and versatile algorithmic method for supervised classification. The basic tree algorithm generates a classification rule by sequentially splitting the data into two buckets. Splits are made between sorted data values of individual variables, with the goal of obtaining pure classes on each side of the split. The inputs for a simple tree classifier commonly include (1) an impurity measure, an indication of the relative diversity among the cases in the terminal nodes; (2) a parameter that sets the minimum number of cases in a node, or the minimum number of observations in a terminal node of the tree; and (3) a complexity measure that controls the growth of a tree, balancing the use of a simple generalizable tree against a more accurate tree tailored to the sample. When applying tree methods, exploring the effects of the input parameters on the tree is instructive; for example, it helps us to assess the stability of the tree model.

Although algorithmic models do not depend on distributional assumptions, that does not mean that every algorithm is suitable for all data. For example, the tree model works best when all variables are independent within each class, because it does not take such dependencies into account. Visualization can help us to determine whether a particular model should be applied. In classification problems, it is useful to explore the cluster structure, comparing the clusters with the classes and looking for evidence of correlation within each class. The plots in Figure 14.2 and Figure 14.4 shows a strong correlation between the variables within each species, which indicates that the tree model may not give good results for the penguins data. We'll show how this is the case with two variables initially, and then extend to the four variables.

The plots in Figure 15.1 show the inadequacies of the tree fit. The background color indicates the class predictions, and thus boundaries produced by the tree fit. They can be seen to be boxy, and missing the elliptical nature of the penguin clusters. This produces errors in the classification of observations which are indefensible. One could always force the tree to fit the data more closely by adjusting the parameters, but the main problem persists: that one is trying to fit elliptical shapes using boxes.

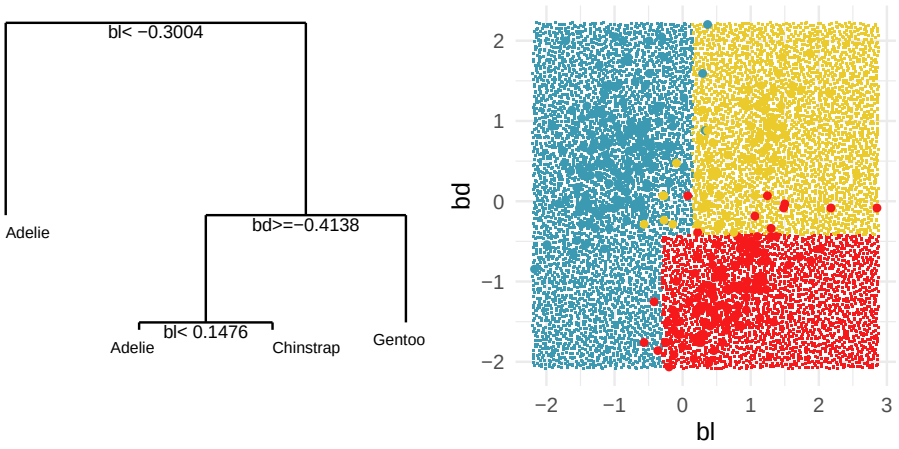
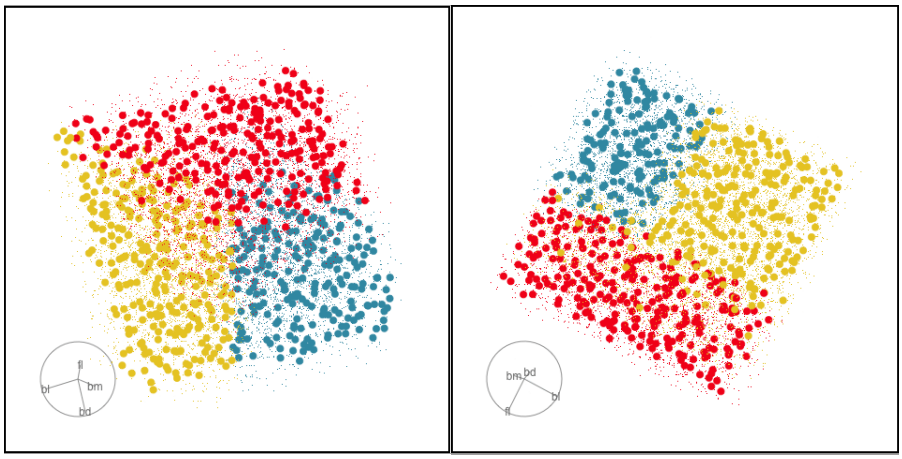


Figure 15.1: The association between variables in the penguins data causes problems for fitting a tree model. Although the model, computed using only bl and bd, is simple (left), the fit is poor (right) because it doesn't adequately utilise combinations of variables.

There are less strict assumptions for a non-parametric model but it is still important to understand the model fit relative to the data.

The boundaries for the tree model on all four variables of the penguins data can be viewed similarly, by predicting a set of points randomly generated in the 4D domain of observed values. Figure 15.2 shows the prediction regions for LDA and a default tree in a slice tour (Laa et al., 2020a). The slice tour is used to help see into the middle of the 4D cube. It slices the cube through the centre of the data, where the boundaries of the regions should meet.

The prediction regions of the default fitted tree are shown in comparison to those from the LDA model. We don't show the tree diagram here, but it makes only six splits of the tree model, which is delightfully simple. However, just like the model fitted to two variables, the result is not adequate for the penguins data. The tree model generates boxy boundaries, whereas the LDA model splits the 4D cube obliquely. The boxy regions don't capture the differences between the elliptically-shaped clusters. Overlaying the observed data on this display would make this clearer, but the boundaries are easier to examine without them.



(a) LDA model (b) Tree model

Figure 15.2: Comparison of the boundaries produced by the LDA (a) and the tree (b) model, using a slice tour. (Here only a single frame is shown.) The tree boundaries are more box-shaped than the LDA boundaries, which does not adequately capture the differences between the elliptically-shaped clusters of the penguins data.

With the penguins data, a tree model may not be a good choice due to the strong correlation between variables. The best separation is in combinations of variables, not the single variable tree splits.

15.2 Random forests

A random forest (Breiman, 2001) is a classifier that is built from multiple trees generated by randomly sampling the cases and the variables. The random sampling (with replacement) of cases has the fortunate effect of creating a training ("in-bag") and a test ("out-of-bag") sample for each tree computed. The class of each case in the out-of-bag sample for each tree is predicted, and the predictions for all trees are combined into a vote for the class identity.

A random forest is a computationally intensive method, a "black box" classifier, but it produces several diagnostics that make the outcome less mysterious.

Some diagnostics that help us to assess the model are the votes, the measure of variable importance, and the proximity matrix.

15.2.1 Examining the votes matrix

Here we show how to use the `randomForest` (Liaw & Wiener, 2002) votes matrix for the penguins data to investigate confusion between classes, and observations which are problematic to classify. The votes matrix can be considered to be predictive probability distribution, where the values for each observation sum to 1. With only three classes the votes matrix is only a 2D object, and thus easy to examine. With four or more classes the votes matrix needs to be examined in a tour.

```
library(randomForest)
library(dplyr)
penguins_rf <- randomForest(species~.,
                            data=penguins_sub[,1:5],
                            importance=TRUE)
```

To examine the votes matrix, we extract the `votes` element from the random forest model object. The first five rows are:

```
head(penguins_rf$votes, 5)
```

```
  Adelie Chinstrap Gentoo
1 0.9860  0.014019      0
2 0.9641  0.035897      0
3 0.9951  0.004878      0
4 1.0000  0.000000      0
5 0.9946  0.005376      0
```

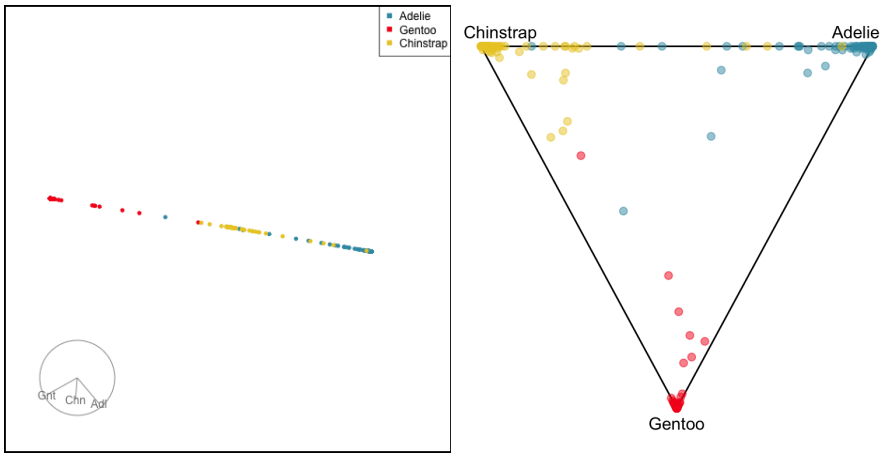
This has three columns corresponding to the three species, but because each row is a set of proportions it is only a 2D object. To reduce the dimension from 3D to the 2D we use a Helmert matrix (Lancaster, 1965). A Helmert matrix has a first row of all 1's. The remaining components of the matrix are 1's in the lower triangle, and 0's in the upper triangle and the diagonal elements are the negative row sum. The rows are usually normalised to have length 1. They are used to create contrasts to test combinations of factor levels for post-testing after Analysis of Variance (ANOVA). For compositional data, like the votes matrix, when the first row is removed a Helmert matrix can be used to reduce the dimension appropriately. For three classes, this will generate the common 2D ternary diagram, but for higher dimensions it will reduce to a $(g-1)$-dimensional simplex. For the penguins data, the Helmert matrix for 3D is

```
geozoo::f_helmert(3)
```

```
          [,1]    [,2]    [,3]
helmert 0.5774  0.5774  0.5774
x       0.7071 -0.7071  0.0000
x       0.4082  0.4082 -0.8165
```

We drop the first row, transpose it, and use matrix multiplication with the votes matrix to get the ternary diagram.

```
# Project 4D into 3D
library(geozoo)
proj <- t(geozoo::f_helmert(3)[-1,])
p_rf_v_p <- as.matrix(penguins_rf$votes) %*% proj
colnames(p_rf_v_p) <- c("x1", "x2")
p_rf_v_p <- p_rf_v_p %>%
  as.data.frame() %>%
  mutate(species = penguins_sub$species)
```



(a) 3D (b) 2D ternary diagram

Figure 15.3: Examining the votes matrix from a random forest fit to the penguins: (a) in a frame from a tour of the 3D, (b) projected into 2D, to make a ternary diagram. In 3D the points can be seen to lie along a 2D plane, which is due to the constraint that the values sum to 1. From the ternary diagram, the classification can be seen to be reasonably well distinguished because points mostly lie at the vertex. There are a few penguins that are confused with a different species, as seen from the few points spread between vertices.

We can use the `geozoo` package to generate the surrounding simplex, which for 2D is a triangle.

The votes matrix reports the proportion of trees each observation is classified as each class. From the tour of the votes matrix, as in Figure 15.3(a), it can be seen to be 2D in 3D space. This is due to the constraint that the three proportions for each observation sum to 1. Using a Helmert matrix, this data can be projected into the 2D space, or more generally the $(g-1)$-dimensional space where it resides, shown in Figure 15.3(b). In 2D this is called a ternary diagram, and in higher dimensions the bounding shapes might be considered to be a simplex. The vertices of this shape correspond to $(1,0,0),(0,1,0),(0,0,1)$ (and analogously for higher dimensions), which represent perfect confidence, that an observation is classified into that group all the time.

What we can see here is a concentration of points in the corners of the triangle indicates that most of the penguins are confidently classified into their correct class. Then there is more separation between the Gentoo and the others, than between Chinstrap and Adelie. That means that as a group Gentoo are more distinguishable. Only one of the Gentoo penguins has substantial confusion, mostly confused as a Chinstrap, but occasionally confused as an Adelie – if it was only ever confused as a Chinstrap it would fall on the edge between Gentoo and Chinstrap. There are quite a few Chinstrap and Adelie penguins confused as each other, with a couple of each more confidently predicted to be the other class. This can be seen because there are points of the wrong colour close to those vertices.

The votes matrix is useful for investigating the fit, but one should remember that there are some structural elements of the penguins data that don't lend themselves to tree models. Although a forest has the capacity to generate non-linear boundaries by combining predictions from multiple trees, it is still based on the boxy boundaries of trees. This makes it less suitable for the penguins data with elliptical classes. You could use the techniques from the previous section to explore the boundaries produced by the forest, and you will find that the are more boxy than the LDA models.

By visualising the votes matrix we can understand which observations are harder to classify, which of the classes are more easily confused with each other.

To examine a vote matrix for a problem with more classes, we will examine the 10 class `fake_trees` data example. The full data has 100 variables, and we have seen from Chapter 7 that reducing to 10 principal components allows the linear branching structure in the data to be seen. Given that the branches correspond to the classes, it will be interesting to see how well the random forest model performs.

```
library(mulgar)
library(dplyr)
library(liminal)
ft_pca <- prcomp(fake_trees[,1:100],
                 scale=TRUE, retx=TRUE)
ft_pc <- as.data.frame(ft_pca$x[,1:10])
ft_pc$branches <- fake_trees$branches
library(randomForest)
ft_rf <- randomForest(branches~., data=ft_pc,
                              importance=TRUE)
```

```
head(ft_rf$votes, 5)
```

```
    0     1    2    3     4    5 6 7     8     9
1 0.9 0.000 0.03 0.00 0.011 0.09 0 0 0.000 0.000
2 0.6 0.000 0.03 0.00 0.005 0.32 0 0 0.000 0.000
3 0.8 0.000 0.07 0.02 0.118 0.03 0 0 0.000 0.011
4 0.9 0.000 0.02 0.00 0.000 0.06 0 0 0.000 0.000
5 0.6 0.006 0.05 0.01 0.035 0.25 0 0 0.006 0.006
```

The votes matrix is 9D, due to the 9 groups. With this many dimensions, if the cluster structure is weak, it will look messy in a tour. However, what we can see in Figure 15.4 is that the structure is relatively simple, and very interesting in that it suggests a strong clustering of classes. Points are coloured by their true class. The lines represent the 8D simplex that bounds the observations, akin to the triangle in the ternary diagram.

Points concentrate at the vertices, which means that most are confidently predicted to be their true class. The most spread of points is along single edges, between pairs of vertices. This means that when there is confusion it is mostly with just one other group. One vertex (0) which has connections to all other vertexes. That is, there are points stretching from this vertex to every other. It means that some observations in every other class can be confused with class 0, and class 0 observations can be confused with every other class. This information suggests that cluster 0 is central to all the other clusters.

Some of this information could also be inferred from the confusion matrix for the model. However visualising the votes matrix provides more intricate details. Here we have seen that the points spread out from a vertex, with fewer and fewer the further one gets. It allows us to see the distribution of points, which is not possible from the confusion matrix alone. The same misclassification rate could be due to a variety of distributions. The visual pattern in the votes matrix is striking, and gives additional information about how the clustering distribution, and shapes of clusters, matches the class labels. It reinforces the clusters are linear extending into different dimensions in the 100D space, but

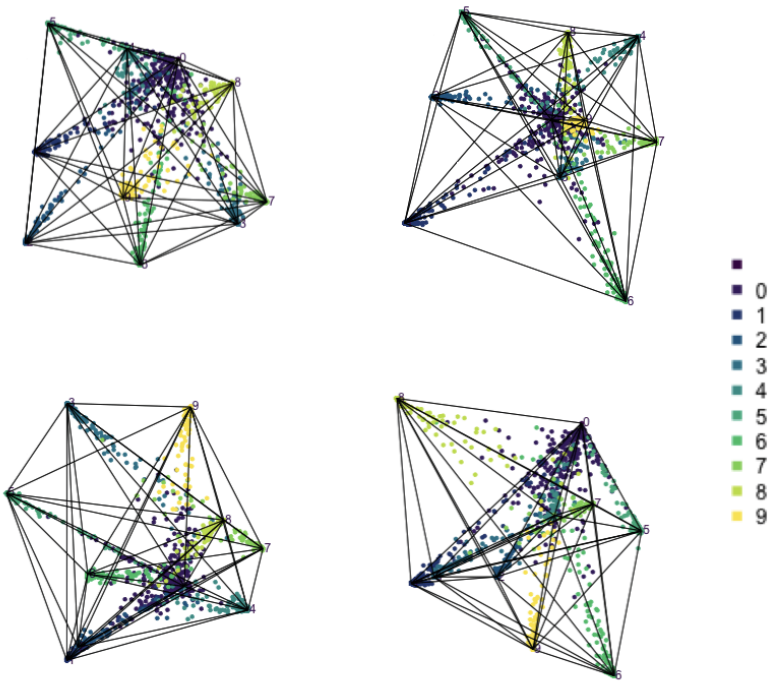


Figure 15.4: Several static views from the tour of the votes matrix. Lines are the edges of the 8D simplex, which bounds the shape. Points mostly concentrate in the vertices, or spread along one of the edges, which means that most observations are clearly belonging to one group, or confused with a single other group. The exception to this is class 0, which spreads in many directions.

really only into about 8D (as we'll see from the variable importance explanation below). We also see that nine of the clusters are all connected to a single cluster.

The votes matrix for the fake trees has a striking geometric structure, with one central cluster connected to all other clusters, each of which is distinct from each other.

15.2.2 Using variable importance

The variable importance score across all classes, and for each class is useful for choosing variables to enter into a tour, to explore class differences. This is particularly so when there are many variables, as in the fake_trees data. We would also expect that this data will have a difference between importance for some classes.

Table 15.1: Variable importance from the random forest fit to the fake trees data, for each of the 9 classes, and using the accuracy and Gini metrics.

Var	0	1	2	3	4	5	6	7	8	9	Acc	Gini
PC1	0.1	0.4	0.5	0.3	0.2	0.5	0.4	0.2	0.3	0.3	0.30	473
PC2	0.1	0.2	0.2	0.5	0.3	0.3	0.2	0.4	0.2	0.3	0.27	381
PC3	0.1	0.1	0.1	0.1	0.5	0.2	0.1	0.1	0.2	0.2	0.17	311
PC4	0.1	0.5	0.1	0.0	0.1	0.0	0.4	0.1	0.1	0.1	0.15	335
PC5	0.1	0.1	0.3	0.1	0.2	0.2	0.1	0.1	0.3	0.2	0.18	333
PC6	0.1	0.2	0.2	0.2	0.0	0.1	0.0	0.3	0.2	0.2	0.16	281
PC7	0.1	0.0	0.1	0.0	0.0	0.1	0.1	0.3	0.1	0.1	0.11	254
PC8	0.1	0.1	0.0	0.2	0.1	0.1	0.0	0.0	0.1	0.3	0.09	228
PC9	0.1	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.1	0.0	0.02	57
PC10	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.01	45

From the variable importance (Table 15.1), we can see that PC9 and PC10 do not substantially contribute. That means the 100D data can be reduced to 8D without losing the information about the cluster structure. PC1 is most important overall, and the order matches the PC order, as might be expected because highest variance corresponds to the most spread clusters. Each cluster has a different set of variables that are important. For example, the variables important for distinguishing cluster 1 are PC1 and PC4, and for cluster 2 they are PC1 and PC5.

Class-wise variable importance helps to find a subspace on which to tour to examine how this class cluster differs from the others.

We can use the accuracy information to choose variables to provide to the tour. Overall, one would sequentially add the variables into a tour based on their accuracy or Gini value. Here it is simply starting with the first three PCs, and then sequentially adding the PCs to examine how distinct the clusters are with and without the extra variable. It can be helpful to focus on a single class against all the others. To do this create a new binary class variable, indicating that the observation belongs to class k or not, as follows:

```
ft_pc <- ft_pc %>%
  mutate(cl1 = factor(case_when(
                  branches == "0" ~ "0",
                  branches == "1" ~ "1",
                  .default = "other"
  )))
```

From Figure 15.5 we can see how cluster 1 is distinct from all of the other observations, albeit with a close connection to the trunk of the tree (cluster 0). The distinction is visible whenever PC4 contributes to the projection, but can be seen clearly with only PC1 and PC4.

