University of Manitoba

Mathematics of Data Science

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Contents

Chapter 1

What is Data Science and why should you care about mathematics as a data scientist?

1.1 What is Data Science?

"Nobody knows" is probably quite an adequate answer to this question. In days of yore (circa 2010), people talked about Big Data, prompting the following declaration, attributed to Dan Ariely (Duke University):

> Big data is like teenage sex: everyone talks about it, nobody really knows how to do it, everyone thinks everyone else is doing it, so everyone claims they are doing it...

The vocabulary has evolved, the term *big data* became *complex data* and more recently, people have been talking about data science. According to Wikipedia (emphasis mine)

> Data science is an **interdisciplinary field** that uses scientific methods, processes, algorithms and systems to extract knowledge and insights from **structured** and **unstructured data**, and apply knowledge and actionable insights from data across a broad range of application domains.
>
> [..] It uses techniques and theories drawn from many fields within the context of **mathematics**, **statistics**, **computer science**, **information science**, and **domain knowledge**.

Data science is nothing new (some statisticians argue it is just another name for statistics), but it has become prominent in recent years as a consequence of the unprecedented mass of information generated and collected by our modern societies.

1.1.1 The data deluge

One speaks of *information explosion* or *data deluge*. See some considerations, e.g., here.

A wide variety of jobs

We have absolutely insane amounts of data and we try to make sense of it. However, except for the more or less fixation of the name, the situation has not improved significantly since the days of Ariely's quote: data science is a hodge-podge that contains everything but the kitchen sink.

To caricature - two main types of data: structured and unstructured - two main branches: statistics and computer science - two main types of jobs: users and developpers

1.2 Why bother about mathematics?

Recall that I said there were two main branches, statistics and computer science, and two main types of jobs: users and developpers. So why a course on Math of Data Science?

In short, if you plan to be a user and are not curious about the *how* and the *why* and can tolerate some errors due to misuse of methods, then you probably do not care about this course.

In other cases, many of the concepts used have their roots in math and to understand where the methods are coming from and, even more importantly, to develop new methods, math is often required

Warning!

We will barely brush the surface here:

- Some techniques from linear algebra - Some graph theory ideas

There is a lot more to see!!!

1.3 Where to go for more information

The Faculty of Science at the University of Manitoba has created the Data Science NEXUS (link).

- Education component - Data Science Undergraduate Program (Fall 2021) - Data Science Master's Program - Master of Business Analytics

- Training (workshops, COOP, internships, etc.)

- Events (conferences, etc.)

1.4 Remark about this document

This document is written in `RSweave`, which is very similar to `Rmarkdown`, but allows to write in native LaTeX. All figures and most data processing is run by `R` at the time of compilation. `R` code is also displayed frequently, when it is novel, in the sense that

it has not been shown before. Otherwise, it is hidden. For example, the code used to generate the first figure is shown; in subsequent figures, code is only shown if additional options are used, etc.

Chapter 2

Getting started – Learning R and collecting data

2.1 Introduction to R and jupyter notebook

In order to illustrate the use of Jupyter Notebook and R, let us prepare for the next lecture using a notebook.

Notebooks run online (here on syzygy.ca). It uses two (mainly) types of "cells". A cell like this one is a text cell. Text is formatted using 'markdown', which is a simple text description language yet has relatively powerful capabilities. See here, for instance, for details.

2.2 Grabing the Canadian census data and putting it into shape

The first steps in analysing data typically involve acquiring it, then putting it into a form that is appropriate for the analysis steps that will follow. The latter step is often called **data wrangling**.

To illustrate the process, let us consider the evolution of the population of Canada through time. For this, we want to find census data. We search the web for "canada historical census data csv", since `csv` (comma separated values) files are very easy to use with `R`. Our search returns a website, here, with a `csv` for 1851 to 1976. We follow the link to Table A2-14, where we find another link (this one), this time to a `csv` file. This is what we use below.

The first step is to read in the data. The function `read.csv` reads in a file, potentially directly from the web. We assign the result to the variable `data_old`. The reason for using the suffix *old* should become clear soon. Note that in order for the link to appear clearly in this text, we first store it in two variable, one for the base url and one for the specific page; this is not a required step by any means. The way we do this, however, is of interest, as it is a process that is often used. Once the two strings are

stored, we paste them one to another using the function `paste0`, which appends all its arguments as a string without adding any space (there is also a function `paste` that does the same thing but with separating spaces).

```
> url_base = "https://www150.statcan.gc.ca/"
> url_page = "n1/en/pub/11-516-x/sectiona/A2_14-eng.csv?st=L7vSnqio"
> url_data = paste0(url_base, url_page)
> data_old = read.csv(url_data)
```

When this is done, it is always a good idea to take a look at the first few rows in the resulting table, to see what things look like. The function `head` shows the first few lines in the argument, eight by default. The call to `knitr::kable` allows to use the function `kable` from the `knitr` library without loading the whole library. The function `kable` formats a table for display in a much better way than `R` does by default.

```
> knitr::kable(head(data_old))
```

```
|  X|Series.A2.14. |Population.of.Canada..by.province..census.dates..1851.to.1976 | X.
|--:|:-------------|:-----------------------------------------------------------|---
| NA|              |                                                            |  N
| NA|Year          |Canada                                                      |  N
| NA|              |                                                            |  N
| NA|              |                                                            |  N
| NA|              |2                                                           |  N
| NA|              |                                                            |  N
```

We use `kable` quite often, actually, so let us load the library (I am assuming it is installed and not using the "safe" way of loading a library explained earlier).

```
> library(knitr)
```

Returning to the data, obviously, this does not make a lot of sense. Take a look at the first few lines in the `csv` file. (This is something you would usually do even before loading the data into `R`.) They take the form

```
,Series A2-14.,"Population of Canada, by province, census dates, 1851 to 1976",,,,,,,,,,,,,,,,
,,,,,,,,,,,,,,,,,,,,,,
,Year,Canada,,Newfound-,Prince,,Nova,New,Quebec,Ontario, Manitoba,,Saskat-,,Alberta,,British,,
,,,,land,Edward,,Scotia,Brunswick,,,,,chewan,,,,Columbia,,Territory,Territories,,
,,,,,Island,,,,,,,,,,,,,,,,
,,2,,3,4,,5,6,7,8,9,,10,,11,,12,,13,14,,
,,,,,,,,,,,,,,,,,,,,,,
```

This is frequent and results from good data storage practice: the first row (and sometimes quite a few more) contains metadata that helps understand what is in the table. However, in the present case, this is not something we care about because we know where the data is coming from, so we can discard this row. The function `read.csv` takes the optional argument `skip=`, which indicates how many lines to skip at the beginning. The second line is also empty, so let us skip it too.

```
> data_old = read.csv(url_data, skip = 2)
```

This gives a slightly better looking table.

```
|  X|Year |Canada     | X.1|Newfound. |Prince  | X.2|Nova    |New       |Quebec    |Ontario
|--:|:----|:----------|---:|:---------|:-------|---:|:-------|:---------|:---------|:---------
| NA|     |           |  NA|land      |Edward  |  NA|Scotia  |Brunswick |          |
| NA|     |           |  NA|          |Island  |  NA|        |          |          |
| NA|     |2          |  NA|3         |4       |  NA|5       |6         |7         |8
| NA|     |           |  NA|          |        |  NA|        |          |          |
| NA|1976 |22,992,604 |  NA|557,725   |118,229 |  NA|828,571 |677,250   |6,234,445 |8,264,465
| NA|     |           |  NA|          |        |  NA|        |          |          |
```

Here, there is the further issue that to make things legible, the table authors used 3 rows (from 2 to 4) to encode for long names (e.g., Prince Edward Island is written over 3 rows). Because we are only interested in the total population of the country and the year, let us get rid of the first 4 rows and of all columns except the second (`Year`) and third (`Canada`). Let us take a look at what we now have, both at the top of the table (using `head()`):

	Year	Canada
5	1976	22,992,604
6		
7	1971	21,568,311
8	1966	20,014,880
9	1961	18,238,247
10	1956	16,080,791

and at the end of the table (using `tail()`):

	Year
24	
25	Includes 485 members of the Royal Canadian Navy whose province of residence is not known.
26	Included with Northwest Territories.
27	For the discussion of the ambiguities and under-enumeration contained in these figures consult the notes
28	see notes to series A15-53.
29	1848 figure.

There are still quite a few remaining issues:

1. there are some empty rows;
2. the last few rows need to be removed too, they contain remarks about the data;
3. the population counts contain commas;
4. it would be better if years were increasing.

