

Interactively exploring high-dimensional data and models in R

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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.
- **Miscellaneous:** The material in this part focuses on examining data from different contexts. This includes multiple time series, longitudinal data. A key pre-processing step is to convert the data into Euclidean space.

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`.¹²

```
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.

¹Mulga 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 **MULT**ivariate **G**raphical **A**nalysis with **R**.

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

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

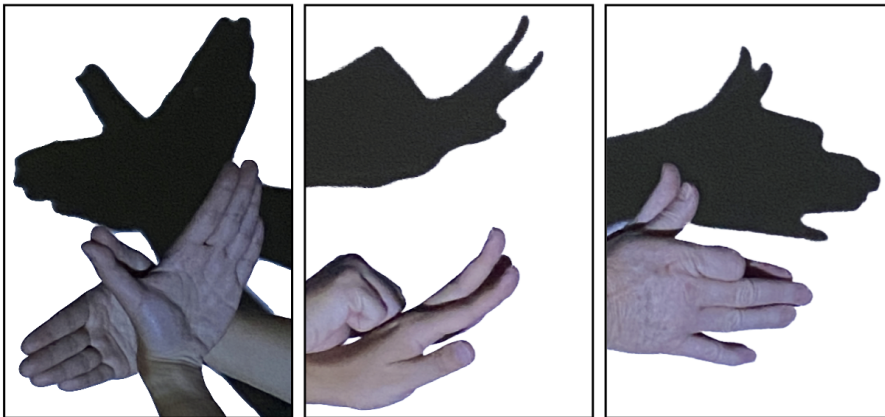
Part I

Introduction

Chapter 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.

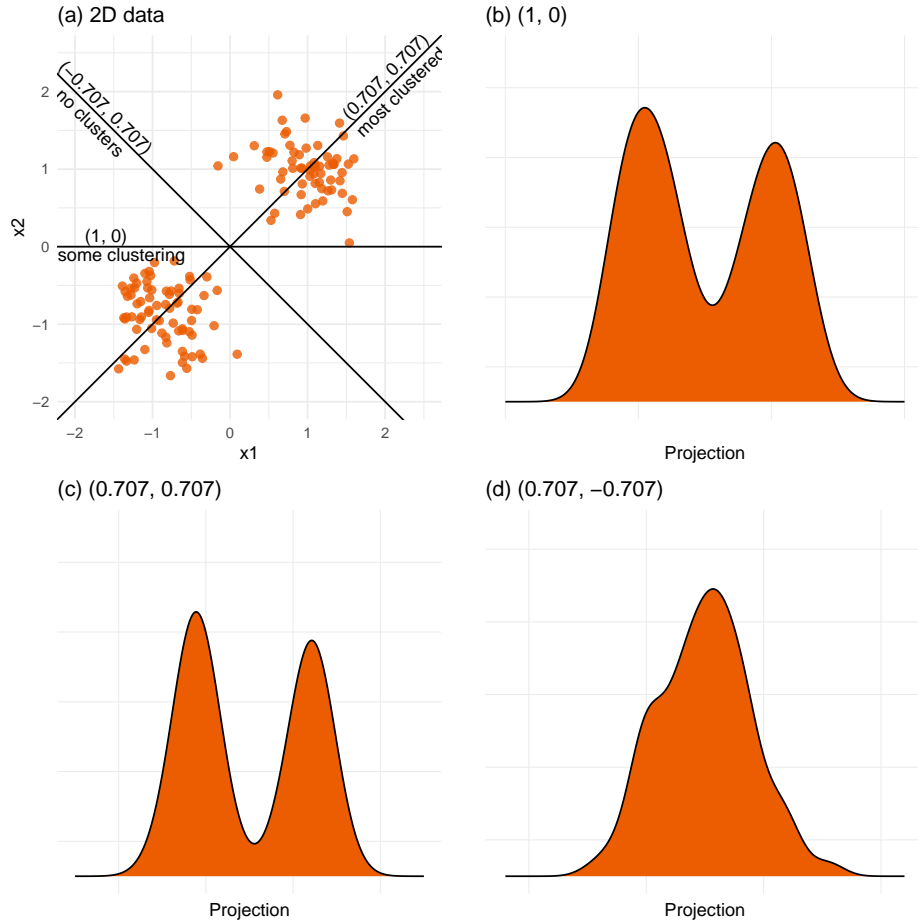


Figure 1.1: How a tour can be used to explore high-dimensional data illustrated using (a) 2D data with two clusters and (b,c,d) 1D projections from a tour shown as a density plot. Imagine spinning a line around the centre of the data plot, with points projected orthogonally onto the line. With this data, when the line is at $x_1=x_2$ $(0.707, 0.707)$ or $(-0.707, -0.707)$ the clustering is the strongest. When it is at $x_1=-x_2$ $(0.707, -0.707)$ there is no clustering.