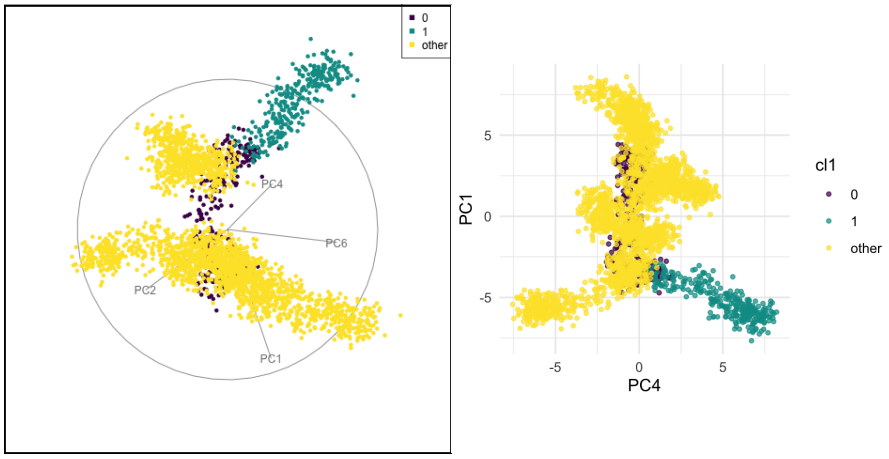


Figure 15.5: Focusing on class 1 in the `fake_trees` data. The most important variables were PC1 and PC4. A combination of PC2 and PC4 reveals the difference between cluster 1 and all the other clusters.

For a problem like this, it can be useful to several classes together. We've chosen to start with class 8 (light green), because from Figure 15.4 it appears to have less connection with class 0, and closer connection with another class. This is class 6 (medium green). A good guess because it has one observation confused with class 8 according to the confusion matrix (printed below).

When we examine these two clusters in association with class 0, we can see

that there is a third cluster that is connected with clusters 6 and 8. It turns out to be cluster 1. It's confusing, because the confusion matrix would suggest that the overlap from all is with cluster 0, but not each other.

```
ft_rf$confusion
```

```
     0   1   2   3   4   5   6   7   8   9 class.error
0  263   4   3   4   3   4   6   2   8   3       0.123
1   13 287   0   0   0   0   0   0   0   0       0.043
2   10   0 288   0   2   0   0   0   0   0       0.040
3    6   0   0 290   0   0   0   3   0   1       0.033
4   12   0   0   0 288   0   0   0   0   0       0.040
5   11   0   0   0   0 289   0   0   0   0       0.037
6   14   0   0   0   0   0 285   0   1   0       0.050
7    6   0   0   4   0   0   0 290   0   0       0.033
8    5   0   0   0   0   0   0   0 295   0       0.017
9    6   0   0   0   0   0   0   1   0 293       0.023
```

From the tour in Figure 15.6 we can see that clusters 1, 6, and 8 share one end of the trunk (cluster 0). Cluster 8 is almost more closely connected with cluster 6, though, than cluster 0. PC1 and PC5 mostly show the distinction between cluster 8 and the rest of the points, but it is clearer if more variables are used.

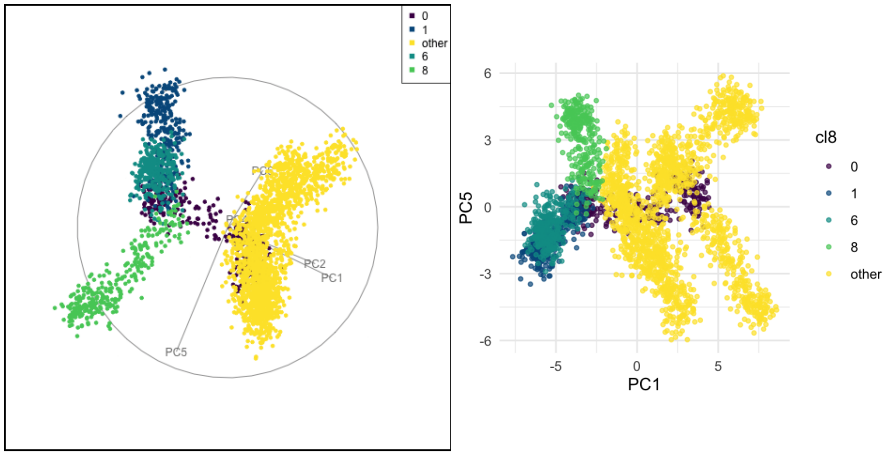


Figure 15.6: Focusing on class 8 in the `fake_trees` data using a tour (left) reveals that it shares an end of cluster 0 with clusters 1 and 6. A combination of PC1 and PC5 reveals that there is a difference between the observations in class 8 relative to 6, 1 and 0 is largely due to PC5 (right).

Although the confusion matrix suggests that class clusters are separated except for class 0, focusing on a few classes and using the variable importance to examine smaller subspaces, reveals they are connected in groups of three to class 0.

Exercises

1. Using a grand tour compare the boundaries from the random forest model on the `penguins` data to that of (a) a default tree model, (b) an LDA model. Is it less boxy than the tree model, but still more boxy than that of the LDA model?
2. Tinker with the parameters of the tree model to force it to fit a tree more closely to the data. Compare the boundaries from this with the default tree, and with the forest model. Is it less boxy than the default tree, but more boxy than the forest model?
3. Fit a random forest model to the `bushfires` data using the `cause` variable as the class. It is a highly imbalanced classification problem. What is the out-of-bag error rate for the forest? Are there some classes that have lower error rate than others? Examine the 4D votes matrix with a tour, and describe the confusion between classes. This is interesting because it is difficult to accurately classify the fire ignition cause, and only some groups are often confused with each other. You should be able to see this from the 3D votes matrix.
4. Fit a forest model to the first 21 PCs of the `sketches` data. Explore the 5D votes matrix. Why does it look star-shaped?
5. Choose a cluster (or group of clusters) from the `fake_trees` data (2, 3, 4, 5, 7, 9) to explore in detail like done in Section 15.2.2. Be sure to choose which PCs are the most useful using a tour, and follow-up by making a scatterplot showing the best distinction between your chosen cluster and the other observations.

16

Support vector machines

A support vector machine (SVM) (Vapnik, 1999) looks for gaps between clusters in the data, based on the extreme observations in each class. In this sense it mirrors the graphical approach described Chapter 7, in which we searched for gaps between groups. It can be viewed as similar to LDA, in that the boundary between classes is a hyperplane. The difference between LDA and SVM is the placement of the boundary. LDA uses the means and covariance matrices of the classes to place the boundary, but SVM uses extreme observations.

The key elements of the SVM model to extract are:

- support vectors
- separating hyperplane.

SVM is widely used for it's ability to fit non-linear classification models in a simple fashion using kernels in the boundary equation. We are focusing on linear methods here because it makes for a useful comparison with how the models differ from those provided by SVM. SVM tends to place the boundary between groups in a gap, if it exists. This is nice from a visual perspective because when we look at differences between classes using a tour, we naturally focus on the gaps. SVM better fits this perception than LDA.

Non-linear SVM models are interesting to examine also. Mostly one would examine the boundaries between classes which can be done in the same way that is documented in the Chapter 14 and Chapter 15.

16.1 Components of the SVM model

To illustrate the approach, we use two simple simulated data examples. Both have only two variables, and two classes. Explaining SVM is easier when there are just two groups. In the first data set the two classes have different covariances matrices, which will cause trouble for LDA, but SVM should see

the gap between the two clusters and place the separating hyperplane in the middle of the gap. In the second data set the two groups are concentric circles, with the inner one solid. A non-linear SVM should be fitted to this data, which should see circular gap between the two classes.

Note that the `svm` function in the `e1071` package will automatically scale observations into the range $[0, 1]$. To make it easier to examine the fitted model, it is best to scale your data first, and then fit the model.

```
library(classifly)
library(e1071)
df1_svm <- svm(cl~., data=df1,
                     probability=TRUE,
                     kernel="linear",
                scale=FALSE)
df1_svm_e <- explore(df1_svm, df1)

df2_svm <- svm(cl~., data=df2,
                     probability=TRUE,
                     kernel="radial")
df2_svm_e <- explore(df2_svm, df2)
```

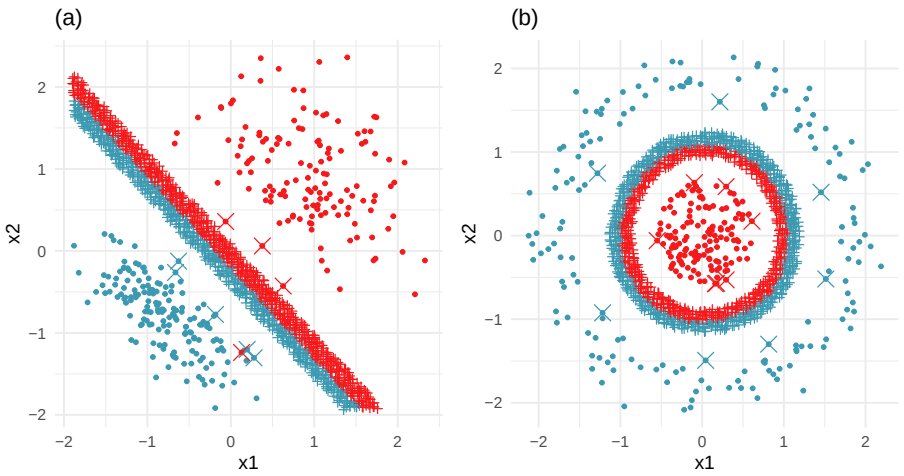


Figure 16.1: SVM classifier fit overlaid on two simulated data examples: (a) groups with different variance-covariance, fitted using a linear kernel, (b) groups with non-linear separation, fitted using a radial kernel. The band of points shown as '+' mark the SVM boundary, and points marked by 'x' are the support vectors used to define the boundary.

Figure 16.1 shows the two data sets and the important aspects of the fitted SVM model for each. The observations are represented by dots, the separating

hyperplane (just a line for 2D) is represented by '+'. Where the two colours merge is the actual location of the boundary between classes. It can be seen that this is located right down the middle of the gap, for both data sets. Even though the boundary is circular for the second data set, in a transformed high-dimensional space it would be linear.

SVMs use a subset of the observations to define the boundary, and these are called the support vectors. For each of the data sets these are marked with 'x'. For the linear boundary, there are nine support vectors, five in one group and four in the other. There is one interesting observation in the red group, which falls on the other side of the boundary. It is marked as a support vector, but its contribution to the fitted hyperplane is limited by a control parameter in the model fitting process.

Linear SVMs can be assessed similarly to regression models. The components of the model are:

1. The points that are the support vectors:

```
df1_svm$index
```

```
[1]  15  45 123 135 155 180 202 239 292
```

2. Their coefficients:

```
df1_svm$coefs
```

```
           [,1]
 [1,]  0.3771240
 [2,]  0.1487726
 [3,]  1.0000000
 [4,]  1.0000000
 [5,]  1.0000000
 [6,] -0.5258966
 [7,] -1.0000000
 [8,] -1.0000000
 [9,] -1.0000000
```

which indicate that all but 15, 45 and 180 are actually bounded support vectors (their coefficients are bounded to magnitude 1).

3. that when used with the intercept:

```
df1_svm$rho
```

```
[1] 0.3520001
```

can be used to compute the equation of the fitted hyperplane.

```
w = t(df1_svm$SV) %*% df1_svm$coefs
w
```

```
       [,1]
x1 -1.501086
x2 -1.356237
```

Giving the equation to be -1.5 x_1+ -1.36 x_2+ -0.35 = 0, or alternatively, x_2 = -1.11 x_1+ -0.26.

which can be used to generate a line to show the boundary with the data.

```
s1 + geom_abline(intercept=df1_svm$rho/w[2],
                 slope=-w[1]/w[2])
```

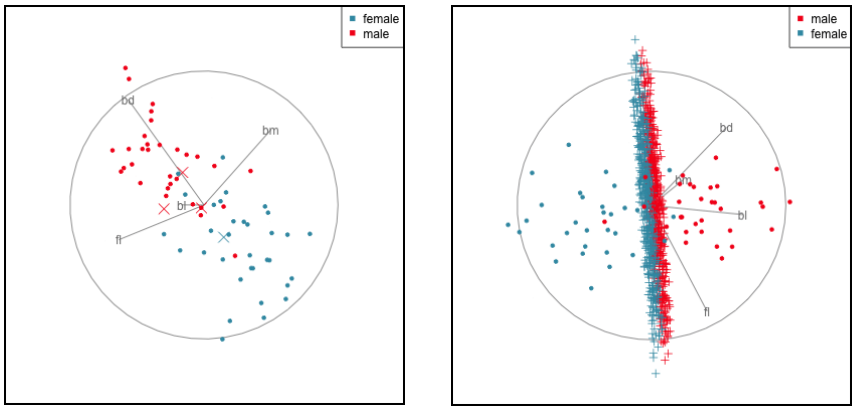
Note that care in scaling of data is important to get the intercept calculated exactly. We have standardised the data, and set the `scale=FALSE` parameter in the `svm` function. The slope calculation is quite robust to the data scaling.

Like LDA, a linear SVM model for two groups can be written using the equation of a hyperplane. The fitted model coefficients are then used to generate points on this plane, to examine the boundary between groups.

16.2 Examining the model components in high-dimensions

For higher dimensions, the procedures are similar, with the hyperplane and support vectors being examined using a tour. Here we examine the model for differentiating male and female Chinstrap penguins. The Chinstrap penguins have a noticeable difference in size of the sexes, unlike the other two species. Working with a two-class problem is easier for explaining SVM, but multi-class calculations can also follow this approach.

```
library(dplyr)
load("data/penguins_sub.rda")
chinstrap <- penguins_sub %>%
  filter(species == "Chinstrap") %>%
  select(-species) %>%
  mutate_if(is.numeric, mulgar:::scale2)
chinstrap_svm <- svm(sex~., data=chinstrap,
                     kernel="linear",
                     probability=TRUE,
                     scale=FALSE)
chinstrap_svm_e <- explore(chinstrap_svm, chinstrap)
```



(a) Support vectors (b) SVM boundary

Figure 16.2: SVM model for distinguishing the sexes of the Chinstrap penguins. The separating hyperplane is 3D, and separates primarily on variables `bl` and `bd`, as seen because these two axes extend out from the plane when it is seen on its side, separating the two groups.

Mark the support vectors by point shape, and examine where these are relative to the difference between groups.

Examining the hyperplane in a grand tour display (Figure 16.2) indicates that two of the variables, `bl` and `bd`, are important for separating the two classes. We can check this interpretation using the radial tour. Using the components from the model, the coefficients of the hyperplane are:

```
t(chinstrap_svm$SV) %*% chinstrap_svm$coefs
```

```
     [,1]
```

```
bl -0.9102439
bd -1.1073475
fl -0.5223364
bm -0.2846370
```

The coefficients for `bl` and `bd` are the largest (in magnitude) which supports the the interpretation that they are most important. This vector can be used to set the starting point for radial tour, once it is normalised. Any orthonormal vector serves to turn this into a 2D projection, to visualise the boundary.

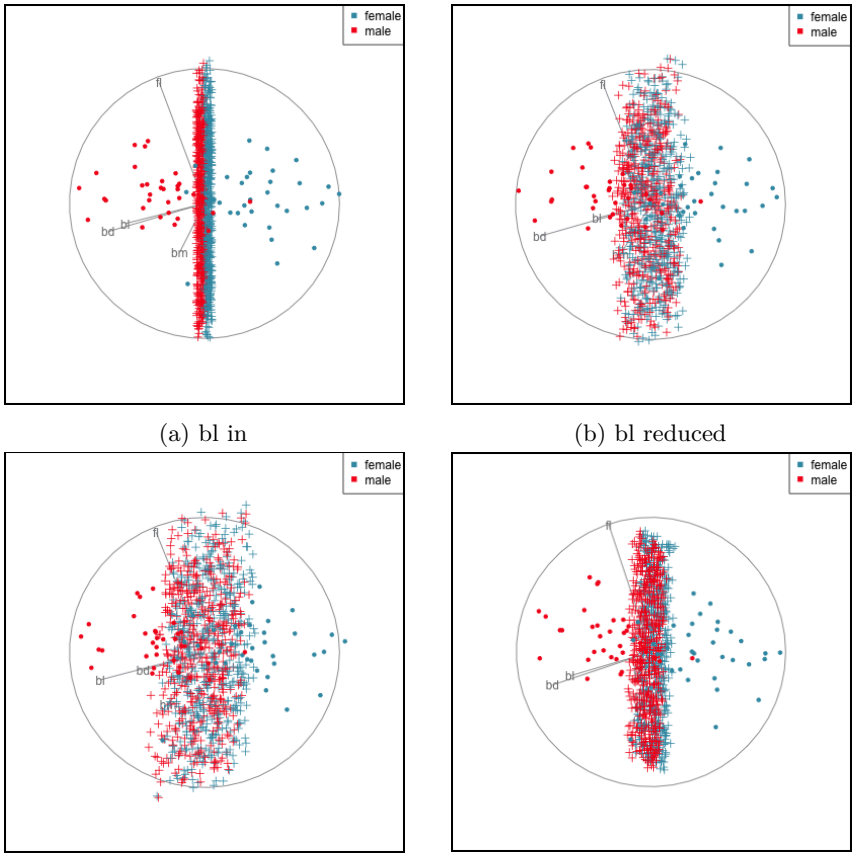
```
set.seed(1022)
prj1 <- mulgar::norm_vec(t(chinstrap_svm$SV) %*%
                           chinstrap_svm$coefs)
prj2 <- basis_random(4, 1)
prj <- orthonormalise(cbind(prj1, prj2))
prj
```

```
         [,1]        [,2]
bl -0.5865081 -0.06412875
bd -0.7135101  0.51192498
fl -0.3365631 -0.77713899
bm -0.1834035 -0.36038216
```

This projection is show in Figure 16.3. You can see the boundary between the two sexes as a clear line, marked by a sample of points on either side. We use the radial tour to remove each of the variables from the projection using the radial tour to examine it's importance on the model, and hence the boundary. If the clear view of the boundary gets jumbled when a variable is removed we infer that this variable is very important for the model (as seen for `bl` and `bd`). If there is little change in the clarity when a variable is removed, then it is less important (as seen for `fl` and `bm`).

Use a radial tour to zero out coefficients defining the separating hyperplane to explore the variable importance.

In this example, we can see that clarity of the boundary changes substantially when either `bl` and `bd` are removed. There is a small change when `fl` and `bm` are removed, so they are less important. This interpretation matches the interpretation that would be made from the magnitude of the coefficients of the hyperplane (printed earlier). They reinforce each other. It is possible that the interpretation of the coefficients could differ after using the radial tour, most likely in terms of simplifying the vector, supporting the forcing some coefficients to zero.



(a) bl in (b) bl reduced

(c) bd reduced (d) bm out

Figure 16.3: Exploring the importance of the four variables to the separating hyperplane using a radial tour to reduce the contribution of each variable to 0, and then back to it's original value: (a) separating hyperplane visible, (b) `bl` contribution reduced, (c) `bd` contribution decreased, (d) `bm` contribution removed. You can see that `bl` and `bd` contribute most to the plane, because when they are removed the plane is no longer on it side marking the boundary. Variables `fl` (not shown) and `bm` contribute a small amount to the separating hyperplane, but it is possible that these two could be removed with only a small effect on the strength of the separation between the sexes.

When we use the radial tour to examine how the different variables contribute to the separating hyperplane between the sexes, we learn that bl and bd are the most important variables. We could (almost) ignore fl and bm for this classification.

Exercises

1. Generate a small subset from the `bushfire` data: we keep the variables `log_dist_cfa`, `log_dist_road` and `cause`, and we select only observations where `cause` is either lightning or arson. Fit a linear SVM model to separate the two classes and show the decision boundary together with the data. Compare to the boundary obtained by LDA and argue how the two models place the separating hyperplane in different ways.
2. We extend this into a multivariate setting by also including `amaxt180` and `amaxt720` as predictors. Fit a linear SVM model and calculate the hyperplane to judge which of these variables are important.
3. Calculate the decision boundary and look at it with a radial tour to see the effect from including individual predictors in a projection. Also explore what happens when rotating out multiple variables together. What can you learn from this?
4. From the `sketches_train` data select all observations of class banana or boomerang For this subset use PCA to find the first 5 PCs. Fit two SVM models: once with linear kernel and once with radial kernel and default value for the gamma parameter. Compare the number of misclassified observations in the training data for the two models.
5. Compute the model predictions and compare the decision boundaries between the linear and radial SVM using a slice tour. Does the shape match what you expect given the respective kernel function?
6. SVM models are defined for separating two classes, but and ensemble of such models can be used when we want to distinguish more than two classes. Look up the documentation of the `svm` function to learn how this works, then fit an SVM model to separate the three penguin species. In this case we primarily use the model predictions to investigate the decision boundaries, you can use `explore` together with the slice tour to do this. You can use different kernels and compare the resulting decision boundaries.