Let us fix these issues.

- For 1 and 2, this is easy: remark that the `Canada` column is empty for both issues. Remark as well (if viewing the data from within RStudio or Jupyter Notebook) that below `Canada` (and `Year`, for that matter), the text *<chr>*. This means that entries in the column are *characters*. Looking for empty content therefore means looking for empty strings. So we want to keep the rows where `Canada` does not equal the empty string.

  ```
  > data_old = data_old[which(data_old$Canada != ""),]
  ```

- To get rid of commas, we just need to substitute an empty chain for ",".

  ```
  > data_old$Canada = gsub(",", "", data_old$Canada)
  ```

- To sort, we find the order for the years and apply it to the entire table.

  ```
  > order_data = order(data_old$Year)
  > data_old = data_old[order_data,]
  ```

- Finally, as remarked above, both the year and the population are strings. This means that in order to plot anything, we will have to indicate that these are numbers, not strings.

  ```
  > data_old$Year = as.numeric(data_old$Year)
  > data_old$Canada = as.numeric(data_old$Canada)
  ```

Let us see what the table looks like now.

	Year	Canada
23	1851	2436297
22	1861	3229633
21	1871	3689257
20	1881	4324810
19	1891	4833239
17	1901	5371315

Row numbers are a little weird (the indicate the number of the row in the table as we originally loaded it), so let us fix this. Note that this is purely cosmetic.

```
> row.names(data_old) = 1:dim(data_old)[1]
```

So we have

Year	Canada
1851	2436297
1861	3229633
1871	3689257
1881	4324810
1891	4833239
1901	5371315
1911	7206643
1921	8787949
1931	10376786
1941	11506655
1951	14009429
1956	16080791
1961	18238247
1966	20014880
1971	21568311
1976	22992604

Note that the row numbers are not show any more: they "make sense" and thus `kable` has "decided" not to show them. This is looking quite good. However, this data only goes to 1976. That is close to 50 years missing, surely there must be more recent data!

Looking around, we find another table here. There is a download csv link on that page (this one), let us see where this leads us. Note that the link is very long so I am not showing the `read.csv` command used. Refer to the `Jupyter Notebook` or `Rmarkdown` files on the GitHub repository to see it. The table is 720KB, so there must be more to this than just the population. To get a sense of that, we could dump the whole data frame. Again, this is too much for lecture notes, refer to the worksheets for details. Let us, nonetheless, take a quick peek inside the file. For this, instead of using `head()`, let us pick 10 rows at random.

```
> idx = sort(sample(1:dim(data_new)[1], 10))
```

giving

	GEOGRAPHY.NAME	CHARACTERISTIC	YEAR.S.	TOTAL
181	Canada	Number of persons aged 65 and over, Canada	1971	1744405.00
959	Prince Edward Island	% of two-person households	1961	20.53
1226	Nova Scotia	% of one-person households	1986	18.55
4178	Oshawa	% of the population aged 65 years and over	2001	10.40
5191	Brantford	Population by single years of age: 86 years	2011	440.00
7026	Saskatchewan	% of five-or-more-person households	2006	9.09
7330	Saskatoon	Population by single years of age: 34 years	2011	3630.00
8028	Edmonton	Population by single years of age: 94 years	2011	485.00
8250	British Columbia	% of one-person households	1966	16.00
9603	Northwest Territories	% of lone-parent families	1966	9.70

This is a very different way of storing the information from the first table, which had, to caricature, columns with the different regions of interest and rows the years. Here, different contain different information. To get a better sense of what we are looking at, let us first look at the columns.

```
> colnames(data_new)
```

```
[1] "GEOGRAPHY.NAME" "CHARACTERISTIC" "YEAR.S."        "TOTAL"
[5] "FLAG_TOTAL"
```

This is a different way of thinking about the data. `GEOGRAPHY.NAME` and `CHARACTERISTIC`, taken as a pair, define an attribute, whose `TOTAL` (value) is then documented for each `YEAR.S` in the table. The column `FLAG_TOTAL` is used to comment on individual data points. By selecting the relevant *geography* and *characteristic*, we therefore get the time series we want. To find what value of *geography* and *characteristic* to use, we parse through the output of, say,

```
unique(data_new$GEOGRAPHY.NAME)
unique(data_new$CHARACTERISTIC)
```

that return the list of distinct (unique) values in both these columns. The output is not shown here because these commands generate a substantial number of results: there are 57 unique geographies and 213 unique characteristics in the table. Looking through these results, we find that the information we want has geography "Canada" and characteristic "Population (in thousands)". In passing, from this we also remark that the population of Canada is expressed in thousands, so once we have selected what we want, we will need to multiply the value by 1,000 in order to have data in the same units as in `data_old`.

There are many ways to select rows. Let us present three different mechanisms.

The basic (and reliable) way Let us proceed as follows: we want the rows where the geography is "Canada" and the characteristic is "Population (in thousands)". Let us find the indices of rows that satisfy the first criterion, those that satisfy the second; if we then intersect these two sets of indices, we have the indices of the rows we are interested in.

```
> idx_CAN = which(data_new$GEOGRAPHY.NAME == "Canada")
> idx_char = which(data_new$CHARACTERISTIC == "Population (in thousands)")
> idx_keep = intersect(idx_CAN, idx_char)
```

Once these indices have been selected, we can retain only those rows in `data_new` that are of interest to us.

```
> data_new = data_new[idx_keep,]
```

Thinking SQL If you have any experience with SQL, a language for maintaining and querying databases, it can be tempting to solve this selection problem using SQL syntax. This is made possible by using the library `sqldf`, which allows to perform SQL queries on data frames.

```
> if (!require("sqldf")) {
+   install.packages("sqldf")
+ }
> query = "SELECT * FROM data_new
+ WHERE `GEOGRAPHY.NAME`='Canada'
+ AND `CHARACTERISTIC`='Population (in thousands)'"
> data_new = sqldf(query)
```

The modern way: `dplyr` `dplyr` is part of the `tidyverse`, an ecosystem of `R` libraries meant to facilitate data manipulation. Personnally, I tend to be more familiar with SQL, but there are similarities. `dplyr` also makes use of the pipe `%>%`, which is extremely powerful when manipulated correctly. (This is the same idea as the unix pipe |.)

Back to our wrangling We want to concatenate this data frame with the one from earlier. To do this, we need the two data frames to have the same number of columns and, actually, the same column names and entry types (notice that `YEAR.S.` in `data_new` is a column of characters). So what remains to do:

1. Rename the columns in the old data (`data_old`) to `year` and `population` (personally, I prefer lowercase column names).

   ```
   > colnames(data_old) = c("year", "population")
   ```

2. Keep only the relevant columns in `data_new` and rename them to match column names in `data_old`.

```
> data_new = data_new[,c("YEAR.S.","TOTAL")]
> colnames(data_new) = c("year", "population")
```

3. Transform year in `data_new` to numbers.

   ```
   > data_new$year = as.numeric(data_new$year)
   ```

4. Multiply population by 1,000 in `data_new`.

   ```
   > data_new$population = data_new$population*1000
   ```

5. We already have data up to and including 1976 in `data_old`, so get rid of that in `data_new`.

   ```
   > data_new = data_new[which(data_new$year>1976),]
   ```

6. Append the rows of `data_new` to those of `data_old`. To simplify later use, we call `data` this aggregated data.

   ```
   > data = rbind(data_old,data_new)
   ```

Let us see what this looks like when all of this is done; see Figure 2.1. For information, the command used to generate Figure 2.1 is the following:

```
plot(data$year, data$population,
     type = "b",
     lwd = 2,
     xlab = "Year",
     ylab = "Population")
```

In case we need the data elsewhere, we save it.

```
> write.csv(data, file = "Canada_census.csv")
```

Saving processed data is usually a good idea. The preprocessing steps we have just carried out can be quite costly computationally in the case of a large data set. Also, the source of the data may move: websites, even institutional ones like Open Data portals, have a tendency to rename files occasionally. Some files come with permanent identifiers that in principle make them impervious to these changes, but this is not yet the norm.