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.)

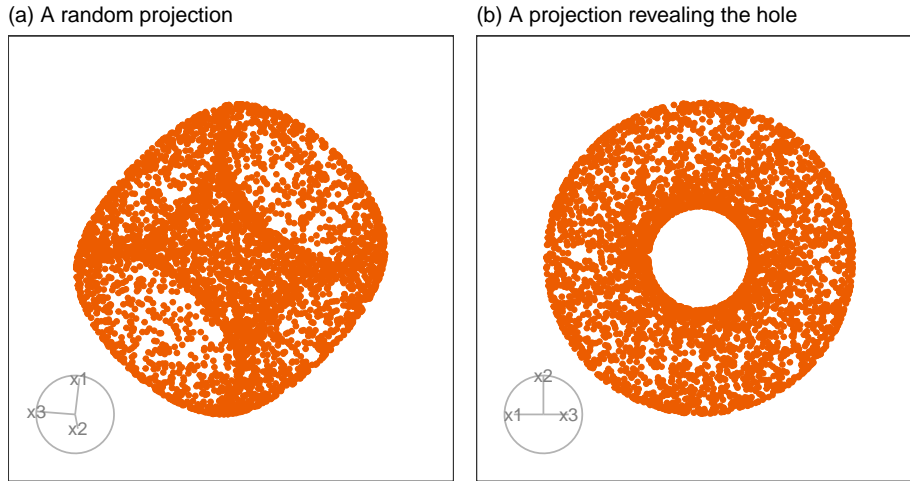


Figure 1.2: How a tour can be used to explore high-dimensional data illustrated by showing a sequence of random 2D projections of 3D data (a). The data has a donut shape with the hole revealed in a single 2D projection (b). Data usually arrives with a given number of observations, and when we plot it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

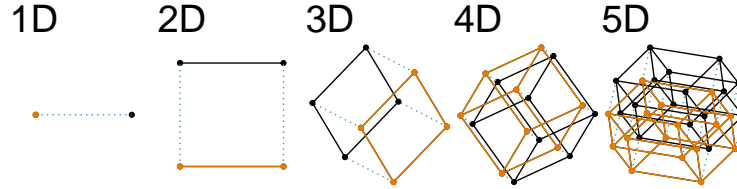


Figure 1.3: Space can be considered to be a high-dimensional cube. Here we have pictured a sequence of increasing dimension cubes, from 1D to 5D, as wireframes, it can be seen that as the dimension increase by one, the cube doubles.

Interestingly, the struggle with imagining high-dimensions this way is described 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 added². 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 (a) and the other has two outliers and a plane (b). Can you see these? One difference in

¹Thanks 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!

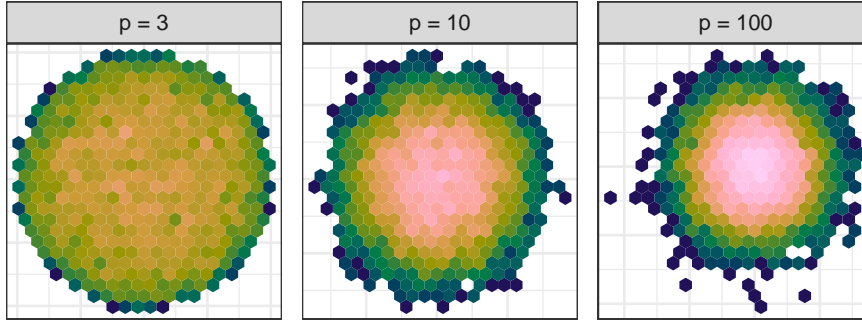


Figure 1.4: Illustration of data crowding in the low-dimensional projection as dimension increases, here from 3, 10, 100. Colour shows the number of points in each hexagon bin (pink is large, navy is small). As dimension increases the points concentrate near the centre.

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 is the effect of dimensionality, with different variance or spread in some directions.