17

Neural networks and deep learning

Neural networks (NN) can be considered to be nested additive (or even ensemble) models where explanatory variables are combined, and transformed through an activation function like a logistic. These transformed combinations are added recursively to yield class predictions. They are considered to be black box models, but there is a growing demand for interpretability. Although interpretability is possible, it can be unappealing to understand a complex model constructed to tackle a difficult classification task. Nevertheless, this is the motivation for the explanation of visualisation for NN models in this chapter.

In the simplest form, we might write the equation for a NN as

$$\hat{y} = f(x) = a_0 + \sum_{h=1}^{s} w_{0h}\phi(a_h + \sum_{i=1}^{p} w_{ih}x_i)$$

where s indicates the number of nodes in the hidden (middle layer), and ϕ is a choice of activation function. In a simple situation where $p = 3$, $s = 2$, and linear output layer, the model could be written as:

$$\begin{aligned}\hat{y} = a_0 + w_{01}\phi(a_1 + w_{11}x_1 + w_{21}x_2 + w_{31}x_3) + \\ w_{02}\phi(a_2 + w_{12}x_1 + w_{22}x_2 + w_{32}x_3)\end{aligned}$$

which is a combination of two (linear) models, each of which could be examined for their role in making predictions.

In practice, a model may have many nodes, and several hidden layers, a variety of activation functions, and regularisation modifications. One should keep in mind the principle of parsimony is important when applying NNs, because it is tempting to make an overly complex, and thus over-parameterised, construction. Fitting NNs is still problematic. One would hope that fitting produces a stable result, whatever the starting seed the same parameter estimates are returned. However, this is not the case, and different, sometimes radically different, results are routinely obtained after each attempted fit (Wickham et al., 2015).

For these examples we use the software `keras` (Allaire & Chollet, 2023) following the installation and tutorial details at https://tensorflow.rstudio.com/tutorials/. Because it is an interface to python it can be tricky to install. If

this is a problem, the example code should be possible to convert to use `nnet` (Venables & Ripley, 2002a) or `neuralnet` (Fritsch et al., 2019). We will use the penguins data to illustrate the fitting, because it makes it easier to understand the procedures and the fit. However, a NN is like using a jackhammer instead of a trowel to plant a seedling, more complicated than necessary to build a good classification model for this data.

17.1 Setting up the model

A first step is to decide how many nodes the NN architecture should have, and what activation function should be used. To make these decisions, ideally you already have some knowledge of the shapes of class clusters. For the penguins classification, we have seen that it contains three elliptically shaped clusters of roughly the same size. This suggests two nodes in the hidden layer would be sufficient to separate three clusters (Figure 17.1). Because the shapes of the clusters are convex, using linear activation ("relu") will also be sufficient. The model specification is as follows:

```
library(keras)
tensorflow::set_random_seed(211)

# Define model
p_nn_model <- keras_model_sequential()
p_nn_model %>%
  layer_dense(units = 2, activation = 'relu',
              input_shape = 4) %>%
  layer_dense(units = 3, activation = 'softmax')
p_nn_model %>% summary

loss_fn <- loss_sparse_categorical_crossentropy(
  from_logits = TRUE)

p_nn_model %>% compile(
  optimizer = "adam",
  loss      = loss_fn,
  metrics   = c('accuracy')
)
```

Note that `tensorflow::set_random_seed(211)` sets the seed for the model fitting so that we can obtain the same result to discuss later. It needs to be

set before the model is defined in the code. The model will also be saved in order to diagnose and make predictions.

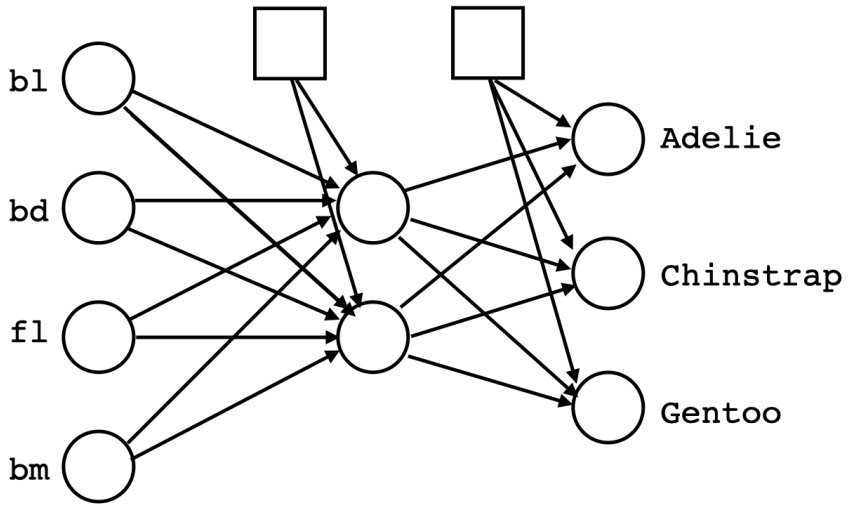
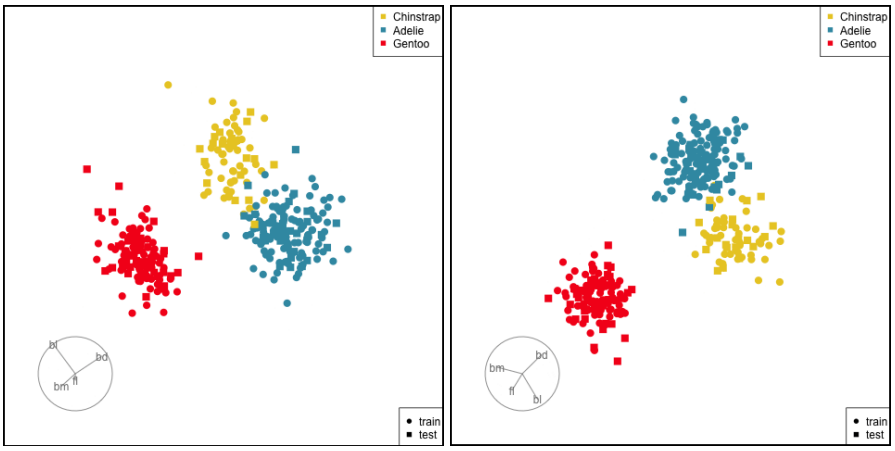


Figure 17.1: Network architecture for the model on the penguins data. The round nodes indicate original or transformed variables, and each arrow connecting these is represented as one of the weights w_{ih} in the definition. The boxes indicate the additive constant entering the nodes, and the corresponding arrows represent the terms a_h.

17.2 Checking the training/test split

Splitting the data into training and test is an essential way to protect against overfitting, for most classifiers, but especially so for the copiously parameterised NNs. The model specified for the penguins data with only two nodes is unlikely to be overfitted, but it is nevertheless good practice to use a training set for building and a test set for evaluation.

Figure 17.8 shows the tour being used to examine the split into training and test samples for the penguins data. Using random sampling, particularly stratified by group, should result the two sets being very similar, as can be seen here. It does happen that several observations in the test set are on the extremes of their class cluster, so it could be that the model makes errors in the neighbourhoods of these points.



(a) Grand tour (b) Guided tour

Figure 17.2: Evaluating the training/test split, where we expect that the two samples should roughly match. There are a few observations in the test set that are on the outer edges of the clusters, which will likely result in the model making an error in these regions. However, the two samples roughly match.

17.3 Fit the model

The data needs to be specially formatted for the model fitted using `keras`. The explanatory variables need to be provided as a `matrix`, and the categorical response needs to be separate, and specified as a `numeric` variable, beginning with 0.

```
# Data needs to be matrix, and response needs to be numeric
p_train_x <- p_train %>%
  select(bl:bm) %>%
  as.matrix()
p_train_y <- p_train %>% pull(species) %>% as.numeric()
p_train_y <- p_train_y-1 # Needs to be 0, 1, 2
p_test_x <- p_test %>%
  select(bl:bm) %>%
  as.matrix()
p_test_y <- p_test %>% pull(species) %>% as.numeric()
p_test_y <- p_test_y-1 # Needs to be 0, 1, 2
```

The specified model is reasonably simple, four input variables, two nodes in the

hidden layer and a three column binary matrix for output. This corresponds to 5+5+3+3+3=19 parameters.

```
Model: "sequential"
_________________________________________________________________
 Layer (type)                Output Shape              Param #
=================================================================
 dense_1 (Dense)             (None, 2)                 10
 dense (Dense)               (None, 3)                 9
=================================================================
Total params: 19 (76.00 Byte)
Trainable params: 19 (76.00 Byte)
Non-trainable params: 0 (0.00 Byte)
_________________________________________________________________
```

```
# Fit model
p_nn_fit <- p_nn_model %>% keras::fit(
  x = p_train_x,
  y = p_train_y,
  epochs = 200,
  verbose = 0
)
```

Because we set the random number seed we will get the same fit each time the code provided here is run. However, if the model is re-fit without setting the seed, you will see that there is a surprising amount of variability in the fits. Setting `epochs = 200` helps to usually get a good fit. One expects that `keras` is reasonably stable so one would not expect the huge array of fits as observed in Wickham et al. (2015) using `nnet`. That this can happen with the simple model used here reinforces the notion that fitting of NN models is fiddly, and great care needs to be taken to validate and diagnose the fit.

Fitting NN models is fiddly, and very different fitted models can result from restarts, parameter choices, and architecture.

The fitted model that we have chosen as the final one has reasonably small loss and high accuracy. Plots of loss and accuracy across epochs showing the change during fitting can be plotted, but we don't show them here, because they are generally not very interesting.

```
p_nn_model %>% evaluate(p_test_x, p_test_y, verbose = 0)
```

```
     loss  accuracy
0.2563850 0.9553571
```

The model object can be saved for later use with:

```
save_model_tf(p_nn_model, "data/penguins_cnn")
```

17.4 Extracting model components

View the individual node models to understand how they combine to produce the overall model.

Because nodes in the hidden layers of NNs are themselves (relatively simple regression) models, it can be interesting to examine these to understand how the model is making it's predictions. Although it's rarely easy, most software will allow the coefficients for the models at these nodes to be extracted. With the penguins NN model there are two nodes, so we can extract the coefficients and plot the resulting two linear combinations to examine the separation between classes.

```
# Extract hidden layer model weights
p_nn_wgts <- keras::get_weights(p_nn_model, trainable=TRUE)
p_nn_wgts
```

```
[[1]]
           [,1]        [,2]
[1,]  0.6216676  1.33304155
[2,]  0.1851478 -0.01596385
[3,] -0.1680396 -0.30432791
[4,] -0.8867414 -0.36627045

[[2]]
[1]  0.12708087 -0.09466381

[[3]]
           [,1]     [,2]       [,3]
[1,] -0.1646167 1.527644 -1.9215064
[2,] -0.7547278 1.555889  0.3210194

[[4]]
[1]  0.4554813 -0.9371488  0.3577386
```

The linear coefficients for the first node in the model are 0.62, 0.19, -0.17, -0.89, and the second node in the model are 1.33, -0.02, -0.3, -0.37. We can use these like we used the linear discriminants in LDA to make a 2D view of the data, where the model is separating the three species. The constants 0.13, -0.09 are not important for this. They are only useful for drawing the location of the boundaries between classes produced by the model.

These two sets of model coefficients provide linear combinations of the original variables. Together, they define a plane on which the data is projected to view the classification produced by the model. Ideally, though this plane should be defined using an orthonormal basis otherwise the shape of the data distribution might be warped. So we orthonormalise this matrix before computing the data projection.

```
# Orthonormalise the weights to make 2D projection
p_nn_wgts_on <- tourr::orthonormalise(p_nn_wgts[[1]])
p_nn_wgts_on
```

```
           [,1]       [,2]
[1,]  0.5593355  0.7969849
[2,]  0.1665838 -0.2145664
[3,] -0.1511909 -0.1541475
[4,] -0.7978314  0.5431528
```

Figure 17.3 shows the data projected into the plane determined by the two linear combinations of the two nodes in the hidden layer. Training and test sets are indicated by empty and solid circles. The three species are clearly different but there is some overlap or confusion for a few penguins. The most interesting aspect to learn is that there is no big gap between the Gentoo and other species, which we know exists in the data. The model has not found this gap, and thus is likely to unfortunately and erroneously confuse some Gentoo penguins, particularly with Adelie.

What we have shown here is a process to use the models at the nodes of the hidden layer to produce a reduced dimensional space where the classes are best separated, at least as determined by the model. The process will work in higher dimensions also.

When there are more nodes in the hidden layer than the number of original variables it means that the space is extended to achieve useful classifications that need more complicated non-linear boundaries. The extra nodes describe the non-linearity. Wickham et al. (2015) provides a good illustration of this in 2D. The process of examining each of the node models can be useful for understanding this non-linear separation, also in high dimensions.

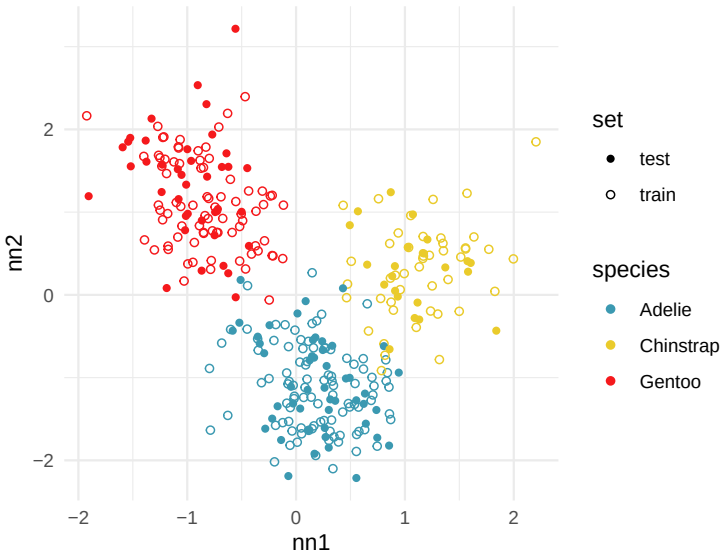


Figure 17.3: Plot of the data in the linear combinations from the two nodes in the hidden layer. The three species are clearly different, although with some overlap between all three. A main issue to notice is that there isn't a big gap between Gentoo and the other species, which we know is there based on our data exploration done in other chapters. This suggests this fitted model is sub-optimal.

17.5 Examining predictive probabilities

When the predictive probabilities are returned by a model, as is done by this NN, we can use a ternary diagram for three class problems, or high-dimensional simplex when there are more classes to examine the strength of the classification. This done in the same way that was used for the votes matrix from a random forest in Section 15.2.1.

```
# Predict training and test set
p_train_pred <- p_nn_model %>%
  predict(p_train_x, verbose = 0)
p_train_pred_cat <- levels(p_train$species)[
  apply(p_train_pred, 1,
        which.max)]
p_train_pred_cat <- factor(
  p_train_pred_cat,
  levels=levels(p_train$species))
table(p_train$species, p_train_pred_cat)
```

```
           p_train_pred_cat
            Adelie Chinstrap Gentoo
  Adelie        92         4      1
  Chinstrap      0        45      0
  Gentoo         1         0     78
```

```
p_test_pred <- p_nn_model %>%
  predict(p_test_x, verbose = 0)
p_test_pred_cat <- levels(p_test$species)[
  apply(p_test_pred, 1,
        which.max)]
p_test_pred_cat <- factor(
  p_test_pred_cat,
  levels=levels(p_test$species))
table(p_test$species, p_test_pred_cat)
```

```
           p_test_pred_cat
            Adelie Chinstrap Gentoo
  Adelie        45         3      1
  Chinstrap      0        23      0
  Gentoo         1         0     39
```

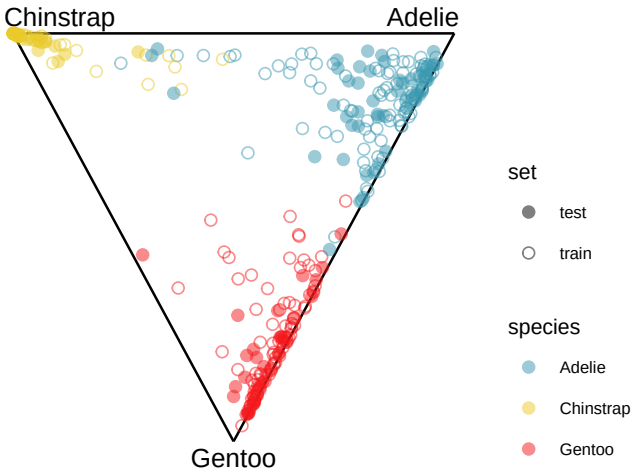


Figure 17.4: Ternary diagram for the three groups of the predictive probabilities of both training ans test sets. From what we already know about the penguins data this fit is not good. Both Chinstrap and Gentoo penguins are confused with Adelie, or at risk of it. Gentoo is very well-separated from the other two species when several variables are used, and this fitted model is blind to it. One useful finding is that there is little difference between training and test sets, so the model has not been over-fitted.

If the training and test sets look similar when plotted in the model space then the model is not suffering from over-fitting.

17.6 Local explanations

It especially important to be able to interpret or explain a model, even more so when the model is complex or black-box'y. A good resource for learning about the range of methods is Molnar (2022). Local explanations provide some information about variables that are important for making the prediction for a particular observation. The method that we use here is Shapley value, as computed using the `kernelshap` package (Mayer & Watson, 2023).

```
# Explanations
# https://www.r-bloggers.com/2022/08/kernel-shap/
library(kernelshap)
library(shapviz)
```

```
p_explain <- kernelshap(
    p_nn_model,
    p_train_x,
    bg_X = p_train_x,
    verbose = FALSE
  )
p_exp_sv <- shapviz(p_explain)
save(p_exp_sv, file="data/p_exp_sv.rda")
```

A Shapley value for an observation indicates how the variable contributes to the model prediction for that observation, relative to other variables. It is an average, computed from the change in prediction when all combinations of presence or absence of other variables. In the computation, for each combination, the prediction is computed by substituting absent variables with their average value, like one might do when imputing missing values.

Figure 17.5 shows the Shapley values for Gentoo observations (both training and test sets) in the penguins data, as a parallel coordinate plot. The values for the single misclassified Gentoo penguin (in the training set) is coloured orange. Overall, the Shapley values don't vary much on `bl`, `bd` and `fl` but they do on `bm`. The effect of other variables is seems to be only important for `bm`.

For the misclassified penguin, the effect of `bm` for all combinations of other variables leads to a decline in predicted value, thus less confidence in it being a Gentoo. In contrast, for this same penguin when considering the effect of `bl` the predicted value increases on average.

If we examine the data Figure 17.6 the explanation makes some sense. The misclassified penguin has an unusually small value on `bm`. That the SHAP value for `bm` was quite different pointed to this being a potential issue with the model, particularly for this penguin. This penguin's prediction is negatively impacted by `bm` being in the model.

17.7 Examining boundaries

Figure 17.7 shows the boundaries for this NN model along with those of the LDA model.

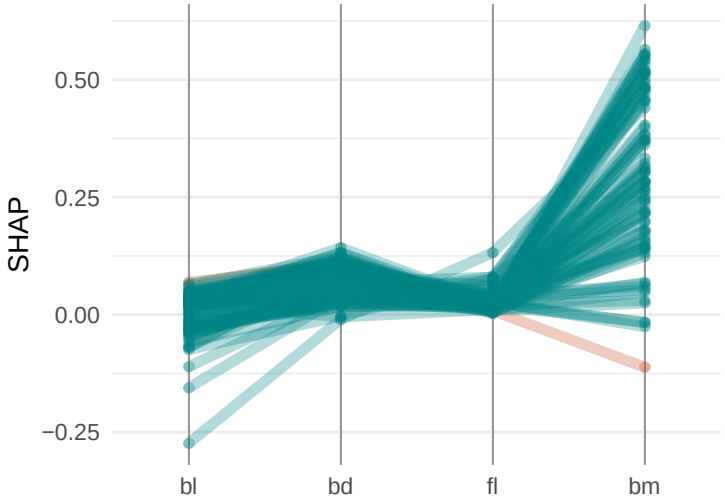


Figure 17.5: SHAP values focused on Gentoo class, for each variable. The one misclassified penguin (orange) has a much lower value for body mass, suggesting that this variable is used differently for the prediction than for other penguins.