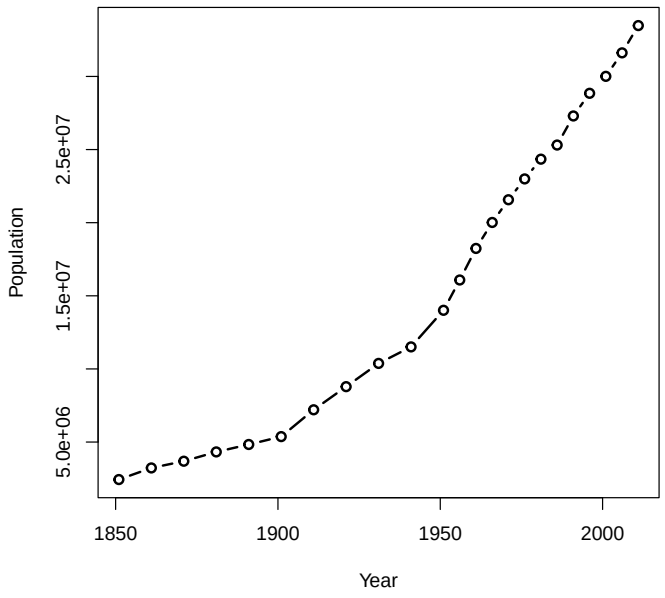


Figure 2.1: Evolution of the population of Canada.

Chapter 3

Least squares problems

In this chapter, we consider several matrix methods useful in Data Science applications, with different purposes in mind. Firstly, explain the principles; secondly, understand why a method works; thirdly, show how to use the method in practice, both "by hand" and using computational software.

We present some matrix theory, focusing on the specific results needed for the topics under consideration. Other required material is found in Appendix A.

To motivate least squares problems, remember the data we gathered in Chapter 2 about the evolution of the population of Canada through time. As we saved that data then, let us load it

```
> data = read.csv("Canada_census.csv")
```

and plot it, with the result shown in Figure 3. A public official, in view of this figure, might be interested in getting a sense of what the population of Canada could be expected to be in, say, 2050. There are several ways to do that. One is to use so-called linear least squares (often called least squares for short), which is what we study here.

3.1 From interpolation to fitting

Let us start with the simplest possible case: if we have just two points, then obviously, it is easy to find the parameters a_0 and a_1 such that the line

$$\ell : \ y = a_0 + a_1 x \tag{3.1}$$

goes through the two points. This is called a problem of **interpolation**. There are several ways to do that, but let us do so in a way that will be an inspiration for later problems.

Suppose the two points are (x_1, y_1) and (x_2, y_2). Since they are on the line ℓ, they must satisfy the equation (3.1), and thus

$$\begin{aligned} y_1 &= a_0 + a_1 x_1 \\ y_2 &= a_0 + a_1 x_2. \end{aligned}$$

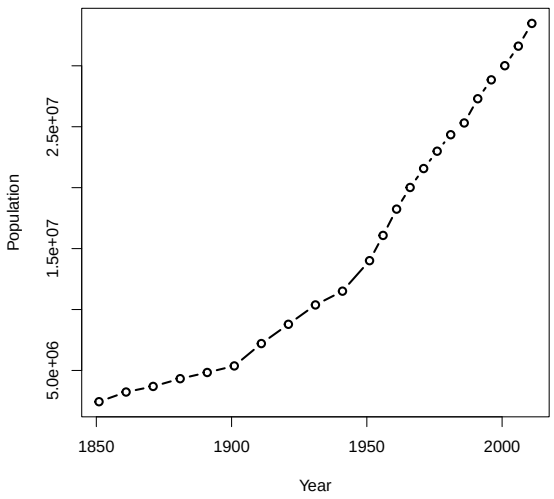


Figure 3.1: Evolution of the population of Canada.

Recall that what we seek are the coefficients a_0, a_1 of ℓ, so we write this as a linear system with unknowns a_0 and a_1:

$$\begin{pmatrix} 1 & x_1 \\ 1 & x_2 \end{pmatrix} \begin{pmatrix} a_0 \\ a_1 \end{pmatrix} = \begin{pmatrix} y_1 \\ y_2 \end{pmatrix},$$

which we write $A\mathbf{x} = \mathbf{b}$ with

$$A = \begin{pmatrix} 1 & x_1 \\ 1 & x_2 \end{pmatrix}, \mathbf{x} = \begin{pmatrix} a_0 \\ a_1 \end{pmatrix} \text{ and } \mathbf{b} = \begin{pmatrix} y_1 \\ y_2 \end{pmatrix}.$$

From Theorem A.62, we know that this system has the unique solution $\mathbf{x} = A^{-1}\mathbf{b}$ if and only if $\det(A) \neq 0$. We easily obtain that $\det(A) = x_2 - x_1$ and thus $\det(A) \neq 0$ (and we have a unique solution) if and only if $x_1 \neq x_2$. This makes sense: if $x_1 = x_2$, this means ℓ is vertical, which cannot be described by an equation such as (3.1).

Let us take a quick look at a numerical example. Suppose we have two points $(1, 3)$ and $(3, 5)$. In `R`, we can for instance create a list and store the values there.

```
> points = list()
> points$x = c(1,2)
> points$y = c(3,5)
```

Recall that matrix inversion in `R` is through the function `solve`, which, when provided with a second (vector) argument, actually computes $A^{-1}\mathbf{b}$, so

```
> A = matrix(c(1,points$x[1],
+              1,points$x[2]),
+            nr = 2, byrow = TRUE)
> coefs = solve(A, points$y)
```

To plot the line with the coefficients we just obtained, we use the function `abline`, which is quite versatile. With an argument `coef=`, it plots the line with these coefficients. So, here, we will add the command `abline(coef = coefs, lwd = 2, col = "red")` after the `plot` command, giving Figure 3.1.

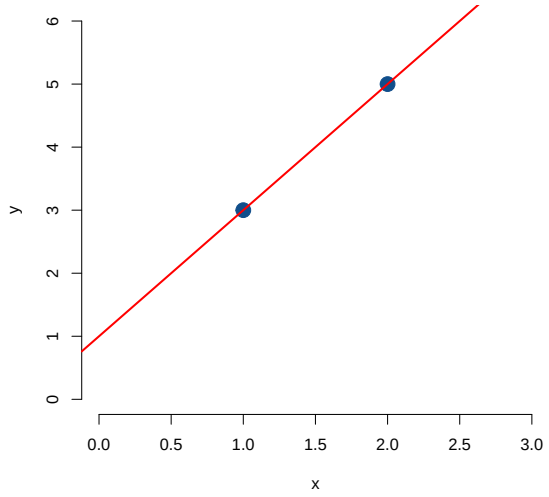


Figure 3.2: Two lonely points and an interpolating line.

However, we rarely have just two points and that is where things get more complicated. Suppose we add a third point, say, $(3, 4)$, to the previous two. So we now have the situation shown in Figure **??** and, clearly, since the points are not colinear, it is impossible to find coefficients a_0, a_1 of a curve $y = a_0 + a_1 x$ that goes through the three points.

Mathematically, this is also obvious. Reason as we did before: we have, now, three points (x_1, y_1), (x_2, y_2) and (x_3, y_3) that must all satisfy the equation (3.1), i.e.,

$$\begin{aligned} y_1 &= a_0 + a_1 x_1 \\ y_2 &= a_0 + a_1 x_2 \\ y_3 &= a_0 + a_1 x_3. \end{aligned}$$

As we did earlier, we write this in the form of a linear system $A\mathbf{x} = \mathbf{b}$ with

$$A = \begin{pmatrix} 1 & x_1 \\ 1 & x_2 \\ 1 & x_3 \end{pmatrix}, \mathbf{x} = \begin{pmatrix} a_0 \\ a_1 \end{pmatrix} \text{ and } \mathbf{b} = \begin{pmatrix} y_1 \\ y_2 \\ y_3 \end{pmatrix}.$$

Here, the matrix A is not square so we cannot rely of Theorem A.62 and instead row-

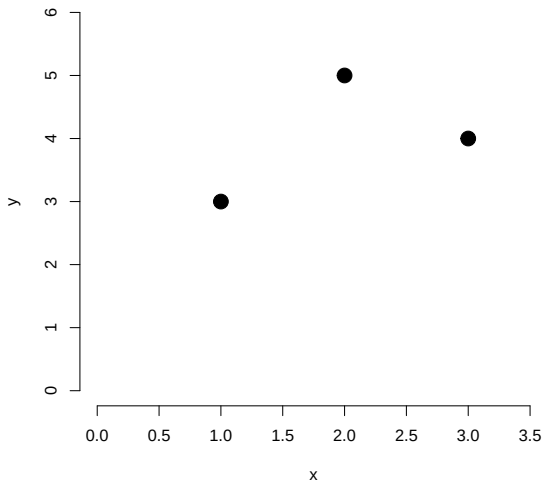


Figure 3.3: A little less ronery!

reduce A. We find

$$A = \begin{pmatrix} 1 & x_1 \\ 1 & x_2 \\ 1 & x_3 \end{pmatrix} \overset{\substack{R_2 \leftarrow R_2 - R_1 \\ R_3 \leftarrow R_3 - R_1}}{\longrightarrow} \begin{pmatrix} 1 & x_1 \\ 0 & x_2 - x_1 \\ 0 & x_3 - x_1 \end{pmatrix}$$

Thus, we have a solution if all three points lie on the same line, i.e., they are colinear. In all other cases, there is no solution.