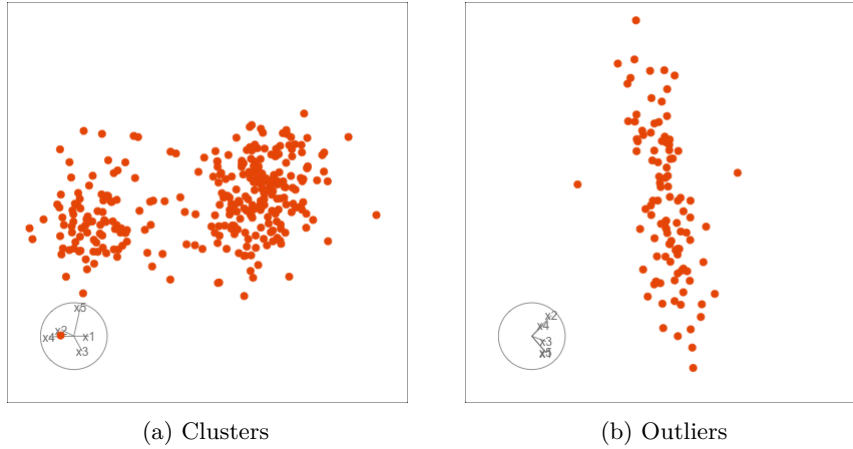


Figure 1.5: Frames from 2D tours on two 5D datasets, with clusters of points in (a) and two outliers with a plane in (b). This figure is best viewed in the HTML version of the book.

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.

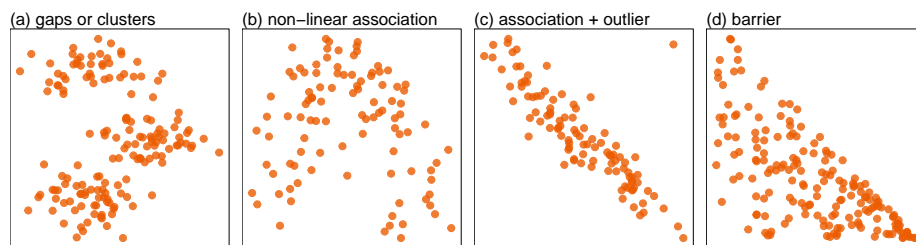


Figure 1.6: Example structures that might be visible in a 2D projection that imply presence of structure in high dimensions. These include clusters, linear and non-linear association, outliers and barriers.

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.
- 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.

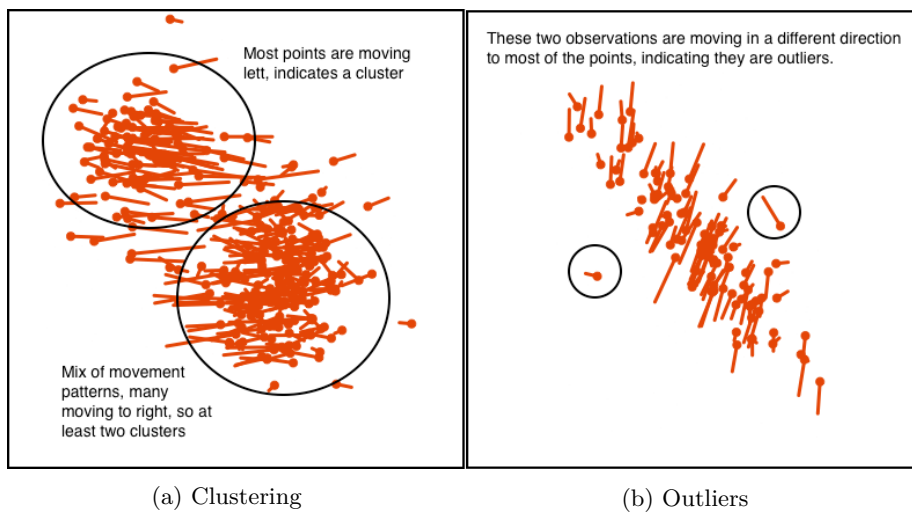


Figure 1.7: The movement of points give further clues about the structure of the data in high-dimensions. In the data with clustering, often we can see a group of points moving differently from the others. Because there are three clusters, you should see three distinct movement patterns. It is similar 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.

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 (Fisher et al., 1973) where a variety of interactive and dynamic tools are used together to explore high dimensional physics data, documented in Fisher 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 hypercube 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`, \dots , `c7` from the `mulgar` package, use the grand tour to view and try to identify structure (outliers, clusters, non-linear relationships).

Chapter 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:

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

where X indicates the the $n \times p$ data matrix, X_j indicates variable $j, j = 1, \dots, p$ 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:

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

A should be an orthonormal matrix, which means that the $\sum_{j=1}^p A_{jk}^2 = 1, k = 1, \dots, d$ (columns represent vectors of length 1) and $\sum_{j=1}^p A_{jk} A_{jl} = 0, k, l = 1, \dots, d; k \neq l$ (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:

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

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?

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