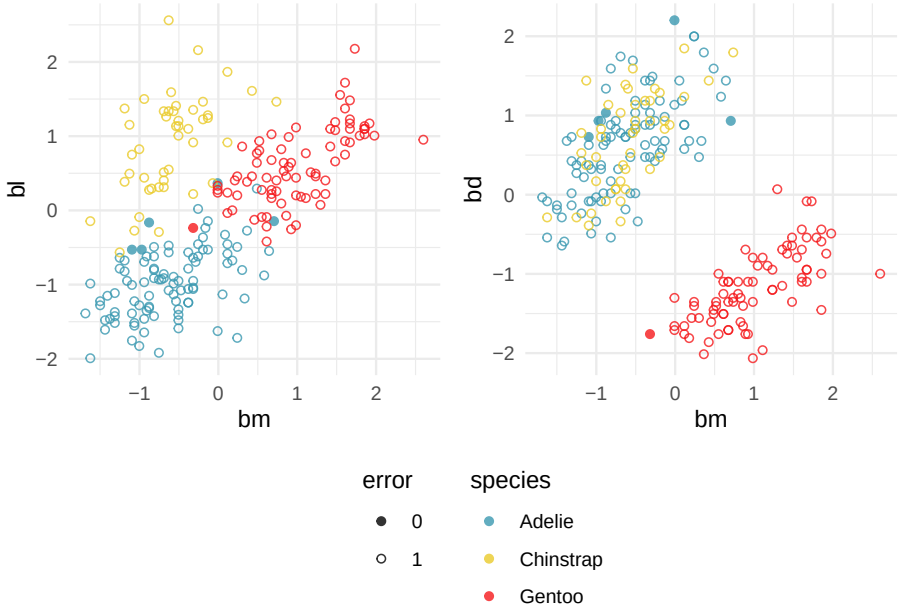


Figure 17.6: Plots of the data to help understand what the SHAP values indicate. The misclassified Gentoo penguin has an unusually low body mass value which makes it appear to be more like an Adelie penguin, particularly when considered in relation to it's bill length.

(a) LDA model

(b) NN model

Figure 17.7: Comparison of the boundaries produced by the LDA (a) and the NN (b) model, using a slice tour.

17.8 Application to a large dataset

To see how these methods apply in the setting where we have a large number of variables, observations and classes we will look at a neural network that predicts the category for the fashion MNIST data. The code for designing and fitting the model is following the tutorial available from https://tensorflow.rstudio.com/tutorials/keras/classification and you can find additional information there. Below we only replicate the steps needed to build the model from scratch. We also note that a similar investigation was presented in Li et al. (2020), with a focus on investigating the model at different epochs during the training.

The first step is to download and prepare the data. Here we scale the observations to range between zero and one, and we define the label names.

```
library(keras)

# download the data
fashion_mnist <- dataset_fashion_mnist()

# split into input variables and response
c(train_images, train_labels) %<-% fashion_mnist$train
c(test_images, test_labels) %<-% fashion_mnist$test
```

```
# for interpretation we also define the category names
class_names = c('T-shirt/top',
                'Trouser',
                'Pullover',
                'Dress',
                'Coat',
                'Sandal',
                'Shirt',
                'Sneaker',
                'Bag',
                'Ankle boot')

# rescaling to the range (0,1)
train_images <- train_images / 255
test_images <- test_images / 255
```

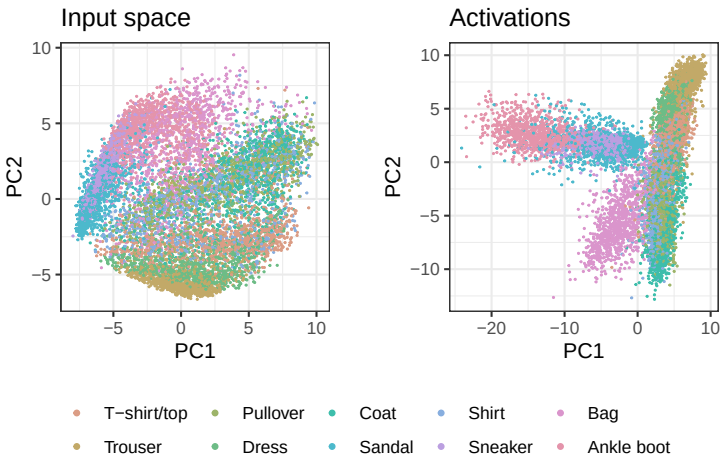
In the next step we define the neural network and train the model. Note that because we have many observations, even a very simple structure returns a good model. And because this example is well-known, we do not need to tune the model or check the validation accuracy.

```
# defining the model
model_fashion_mnist <- keras_model_sequential()
model_fashion_mnist %>%
  # flatten the image data into a long vector
  layer_flatten(input_shape = c(28, 28)) %>%
  # hidden layer with 128 units
  layer_dense(units = 128, activation = 'relu') %>%
  # output layer for 10 categories
  layer_dense(units = 10, activation = 'softmax')

model_fashion_mnist %>% compile(
  optimizer = 'adam',
  loss = 'sparse_categorical_crossentropy',
  metrics = c('accuracy')
)

# fitting the model, if we did not know the model yet we
# would add a validation split to diagnose the training
model_fashion_mnist %>% fit(train_images,
              train_labels,
              epochs = 5)
save_model_tf(model_fashion_mnist, "data/fashion_nn")
```

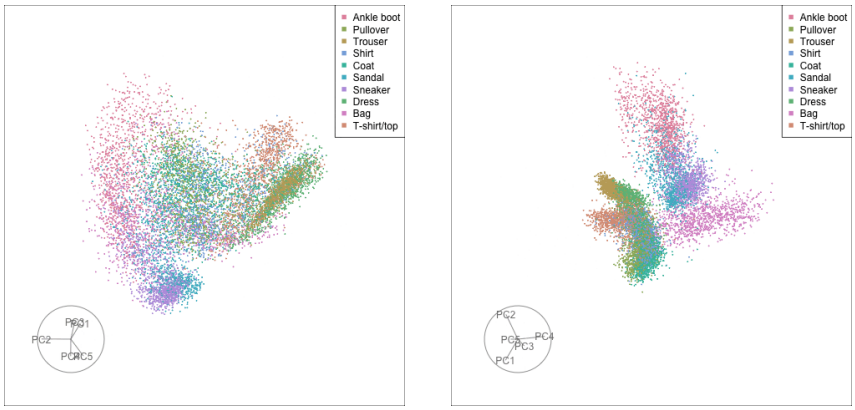
We have defined a flat neural network with a single hidden layer with 128

nodes. To investigate the model we can start by comparing the activations to the original input data distribution. Since both the input space and the space of activations is large, and they are of different dimensionality, we will first use principal component analysis. This simplifies the analysis, and in general we do not need the original pixel or hidden node information for the interpretation here. The comparison is using the test-subset of the data.

```
# get the fitted model
model_fashion_mnist <- load_model_tf("data/fashion_nn")
# observed response labels in the test set
test_tags <- factor(class_names[test_labels + 1],
                    levels = class_names)

# calculate activation for the hidden layer, this can be done
# within the keras framework
activations_model_fashion <- keras_model(
  inputs = model_fashion_mnist$input,
  outputs = model_fashion_mnist$layers[[2]]$output
)
activations_fashion <- predict(
  activations_model_fashion,
  test_images, verbose = 0)

# PCA for activations
activations_pca <- prcomp(activations_fashion)
activations_pc <- as.data.frame(activations_pca$x)

# PCA on the original data
# we first need to flatten the image input
test_images_flat <- test_images
dim(test_images_flat) <- c(nrow(test_images_flat), 784)
images_pca <- prcomp(as.data.frame(test_images_flat))
images_pc <- as.data.frame(images_pca$x)
```



Looking only at the first two principal components we note some clear differences from the transformation in the hidden layer. The observations seem to be more evenly spread in the input space, while in the activations space we notice grouping along specific directions. In particular the category "Bag" appears to be most different from all other classes, and the non-linear transformation in the activations space shows that they are clearly different from the shoe categories, while in the input space we could note some overlap in the linear projection. To better identify differences between other groups we will use the tour on the first five principal components.



(a) Input space (b) Activations

Figure 17.8: Comparison of the test observations in the first five principal components of the input space (left) and in the hidden layer activations (right). The activation function results in more clearly defined grouping of the different classes.

As with the first two principal components we get a much more spread out

distribution in the original space. Nevertheless we can see differences between the classes, and that some groups are varying along specific directions in that space. Overall the activations space shows tighter clusters as expected after including the ReLU activation function, but the picture is not as neat as the first two principal components would suggest. While certain groups appear very compact even in this larger subspace, others vary quite a bit within part of the space. For example we can clearly see the "Bag" observations as different from all other images, but also notice that there is a large variation within this class along certain directions.

Finally we will investigate the model performance through the misclassifications and uncertainty between classes. We start with the error matrix for the test observations. To fit the error matrix we use the numeric labels, the ordering is as defined above for the labels.

```
fashion_test_pred <- predict(model_fashion_mnist,
                             test_images, verbose = 0)
fashion_test_pred_cat <- levels(test_tags)[
  apply(fashion_test_pred, 1,
        which.max)]
predicted <- factor(
  fashion_test_pred_cat,
  levels=levels(test_tags)) %>%
  as.numeric() - 1
observed <- as.numeric(test_tags) -1
table(observed, predicted)
```

```
        predicted
observed   0   1   2   3   4   5   6   7   8   9
       0 128   0  84 719  10   0  51   7   1   0
       1   0  42  15 941   0   0   0   2   0   0
       2   6   0 824  38 121   0   3   8   0   0
       3   1   0  14 976   8   0   1   0   0   0
       4   1   0 205 181 605   0   0   8   0   0
       5   1   0   0   2   0  77   0 902   1  17
       6  24   0 231 282 405   0  44  12   2   0
       7   0   0   0   0   0   0   0 1000   0   0
       8  17   1  78 102  49   0   5 730  16   2
       9   0   0   0   2   0   0   0 947   0  51
```

From this we see that the model mainly confuses certain categories with each other, and within expected groups (e.g. different types of shoes can be confused with each other, or different types of shirts). We can further investigate this by visualizing the full probability matrix for the test observations, to see which categories the model is uncertain about.

For this data using explainers like SHAP is not so interesting, since the individual pixel contribution to a prediction are typically not of interest. With image classification a next step might be to further investigate which part of the image is important for a prediction, and this can be visualized as a heat map placed over the original image. This is especially interesting in the case of difficult or misclassified images. This however is beyond the scope of this book.

Exercises

1. The problem with the NN model fitted to the penguins is that the Gentoo are poorly classified, when they should be perfectly predictable due to the big gap between class clusters. Re-fit the NN to the penguins data, to find a better model that appropriately perfectly predicts Gentoo penguins. Support this by plotting the model (using the hidden layer), and the predictive probabilities as a ternary plot. Do the SHAP values also support that `bd` plays a stronger role in your best model? (`bd` is the main variable for distinguishing Gentoo's from the other species, particularly when used with `fl` or `bl`.)
2. For the fashion MNIST data we have seen that certain categories are more likely to be confused with each other. Select a subset of the data including only the categories Ankle boot, Sneaker and Sandal and see if you can reproduce the analysis of the penguins data in this chapter with this subset.
3. XXX fake trees, can we think about the number of nodes and make it work with a simple NN similar to penguins data?
4. The sketches data could also be considered a classic image classification problem, and we have seen that we can get a reasonable accuracy with a random forest model. Because we only have a smaller number of observations (compared to the fashion MNIST data) when fitting a neural network we need to be very careful not to overfit the training data. Try fitting a flat neural network (similar to what we did for the fashion MNIST data) and check the test accuracy of the model.
5. Challenge: try to design a more accurate neural network for the sketches data. Here you can investigate using a convolutional neural network in combination with data augmentation. In addition, using batch normalization should improve the model performance.

18

Exploring misclassifications

18.1 Errors for a single model

To examine misclassifications, we can create a separate variable that identifies the errors or not. Constructing this for each class, and exploring in small steps is helpful. Let's do this using the random forest model for the penguins fit. The random forest fit has only a few misclassifications. There are four Adelie penguins confused with Chinstrap, and similarly four Chinstrap confused with Adelie. There is one Gentoo penguin confused with a Chinstrap. This is interesting, because the Gentoo cluster is well separated from the clusters of the other two penguin species.

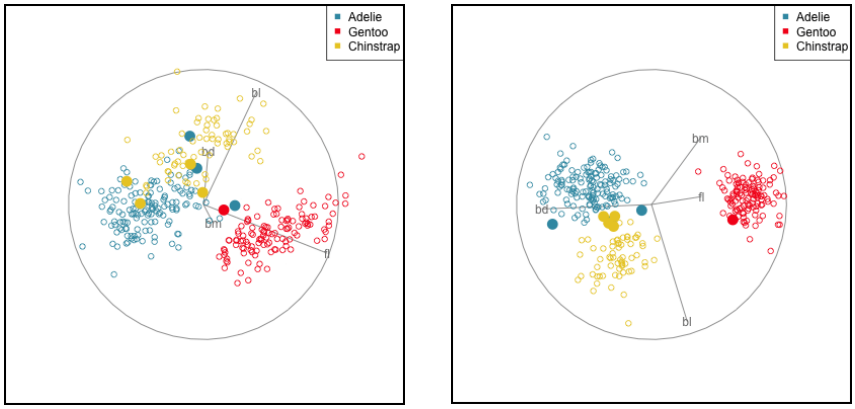
```
penguins_rf$confusion
```

```
          Adelie Chinstrap Gentoo class.error
Adelie       143         3      0 0.020547945
Chinstrap      4        64      0 0.058823529
Gentoo         0         1    118 0.008403361
```

```
penguins_errors <- penguins_sub %>%
  mutate(err = ifelse(penguins_rf$predicted !=
                        penguins_rf$y, 1, 0))
```

Figure 18.1 shows a grand tour, and a guided tour, of the penguins data, where the misclassifications are marked by an asterisk. (If the gifs are too small to see the different glyphs, you can zoom in to make the figures larger.) It can be seen that the one Gentoo penguin that is mistaken for a Chinstrap by the forest model is always moving with its other Gentoo (yellow) family. It can occasionally be seen to be on the edge of the group, closer to the Chinstraps, in some projections in the grand tour. But in the final projection from the guided tour it is hiding well among the other Gentoos. This is an observation where a mistake has been made because of the inadequacies of the forest algorithm. Forests are only as good as the trees they are constructed from, and we have seen from Section 15.1 that the splits only on single variables

done by trees does not adequately utilise the covariance structure in each class. They make mistakes based on the boxy nature of the boundaries. This can carry through to the forests model. Even though many trees are combined to generate smoother boundaries, forests do not effectively utilise covariance in clusters either. The other mistakes, where Chinstrap are predicted to be Adelie, and vice versa, are more sensible. These mistaken observations can be seen to lie in the border region between the two clusters, and reflect genuine uncertainty about the classification of penguins in these two species.



(a) Grand tour (b) Guided tour

Figure 18.1: Examining the misclassified cases (marked as asterisks) from a random forest fit to the penguins data. The one Gentoo penguin mistaken for a Chinstrap is a mistake made because the forest method suffers from the same problems as trees - cutting on single variables rather than effectively using covariance structure. The mistakes between the Adelie and Chinstrap penguins are more sensible because all of these observations lie is the bordering regions between the two clusters.

Some errors are reasonable because there is overlap between the class clusters. Some errors are not reasonable because the model used is inadequate.

18.2 Comparison between LDA and CNN

18.3 Constructing data to diagnose your model

18.4 Explainability

Exercises

1. Examine misclassifications from a random forest model for the fake_trees data between cluster 1 and 0, using the
   a. principal components
   b. votes matrix. Describe where these errors relative to their true and predicted class clusters. When examining the simplex, are the misclassifications the points that are furthest from any vertices?
2. Examine the misclassifications for the random forest model on the sketches data, focusing on cactus sketches that were mistaken for bananas. Follow up by plotting the images of these errors, and describe whether the classifier is correct that these sketches are so poor their true cactus or banana identity cannot be determined.
3. How do the errors from the random forest model compare with those of your best fitting CNN model? Are the the corresponding images poor sketches of cacti or bananas?
4. Now examine the misclassifications of the sketches data in the
   a. votes matrix from the random forest model
   b. predictive probability distribution from the CNN model, using the simplex approach. Are they as expected, points lying in the middle or along an edge of the simplex?

References

Abbott, E. (1884). *Flatland: A romance of many dimensions*. Dover Publications.

Ahlberg, C., Williamson, C., & Shneiderman, B. (1991). Dynamic Queries for Information Exploration: An Implementation and Evaluation. *ACM CHI '92 Conference Proceedings*, 619–626.

Allaire, J., & Chollet, F. (2023). *Keras: R interface to 'keras'*. https://CRAN.R-project.org/package=keras

Anderson, E. (1957). A Semigraphical Method for the Analysis of Complex Problems. *Proceedings of the National Academy of Science, 13*, 923–927.

Andrews, D. F. (1972). Plots of High-dimensional Data. *Biometrics*, *28*, 125–136.

Andrews, D. F., Gnanadesikan, R., & Warner, J. L. (1971). Transformations of Multivariate Data. *Biometrics*, *27*, 825–840.

Anselin, L., & Bao, S. (1997). Exploratory Spatial Data Analysis Linking SpaceStat and ArcView. In M. M. Fischer & A. Getis (Eds.), *Recent Developments in Spatial Analysis* (pp. 35–59). Springer.

Arnold, J. B. (2021). *Ggthemes: Extra themes, scales and geoms for ggplot2*. https://github.com/jrnold/ggthemes

ASA Statistical Graphics Section. (2023). *Video Library*. https://community.amstat.org/jointscsg-section/media/videos.

Asimov, D. (1985). The Grand Tour: A Tool for Viewing Multidimensional Data. *SIAM Journal of Scientific and Statistical Computing*, *6*(1), 128–143.

Auguie, B. (2017). *gridExtra: Miscellaneous functions for "grid" graphics*. https://CRAN.R-project.org/package=gridExtra

Australian Bureau of Agricultural and Resource Economics and Sciences. (2018). *Forests of Australia*. https://www.agriculture.gov.au/abares/forestsaustralia/forest-data-maps-and-tools/spatial-data/forest-cover

Becker, R. A., & Chambers, J. M. (1984). *S: An environment for data analysis and graphics*. Wadsworth.

Becker, R. A., & Cleveland, W. S. (1988). Brushing Scatterplots. In W. S. Cleveland & M. E. McGill (Eds.), *Dynamic graphics for statistics* (pp. 201–224). Wadsworth.

Becker, R., Cleveland, W. S., & Shyu, M.-J. (1996). The Visual Design and Control of Trellis Displays. *Journal of Computational and Graphical Statistics*, *6*(1), 123–155.

Bederson, B. B., & Schneiderman, B. (2003). *The craft of information visualization: Readings and reflections*. Morgan Kaufmann.

Bellman, R. (1961). *Adaptive control processes : A guided tour*.

Bickel, P. J., Kur, G., & Nadler, B. (2018). Projection pursuit in high dimensions. *Proceedings of the National Academy of Sciences*, *115*, 9151–9156. https://doi.org/10.1073/pnas.1801177115

Bishop, C. M. (2006). *Pattern Recognition and Machine Learning*. Springer.

Boehmke, B., & Greenwell, B. M. (2019). *Hands-on machine learning with r (1st ed.)*. Chapman; Hall/CRC. https://doi.org/10.1201/9780367816377

Boelaert, J., Ollion, E., & Sodoge, J. (2022). *aweSOM: Interactive self-organizing maps*. https://CRAN.R-project.org/package=aweSOM

Bonneau, G.-P., Ertl, T., & Nielson, G. M. (Eds.). (2006). *Scientific visualization: The visual extraction of knowledge from data*. Springer.

Borg, I., & Groenen, P. J. F. (2005). *Modern Multidimensional Scaling*. Springer.