So we ask if we can do the next-best thing, which would be to drive a line "as close to as possible" (whatever that means) to the three points, which becomes a problem of **fitting**.

3.2 Least squares problems

We have just established that, given more than two points, the problem we need to consider is that of driving a line as close to as possible to the points. The first problem is to define what we mean by "as close to as possible". From earlier Linear Algebra, you should remember that the shortest distance between a point and a line is the orthogonal projection of the point onto the line. So, given values of a_0 and a_1, we could create the resulting line $y = a_0 + a_1 x$ and compute the distance from the line to each of the three points, sum these distances. Let us do that numerically. To do this, we use projections (Section A.3.7) and more specifically, (A.2).

There is one obvious issue with the previous method: if instead of straight line, we use a more complex curve, then projecting onto the curve becomes more complicated. Indeed, firstly, we need to use the tangent to the curve (and hence need to consider

the derivative of the curve), but also there are no guarantees of uniqueness of the point being the closest to the curve.

Hence, instead of the projection onto the curve, we use another approach that considers the distance between the data points (the known points) and what value we "predict" that point should have when we use the curve that we find.

For future use, let me define a function that returns the value of (3.1):

```
> my_line = function(x, a_0, a_1) {
+     return(a_0 + a_1*x)
+ }
```

In Figure 3.2, you can see the situation when $a_0 = 3.5$ and $a_1 = 0.4$, with the distance being the length of the blue line segments between the red and black dots.

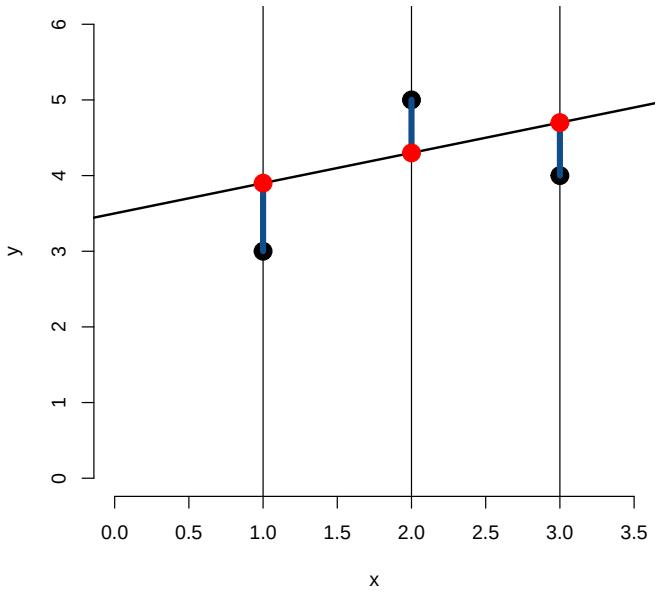


Figure 3.4: Distance between the (given) data points, in black, and the value predicted for the data points if using a line with coefficients $a_0 = 3.5$ and $a_1 = 0.4$.

The location of the black points in Figure 3.2 is easily found: given parameters a_0 and a_1 and the line equation (3.1), they have the same x coordinates as the data points and y coordinates given by, at $x_1 = 1$,

$$\tilde{y}_1 = a_0 + a_1 x_1 = a_0 + a_1,$$

at $x_2 = 2$,

$$\tilde{y}_2 = a_0 + a_1 x_2 = a_0 + 2a_1$$

and at $x_3 = 3$,

$$\tilde{y}_3 = a_0 + a_1 x_3 = a_0 + 3a_1.$$

Consider x_1, for instance. The error we made by using the line with coefficients (a_0, a_1) is $\varepsilon_1 = y_1 - \tilde{y}_1$, where the sign indicates whether we under-estimated or over-estimated the value. We can then form the **error vector**

$$\mathbf{e} = (\varepsilon_1, \varepsilon_2, \varepsilon_3). \tag{3.2}$$

The norm $\|\mathbf{e}\|$ of $\mathbf{e}$ then gives a measure of the overall error we made with our choice of a_0, a_1. Different norms can be used, which will pick up on different characteristics, but in linear least squares, we use the Euclidean norm

$$\|\mathbf{e}\| = \sqrt{\varepsilon_1^2 + \varepsilon_2^2 + \varepsilon_3^2},$$

because this norm has very useful properties. Our objective is then to find the coefficients a_0, a_1 such that $\|\mathbf{e}\|$ is minimal. This problem generalises of course to an arbitrary number of data points, giving rise to the following definition.

Definition 3.1 (Linear least squares problem)**.** *Given a collection $(x_1, y_1), \ldots, (x_n, y_n)$ of data points, find the coefficients a_0, a_1 of the line $y = a_0 + a_1 x$ such that the error*

$$\|\mathbf{e}\| = \sqrt{\varepsilon_1^2 + \cdots + \varepsilon_n^2} = \sqrt{(y_1 - \tilde{y}_1)^2 + \cdots + (y_n - \tilde{y}_n)^2} \tag{3.3}$$

is minimal, where $\tilde{y}_i = a_0 + a_1 x_i$ for $i = 1, \ldots, n$.

Before continuing, let us write a function to compute the error when the norm is the Euclidean norm. This function expects that `points` are a list, as we have been using this far.

```
> error = function(a_0, a_1, points) {
+     y_tilde = my_line(points$x, a_0 = a_0, a_1 = a_1)
+     e = points$y - y_tilde
+     return(sqrt(sum(e^2)))
+ }
```

Using it on a couple of different parameter values gives the following.

```
> error(a_0 = 3.5, a_1 = 0.4, points)

[1] 1.337909

> error(a_0 = 3, a_1 = 0.5, points)

[1] 1.224745
```

Of course, it would be Sisyphean to undertake to find a solution by hand: we do not know that a solution to the problem exists and even if it does, a trial and error approach could prove quite lengthy.

3.3 Solving by brute force using a genetic algorithm

We want to minimise the error (3.3). Let us set aside for now the issue of existence of a minimal value for the expression and try to find a numerical solution to this **minimisation problem**, which falls within the larger category of **optimisation problems**. There are many algorithms available to perform optimisation, with probably the most well known being the (deterministic) gradient descent algorithm. Here, we will use a *stochastic* optimisation method called a **genetic algorithm**. The idea is to use a mechanism mimicking evolution's drive towards higher *fitness*. As such, genetic algorithms study the maximisation of functions, but we will see that it is very easy to use them as well with the goal of minimising functions.

The "philosophy" of the genetic algorithm is as follows. Suppose we have a scalar-valued function $f : \mathbb{R}^n \to \mathbb{R}$ of several variables.

1. A point $\mathbf{x} \in \mathbb{R}^n$ is a *gene*.
2. The function value $f(\mathbf{x})$ is the fitness of the gene $\mathbf{x} \in \mathbb{R}^n$.
3. Initiate the algorithm with N (the population size) random genes $\mathbf{x}_1, \ldots, \mathbf{x}_N$.
4. Repeat the following steps for the specified number of generations.
   (a) Evaluate the fitness $f(\mathbf{x}_1), \ldots, f(\mathbf{x}_N)$ of all the genes in the population.
   (b) Keep a certain number of the best performing genes, i.e., the ones with higher fitness.
   (c) To prepare the population for the next generation $i + 1$, keep these best performing genes and throw in some new genes. Some of these new genes may be random as initially, but most are obtained by using "genetic operations" on the best performing genes in the current generation: crossover, mutations, etc.

This algorithm is known to have good convergence properties. It is also less prone to being stuck at local maxima, because of the stochasticity of the process. Also, this algorithm is highly parallelisable: in a given generation, fitness evaluations are completely independent, i.e., they do not require to know the results of the other evaluations. This means that if you can devote a number of computing cores to the task, they can run independently, greatly speeding up the process.