Breiman, L. (2001). Random Forests. *Machine Learning*, *45*(1), 5–32.

Breiman, L., Cutler, A., Liaw, A., & Wiener, M. (2022). *randomForest: Breiman and cutler's random forests for classification and regression*. https://www.stat.berkeley.edu/~breiman/RandomForests/

Breiman, L., Friedman, J., Olshen, C., & Stone, C. (1984). *Classification and Regression Trees*. Wadsworth; Brooks/Cole.

Buja, A. (1996). Interactive Graphical Methods in the Analysis of Customer Panel Data: Comment. *Journal of Business & Economic Statistics*, *14*(1), 128–129.

Buja, A., & Asimov, D. (1986). Grand Tour Methods: An Outline. *Computing Science and Statistics*, *17*, 63–67.

Buja, A., Asimov, D., Hurley, C., & McDonald, J. A. (1988). Elements of a Viewing Pipeline for Data Analysis. In W. S. Cleveland & M. E. McGill (Eds.), *Dynamic graphics for statistics* (pp. 277–308). Wadsworth.

Buja, A., Cook, D., Asimov, D., & Hurley, C. (1997). *Dynamic Projections in High-Dimensional Visualization: Theory and Computational Methods*. AT&T Labs.

Buja, A., Cook, D., Asimov, D., & Hurley, C. (2005). Computational Methods for High-Dimensional Rotations in Data Visualization. In C. R. Rao, E. J. Wegman, & J. L. Solka (Eds.), *Handbook of statistics: Data mining and visualization* (pp. 391–414). Elsevier/North-Holland.

Buja, A., Cook, D., & Swayne, D. (1996). Interactive High-Dimensional Data Visualization. *Journal of Computational and Graphical Statistics*, *5*(1), 78–99.

Buja, A., Hurley, C., & McDonald, J. A. (1986). A Data Viewer for Multivariate Data. *Computing Science and Statistics*, *17*(1), 171–174.

Buja, A., & Swayne, D. F. (2002). Visualization Methodology for Multidimensional Scaling. *Journal of Classification*, *19*(1), 7–43.

Buja, A., Swayne, D. F., Littman, M. L., Dean, N., Hofmann, H., & Chen, L. (2008). Data visualization with multidimensional scaling. *Journal of*

Computational and Graphical Statistics, *17*(2), 444–472. https://doi.org/10.1198/106186008X318440

Buja, A., & Tukey, P. (Eds.). (1991). *Computing and Graphics in Statistics*. Springer-Verlag.

Card, S. K., Mackinlay, J. D., & Schneiderman, B. (1999). *Readings in information visualization*. Morgan Kaufmann Publishers.

Carr, D. B., Wegman, E. J., & Luo, Q. (1996). *ExplorN: Design Considerations Past and Present* (Technical Report No. 129). Center for Computational Statistics, George Mason University.

Chatfield, C. (1995). *Problem solving: A statistician's guide*. Chapman; Hall/CRC Press.

Chen, C., Härdle, W., & Unwin, A. (Eds.). (2006). *Handbook of computational statistics (volume III) data visualization*. Springer.

Chen, C.-H., Härdle, W., & Unwin, A. (Eds.). (2007). *Handbook of Data Visualization*. Springer.

Cheng, B., & Titterington, M. (1994). Neural Networks: A Review from a Statistical Perspective. *Statistical Science*, *9*(1), 2–30.

Cheng, J., & Sievert, C. (2021). *Crosstalk: Inter-widget interactivity for HTML widgets*. https://rstudio.github.io/crosstalk/

Chernoff, H. (1973). The Use of Faces to Represent Points in k-dimensional Space Graphically. *Journal of the American Statistical Association*, *68*, 361–368.

Cleveland, W. S. (1979). Robust Localy Weighted Regression and Smoothing Scatterplots. *Journal of American Statistics Association*, *74*, 829–836.

Cleveland, W. S. (1993). *Visualizing Data*. Hobart Press.

Cleveland, W. S., & McGill, M. E. (Eds.). (1988). *Dynamic graphics for statistics*. Wadsworth.

Cook, D., & Buja, A. (1997). Manual Controls For High-Dimensional Data Projections. *Journal of Computational and Graphical Statistics*, *6*(4), 464–480.

Cook, D., Buja, A., & Cabrera, J. (1993). Projection Pursuit Indexes Based on Orthonormal Function Expansions. *Journal of Computational and Graphical Statistics*, *2*(3), 225–250.

Cook, D., Buja, A., Cabrera, J., & Hurley, C. (1995a). Grand Tour and Projection Pursuit. *Journal of Computational and Graphical Statistics*, *4*(3), 155–172.

Cook, D., Buja, A., Cabrera, J., & Hurley, C. (1995b). Grand Tour and Projection Pursuit. *Journal of Computational and Graphical Statistics*, *4*(3), 155–172.

Cook, D., Hofmann, H., Lee, E.-K., Yang, H., Nikolau, B., & Wurtele, E. (2007). Exploring Gene Expression Data, Using Plots. *Journal of Data Science*, *5*(2), 151–182.

Cook, D., & Laa, U. (2023). *Mulgar: Functions for pre-processing data for multivariate data visualisation using tours*. https://dicook.github.io/mulgar/

Cook, D., Lee, E.-K., Buja, A., & Wickham, H. (2006). Grand Tours, Projection

Pursuit Guided Tours and Manual Controls. In C.-H. Chen, W. Härdle, & A. Unwin (Eds.), *Handbook of Data Visualization*. Springer.

Cook, D., Majure, J. J., Symanzik, J., & Cressie, N. (1996). Dynamic Graphics in a GIS: Exploring and Analyzing Multivariate Spatial Data using Linked Software. *Computational Statistics: Special Issue on Computer Aided Analyses of Spatial Data*, *11*(4), 467–480.

Cook, D., & Swayne, D. F. (2007). *Interactive and dynamic graphics for data analysis: With R and GGobi*. Springer-Verlag. https://doi.org/10.1007/978-0-387-71762-3

Cortes, C., Pregibon, D., & Volinsky, C. (2003). Computational Methods for Dynamic Graphs. *Journal of Computational & Graphical Statistics*, *12*(4), 950–970.

Cortes, C., & Vapnik, V. N. (1995). Support-Vector Networks. *Machine Learning*, *20*(3), 273–297.

d'Ocagne, M. (1885). *Coordonnées Parallèles et Axiales: Méthode de transformation géométrique et procédé nouveau de calcul graphique déduits de la considération des coordonnées paralléles*. Gauthier-Villars.

Dalgaard, P. (2002). *Introductory statistics with R*. Springer.

Dasu, T., Swayne, D. F., & Poole, D. (2005). Grouping Multivariate Time Series: A Case Study. *Proceedings of the IEEE Workshop on Temporal Data Mining: Algorithms, Theory and Applications, in Conjunction with the Conference on Data Mining, Houston, November 27, 2005*, 25–32.

de Vries, A., & Ripley, B. D. (2022). *Ggdendro: Create dendrograms and tree diagrams using ggplot2*. https://github.com/andrie/ggdendro

Department of Environment, Land, Water & Planning. (2019). *Fire Origins - Current and Historical*. https://discover.data.vic.gov.au/dataset/fire-origins-current-and-historical

Department of Environment, Land, Water & Planning. (2020a). *CFA - Fire Station*. https://discover.data.vic.gov.au/dataset/cfa-fire-station-vmfeat-geomark_point

Department of Environment, Land, Water & Planning. (2020b). *Recreation Sites*. https://discover.data.vic.gov.au/dataset/recreation-sites

Diaconis, P., & Freedman, D. (1984b). Asymptotics of Graphical Projection Pursuit. *Annals of Statistics*, *12*, 793–815.

Diaconis, P., & Freedman, D. (1984a). Asymptotics of graphical projection pursuit. *Annals of Statistics*, *12*(3), 793–815. https://doi.org/10.1214/aos/1176346703

Dolnicar, S., Grün, B., & Leisch, F. (2018). *Market segmentation analysis: Understanding it, doing it, and making it useful* (pp. 11–22). https://doi.org/10.1007/978-981-10-8818-6_2

Dykes, J., MacEachren, A. M., & Kraak, M.-J. (2005). *Exploring geovisualization*. Elsevier.

Everitt, B. S., Landau, S., & Leese, M. (2001). *Cluster Analysis (4th ed)*. Edward Arnold.

Fienberg, S. E. (1979). Graphical Methods in Statistics. *Journal of American Statistical Association*, *33*(4), 165–178.

Fisher, R. A. (1936b). The Use of Multiple Measurements in Taxonomic Problems. *Annals of Eugenics*, *7*, 179–188.

Fisher, R. A. (1936a). The use of multiple measurements in taxonomic problems. *Annals of Eugenics*, *7*(2), 179–188. https://doi.org/10.1111/j.1469-1809.1936.tb02137.x

Fisher, R. A. (1938). The Statistical Utilization of Multiple Measurements. *Annals of Eugenics*, *8*, 376–386.

Fisherkeller, M. A., Friedman, J. H., & Tukey, J. W. (1973). *PRIM-9, an interactive multidimensional data display and analysis system*. https://www.youtube.com/watch?v=B7XoW2qiFUA

Fisherkeller, M. A., Friedman, J. H., & Tukey, J. W. (1974). PRIM-9, an interactive multidimensional data display and analysis system. In W. S. Cleveland (Ed.), *The collected works of john w. Tukey: Graphics 1965-1985, volume v* (pp. 340–346).

Forbes, J., Cook, D., & Hyndman, R. J. (2020). Spatial modelling of the two-party preferred vote in australian federal elections: 2001–2016. *Australian & New Zealand Journal of Statistics*, *62*(2), 168–185. https://doi.org/https://doi.org/10.1111/anzs.12292

Ford, B. J. (1992). *Images of science: A history of scientific illustration*. The British Library.

Forgy, E. (1965). Cluster analysis of multivariate data: Efficiency versus interpretability of classification. *Biometrics*, *21*(3), 768–769.

Fraley, C., & Raftery, A. E. (2002). Model-based Clustering, Discriminant Analysis, Density Estimation. *Journal of the American Statistical Association*, *97*, 611–631.

Fraley, C., Raftery, A. E., & Scrucca, L. (2022). *Mclust: Gaussian mixture modelling for model-based clustering, classification, and density estimation*. https://mclust-org.github.io/mclust/

Friedman, J. H. (1987). Exploratory Projection Pursuit. *Journal of American Statistical Association*, *82*, 249–266.

Friedman, J. H., & Tukey, J. W. (1974). A Projection Pursuit Algorithm for Exploratory Data Analysis. *IEEE Transactions on Computing C*, *23*, 881–889.

Friendly, M., & Denis, D. J. (2004). *Milestones in the history of thematic cartography, statistical graphics, and data visualization*. http://www.math.yorku.ca/SCS/Gallery/milestone/.

Fritsch, S., Guenther, F., & Wright, M. N. (2019). *Neuralnet: Training of neural networks*. https://CRAN.R-project.org/package=neuralnet

Furnas, G. W., & Buja, A. (1994). Prosection Views: Dimensional Inference Through Sections and Projections. *Journal of Computational and Graphical Statistics*, *3*(4), 323–385.

Gabriel, K. R. (1971). The Biplot Graphical Display of Matrices with Applications to Principal Component Analysis. *Biometrika*, *58*, 453–467.

Gentle, J. E., Härdle, W., & Mori, Y. (Eds.). (2004). *Handbook of computational statistics: Concepts and methods*. Springer.

Giordani, P., Ferraro, M. B., & Martella, F. (2020). *An introduction to clustering with r*. Springer Singapore. https://doi.org/10.1007/978-981-13-0553-5

Glover, D. M., & Hopke, P. K. (1992). Exploration of Multivariate Chemical Data by Projection Pursuit. *Chemometrics and Intelligent Laboratory Systems*, *16*, 45–59.

Good, P. (2005). *Permutation, Parametric, and Bootstrap Tests of Hypotheses*. Springer.

Gower, J. C., & Hand, D. J. (1996). *Biplots*. Chapman; Hall.

Hajibaba, H., Karlsson, L., & Dolnicar, S. (2016). Residents open their homes to tourists when disaster strikes. *Journal of Travel Research*, *56*(8), 1065–1078.

Hansen, C., & Johnson, C. R. (2004). *Visualization handbook*. Academic Press.

Harrison, P. (2023a). *Langevitour: Langevin tour*. https://logarithmic.net/langevitour/

Harrison, P. (2023b). Langevitour: Smooth interactive touring of high dimensions, demonstrated with scRNA-seq data. *The R Journal*, *15*(2), 206–219. https://doi.org/10.32614/RJ-2023-046

Hart, C., & Wang, E. (2022). *Detourr: Portable and performant tour animations*. https://casperhart.github.io/detourr/

Hartigan, J. A., & Kleiner, B. (1981). Mosaics for Contingency Tables. *Computer Science and Statistics: Proceedings of the 13th Symposium on the Interface*, 268–273.

Hartigan, J., & Kleiner, B. (1984). A Mosaic of Television Ratings. *The American Statistician*, *38*, 32–35.

Haslett, J., Bradley, R., Craig, P., Unwin, A., & Wills, G. (1991). Dynamic Graphics for Exploring Spatial Data with Application to Locating Global and Local Anomalies. *The American Statistician*, *45*(3), 234–242.

Hastie, T., Tibshirani, R., & Friedman, J. (2001). *The Elements of Statistical Learning*. Springer.

Hennig, C., Meila, M., Murtagh, F., & Rocci, R. (Eds.). (2015). *Handbook of cluster analysis*. Chapman; Hall/CRC. https://doi.org/10.1201/b19706

Hofmann, H. (2001). *Graphical Tools for the Exploration of Multivariate Categorical Data*. Books on Demand.

Hofmann, H. (2003). Constructing and Reading Mosaicplots. *Computational Statistics and Data Analysis*, *43*(4), 565–580.

Hofmann, H., & Theus, M. (1998). Selection Sequences in MANET. *Computational Statistics*, *13*(1), 77–87.

Horikoshi, M., & Tang, Y. (2018). *Ggfortify: Data visualization tools for statistical analysis results*. https://CRAN.R-project.org/package=ggfortify

Horikoshi, M., & Tang, Y. (2023). *Ggfortify: Data visualization tools for statistical analysis results*. https://github.com/sinhrks/ggfortify

Horst, A., Hill, A., & Gorman, K. (2022). *Palmerpenguins: Palmer archipelago (antarctica) penguin data*. https://CRAN.R-project.org/package=palmerpenguins

Hotelling, H. (1933). Analysis of a complex of statistical variables into principal components. *Journal of Educational Psychology*, *24*(6), 417--441. https://doi.org/10.1037/h0071325

Huber, P. J. (1985). Projection Pursuit (with discussion). *Annals of Statistics*, *13*, 435–525.

Hurley, C. (1987). *The data viewer: An interactive program for data analysis* [PhD thesis]. University of Washington.

Iannone, R., Cheng, J., Schloerke, B., Hughes, E., Lauer, A., & Seo, J. (2023). *Gt: Easily create presentation-ready display tables*. https://CRAN.R-project.org/package=gt

Ihaka, R., & Gentleman, R. (1996). R: A Language for Data Analysis and Graphics. *Journal of Computational and Graphical Statistics*, *5*, 299–314.

Ihaka, R., Murrell, P., Hornik, K., Fisher, J. C., Stauffer, R., Wilke, C. O., McWhite, C. D., & Zeileis, A. (2023). *Colorspace: A toolbox for manipulating and assessing colors and palettes*. https://CRAN.R-project.org/package=colorspace

Inselberg, A. (1985). The Plane with Parallel Coordinates. *The Visual Computer*, *1*, 69–91.

Iowa State University. (2020). *ASOS-AWOS-METAR data download*. https://mesonet.agron.iastate.edu/request/download.phtml?network=AU___ASOS

Johnson, D., & Travis, J. (2007). *Flatland: The movie*. https://round-drum-w7xh.squarespace.com/our-story.

Johnson, R. A., & Wichern, D. W. (2002). *Applied multivariate statistical analysis (5th ed)*. Prentice-Hall.

Jolliffe, I. T., & Cadima, J. (2016). Principal component analysis: A review and recent developments. *Phil. Trans. R. Soc. A.*, *374*, 20150202. https://doi.org/10.1098/rsta.2015.0202

Jones, M. C., & Sibson, R. (1987). What is Projection Pursuit? (With discussion). *Journal of the Royal Statistical Society, Series A*, *150*, 1–36.

Kassambara, A. (2017). *Practical guide to cluster analysis in r: Unsupervised machine learning*. STHDA.

Kassambara, A. (2023). *Ggpubr: ggplot2 based publication ready plots*. https://rpkgs.datanovia.com/ggpubr/

Kohonen, T. (2001). *Self-Organizing Maps (3rd ed)*. Springer.

Koschat, M. A., & Swayne, D. F. (1996). Interactive Graphical Methods in the Analysis of Customer Panel Data (with discussion). *Journal of Business and Economic Statistics*, *14*(1), 113–132.

Krijthe, J. (2022). *Rtsne: T-distributed stochastic neighbor embedding using a barnes-hut implementation*. https://github.com/jkrijthe/Rtsne

Kruskal, J. B. (1964a). Multidimensional Scaling by Optimizing Goodness of Fit to a Nonmetric Hypothesis. *Psychometrika*, *29*, 1–27.

Kruskal, J. B. (1964b). Nonmetric Multidimensional Scaling: A Numerical Method. *Psychometrika*, *29*, 115–129.

Kruskal, J. B., & Wish, M. (1978). *Multidimensional Scaling*. Sage Publications.

Kuhn, M., & Wickham, H. (2020). *Tidymodels: A collection of packages for modeling and machine learning using tidyverse principles*. https://www.tidymodels.org

Kuhn, M., & Wickham, H. (2023). *Tidymodels: Easily install and load the tidymodels packages*. https://CRAN.R-project.org/package=tidymodels

Laa, U., Cook, D., & Lee, S. (2022). Burning sage: Reversing the curse of dimensionality in the visualization of high-dimensional data. *Journal of Computational and Graphical Statistics*, *31*(1), 40–49. https://doi.org/10.1080/10618600.2021.1963264

Laa, U., Cook, D., & Valencia, G. (2020a). A slice tour for finding hollowness in high-dimensional data. *Journal of Computational and Graphical Statistics*, *29*(3), 681–687. https://doi.org/10.1080/10618600.2020.1777140

Laa, U., Cook, D., & Valencia, G. (2020b). A slice tour for finding hollowness in high-dimensional data. *Journal of Computational and Graphical Statistics*, *29*(3), 681–687. https://doi.org/10.1080/10618600.2020.1777140

Lancaster, H. O. (1965). The helmert matrices. *The American Mathematical Monthly*, *72*(1), 4–12.

Laurent, S. (2023). *Cxhull: Convex hull*. https://github.com/stla/cxhull

Lee, E.-K. (2018). PPtreeViz: An r package for visualizing projection pursuit classification trees. *Journal of Statistical Software*, *83*(8), 1–30. https://doi.org/10.18637/jss.v083.i08

Lee, E.-K., & Cook, D. (2009). A projection pursuit index for large p small n data. *Statistics and Computing*, *20*, 381–392. https://doi.org/10.1007/s11222-009-9131-1

Lee, E.-K., Cook, D., Klinke, S., & Lumley, T. (2005). Projection Pursuit for Exploratory Supervised Classification. *Journal of Computational and Graphical Statistics*, *14*(4), 831–846.

Lee, S. (2021). *Liminal: Multivariate data visualization with tours and embeddings*. https://CRAN.R-project.org/package=liminal

Lee, S., Cook, D., Silva, N. da, Laa, U., Spyrison, N., Wang, E., & Zhang, H. S. (2022). The state-of-the-art on tours for dynamic visualization of high-dimensional data. *WIREs Computational Statistics*, *14*(4), e1573. https://doi.org/10.1002/wics.1573

Lee, Y. D., Cook, D., Park, J., & Lee, E.-K. (2013). PPtree: Projection pursuit classification tree. *Electronic Journal of Statistics*, *7*(none), 1369–1386. https://doi.org/10.1214/13-EJS810

Leisch, F., & Gruen, B. (2023). *CRAN task view: Cluster analysis & finite mixture models*. https://cran.r-project.org/web/views/Cluster.html.

Leisch, F., & Grün, B. (2020). *MSA: Market segmentation analysis*.

Li, M., Zhao, Z., & Scheidegger, C. (2020). Visualizing neural networks with the grand tour. *Distill*. https://doi.org/10.23915/distill.00025

Liaw, A., & Wiener, M. (2002). Classification and regression by randomForest. *R News*, *2*(3), 18–22. https://CRAN.R-project.org/doc/Rnews/

Littman, M. L., Swayne, D. F., Dean, N., & Buja, A. (1992). Visualizing

the Embedding of Objects in Euclidean Space. *Computing Science and Statistics: Proceedings of the 24th Symposium on the Interface*, 208–217.

Lloyd, S. (1982). Least squares quantization in PCM. *IEEE Transactions on Information Theory*, *28*(2), 129–137. https://doi.org/10.1109/TIT.1982.1056489

Longley, P. A., Maguire, D. J., Goodchild, M. F., & Rhind, D. W. (2005). *Geographic information systems and science*. John Wiley & Sons.

Loperfido, N. (2018). Skewness-based projection pursuit: A computational approach. *Computational Statistics & Data Analysis*, *120*, 42–57. https://doi.org/https://doi.org/10.1016/j.csda.2017.11.001

Maaten, L. van der, & Hinton, G. (2008). Visualizing data using t-SNE. *J. Mach. Learn. Res.*, *9*(Nov), 2579–2605. http://www.jmlr.org/papers/v9/vandermaaten08a.html

MacQueen, J. B. (1967). Some methods for classification and analysis of multivariate observations. In L. M. L. Cam & J. Neyman (Eds.), *Proc. Of the fifth berkeley symposium on mathematical statistics and probability* (Vol. 1, pp. 281–297). University of California Press.

Maindonald, J., & Braun, J. (2003). *Data analysis and graphics using r - an example-based approach*. Cambridge University Press.

Martin, E. (1965). *Flatland*. http://www.der.org/films/flatland.html.

Mayer, M., & Watson, D. (2023). *Kernelshap: Kernel SHAP*. https://CRAN.R-project.org/package=kernelshap

McFarlane, M., & Young, F. W. (1994). Graphical Sensitivity Analysis for Multidimensional Scaling. *Journal of Computational and Graphical Statistics*, *3*, 23–33.

McInnes, L., Healy, J., & Melville, J. (2018). *UMAP: Uniform manifold approximation and projection for dimension reduction*. http://arxiv.org/abs/1802.03426

McNeil, D. (1977). *Interactive Data Analysis*. John Wiley & Sons.

McVicar, T. (2011). *Near-surface wind speed. v10. CSIRO. Data collection*. https://doi.org/10.25919/5c5106acbcb02

Meyer, D., Dimitriadou, E., Hornik, K., Weingessel, A., & Leisch, F. (2023). *e1071: Misc functions of the department of statistics, probability theory group (formerly: E1071), TU wien*. https://CRAN.R-project.org/package=e1071

Milborrow, S. (2022). *Rpart.plot: Plot rpart models: An enhanced version of plot.rpart*. http://www.milbo.org/rpart-plot/index.html

Mock, T. (2022). *gtExtras: Extending gt for beautiful HTML tables*. https://CRAN.R-project.org/package=gtExtras

Molnar, C. (2022). *Interpretable machine learning: A guide for making black box models explainable (2nd ed)*. https://christophm.github.io/interpretable-ml-book/.

Moon, K. R., Dijk, D. van, Wang, Z., Gigante, S., Burkhardt, D. B., Chen, W. S., Yim, K., Elzen, A. van den, Hirn, M. J., Coifman, R. R., Ivanova, N. B., Wolf, G., & Krishnaswamy, S. (2019). Visualizing structure and

transitions for biological data exploration. *Nature Biotechnology*, *37*, 1482–1492. https://doi.org/10.1038/s41587-019-0336-3

Murrell, P. (2005). *R graphics*. Chapman & Hall/CRC.

OpenStreetMap contributors. (2020). *Planet dump retrieved from https://planet.osm.org* .https://www.openstreetmap.org.

Pearson, K. (1901). LIII. On lines and planes of closest fit to systems of points in space. *The London, Edinburgh, and Dublin Philosophical Magazine and Journal of Science*, *2*(11), 559–572. https://doi.org/10.1080/14786440109462720

Pedersen, T. L. (2023). *Patchwork: The composer of plots*. https://CRAN.R-project.org/package=patchwork

Perisic, I., & Posse, C. (2005). Projection pursuit indices based on the empirical distribution function. *Journal of Computational and Graphical Statistics*, *14*(3), 700–715. https://doi.org/10.1198/106186005X69440

Polzehl, J. (1995). Projection Pursuit Discriminant Analysis. *Computational Statistics and Data Analysis*, *20*, 141–157.

Posse, C. (1992). Projection Pursuit Discriminant Analysis for Two Groups. *Communications in Statistics, Part A – Theory and Methods*, *21*, 1–19.

Posse, C. (1995). Tools for Two-dimensional Projection Pursuit. *Journal of Computational and Graphical Statistics*, *4*(2), 83–100.

P-Tree System. (2020). *JAXA Himawari Monitor - User's Guide*. https://www.eorc.jaxa.jp/ptree/userguide.html

R Core Team. (2023). *R: A language and environment for statistical computing*. R Foundation for Statistical Computing. https://www.R-project.org/

Rao, C. R. (1948). The Utilization of Multiple Measurements in Problems of Biological Classification (with discussion). *Journal of the Royal Statistical Society, Series B*, *10*, 159–203.

Rao, C. R. (Ed.). (1993). *Handbook of Statistics, Vol. 9*. Elsevier Science Publishers.

Rao, C. R., Wegman, E. J., & Solka, J. L. (Eds.). (2006). *Handbook of Statistics: Data Mining and Visualization*. Elsevier/North-Holland.

Ripley, B. (1996). *Pattern Recognition and Neural Networks*. Cambridge University Press.

Ripley, B. (2023a). *MASS: Support functions and datasets for venables and ripley's MASS*. http://www.stats.ox.ac.uk/pub/MASS4/

Ripley, B. (2023b). *Nnet: Feed-forward neural networks and multinomial log-linear models*. http://www.stats.ox.ac.uk/pub/MASS4/

Rothkopf, E. Z. (1957). A Measure of Stimulus Similarity and Errors in Some Paired-associate Learning Tasks. *Journal of Experimental Psychology*, *53*, 94–101.

Schloerke, B. (2016). *Geozoo: Zoo of geometric objects*. https://CRAN.R-project.org/package=geozoo

Schloerke, B., Cook, D., Larmarange, J., Briatte, F., Marbach, M., Thoen, E., Elberg, A., & Crowley, J. (2023). *GGally: Extension to ggplot2*. https://ggobi.github.io/ggally/

Scrucca, L., Fop, M., Murphy, T. B., & Raftery, A. E. (2016). mclust 5: Clustering, classification and density estimation using Gaussian finite mixture models. *The R Journal*, *8*(1), 289–317. https://doi.org/10.32614/RJ-2016-021

Shepard, R. N. (1962). The Analysis of Proximities: Multidimensional Scaling with an Unknown Distance Function, I and II. *Psychometrika*, *27*, 125-139 and 219-246.

Sievert, C. (2020). *Interactive web-based data visualization with r, plotly, and shiny*. Chapman; Hall/CRC. https://plotly-r.com

Sievert, C., Parmer, C., Hocking, T., Chamberlain, S., Ram, K., Corvellec, M., & Despouy, P. (2023). *Plotly: Create interactive web graphics via plotly.js*. https://CRAN.R-project.org/package=plotly

Sjoberg, D. D., Larmarange, J., Curry, M., Lavery, J., Whiting, K., & Zabor, E. C. (2023). *Gtsummary: Presentation-ready data summary and analytic result tables*. https://CRAN.R-project.org/package=gtsummary

Sjoberg, D. D., Whiting, K., Curry, M., Lavery, J. A., & Larmarange, J. (2021). Reproducible summary tables with the gtsummary package. *The R Journal*, *13*, 570–580. https://doi.org/10.32614/RJ-2021-053

Slowikowski, K. (2023). *Ggrepel: Automatically position non-overlapping text labels with ggplot2*. https://github.com/slowkow/ggrepel

Sparks, A. H., Carroll, J., Goldie, J., Marchiori, D., Melloy, P., Padgham, M., Parsonage, H., & Pembleton, K. (2020). *bomrang: Australian government bureau of meteorology (BOM) data client*. https://CRAN.R-project.org/package=bomrang

Spence, R. (2007). *Information visualization: Design for interaction*. Prentice Hall.

Stauffer, R., Mayr, G. J., Dabernig, M., & Zeileis, A. (2009). Somewhere over the rainbow: How to make effective use of colors in meteorological visualizations. *Bulletin of the American Meteorological Society*, *96*(2), 203–216. https://doi.org/10.1175/BAMS-D-13-00155.1

Sutherland, P., Rossini, A., Lumley, T., Lewin-Koh, N., Dickerson, J., Cox, Z., & Cook, D. (2000b). Orca: A Visualization Toolkit for High-Dimensional Data. *Journal of Computational and Graphical Statistics*, *9*(3), 509–529.

Sutherland, P., Rossini, A., Lumley, T., Lewin-Koh, N., Dickerson, J., Cox, Z., & Cook, D. (2000a). Orca: A visualization toolkit for high-dimensional data. *Journal of Computational and Graphical Statistics*, *9*(3), 509–529. https://doi.org/10.1080/10618600.2000.10474896

Swayne, D. F., Buja, A., & Temple Lang, D. (2004). Exploratory visual analysis of graphs in GGobi. In J. Antoch (Ed.), *CompStat: Proceedings in computational statistics, 16th symposium*. Physica-Verlag.

Swayne, D. F., Cook, D., & Buja, A. (1992). XGobi: Interactive Dynamic Graphics in the X Window System with a Link to S. *American Statistical Association 1991 Proceedings of the Section on Statistical Graphics*, 1–8.

Swayne, D. F., Cook, D., & Buja, A. (1998). XGobi: Interactive dynamic data visualization in the x window system. *Journal of Computational and*

Graphical Statistics, *7*(1), 113–130. https://doi.org/10.1080/10618600.1998.10474764

Swayne, D. F., & Klinke, S. (1998). Editorial commentary. *Computational Statistics: Special Issue on The Use of Interactive Graphics*, *14*(1).

Swayne, D. F., Temple Lang, D., Buja, A., & Cook, D. (2003). GGobi: Evolving from XGobi into an Extensible Framework for Interactive Data Visualization. *Computational Statistics & Data Analysis*, *43*, 423–444.

Swayne, D., & Buja, A. (1998). Missing Data in Interactive High-Dimensional Data Visualization. *Computational Statistics*, *13*(1), 15–26.

Symanzik, J. (2002). New applications of the image grand tour. *Computing Science and Statistics*, *34*, 500--512. https://math.usu.edu/symanzik/papers/2002_interface.pdf

Symanzik, J. (2004). Interactive and Dynamic Graphics. In J. E. Gentle, W. Härdle, & Y. Mori (Eds.), *Handbook of computational statistics: Concepts and methods* (pp. 293–336). Springer.

Takatsuka, M., & Gahegan, M. (2002). GeoVISTA Studio: A Codeless Visual Programming Environment for Geoscientific Data Analysis and Visualization. *The Journal of Computers and Geosciences*, *28*(10), 1131–1144.

Tang, Y., Horikoshi, M., & Li, W. (2016). Ggfortify: Unified interface to visualize statistical result of popular r packages. *The R Journal*, *8*(2), 474–485. https://doi.org/10.32614/RJ-2016-060

Tarpey, T., Li, L., & Flury, B. (1995). Principal points and self–consistent points of elliptical distributions. *The Annals of Statistics*, *23*, 103–112.

Temple Lang, D., Swayne, D., Wickham, H., & Lawrence, M. (2006). *`rggobi`: An Interface between R and GGobi*. `http://www.R-project.org`.

Therneau, T., & Atkinson, B. (2023). *Rpart: Recursive partitioning and regression trees*. https://CRAN.R-project.org/package=rpart

Theus, M. (2002). Interactive Data Visualization Using Mondrian. *Journal of Statistical Software*, *7*(11), http://www.jstatsoft.org.

Theus, M., Hofmann, H., & Wilhelm, A. F. X. (1998). Selection Sequences – Interactive Analysis of Massive Data Sets. *Computing Science and Statistics*, *29*(1), 439–444.

Thompson, G. L. (1993). Generalized Permutation Polytopes and Exploratory Graphical Methods for Ranked Data. *The Annals of Statistics*, *21*, 1401–1430.

Tierney, L. (1991). *LispStat: An Object-Orientated Environment for Statistical Computing and Dynamic Graphics*. John Wiley & Sons.

Tierney, N., & Cook, D. (2023a). Expanding tidy data principles to facilitate missing data exploration, visualization and assessment of imputations. *Journal of Statistical Software*, *105*(7), 1–31. https://doi.org/10.18637/jss.v105.i07

Tierney, N., & Cook, D. (2023b). Expanding tidy data principles to facilitate missing data exploration, visualization and assessment of imputations. *Journal of Statistical Software*, *105*(7), 1–31. https://doi.org/10.18637/jss.v105.i07

Tierney, N., Cook, D., McBain, M., & Fay, C. (2023). *Naniar: Data structures, summaries, and visualisations for missing data*. https://github.com/njtierney/naniar

Torgerson, W. S. (1952). Multidimensional Scaling. 1. Theory and Method. *Psychometrika*, *17*, 401–419.

Tufte, E. (1983). *The visual display of quantitative information*. Graphics Press.

Tufte, E. (1990). *Envisioning information*. Graphics Press.

Tukey, J. W. (1965). The Technical Tools of Statistics. *The American Statistician*, *19*, 23–28.

Unwin, A. R., Hawkins, G., Hofmann, H., & Siegl, B. (1996). Interactive Graphics for Data Sets with Missing Values - MANET. *Journal of Computational and Graphical Statistics*, *5*(2), 113–122.

Unwin, A., Hofmann, H., & Wilhelm, A. (2002). Direct Manipulation Graphics for Data Mining. *Journal of Image and Graphics*, *2*(1), 49–65.

Unwin, A., Theus, M., & Hofmann, H. (2006). *Graphics of Large Datasets: Visualizing a Million*. Springer.

Unwin, A., Volinsky, C., & Winkler, S. (2003). Parallel Coordinates for Exploratory Modelling Analysis. *Comput. Stat. Data Anal.*, *43*(4), 553–564. https://doi.org/{\tt http://dx.doi.org/10.1016/S0167-9473(02)00292-X}

Urbanek, S., & Theus, M. (2003). iPlots: High Interaction Graphics for R. In K. Hornik, F. Leisch, & A. Zeileis (Eds.), *Proceedings of the 3rd international workshop on distributed statistical computing (DSC 2003)*.

Vaidyanathan, R., Xie, Y., Allaire, J., Cheng, J., Sievert, C., & Russell, K. (2023). *Htmlwidgets: HTML widgets for r*. https://github.com/ramnathv/htmlwidgets

van der Maaten, L. J. P. (2014). Accelerating t-SNE using tree-based algorithms. *Journal of Machine Learning Research*, *15*, 3221–3245.

van der Maaten, L. J. P., & Hinton, G. E. (2008). Visualizing high-dimensional data using t-SNE. *Journal of Machine Learning Research*, *9*, 2579–2605.

Vapnik, V. N. (1999). *The Nature of Statistical Learning Theory*. Springer.

Velleman, P. F., & Velleman, A. Y. (1985). *Data desk handbook*. Data Description, Inc.

Venables, W. N., & Ripley, B. (2002a). *Modern Applied Statistics with S*. Springer-Verlag.

Venables, W. N., & Ripley, B. D. (2002b). *Modern applied statistics with s* (Fourth). Springer. https://www.stats.ox.ac.uk/pub/MASS4/

Venables, W. N., & Ripley, B. D. (2002c). *Modern applied statistics with s* (Fourth). Springer. https://www.stats.ox.ac.uk/pub/MASS4/

Wainer, H. (2000). *Visual Revelations (2nd ed)*. LEA, Inc.

Wainer, H., & Spence, I. (eds). (2005a). *The Commercial and Political Atlas, Representing, by means of Stained Copper-Plate Charts, The Progress of the Commerce, Revenues, Expenditure, and Debts of England, during the whole of the Eighteenth Century, by William Playfair*. Cambridge University Press.

Wainer, H., & Spence, I. (eds). (2005b). *The Statistical Breviary; Shewing on a Principle entirely new, the resources of every state and kingdom in Europe; illustrated with Stained Copper-Plate Charts, representing the physical powers of each distinct nation with ease and perspicuity by William Playfair*. Cambridge University Press.

Wang, P. C. C. (Ed.). (1978). *Graphical Representation of Multivariate Data*. Academic Press.

Wegman, E. (1990). Hyperdimensional Data Analysis Using Parallel Coordinates. *Journal of American Statistics Association*, *85*, 664–675.

Wegman, E. J. (1991). *The Grand Tour in k-Dimensions* (Technical Report No. 68). Center for Computational Statistics, George Mason University.

Wegman, E. J., & Carr, D. B. (1993). *Statistical Graphics and Visualization* (C. R. Rao, Ed.; pp. 857–958). Elsevier Science Publishers.

Wegman, E. J., Poston, W. L., & Solka, J. L. (1998). Image Grand Tour. *Automatic Target Recognition VIII - Proceedings of SPIE, 3371*, 286–294.

Wehrens, R., & Buydens, L. M. C. (2007). Self- and super-organizing maps in R: The kohonen package. *Journal of Statistical Software*, *21*(5), 1–19. https://doi.org/10.18637/jss.v021.i05

Wehrens, R., & Kruisselbrink, J. (2018). Flexible self-organizing maps in kohonen 3.0. *Journal of Statistical Software*, *87*(7), 1–18. https://doi.org/10.18637/jss.v087.i07

Wehrens, R., & Kruisselbrink, J. (2023). *Kohonen: Supervised and unsupervised self-organising maps*. https://CRAN.R-project.org/package=kohonen

Wickham, H. (2016). *ggplot2: Elegant graphics for data analysis*. Springer-Verlag New York. https://ggplot2.tidyverse.org

Wickham, H. (2022). *Classifly: Explore classification models in high dimensions*. http://had.co.nz/classifly

Wickham, H., Chang, W., Henry, L., Pedersen, T. L., Takahashi, K., Wilke, C., Woo, K., Yutani, H., Dunnington, D., & van den Brand, T. (2024). *ggplot2: Create elegant data visualisations using the grammar of graphics*. https://CRAN.R-project.org/package=ggplot2

Wickham, H., & Cook, D. (2024). *Tourr: Tour methods for multivariate data visualisation*. https://github.com/ggobi/tourr

Wickham, H., Cook, D., & Hofmann, H. (2015). Visualizing statistical models: Removing the blindfold. *Statistical Analysis and Data Mining: The ASA Data Science Journal*, *8*(4), 203–225. https://doi.org/10.1002/sam.11271

Wickham, H., Cook, D., Hofmann, H., & Buja, A. (2011a). Tourr: An R Package for Exploring Multivariate Data with Projections. *Journal of Statistical Software*, *40*(2). https://doi.org/10.18637/jss.v040.i02

Wickham, H., Cook, D., Hofmann, H., & Buja, A. (2011b). tourr: An R package for exploring multivariate data with projections. *Journal of Statistical Software*, *40*(2), 1–18. https://doi.org/10.18637/jss.v040.i02

Wickham, H., François, R., Henry, L., Müller, K., & Vaughan, D. (2023). *Dplyr: A grammar of data manipulation*. https://CRAN.R-project.org/package=dplyr

Wickham, H., Hester, J., & Bryan, J. (2023). *Readr: Read rectangular text data*. https://CRAN.R-project.org/package=readr

Wilhelm, A. F. X., Wegman, E. J., & Symanzik, J. (1999). Visual Clustering and Classification: The Oronsay Particle Size Data Set Revisited. *Computational Statistics: Special Issue on Interactive Graphical Data Analysis*, *14*(1), 109–146.

Wilkinson, L. (2005). *The grammar of graphics*. Springer.

Wills, G. (1999). NicheWorks – Interactive Visualization of Very Large Graphs. *Journal of Computational and Graphical Statistics*, *8*(2), 190–212.