In `R`, there are several libraries implementing genetic algorithms; `GA` is probably a good place to start. Additionally, `ga`, the main function in that library, makes it almost trivial to parallelise your code, as I will demonstrate later. Assuming the library is installed and loaded, running the algorithm is really simple for the problem we are considering.

```
> GA = ga(type = "real-valued",
+         fitness = function(x) -error(a_0 = x[1], a_1 = x[2], points),
+         lower = c(0, -1), upper = c(10, 1),
+         suggestions = c(a_0 = 3.5, a_1 = 0.4),
+         popSize = 200, maxiter = 150,
+         monitor = FALSE)
```

Let me detail the function call above, as the components can be a little confusing. As explained, genetic algorithms are *maximisers*, so in order to minimise the error, for `fitness` (the function that computes the fitness), we use `function(x) -error(a_0 = x[1], a_1 = x[2], points)`. Note that if `error()` had only depended on `x` and not also on `points`, we could have used `fitness = -error(a_0 = x[1], a_1 = x[2])`; the reason for using `function(x)` is that `error()` is a function of several variables, only a subset of which are of interest to `ga` for its computations.

`lower` and `upper` are lower and upper bounds for the (random) values of parameters. They are vectors that must have the same length; they also determine the size of the genes, i.e., the number of parameters with respect to which we are optimising. `lower`, `upper` and `fitness` are the only required arguments to the function.

Given `lower` and `upper`, those gene components that are chosen at random are chosen at random uniformly between the lower and upper bound. For instance, the call above says that we seek $a_0 \in [0, 10]$ and $a_1 \in [-1, 1]$. There are instances when we want to hasard guesses as to the parameter values; these guesses can be given to the function as a matrix (or a vector if there is only one). Above, I have added the values I used for the figures above, as they did not look too bad.

Finally, `popSize` and `maxiter` have default values of 50 and 100, respectively, which I have increased here just to point out their role. `popSize` is the size of the population, i.e., the number of genes that are evaluated at each generation, while `maxiter` is the maximum number of generations for which the algorithm is run. Increasing both values from their defaults might help with some problems, but they might also vastly increase the run time. And `monitor` is set to `FALSE` to suppress any output from the function, otherwise progress is shown for each generation.

Using the command `plot(GA)`, where `GA` is the result obtained above, gives a visual representation of the behaviour of the algorithm, showing how the mean fitness, minimum and maximum fitness vary through generations. Give it a try (this is not shown here). The result of using `ga` is a so-called S4 object, so accessing the result is done using @ rather than $. The most useful part of the return value is of course the parameters we are looking for, which are returned as follows.

```
> GA@solution

           x1        x2
[1,] 2.999788 0.5001439
```

You could also see the value of the fitness at that solution by looking at `GA@fitnessValue`.

3.4 How about a little finesse?

We just saw how to minimise $\|e\|$ by brute force using a genetic algorithm. Let us now see what mathematics can tell us about this.

For a data point $i = 1, \dots, n$, because of the form of (3.1), the error can be written as

$$\varepsilon_i = y_i - \tilde{y}_i = y_i - (a_0 + a_1 x_i).$$

Do this for all data points,

$$\begin{aligned} \varepsilon_1 &= y_1 - (a_0 + a_1 x_1) \\ &\vdots \\ \varepsilon_n &= y_n - (a_0 + a_1 x_n) \end{aligned}$$

and rewrite in matrix form. This allows to reformulate the problem as follows.

Definition 3.2 (Least squares for an affine function)**.** *Given a set of data points*

$$(x_1, y_1), \dots, (x_n, y_n), \tag{3.4}$$

define the vectors

$$\mathbf{b} = \begin{pmatrix} y_1 \\ \vdots \\ y_n \end{pmatrix} \text{ and } \mathbf{x} = \begin{pmatrix} a_0 \\ a_1 \end{pmatrix} \tag{3.5}$$

and the matrix

$$A = \begin{pmatrix} 1 & x_1 \\ \vdots & \vdots \\ 1 & x_n \end{pmatrix}. \tag{3.6}$$

Let the error vector $\mathbf{e} = (\varepsilon_1, \dots, \varepsilon_n)^T$ *be defined as*

$$\mathbf{e} = \mathbf{b} - A\mathbf{x}. \tag{3.7}$$

Find $\mathbf{x}$ *such that* $\|\mathbf{e}\|$ *is minimum.*

Note that this is where the complication comes from. Finding $\mathbf{e} = \mathbf{b} - A\mathbf{x}$ is trivial: since $\mathbf{b}$ and A are given, plugging in any value of $\mathbf{x}$ gives a resulting value of $\mathbf{e}$. However, what we seek here is $\mathbf{x}$ that minimises $\|\mathbf{e}\|$, i.e., of all possible values of $\mathbf{x}$, i.e., here, $\mathbb{R}^2$, we want the one or the ones that make $\|\mathbf{e}\|$ the smallest possible. To solve the problem, we need a few more tools.

Definition 3.3 (Least squares solution)**.** *Let* $A \in \mathcal{M}_{mn}$ *and* $\mathbf{b} \in \mathbb{R}^m$*. A* ***least squares solution*** *of* $A\mathbf{x} = \mathbf{b}$ *is a vector* $\tilde{\mathbf{x}} \in \mathbb{R}^n$ *such that*

$$\forall \mathbf{x} \in \mathbb{R}^n, \quad \|\mathbf{b} - A\tilde{\mathbf{x}}\| \leq \|\mathbf{b} - A\mathbf{x}\|. \tag{3.8}$$

In other words, if we denote $\tilde{\mathbf{e}}$ the error corresponding to a least squares solution, $\tilde{\mathbf{e}}$ is such that $\tilde{\mathbf{e}} \leq \mathbf{e}$ for all $\mathbf{x}$.

Definition 3.4 (Best approximation)**.** *Let V be a vector space, $W \subseteq V$ and $\mathbf{v} \in V$. The **best approximation** to $\mathbf{v}$ in W is $\tilde{\mathbf{v}} \in W$ such that*

$$\forall \mathbf{w} \in W, \mathbf{w} \neq \tilde{\mathbf{v}}, \quad \|\mathbf{v} - \tilde{\mathbf{v}}\| < \|\mathbf{v} - \mathbf{w}\|. \tag{3.9}$$

Theorem 3.5 (Best approximation theorem)**.** *Let V be a vector space with an inner product, $W \subset V$ and $\mathbf{v} \in V$. Then $\mathsf{proj}_W(\mathbf{v})$ is the best approximation to $\mathbf{v}$ in W*

Let us reformulate this result even more explicitly in terms of projections.

Theorem 3.6 (Best approximation theorem)**.** *Let V be a vector space with an inner product, $W \subset V$ and $\mathbf{v} \in V$. Then $\mathsf{proj}_W(\mathbf{v}) \in W$ is the best approximation to $\mathbf{v}$ in W, i.e.,*

$$\forall \mathbf{w} \in W, \mathbf{w} \neq \mathsf{proj}_W(\mathbf{v}), \quad \|\mathbf{v} - \mathsf{proj}_W(\mathbf{v})\| < \|\mathbf{v} - \mathbf{w}\|$$

We then have the following theorem.

Theorem 3.7 (Least squares theorem)**.** *Let $A \in \mathcal{M}_{mn}$ and $\mathbf{b} \in \mathbb{R}^m$. Then*

1. *$A\mathbf{x} = \mathbf{b}$ always has at least one least squares solution $\tilde{\mathbf{x}}$*
2. *$\tilde{\mathbf{x}}$ least squares solution to $A\mathbf{x} = \mathbf{b} \iff \tilde{\mathbf{x}}$ is a solution to the **normal equations** $A^T A\tilde{\mathbf{x}} = A^T\mathbf{b}$*
3. *A has linearly independent columns $\iff A^TA$ invertible. In this case, the least squares solution is unique and*

$$\tilde{\mathbf{x}} = \left(A^T A\right)^{-1} A^T\mathbf{b}.$$

Before we prove this, let us consider what Theorem 3.7 says. The first point stipulates that we are always be able to find a least squares solution. The second provides us with a way to construct least squares solutions that always works. The third condition then says that under stricter conditions, the least squares is unique.