Xie, Y., Hofmann, H., & Cheng, X. (2014). Reactive Programming for Interactive Graphics. *Statistical Science*, *29*(2), 201–213. https://doi.org/10.1214/14-STS477

Young, F. W., Valero-Mora, P. M., & Friendly, M. (2006). *Visual Statistics: Seeing Data with Dynamic Interactive Graphics*. John Wiley & Sons.

Zeileis, A., Fisher, J. C., Hornik, K., Ihaka, R., McWhite, C. D., Murrell, P., Stauffer, R., & Wilke, C. O. (2020). colorspace: A toolbox for manipulating and assessing colors and palettes. *Journal of Statistical Software*, *96*(1), 1–49. https://doi.org/10.18637/jss.v096.i01

Zeileis, A., Hornik, K., & Murrell, P. (2009). Escaping RGBland: Selecting colors for statistical graphics. *Computational Statistics & Data Analysis*, *53*(9), 3259–3270. https://doi.org/10.1016/j.csda.2008.11.033

Zhang, C., Ye, J., & Wang, X. (2023). A computational perspective on projection pursuit in high dimensions: Feasible or infeasible feature extraction. *International Statistical Review*, *91*(1), 140–161. https://doi.org/10.1111/insr.12517

Zhang, H. S., Cook, D., Laa, U., Langrené, N., & Menéndez, P. (2021). Visual diagnostics for constrained optimisation with application to guided tours. *The R Journal*, *13*(2), 624–641. https://doi.org/10.32614/RJ-2021-105

Zhang, H. S., Cook, D., Laa, U., Langrené, N., & Menéndez, P. (2022). *Ferrn: Facilitate exploration of touRR optimisatioN*. https://github.com/huizezhang-sherry/ferrn/

Zhu, H. (2021). *kableExtra: Construct complex table with kable and pipe syntax*. https://CRAN.R-project.org/package=kableExtra

A

Toolbox

A.1 Using tours in the `tourr` package

A.1.1 Installation

You can install the released version of `tourr` from CRAN with:

```
install.packages("tourr")
```

and the development version from the GitHub repo with:

```
# install.packages("remotes")
remotes::install_github("ggobi/tourr")
```

A.1.2 Getting started

To run a tour in R, use one of the animate functions. The following code will show a 2D tour displayed as a scatterplot on a 6D data set with three labelled classes.

```
animate_xy(flea[,-7], col=flea$species)
```

Wickham et al. (2011a) remains a good reference for learning more about this package. The package website has a list of current functionality.

A.1.3 Different tours

The two main components of the tour algorithm are the projection dimension which affects the choice of display to use, and the algorithm that delivers the projection sequence. The primary functions for these two parts are

1. For display of different projection dimensions:

- `display_dist()`: choice of density, histogram or average shifted histogram (ash) display of the 1D projections.
- `display_xy()`, `display_density2d()`, `display_groupxy()`, `display_pca()`, `display_sage()`, `display_slice()`, `display_trails()`: choices in display of 2D projections.
- `display_depth()`, `display_stereo()`: choices to display 3D projections.
- `display_pcp()`, `display_scatmat()`, `display_stars()`, `display_faces()`: choices for displaying three or more variables.
- `display_image()`: to use with multispectral images, where different combinations of spectral bands are displayed. See E. J. Wegman et al. (1998) and Symanzik (2002) for applications.
- `display_andrews()`: 1D projections as Andrews curves.

2. To change the way projections are delivered:

- `grand_tour()`: Smooth sequence of random projections to view all possible projections as quickly as possible. Good for getting an overview of the high-dimensional data, especially when you don't know what you are looking for.
- `guided_tour()`: Follow a projection pursuit optimisation to find projections that have particular patterns. This is used when you want to learn if the data has particular patterns, such as clustering or outliers. Use the `holes()` index to find projections with gaps that allow one to see clusters, or `lda_pp()` or `pda_pp()` when class labels are known and you want to find the projections where the clusters are separated.
- `little_tour()`: Smoothly interpolate between pairs of variables, to show all the marginal views of the data.
- `local_tour()`: Makes small movements around a chosen projections to explore a small neighbourhood. Very useful to learn if small distances away from a projection change the pattern substantially or not.
- `radial_tour()`: Interpolates a chosen variable out of the projection, and then back into the projection. This is useful for assessing importance of variables to pattern in a projection. If the pattern changes a lot when the variable is rotated out, then the variable is important for producing it.
- `dependendence_tour()`: Delivers two sequences of 1D grand tours, to examine associations between two sets of variables. This is useful for displaying two groups of variables as in multiple regression, or multivariate regression or canonical correlation analysis, as two independent 1D projections.
- `frozen_tour()`: This is an interesting one! it allows the coefficient for some variables to be fixed, and others to vary.

A.1.4 The importance of scale

Scaling of multivariate data is really important in many ways. It affects most model fitting, and can affect the perception of patterns when data is visualised. Here we describe a few scaling issues to take control of when using tours.

Pre-processing data

It is generally useful to standardise your data to have mean 0 and variance-covariance equal to the identity matrix before using the tour. We use the tour to discover associations between variables. Characteristics of single variables should be examined and understood before embarking on looking for high-dimensional structure.

The `rescale` parameter in the `animate()` function will scale all variables to range between 0 and 1, prior to starting the tour. This will force all to have the same range. It is the default, and without this data with different ranges across variable may have some strange patterns. If you have already scaled the data yourself, even if using a different scaling such as using standardised variables you should set `rescale=FALSE`.

A more severe transformation that can be useful prior to starting a tour is to **sphere** the data. This is also an option in the `animate()` function, but is `FALSE` by default. Sphering is the same as conducting a principal component analysis, and using the principal components as the variables. It removes all linear association between variables! This can be especially useful if you want to focus on finding non-linear associations, including clusters, and outliers.

Scaling to fit into plot region

The `half_range` parameter in most of the display types sets the range used to scale the data into the plot. It is estimated when a tour is started, but you may need to change it if you find that the data keeps escaping the plot window or is not fully using the space. Space expands exponentially as dimension increases, and the estimation takes this into account. However, different distributions of data points lead to different variance of observations in high-dimensional space. A skewed distribution will be more varied than a normal distribution. It is hard to estimate precisely how the data should be scaled so that it fits nicely into the plot space for all projections viewed.

The `center` parameter is used to centre each projection by setting the mean to be at the middle of the plot space. With different distributions the mean of the data can vary around the plot region, and this can be distracting. Fixing the mean of each projection to always be at the center of the plot space makes it easier to focus on other patterns.

A.1.5 Saving your tour

The functions `save_history()` and `planned_tour()` allow the tour path to be pre-computed, and re-played in your chosen way. The tour path is saved as a list of projection vectors, which can also be passed to external software for displaying tours easily. Only a minimal set of projections is saved, by default, and a full interpolation path of projections can always be generated from it using the `interpolate()` function.

Versions and elements of tours can be saved for publication using a variety of functions:

- `render_gif()`: Save a tour as an animated gif, using the `gifski` package.
- `render_proj()`: Save an object that can be used to produce a polished rendering of a single projection, possibly with `ggplot`.
- `render_anim()`: Creates an object containing a sequence of projections that can be used with `plotly()` to produce an HTML animation, with interactive control.

A.1.6 Understanding your tour path

Figure A.1 shows tour paths on 3D data spaces. For 1D projections the space of all possible projections is a p-dimensional sphere Figure A.1a. For 2D projections the space of all possible projections is a $p \times 2$-dimensional torus Figure A.1b! The geometry is elegant.

In these figures, the space is represented by the light colour, and is constructed by simulating a large number of random projections. The two darker colours indicate paths generated by a grand tour and a guided tour. The grand tour will cover the full space of all possible projections if allowed to run for some time. The guided tour will quickly converge to an optimal projection, so will cover only a small part of the overall space.

```
library(ferrn)
library(tourr)
library(geozoo)
library(dplyr)
library(purrr)
```

(a) 1D tour paths (b) 2D tour paths

Figure A.1: Grand and guided tour paths of 1D and 2D projections of 3D data. The light points represent the space of all 1D and 2D projections respectively. You can see the grand tour is more comprehensively covering the space, as expected, whereas the guided tour is more focused, and quickly moves to the best projection.

A.2 What not to do

A.2.1 Discrete and categorical data

Tour methods are for numerical data, particularly real-valued measurements. If your data is numerical, but discrete the data can look artificially clustered. Figure A.2 shows an example. The data is numeric but discrete, so it is ok to examine it in a tour. In this example, there will be overplotting of observations and the artificial clustering (plot a). It can be helpful to jitter observations, by adding a small amount of noise (plot b). This helps to remove the artificial clustering, but preserve the main pattern which is the strong linear association. Generally, jittering is a useful tool for working with discrete data, so that you can focus on examining the multivariate association. If the data is categorical, with no natural ordering of categories, the tour is not advised.

```
set.seed(430)
df <- data.frame(x1 = sample(1:6, 107, replace=TRUE)) %>%
          mutate(x2 = x1 + sample(1:2, 107, replace=TRUE),
                 x3 = x1 - sample(1:2, 107, replace=TRUE),
                 x4 = sample(1:3, 107, replace=TRUE))
animate_xy(df)
render_gif(df,
           grand_tour(),
           display_xy(),
           gif_file = "gifs/discrete_data.gif",
           frames = 100,
           width = 300,
           height = 300)
```

```
dfj <- df %>%
  mutate(x1 = jitter(x1, 2),
         x2 = jitter(x2, 2),
         x3 = jitter(x3, 2),
         x4 = jitter(x4, 2))
animate_xy(dfj)
render_gif(dfj,
           grand_tour(),
           display_xy(),
           gif_file = "gifs/jittered_data.gif",
           frames = 100,
           width = 300,
           height = 300)
```

(a) Discrete data (b) Jittered data

Figure A.2: Discrete data can look like clusters, which is misleading. Adding a small amount of jitter (random number) can help. The noise is not meaningful but it could allow the viewer to focus on linear or non-linear association between variables without being distracted by artificial clustering.

A.2.2 Missing values

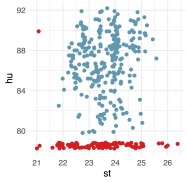
```
library(naniar)
library(ggplot2)
library(colorspace)
data("oceanbuoys")
ob_p <- oceanbuoys %>%
  filter(year == 1993) %>%
  ggplot(aes(x = air_temp_c,
             y = humidity)) +
     geom_miss_point() +
  scale_color_discrete_divergingx(palette="Zissou 1") +
  theme_minimal() +
  theme(aspect.ratio=1)
```

```
ob_nomiss_below <- oceanbuoys %>%
  filter(year == 1993) %>%
  rename(st = sea_temp_c,
         at = air_temp_c,
         hu = humidity) %>%
  select(st, at, hu) %>%
  rowwise() %>%
  mutate(anymiss = factor(ifelse(naniar:::any_na(c(st, at, hu)), TRUE, FALSE))) %>%
  add_shadow(st, at, hu) %>%
  impute_below_if(.predicate = is.numeric)
ob_nomiss_mean <- oceanbuoys %>%
  filter(year == 1993) %>%
  rename(st = sea_temp_c,
         at = air_temp_c,
         hu = humidity) %>%
  select(st, at, hu) %>%
  rowwise() %>%
  mutate(anymiss = factor(ifelse(naniar:::any_na(c(st, at, hu)), TRUE, FALSE))) %>%
  add_shadow(st, at, hu) %>%
  impute_mean_if(.predicate = is.numeric)
ob_p_below <- ob_nomiss_below %>%
  ggplot(aes(x=st, y=hu, colour=anymiss)) +
  geom_point() +
  scale_color_discrete_divergingx(palette="Zissou 1") +
  theme_minimal() +
  theme(aspect.ratio=1, legend.position = "None")
ob_p_mean <- ob_nomiss_mean %>%
  ggplot(aes(x=st, y=hu, colour=anymiss)) +
  geom_point() +
  scale_color_discrete_divergingx(palette="Zissou 1") +
  theme_minimal() +
  theme(aspect.ratio=1, legend.position = "None")
```

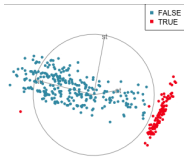
```
animate_xy(ob_nomiss_below[,1:3], col=ob_nomiss$anymiss)
render_gif(ob_nomiss_below[,1:3],
           grand_tour(),
           display_xy(col=ob_nomiss_below$anymiss),
           gif_file = "gifs/missing_values1.gif",
           frames = 100,
           width = 300,
           height = 300)
render_gif(ob_nomiss_mean[,1:3],
           grand_tour(),
           display_xy(col=ob_nomiss_mean$anymiss),
```

```
          gif_file = "gifs/missing_values2.gif",
          frames = 100,
          width = 300,
          height = 300)
```

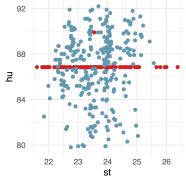
Missing values can also pose a problem for high-dimensional visualisation, but they shouldn't just be ignored or removed. Methods used in 2D to display missings as done in the `naniar` package (N. Tierney & Cook, 2023a) like placing them below the complete data don't translate well to high dimensions. Figure A.3 illustrates this. It leads to artificial clustering of observations Figure A.3b. It is better to impute the values, and mark them with colour when plotting. The cases are then included in the visualisation so we can assess the multivariate relationships, and also obtain some sense of how these cases should be handled, or imputed. In the example in Figure A.3d we imputed the values simply, using the mean of the complete cases. We can see this is not an ideal approach for imputation for this data because some of the imputed values are outside the domain of the complete cases.



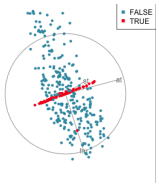
(a) Missings below in 2-D



(b) Missings below in high-D



(c) Missings imputed in 2-D



(d) Missings imputed in high-D

Figure A.3: Ways to visualise missings for 2D don't transfer to higher dimensions. When the missings are set at 10% below the complete cases it appears to be clustered data when viewed in a tour (b). It is better to impute the value, and use colour to indicate that it is originally a missing value (d).

A.2.3 Context such as time and space

We occasionally hear statements like "time is the fourth dimension" or "space is the fifth dimension". This is not a useful way to think about dimensionality.

If you have data with spatial or temporal context, we recommend avoiding

using the time index or the spatial coordinates along with the multiple variables in the tour. Time and space are different types of variables, and should not be combined with the multivariate measurements.

For multivariate temporal data, we recommend using a dependence tour, where one axis is reserved for the time index, and the other axis is used to tour on the multiple variables. For spatial data, we recommend using an image tour, where horizontal and vertical axes are used for spatial coordinates and colour of a tile is used for the tour of multiple variables.

A.3 Tours in other software

There are tours available in various software packages. For most examples we use the `tourr` package, but the same purpose could be achieved by using other software. We also use some of the software this book, when the `tourr` package is not up for the task. For information about these packages, their websites are the best places to start

- liminal: to combine tours with (non-linear) dimension reduction algorithms.
- detourr: animations for {tourr} using `htmlwidgets` for performance and portability.
- langevitour: HTML widget that randomly tours projections of a high-dimensional dataset with an animated scatterplot.
- woylier: alternative method for generating a tour path by interpolating between d-D frames in p-D space rather than d-D planes.
- spinifex: manual control of dynamic projections of numeric multivariate data.
- ferrn: extracts key components in the data object collected by the guided tour optimisation, and produces diagnostic plots.

A.4 Supporting software

- classifly: This package is used heavily for supervised classification.

The `explore()` function is used to explore the classification model. It will predict the class of a sample of points in the predictor space (`.TYPE=simulated`), and return this in a data frame with the observed data (`.TYPE=actual`). The variable `.BOUNDARY` indicates that a point is within a small distance of the

classification boundary, when the value is `FALSE`. The variable `.ADVANTAGE` gives an indication of the confidence with which an observation is predicted, so can also be used to select simulated points near the boundary.

B

Data

This chapter describes the datasets used throughout the book as listed in Table B.1.

Table B.1: List of data sets and their sources used in the book examples.

Name	Description	Analysis
aflw	Player statistics from the AFLW	clustering, dimension reduction
bushfires	Multivariate spatio-temporal data for locations of bushfires	clustering, classification with RF
Australian election data	Socioecenomic characteristics of Australian electorates	dimension reduction, multicollinearity
penguins	Measure four physical characteristics of three species of penguins	classification, and clustering
pisa	OECD programme for international student assessment data	dimension reduction, regression
sketches	Google's Quickdraw data	neural networks, classification
multicluster	Simulated data used to show various cluster examples	clustering
fake trees	Simulated data showing branching structure	clustering, dimension reduction
plane and box	Simulated data showing hyper-planes	dimension reduction
clusters, clusters_nonlin, simple_clusters	Simulated data with various clustering	clustering
c1-c7	Simulated data with various clustering, challenge data	clustering
fashion MNIST	Collection of apparel images	classification

B.1 Australian Football League Women

Description

The `aflw` data is from the 2021 Women's Australian Football League. These are average player statistics across the season, with game statistics provided by the fitzRoy package. If you are new to the game of AFL, there is a nice explanation on Wikipedia.

Variables

```
Rows: 381
Columns: 35
$ id              <chr> "CD_I1001678", "CD_I1001679", "CD_I1~
$ given_name      <chr> "Jordan", "Brianna", "Jodie", "Ebony~
$ surname         <chr> "Zanchetta", "Green", "Hicks", "Anto~
$ number          <int> 2, 3, 5, 12, 60, 21, 22, 23, 35, 14,~
$ team            <chr> "Brisbane Lions", "West Coast Eagles~
$ position        <chr> "INT", "INT", "HFFR", "WL", "RK", "B~
$ time_pct        <dbl> 63.00000, 61.25000, 76.50000, 74.900~
$ goals           <dbl> 0.0000000, 0.0000000, 0.0000000, 0.1~
$ behinds         <dbl> 0.0000000, 0.0000000, 0.5000000, 0.4~
$ kicks           <dbl> 5.000000, 2.500000, 3.750000, 8.8000~
$ handballs       <dbl> 2.500000, 3.750000, 3.000000, 3.6000~
$ disposals       <dbl> 7.500000, 6.250000, 6.750000, 12.400~
$ marks           <dbl> 1.5000000, 0.2500000, 1.0000000, 3.7~
$ bounces         <dbl> 0.0000000, 0.0000000, 0.0000000, 0.6~
$ tackles         <dbl> 3.000000, 2.250000, 2.250000, 3.9000~
$ contested       <dbl> 3.500000, 2.250000, 3.500000, 5.7000~
$ uncontested     <dbl> 3.500000, 4.500000, 3.000000, 7.0000~
$ possessions     <dbl> 7.000000, 6.750000, 6.500000, 12.700~
$ marks_in50      <dbl> 1.0000000, 0.0000000, 0.2500000, 0.5~
$ contested_marks <dbl> 1.0000000, 0.0000000, 0.0000000, 0.4~
$ hitouts         <dbl> 0.000000, 0.000000, 0.000000, 0.0000~
$ one_pct         <dbl> 0.0000000, 1.5000000, 0.5000000, 1.2~
$ disposal        <dbl> 60.25000, 67.15000, 37.20000, 65.960~
$ clangers        <dbl> 2.000000, 0.500000, 2.500000, 3.1000~
$ frees_for       <dbl> 1.0000000, 0.5000000, 0.2500000, 2.5~
$ frees_against   <dbl> 1.0000000, 0.5000000, 1.2500000, 1.3~
$ rebounds_in50   <dbl> 0.0000000, 0.5000000, 0.2500000, 1.1~
$ assists         <dbl> 0.00000000, 0.00000000, 0.00000000, ~
$ accuracy        <dbl> 0.00000, 0.00000, 0.00000, 5.00000, ~
```

```
$ turnovers       <dbl> 1.500000, 1.000000, 2.500000, 4.0000~
$ intercepts      <dbl> 2.0000000, 2.0000000, 0.5000000, 5.3~
$ tackles_in50    <dbl> 0.5000000, 0.0000000, 0.7500000, 0.5~
$ shots           <dbl> 0.5000000, 0.0000000, 0.7500000, 1.0~
$ metres          <dbl> 72.50000, 58.50000, 76.00000, 225.90~
$ clearances      <dbl> 0.5000000, 0.2500000, 1.2500000, 0.4~
```

Purpose

The primary analysis is to summarise the variation using principal component analysis, which gives information about relationships between the statistics or skills sets common in players. One also might be tempted to cluster the players, but there are no obvious clusters so it could be frustrating. At best one could partition the players into groups, while recognising there are no absolutely distinct and separated groups.