Proof. Let us find the least squares solution $\forall \mathbf{x} \in \mathbb{R}^n$, $A\mathbf{x}$ is a vector in the **column space** of A (the space spanned by the vectors making up the columns of A)

Since $\mathbf{x} \in \mathbb{R}^n$, $A\mathbf{x} \in \mathsf{col}(A)$. This implies that the least squares solution of $A\mathbf{x} = \mathbf{b}$ is a vector $\tilde{\mathbf{y}} \in \mathsf{col}(A)$ such that

$$\forall \mathbf{y} \in \mathsf{col}(A), \quad \|\mathbf{b} - \tilde{\mathbf{y}}\| \leq \|\mathbf{b} - \mathbf{y}\|.$$

This looks very much like Best approximation and Best approximation theorem

Putting things together We just stated: The least squares solution of $A\mathbf{x} = \mathbf{b}$ is a vector $\tilde{\mathbf{y}} \in \mathsf{col}(A)$ s.t.

$$\forall \mathbf{y} \in \mathsf{col}(A), \quad \|\mathbf{b} - \tilde{\mathbf{y}}\| \leq \|\mathbf{b} - \mathbf{y}\|$$

$\implies W = \mathsf{col}(A)$, $\mathbf{v} = \mathbf{b}$ and $\tilde{\mathbf{y}} = \mathsf{proj}_{\mathsf{col}(A)}(\mathbf{b})$

So if $\tilde{\mathbf{x}}$ is a least squares solution of $A\mathbf{x} = \mathbf{b}$, then

$$\tilde{\mathbf{y}} = A\tilde{\mathbf{x}} = \mathsf{proj}_{\mathsf{col}(A)}(\mathbf{b})$$

We have

$$\mathbf{b} - A\tilde{\mathbf{x}} = \mathbf{b} - \mathsf{proj}_{\mathsf{col}(A)}(\mathbf{b}) = \mathsf{perp}_{\mathsf{col}(A)}(\mathbf{b})$$

and it is easy to show that

$$\mathsf{perp}_{\mathsf{col}(A)}(\mathbf{b}) \perp \mathsf{col}(A)$$

So for all columns $\mathbf{a}_i$ of A

$$\mathbf{a}_i \cdot (\mathbf{b} - A\tilde{\mathbf{x}}) = 0$$

which we can also write as $\mathbf{a}_i^T(\mathbf{b} - A\tilde{\mathbf{x}}) = 0$

For all columns $\mathbf{a}_i$ of A,

$$\mathbf{a}_i^T(\mathbf{b} - A\tilde{\mathbf{x}}) = 0$$

This is equivalent to saying that

$$A^T(\mathbf{b} - A\tilde{\mathbf{x}}) = \mathbf{0}$$

We have

$$\begin{aligned} A^T(\mathbf{b} - A\tilde{\mathbf{x}}) = \mathbf{0} &\iff A^T\mathbf{b} - A^TA\tilde{\mathbf{x}} = \mathbf{0} \\ &\iff A^T\mathbf{b} = A^TA\tilde{\mathbf{x}} \\ &\iff A^TA\tilde{\mathbf{x}} = A^T\mathbf{b} \end{aligned}$$

The latter system constitutes the **normal equations** for $\tilde{\mathbf{x}}$

We have seen 1 and 2, we will not show 3 (it is not hard) □

3.5 Fitting something more complicated

Suppose we want to fit something a bit more complicated, because the data does not seem to be really distributed along a straight line. For instance, instead of the affine function

$$y = a_0 + a_1x,$$

suppose we want to fit the quadratic

$$y = a_0 + a_1x + a_2x^2$$

or even the exponential

$$y = k_0e^{k_1x}.$$

How should we proceed?

3.5.1 Fitting the quadratic

We have the data points $(x_1, y_1), (x_2, y_2), \ldots, (x_n, y_n)$ and want to fit

$$y = a_0 + a_1 x + a_2 x^2.$$

At (x_1, y_1),

$$\tilde{y}_1 = a_0 + a_1 x_1 + a_2 x_1^2.$$

$\vdots$

At (x_n, y_n),

$$\tilde{y}_n = a_0 + a_1 x_n + a_2 x_n^2.$$

In terms of the error

$$\begin{aligned} \varepsilon_1 &= y_1 - \tilde{y}_1 = y_1 - (a_0 + a_1 x_1 + a_2 x_1^2) \\ &\vdots \\ \varepsilon_n &= y_n - \tilde{y}_n = y_n - (a_0 + a_1 x_n + a_2 x_n^2) \end{aligned}$$

i.e.,

$$\mathbf{e} = \mathbf{b} - A\mathbf{x}$$

where

$$\mathbf{e} = \begin{pmatrix} \varepsilon_1 \\ \vdots \\ \varepsilon_n \end{pmatrix}, A = \begin{pmatrix} 1 & x_1 & x_1^2 \\ \vdots & \vdots & \vdots \\ 1 & x_n & x_n^2 \end{pmatrix}, \mathbf{x} = \begin{pmatrix} a_0 \\ a_1 \\ a_2 \end{pmatrix} \text{ and } \mathbf{b} = \begin{pmatrix} y_1 \\ \vdots \\ y_n \end{pmatrix}$$

Theorem 3.7 applies, with here $A \in \mathcal{M}_{n3}$ and $\mathbf{b} \in \mathbb{R}^n$

Recall that the points are (1,3), (2,5) and (3,4). Let us fit $y = a_0 + a_1 x + a_2 x^2$. The matrix A takes the form

$$A = \begin{pmatrix} 1 & x_1 & x_1^2 \\ \vdots & \vdots & \vdots \\ 1 & x_n & x_n^2 \end{pmatrix}$$

b takes the form

$$b = \begin{pmatrix} y_1 \\ \vdots \\ y_n \end{pmatrix}$$

3.5.2 Fitting the exponential

Things are a bit more complicated when trying to fit the data to an exponential function $y = k_0 \exp(k_1 x)$. Indeed, proceeding as we did before, we get the system

$$\begin{aligned} y_1 &= k_0 e^{k_1 x_1} \\ &\vdots \\ y_n &= k_0 e^{k_1 x_n}. \end{aligned}$$

The $e^{k_1 x_i}$ are nonlinear terms, they cannot be put in a matrix. However, this can be transformed into a form more amenable to the technique we already used. Indeed, take the ln of both sides of the equation $y_i = k_0 \exp(k_1 x_i)$:

$$\begin{aligned} \ln(y_i) &= \ln(k_0 e^{k_1 x_i}) \\ &= \ln(k_0) + \ln(e^{k_1 x_i}) \\ &= \ln(k_0) + k_1 x_i. \end{aligned}$$

If $y_i, k_0 > 0$, then their ln are defined and we are back essentially to the affine case, with the system being

$$\mathbf{y} = A\mathbf{x} + \mathbf{b}$$

where

$$A = \begin{pmatrix} x_1 \\ \vdots \\ x_n \end{pmatrix}, \mathbf{x} = \begin{pmatrix} k_1 \end{pmatrix}, \mathbf{b} = \begin{pmatrix} \ln(k_0) \end{pmatrix} \text{ and } \mathbf{y} = \begin{pmatrix} \ln(y_1) \\ \vdots \\ \ln(y_n) \end{pmatrix}.$$

Chapter 4

Matrix factorisations

Matrix factorisations, which are known under many different other names, are theoretical results and algorithms that allow to write matrices typically as the product of several matrices with specified forms. The matrices in the factorisation usually have known properties that make them much easier to perform computations with.

There are several different types of factorisations. Here, we study two: the QR factorisation and the SVD. Both have many applications in their own right, but we also return later to the problem of least squares. Then, we present another dimensionality reduction technique, principal component analysis (PCA).

Before we start, though, we need to learn a little about *orthogonal sets* and *orthogonal matrices*.

4.1 Orthogonal matrices

Definition 4.1 (Orthogonal set of vectors)**.** *The set of vectors* $\{\mathbf{v}_1, \dots, \mathbf{v}_k\} \in \mathbb{R}^n$ *is an* ***orthogonal set*** *if*

$$\forall i, j = 1, \dots, k, \quad i \neq j \implies \mathbf{v}_i \bullet \mathbf{v}_j = 0$$

Theorem 4.2. $\{\mathbf{v}_1, \dots, \mathbf{v}_k\} \in \mathbb{R}^n$ *with* $\forall i$, $\mathbf{v}_i \neq \mathbf{0}$*, orthogonal set* $\implies$ $\{\mathbf{v}_1, \dots, \mathbf{v}_k\} \in \mathbb{R}^n$ *linearly independent.*

Proof. Assume $\{\mathbf{v}_1, \dots, \mathbf{v}_k\}$ orthogonal set with $\mathbf{v}_i \neq \mathbf{0}$ for all $i = 1, \dots, k$. Recall $\{\mathbf{v}_1, \dots, \mathbf{v}_k\}$ is LI if

$$c_1\mathbf{v}_1 + \cdots + c_k\mathbf{v}_k = \mathbf{0} \iff c_1 = \cdots = c_k = 0$$

So assume $c_1, \dots, c_k \in \mathbb{R}$ are s.t. $c_1\mathbf{v}_1 + \cdots + c_k\mathbf{v}_k = \mathbf{0}$. Recall that $\forall \mathbf{x} \in \mathbb{R}^k$, $\mathbf{0}_k \bullet \mathbf{x} = 0$. So for some $\mathbf{v}_i \in \{\mathbf{v}_1, \dots, \mathbf{v}_k\}$

$$\begin{aligned} 0 &= \mathbf{0} \bullet \mathbf{v}_i \\ &= (c_1\mathbf{v}_1 + \cdots + c_k\mathbf{v}_k) \bullet \mathbf{v}_i \\ &= c_1\mathbf{v}_1 \bullet \mathbf{v}_i + \cdots + c_k\mathbf{v}_k \bullet \mathbf{v}_i \end{aligned} \tag{4.1}$$

As $\{\mathbf{v}_1, \ldots, \mathbf{v}_k\}$ orthogonal, $\mathbf{v}_j \bullet \mathbf{v}_i = 0$ when $i \neq j$, (4.1) reduces to

$$c_i \mathbf{v}_i \bullet \mathbf{v}_i = 0 \iff c_i \|\mathbf{v}_i\|^2 = 0$$

As $\mathbf{v}_i \neq 0$ for all i, $\|\mathbf{v}_i\| \neq 0$ and so $c_i = 0$. This is true for all i, hence the result. □

Definition 4.3 (Orthogonal basis)**.** *Let S be a basis of the subspace $W \subset \mathbb{R}^n$ composed of an orthogonal set of vectors. We say S is an* ***orthogonal basis*** *of W*

Example – Vectors of the standard basis of $\mathbb{R}^3$ For $\mathbb{R}^3$, we denote

$$\mathbf{i} = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}, \quad \mathbf{j} = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} \text{ and } \mathbf{k} = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}.$$

For $\mathbb{R}^k$, $k > 3$, we denote them $\mathbf{e}_i$. Clearly, $\{\mathbf{i}, \mathbf{j}\}$, $\{\mathbf{i}, \mathbf{k}\}$, $\{\mathbf{j}, \mathbf{k}\}$ and $\{\mathbf{i}, \mathbf{j}, \mathbf{k}\}$ are orthogonal sets. The standard basis vectors are also $\neq \mathbf{0}$, so the sets are linearly independent. And

$$\{\mathbf{i}, \mathbf{j}, \mathbf{k}\}$$

is an orthogonal basis of $\mathbb{R}^3$ since it spans $\mathbb{R}^3$ and is linearly independent. Then any point (or vector) $(c_1, c_2, c_3) \in \mathbb{R}^3$ can be written as

$$\begin{pmatrix} c_1 \\ c_2 \\ c_3 \end{pmatrix} = c_1 \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} + c_2 \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} + c_3 \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} = c_1\mathbf{i} + c_2\mathbf{j} + c_3\mathbf{k},$$

with this linear combination being unique.

There is an orthonormal version of these definitions and results.

Definition 4.4 (Orthonormal set)**.** *The set of vectors $\{\mathbf{v}_1, \ldots, \mathbf{v}_k\} \in \mathbb{R}^n$ is an* ***orthonormal set*** *if it is an orthogonal set and furthermore*

$$\forall i = 1, \ldots, k, \quad \|\mathbf{v}_i\| = 1.$$

Definition 4.5 (Orthonormal basis)**.** *A basis of the subspace $W \subset \mathbb{R}^n$ is an* ***orthonormal basis*** *if the vectors composing it are an orthonormal set.*

$\{\mathbf{v}_1, \ldots, \mathbf{v}_k\} \in \mathbb{R}^n$ is orthonormal if

$$\mathbf{v}_i \bullet \mathbf{v}_j = \begin{cases} 1 & \text{if } i = j \\ 0 & \text{otherwise.} \end{cases}$$

Theorem 4.6. *Let $Q \in \mathcal{M}_{mn}$. The columns of Q form an orthonormal set if and only if*

$$Q^T Q = \mathbb{I}_n$$

Definition 4.7 (Orthogonal matrix)**.** *$Q \in \mathcal{M}_n$ is an **orthogonal matrix** if its columns form an orthonormal set*

So $Q \in \mathcal{M}_n$ orthogonal if $Q^TQ = \mathbb{I}$, i.e., $Q^T = Q^{-1}$

Theorem 4.8 (NSC for orthogonality)**.** *$Q \in \mathcal{M}_n$ orthogonal $\iff$ $Q^{-1} = Q^T$*

Theorem 4.9 (Orthogonal matrices "encode" isometries)**.** *Let $Q \in \mathcal{M}_n$. The following are equivalent.*

1. *Q orthogonal.*
2. *$\forall \mathbf{x} \in \mathbb{R}^n$, $\|Q\mathbf{x}\| = \|\mathbf{x}\|$.*
3. *$\forall \mathbf{x}, \mathbf{y} \in \mathbb{R}^n$, $Q\mathbf{x} \bullet Q\mathbf{y} = \mathbf{x} \bullet \mathbf{y}$.*

Theorem 4.10. *Let $Q \in \mathcal{M}_n$ be orthogonal. Then*

1. *The rows of Q form an orthonormal set.*
2. *Q^{-1} orthogonal.*
3. *$\det Q = \pm 1$.*
4. *$\forall \lambda \in \sigma(Q)$, $|\lambda| = 1$.*
5. *If $Q_2 \in \mathcal{M}_n$ also orthogonal, then QQ_2 orthogonal.*

Proof. (Proof of 4 in Theorem 4.10) All statements in Theorem 4.10 are easy, but let's focus on 4

Let λ be an eigenvalue of $Q \in \mathcal{M}_n$ orthogonal, i.e., $\exists \mathbb{R}^n \ni \mathbf{x} \neq \mathbf{0}$ s.t.

$$Q\mathbf{x} = \lambda\mathbf{x}$$

Take the norm on both sides

$$\|Q\mathbf{x}\| = \|\lambda\mathbf{x}\|$$

From 2 in Theorem 4.9, $\|Q\mathbf{x}\| = \|\mathbf{x}\|$ and from the properties of norms, $\|\lambda\mathbf{x}\| = |\lambda| \, \|\mathbf{x}\|$, so we have

$$\|Q\mathbf{x}\| = \|\lambda\mathbf{x}\| \iff \|\mathbf{x}\| = |\lambda| \, \|\mathbf{x}\| \iff 1 = |\lambda|$$

(we can divide by $\|\mathbf{x}\|$ since $\mathbf{x} \neq \mathbf{0}$ as an eigenvector) □

4.2 The Gram-Schmidt orthonormalisation procedure

We could spend a long time on these interesting notions, but we need to get back to the QR decomposition. What this aims to do is to construct an orthogonal basis for a subspace $W \subset \mathbb{R}^n$. To do this, we use the *Gram-Schmidt orthogonalisation process*, which turns a basis of W into an orthogonal basis of W.

4.2.1 Projections onto subspaces

Definition 4.11 (Orthogonal projection onto a subspace)**.** *$W \subset \mathbb{R}^n$ a subspace and $\{\mathbf{u}_1, \ldots, \mathbf{u}_k\}$ an orthogonal basis of W. $\forall \mathbf{v} \in \mathbb{R}^n$, the **orthogonal projection** of $\mathbf{v}$ **onto** W is*

$$\mathsf{proj}_W(\mathbf{v}) = \frac{\mathbf{u}_1 \bullet \mathbf{v}}{\|\mathbf{u}_1\|^2}\mathbf{u}_1 + \cdots + \frac{\mathbf{u}_k \bullet \mathbf{v}}{\|\mathbf{u}_k\|^2}\mathbf{u}_k$$

Definition 4.12 (Component orthogonal to a subspace)**.** *$W \subset \mathbb{R}^n$ a subspace and $\{\mathbf{u}_1, \ldots, \mathbf{u}_k\}$ an orthogonal basis of W. $\forall \mathbf{v} \in \mathbb{R}^n$, the **component** of $\mathbf{v}$ **orthogonal to** W is*

$$\mathsf{perp}_W(\mathbf{v}) = \mathbf{v} - \mathsf{proj}_W(\mathbf{v})$$

4.2.2 The Gram-Schmidt process

Theorem 4.13. *$W \subset \mathbb{R}^n$ a subset and $\{\mathbf{x}_1, \ldots, \mathbf{x}_k\}$ a basis of W. Let*

$$\begin{aligned}
\mathbf{v}_1 &= \mathbf{x}_1 \\
\mathbf{v}_2 &= \mathbf{x}_2 - \frac{\mathbf{v}_1 \bullet \mathbf{x}_2}{\|\mathbf{v}_1\|^2}\mathbf{v}_1 \\
\mathbf{v}_3 &= \mathbf{x}_3 - \frac{\mathbf{v}_1 \bullet \mathbf{x}_3}{\|\mathbf{v}_1\|^2}\mathbf{v}_1 - \frac{\mathbf{v}_2 \bullet \mathbf{x}_3}{\|\mathbf{v}_2\|^2}\mathbf{v}_2 \\
&\vdots \\
\mathbf{v}_k &= \mathbf{x}_k - \frac{\mathbf{v}_1 \bullet \mathbf{x}_k}{\|\mathbf{v}_1\|^2}\mathbf{v}_1 - \cdots - \frac{\mathbf{v}_{k-1} \bullet \mathbf{x}_k}{\|\mathbf{v}_{k-1}\|^2}\mathbf{v}_{k-1}
\end{aligned}$$

and

$$W_1 = \mathsf{span}(\mathbf{x}_1), W_2 = \mathsf{span}(\mathbf{x}_1, \mathbf{x}_2), \ldots, W_k = \mathsf{span}(\mathbf{x}_1, \ldots, \mathbf{x}_k)$$