Source

See the information provided with the fitzRoy package.

Pre-processing

The code for downloading and pre-processing the data is available at the mulgar website in the `data-raw` folder. The data provided by the fitzRoy package was pre-processed to reduce the variables to only those that relate to player skills and performance. It is possible that using some transformations on the variables would be useful to make them less skewed.

B.2 Bushfires

Description

This data was collated by Weihao (Patrick) Li as part of his Honours research at Monash University. It contains fire ignitions as detected from satellite hotspots, and processed using the spotoroo package, augmented with measurements on weather, vegetation, proximity to human activity. The cause variable is predicted based on historical fire ignition data collected by County Fire Authority personnel.

Variables

```
Rows: 1,021
Columns: 60
$ id          <dbl> 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12,~
$ lon         <dbl> 141.1300, 141.3000, 141.4800, 147.1600~
$ lat         <dbl> -37.13000, -37.65000, -37.35000, -37.8~
$ time        <date> 2019-10-01, 2019-10-01, 2019-10-02, 2~
$ FOR_CODE    <dbl> 41, 41, 91, 44, 0, 44, 0, 102, 0, 91, ~
$ FOR_TYPE    <chr> "Eucalypt Medium Woodland", "Eucalypt ~
$ FOR_CAT     <chr> "Native forest", "Native forest", "Com~
$ COVER       <dbl> 1, 1, 4, 2, 6, 2, 6, 5, 6, 4, 2, 1, 2,~
$ HEIGHT      <dbl> 2, 2, 4, 2, 6, 2, 6, 5, 6, 4, 3, 2, 3,~
$ FOREST      <dbl> 1, 1, 1, 1, 0, 1, 0, 1, 0, 1, 1, 1, 1,~
$ rf          <dbl> 0.0, 0.0, 15.4, 4.8, 6.0, 11.6, 11.6, ~
$ arf7        <dbl> 5.0857143, 2.4000000, 2.4000000, 0.714~
$ arf14       <dbl> 2.8142857, 1.7428571, 1.8000000, 1.671~
$ arf28       <dbl> 1.9785714, 1.5357143, 1.5357143, 3.785~
$ arf60       <dbl> 2.3033333, 1.7966667, 1.7966667, 4.000~
$ arf90       <dbl> 1.2566667, 1.0150000, 1.0150000, 2.960~
$ arf180      <dbl> 0.9355556, 0.8444444, 0.8444444, 2.358~
$ arf360      <dbl> 1.3644444, 1.5255556, 1.5255556, 1.727~
$ arf720      <dbl> 1.3011111, 1.5213889, 1.5213889, 1.711~
$ se          <dbl> 3.8, 4.6, 14.2, 23.7, 23.8, 16.8, 18.0~
$ ase7        <dbl> 18.02857, 18.50000, 21.41429, 23.08571~
$ ase14       <dbl> 17.03571, 17.44286, 18.03571, 19.17143~
$ ase28       <dbl> 19.32857, 18.47500, 19.33929, 18.23571~
$ ase60       <dbl> 20.38644, 19.99153, 20.39492, 19.90847~
$ ase90       <dbl> 22.54118, 21.93193, 22.04370, 20.59328~
$ ase180      <dbl> 20.79106, 19.93966, 19.99385, 19.11006~
$ ase360      <dbl> 15.55153, 14.83259, 14.87883, 14.69276~
$ ase720      <dbl> 15.52350, 14.75049, 14.77427, 14.53463~
$ maxt        <dbl> 21.3, 17.8, 15.4, 20.8, 19.8, 15.8, 19~
$ amaxt7      <dbl> 22.38571, 20.44286, 22.21429, 24.21429~
$ amaxt14     <dbl> 21.42857, 19.72857, 19.86429, 21.80000~
$ amaxt28     <dbl> 20.71071, 19.10000, 19.18929, 19.75000~
$ amaxt60     <dbl> 24.02667, 22.28000, 22.38667, 22.93167~
$ amaxt90     <dbl> 27.07750, 25.77667, 25.89833, 24.93667~
$ amaxt180    <dbl> 26.92000, 25.92722, 25.98500, 24.84056~
$ amaxt360    <dbl> 21.55389, 20.79778, 20.81333, 20.21972~
$ amaxt720    <dbl> 21.47750, 20.57222, 20.57694, 20.13153~
$ mint        <dbl> 9.6, 9.0, 7.3, 7.7, 8.3, 8.3, 6.1, 5.9~
$ amint7      <dbl> 9.042857, 7.971429, 9.171429, 10.32857~
$ amint14     <dbl> 9.928571, 9.235714, 9.421429, 10.00714~
$ amint28     <dbl> 8.417857, 7.560714, 7.353571, 8.671429~
```

```
$ amint60       <dbl> 11.156667, 9.903333, 9.971667, 10.9716~
$ amint90       <dbl> 11.96667, 10.81250, 10.87833, 12.49000~
$ amint180      <dbl> 11.96778, 11.01056, 11.02000, 12.41944~
$ amint360      <dbl> 9.130556, 8.459722, 8.448333, 9.588611~
$ amint720      <dbl> 8.854861, 8.266250, 8.254028, 9.674861~
$ dist_cfa      <dbl> 9442.206, 6322.438, 7957.374, 7790.785~
$ dist_camp     <dbl> 50966.485, 6592.893, 31767.235, 8816.2~
$ ws            <dbl> 1.263783, 1.263783, 1.456564, 5.424445~
$ aws_m0        <dbl> 2.644795, 2.644795, 2.644795, 5.008369~
$ aws_m1        <dbl> 2.559202, 2.559202, 2.559202, 5.229680~
$ aws_m3        <dbl> 2.446211, 2.446211, 2.446211, 5.386005~
$ aws_m6        <dbl> 2.144843, 2.144843, 2.144843, 5.132617~
$ aws_m12       <dbl> 2.545008, 2.545008, 2.548953, 5.045297~
$ aws_m24       <dbl> 2.580671, 2.580671, 2.584047, 5.081100~
$ dist_road     <dbl> 498.75145, 102.22032, 1217.22446, 281.~
$ log_dist_cfa  <dbl> 9.152945, 8.751860, 8.981854, 8.960697~
$ log_dist_camp <dbl> 10.838924, 8.793748, 10.366191, 9.0843~
$ log_dist_road <dbl> 6.212108, 4.627130, 7.104329, 5.640813~
$ cause         <chr> "lightning", "lightning", "lightning",~
```

Purpose

The primary goal is to predict the cause of the bushfire using the weather and distance from human activity variables provided.

Source

Collated data was part of Weihao Li's Honours thesis, which is not publicly available. The hotspots data was collected from P-Tree System (2020), climate data was taken from the Australian Bureau of Meteorology using the `bomrang` package (Sparks et al., 2020), wind data from McVicar (2011) and Iowa State University (2020), vegetation data from Australian Bureau of Agricultural and Resource Economics and Sciences (2018), distance from roads calculated using OpenStreetMap contributors (2020), CFA stations from Department of Environment, Land, Water & Planning (2020a), and campsites from Department of Environment, Land, Water & Planning (2020b). The cause was predicted from training data provided by Department of Environment, Land, Water & Planning (2019).

Pre-processing

The 60 variables are too many to view with a tour, so it should be pre-processed using principal component analysis. The categorical variables of FOR_TYPE and FOR_CAT are removed. It would be possible to keep these if they are converted to dummy (binary variables).

B.3 Australian election data

Description

This is data from a study on the relationship between voting patterns and socio-demographic characteristics of Australian electorates reported in Forbes et al. (2020). These are the predictor variables upon which voting percentages are modelled. There are two years of data in `oz_election_2001` and `oz_election_2016`.

Variables

```
load("data/oz_election_2001.rda")
load("data/oz_election_2016.rda")
glimpse(oz_election_2001)
```

Purpose

The tour is used to check for multicollinearity between predictors, that might adversely affect the linear model fit.

Source

The data was compiled from Australian Electoral Commission (AEC) and the Australian 38 Bureau of Statistics (ABS). Code to construct the data, and the original data are available at https://github.com/jforbes14/eechidna-paper.

Pre-processing

Considerable pre-processing was done to produce these data sets. The original data was wrangled into tidy form, some variables were log transformed to reduce skewness, and a subset of variables was chosen.

B.4 Palmer penguins

```
library(palmerpenguins)
penguins <- penguins %>%
  na.omit() # 11 observations out of 344 removed
# use only vars of interest, and standardise
# them for easier interpretation
penguins_sub <- penguins %>%
  select(bill_length_mm,
         bill_depth_mm,
         flipper_length_mm,
         body_mass_g,
         species,
         sex) %>%
  mutate(across(where(is.numeric),  ~ scale(.)[,1])) %>%
  rename(bl = bill_length_mm,
         bd = bill_depth_mm,
         fl = flipper_length_mm,
         bm = body_mass_g)
save(penguins_sub, file="data/penguins_sub.rda")
```

Description

This data measure four physical characteristics of three species of penguins.

Variables

Name	Description
`bl`	a number denoting bill length (millimeters)
`bd`	a number denoting bill depth (millimeters)

Name	Description
`fl`	an integer denoting flipper length (millimeters)
`bm`	an integer denoting body mass (grams)
`species`	a factor denoting penguin species (Adélie, Chinstrap and Gentoo)

Purpose

The primary goal is to find a combination of the four variables where the three species are distinct. This is also a useful data set to illustrate cluster analysis.

Source

Details of the penguins data can be found at https://allisonhorst.github.io/palmerpenguins/, and Horst et al. (2022) is the package source.

Pre-processing

The data is loaded from the `palmerpenguins` package. The four physical measurement variables and the species are selected, and the penguins with missing values are removed. Variables are standardised, and their names are shortened.

```
library(palmerpenguins)
penguins <- penguins %>%
  na.omit() # 11 observations out of 344 removed
# use only vars of interest, and standardise
# them for easier interpretation
penguins_sub <- penguins[,c(3:6, 1)] %>%
  mutate(across(where(is.numeric),  ~ scale(.)[,1])) %>%
  rename(bl = bill_length_mm,
         bd = bill_depth_mm,
         fl = flipper_length_mm,
         bm = body_mass_g) %>%
  as.data.frame()
save(penguins_sub, file="data/penguins_sub.rda")
```

B.5 Program for International Student Assessment

Description

The `pisa` data contains plausible scores for math, reading and science of Australian and Indonesian students from the 2018 testing cycle. The plausible scores are simulated from a model fitted to the original data, to preserve privacy of the students.

Variables

Name	Description
`CNT`	country, either AUS for Australia or IDN for Indonesia
`PV1MATH-PV10MATH`	plausible scores for math
`PV1READ-PV10READ`	plausible scores for reading
`PV1SCIE-PV10SCIE`	plausible scores for science

Purpose

Primarily this data is useful as an example for dimension reduction.

Source

The full data is available from https://www.oecd.org/pisa/. There are records of the student test scores, along with survey data from the students, their households and their schools.

Pre-processing

The data was reduced to country and the plausible scores, and filtered to the two countries. It may be helpful to know that the SPSS format data was used, and was read into R using the `read_sav()` function in the `haven` package.

B.6 Sketches

Description

This data is a subset of images from https://quickdraw.withgoogle.com. The subset was created using the quickdraw R package at https://huizezhang-sherry.github.io/quickdraw/. It has 6 different groups: banana, boomerang, cactus, flip flops, kangaroo. Each image is 28x28 pixels. The `sketches_train` data would be used to train a classification model, and the unlabelled `sketches_test` can be used for prediction.

Variables

Name	Description
`V1-V784`	grey scale 0-255
`word`	what the person was asked to draw, NA in the test data
`id`	unique id for each sketch

Purpose

Primarily this data is useful as an example for supervised classification, and also dimension reduction.

Source

The full data is available from https://quickdraw.withgoogle.com.

Pre-processing

It is typically useful to pre-process this data into principal components. This code can also be useful for plotting one of the sketches in a recognisable form:

```
library(mulgar)
library(ggplot2)
data("sketches_train")
set.seed(77)
x <- sketches_train[sample(1:nrow(sketches_train), 1), ]
```

```
xm <- data.frame(gry=t(as.matrix(x[,1:784])),
        x=rep(1:28, 28),
        y=rep(28:1, rep(28, 28)))
ggplot(xm, aes(x=x, y=y, fill=gry)) +
  geom_tile() +
  scale_fill_gradientn(colors = gray.colors(256,
                                      start = 0,
                                      end = 1,
                                      rev = TRUE )) +
  ggtitle(x$word) +
  theme_void() +
    theme(legend.position="none")
```

Figure B.1: One of the sketches in the subset of training data.

B.7 `multicluster`

```
library(mulgar)
data("multicluster")
```

Description

This data has 10 numeric variables, and a class variable labelling groups.

Variables

Name	Description
`group`	cluster label
`x1-x10`	numeric variables

Purpose

The primary goal is to find the different clusters.

Source

This data is originally from http://ifs.tuwien.ac.at/dm/download/multiChallenge-matrix.txt, and provided as a challenge for non-linear dimension reduction.It was used as an example in Lee, Laa, Cook (2023) https://doi.org/10.52933/jdssv.v2i3.

B.8 `clusters`, `clusters_nonlin`, `simple_clusters`

```
library(mulgar)
data("clusters")
data("clusters_nonlin")
data("simple_clusters")
```

Description

This data has a various number of numeric variables, and a class variable labelling the clusters.

Variables

Name	Description
`x1-x5`	numeric variables
`cl`	cluster label

Purpose

The primary goal is to find the different clusters.

Source

Simulated using the code in the `simulate.R` file of the `data-raw` directory of the `mulgar` package.

B.9 plane, plane_nonlin, box

```
library(mulgar)
data("plane")
data("plane_nonlin")
data("box")
```

Description

This data has a various number of numeric variables.

Variables

Name	Description
`x1-x5`	numeric variables

Purpose

The primary goal is to understand how many dimensions the data spreads out.

Source

Simulated using the code in the `simulate.R` file of the `data-raw` directory of the `mulgar` package.

B.10 c1 - c7

```
library(mulgar)
data("c1")
```

```
Warning in data("c1"): data set 'c1' not found
```

```
# Load others similarly
```

Description

This data has a various number of numeric variables, and a variety of cluster shapes.

Variables

Name	Description
x1, x2, ...	numeric variables

Purpose

The primary goal is to detect the different clusters.

Source

These are challenge data sets, so the code to simulate them is not made available.

B.11 Fashion MNIST

Description

This data is a subset of images from https://github.com/zalandoresearch/fashion-mnist. Each image is 28x28 grayscale image. The training set has 60,000 images, and the test set has 10,000 images.

Variables

Name	Description
`x`	arrays of grey scale values 0-255
`y`	label 0-9, corresponding to T-shirt/top, Trouser, Pullover, Dress, Coat, Sandal, Shirt, Sneaker, Bag, Ankle boot

Purpose

Primarily this data is useful as an example for neural network modeling, following the tutorial at https://tensorflow.rstudio.com/tutorials/keras/classification.

Source

The data is available from https://github.com/zalandoresearch/fashion-mnist.

C

Links to Book Code and Additional Data

The code and data and an RStudio project can be downloaded with

```
usethis::use_zip(url="https://dicook.github.io/mulgar_book/code_and_data.zip")
```

Alternatively, individual files can be downloaded from the links below.

C.1 Additional data

Table C.1 lists additional data available on the book web site at https://dicook.github.io/mulgar_book/data.

Table C.1: Links to other data sets used on the book.

Filename	Description	Chapter
`aflw_pct.rda`	Saved 2D tour path for the aflw data	4
`detourr_penguins.csv`	Saved clusters of the penguins data from detourr	7
`fake_trees_sb.csv`	Saved clusters of the fake trees data from detourr	7
`penguins_sub.rda`	Tidied penguins data	5, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 17
`penguins_tour_path.rda`	Saved 2D tour path for penguins data	1, 8, 10, 13, 14, 15
`risk_MSA.rds`	risk survey	12
`penguins_cnn`	penguins NN model	17
`fashion_cnn`	fashion MNST NN model	17
`p_exp_sv.rda`	penguins SHAP values	17

C.2 Code files

Table C.2 lists additional data available on the book web site at https://dicook.github.io/mulgar_book/code.

Table C.2: Links to code used on the book.

Filename	Chapter
`1-intro.R`	1 Picturing high dimensions
`2-notation.R`	2 Notation conventions and R objects
`3-overview-dimred.R`	3 Overview of dimension reduction
`4-pca.R`	4 Principal component analysis
`5-nldr.R`	5 Non-linear dimension reduction
`6-overview-clust.R`	6 Overview of clustering
`7-spin-and-brush.R`	7 Spin-and-brush approach
`8-hierarchical.R`	8 Hierarchical clustering
`9-kmeans.R`	9 k-means clustering
`10-model-based.R`	10 Model-based clustering
`11-som.R`	11 Self-organizing maps
`12-summary-clust.R`	12 Summarising and comparing clustering results
`13-intro-class.R`	13 Overview of supervised classification
`14-lda.R`	14 Linear discriminant analysis
`15-forests.R`	15 Trees and forests
`16-svm.R`	16 Support vector machines
`17-nn.R`	17 Neural networks and deep learning
`18-summary-class.R`	18 Exploring misclassifications
`NA`	A Toolbox

D

Glossary

Term	Synonyms	Description
variable	feature, attribute	a characteristic, number or quantity that can be measured
observations	cases, items, experimental units, observational units, records, statistical units, instances, examples	individuals on which the observations are made
data set	data, file	collection of observations made on one or more variables
response	target	variable that one wishes to predict
predictor	independent variable, feature	variables used to produce a mode to predict the response
similarity	correlation	a measure ranging between 0 and 1, with 1 indicating that the cases are closer
dissimilarity	distance	a measure where a smaller number means the cases are closer
principal component analysis (PCA)	empirical orthogonal functions, eigenvalue decomposition	summarise a high-dimensional variance-covariance using an orthonormal matrix and set of variances. Related methods include factor analysis, multidimensional scaling.
linear discriminant analysis (LDA)	Fisher's linear discriminant	reduce the dimension to the space where the classes are most separated relative to the class means and pooled variance-covariance.
self-organising map (SOM)	Kohonen map	use a grid-constrained set of means to cluster high-dimensional data, and also provide a 2D view of the clusters

Index

Bayes Information Criterion (BIC), 110
brushing
  persistent, 69, 75

classification
  ANN architecture, 162
  boundaries, 138
  confusion matrix, 150, 179
  discriminant space, 130, 139
  Fitting a NN, 164
  hidden layers, 166
  linear discriminant analysis (LDA), 129
  local explanations, 170
  logistic regression, 133
  misclassification, 179
  multivariate analysis of variance (MANOVA), 129
  neural networks, 161
  pooled variance-covariance, 135
  predictive probabilities, 169
  predictive probability distribution, 144
  quadratic discriminant analysis (QDA), 133
  random forest, 143
  separating hyperplane, 157
  supervised, 127
  support vector machines (SVM), 153
  support vectors, 157
  training/test split, 163
  trees, 141
  variable importance, 149
  variance-covariance, 133
  vote matrix, 144, 146
  XAI, 170
cluster analysis
  algorithms, 81, 103
  confusion table, 119
  dendrogram, 81
  hierarchical, 81
  intercluster distance (linkage), 81
  interpoint distance, 69, 70, 72
  k-means, 103
  model-based, 109, 129
  nuisance variable, 69
  self-organizing maps (SOM), 115
  spin-and-brush, 69, 75

data
  aflw, 42, 49
  bushfires, 133
  fake trees, 64, 146, 147
  fashion MNIST, 173
  pisa, 40, 49
detourr, 62
dimension reduction
  coefficients, 39
  eigenvalue, 37
  eigenvector, 37
  interpretation, 45
  principal component analysis (PCA), 37
  principal components, 39
  scree plot, 38, 44
  t-SNE, 59
  UMAP, 59

dimensionality, 13, 15
    crowding, 16
    curse of, 16

feature, 13

liminal, 62

model-in-the-data-space, 47

nonlinearity, 53

outliers, 52

parallel coordinate plot, 70
pooled variance-covariance, 135
projection, 13
    1D, 13
    2D, 15

ternary diagram, 144
tour, 75
    radial, 158
    slice, 138, 142, 171

variable, 13
variance-covariance, 133