Then $\forall i = 1, \ldots, k$, $\{\mathbf{v}_1, \ldots, \mathbf{v}_i\}$ orthogonal basis for W_i

4.3 The QR factorisation

Theorem 4.14. *Let $A \in \mathcal{M}_{mn}$, with A having linearly independent. Then A can be factored as*

$$A = QR, \tag{4.2}$$

where $Q \in \mathcal{M}_{mn}$ has orthonormal columns and $R \in \mathcal{M}_n$ is a nonsingular upper triangular matrix.

4.3.1 Back to least squares

So what was the point of all that..?

Theorem 4.15 (Least squares with QR factorisation)**.** *$A \in \mathcal{M}_{mn}$ with LI columns, $\mathbf{b} \in \mathbb{R}^m$. If $A = QR$ is a QR factorisation of A, then the unique least squares solution $\tilde{\mathbf{x}}$ of $A\mathbf{x} = \mathbf{b}$ is*

$$\tilde{\mathbf{x}} = R^{-1}Q^T\mathbf{b}$$

Proof of Theorem 4.15 A has LI columns so

- least squares $A\mathbf{x} = \mathbf{b}$ has unique solution $\tilde{\mathbf{x}} = (A^TA)^{-1}A^T\mathbf{b}$
- by Theorem 4.14, A can be written as $A = QR$ with $Q \in \mathcal{M}_{mn}$ with orthonormal columns and $R \in \mathcal{M}_n$ nonsingular and upper triangular

So

$$\begin{aligned} A^TA\tilde{\mathbf{x}} = A^T\mathbf{b} &\implies (QR)^TQR\tilde{\mathbf{x}} = (QR)^T\mathbf{b} \\ &\implies R^TQ^TQR\tilde{\mathbf{x}} = R^TQ^T\mathbf{b} \\ &\implies R^T\mathbb{I}_nR\tilde{\mathbf{x}} = R^TQ^T\mathbf{b} \\ &\implies R^TR\tilde{\mathbf{x}} = R^TQ^T\mathbf{b} \\ &\implies (R^T)^{-1}R\tilde{\mathbf{x}} = (R^T)^{-1}R^TQ^T\mathbf{b} \\ &\implies R\tilde{\mathbf{x}} = Q^T\mathbf{b} \\ &\implies \tilde{\mathbf{x}} = R^{-1}Q^T\mathbf{b} \end{aligned}$$

4.4 The singular values decomposition (SVD)

The singular value decomposition, known mostly by its acronym SVD, is another type of factorisation.

Definition 4.16 (Singular value)**.** *Let $A \in \mathcal{M}_{mn}(\mathbb{R})$. The **singular values** of A are the real numbers*

$$\sigma_1 \geq \sigma_2 \geq \cdots \sigma_n \geq 0$$

that are the square roots of the eigenvalues of A^TA.

Recall that $\forall A \in \mathcal{M}_{mn}$, the matrix A^TA is symmetric (see Theorem A.31). Since A is real, there furthermore holds that A^TA has all its eigenvalues real and nonnegative (by Theorem A.33). (Note that the proofs of these results are important, so refer to Section A.6.1 for details.) As a consequence, this definition is valid (it would not were some of the eigenvalues complex).

Theorem 4.17 (Singular value decomposition)**.** *$A \in \mathcal{M}_{mn}$ with singular values $\sigma_1 \geq \cdots \geq \sigma_r > 0$ and $\sigma_{r+1} = \cdots = \sigma_n = 0$. Then there exists $U \in \mathcal{M}_m$ orthogonal, $V \in \mathcal{M}_n$ orthogonal and a block matrix $\Sigma \in \mathcal{M}_{mn}$ taking the form*

$$\Sigma = \begin{pmatrix} D & 0_{r,n-r} \\ 0_{m-r,r} & 0_{m-r,n-r} \end{pmatrix},$$

where

$$D = \mathsf{diag}(\sigma_1, \ldots, \sigma_r) \in \mathcal{M}_r$$

such that

$$A = U\Sigma V^T.$$

Note that by construction, U and V^T are *rotation* or *reflection* matrices, while Σ is a *scaling* matrix.

Definition 4.18. *We call a factorisation as in Theorem 4.17 the* ***singular value decomposition*** *of A. The columns of U and V are, respectively, the* ***left*** *and* ***right singular vectors*** *of A.*

The following result tells us how we can reconstruct the original matrix from its SVD. This is useful in the image compression example of Section 4.5.

Theorem 4.19 (Outer product form of the SVD)**.** *$A \in \mathcal{M}_{mn}$ with singular values $\sigma_1 \geq \cdots \geq \sigma_r > 0$ and $\sigma_{r+1} = \cdots = \sigma_n = 0$, $\mathbf{u}_1, \ldots, \mathbf{u}_r$ and $\mathbf{v}_1, \ldots, \mathbf{v}_r$, respectively, left and right singular vectors of A corresponding to these singular values. Then*

$$A = \sigma_1 \mathbf{u}_1 \mathbf{v}_1^T + \cdots + \sigma_r \mathbf{u}_r \mathbf{v}_r^T.$$

4.4.1 Computing the SVD (case of $\neq$ eigenvalues)

To compute the SVD, we use the following result

Theorem 4.20. *Let $A \in \mathcal{M}_n$ symmetric, $(\lambda_1, \mathbf{u}_1)$ and $(\lambda_2, \mathbf{u}_2)$ be eigenpairs, assuming that $\lambda_1 \neq \lambda_2$. Then $\mathbf{u}_1 \bullet \mathbf{u}_2 = 0$*

Proof. Let $A \in \mathcal{M}_n$ be symmetric, $(\lambda_1, \mathbf{u}_1)$ and $(\lambda_2, \mathbf{u}_2)$ be eigenpairs of A with $\lambda_1 \neq \lambda_2$. Then we have

$$\begin{aligned}
\lambda_1(\mathbf{v}_1 \bullet \mathbf{v}_2) &= (\lambda_1 \mathbf{v}_1) \bullet \mathbf{v}_2 \\
&= A\mathbf{v}_1 \bullet \mathbf{v}_2 \\
&= (A\mathbf{v}_1)^T \mathbf{v}_2 \\
&= \mathbf{v}_1^T A^T \mathbf{v}_2 \\
&= \mathbf{v}_1^T (A\mathbf{v}_2) [A \text{ symmetric so } A^T = A] \\
&= \mathbf{v}_1^T (\lambda_2 \mathbf{v}_2) \\
&= \lambda_2 (\mathbf{v}_1^T \mathbf{v}_2) \\
&= \lambda_2 (\mathbf{v}_1 \bullet \mathbf{v}_2).
\end{aligned}$$

It follows that $(\lambda_1 - \lambda_2)(\mathbf{v}_1 \bullet \mathbf{v}_2) = 0$. However, since $\lambda_1 \neq \lambda_2$, this means that $\mathbf{v}_1 \bullet \mathbf{v}_2 = 0$. □

4.4.2 Computing the SVD (case of $\neq$ eigenvalues)

If all eigenvalues of A^TA are distinct, we can use Theorem 4.20

1. Compute $A^TA \in \mathcal{M}_n$
2. Compute eigenvalues $\lambda_1, \ldots, \lambda_n$ of A^TA; order them as $\lambda_1 > \cdots > \lambda_n \geq 0$ ($>$ not $\geq$ since $\neq$)
3. Compute singular values $\sigma_1 = \sqrt{\lambda_1}, \ldots, \sigma_n = \sqrt{\lambda_n}$
4. Diagonal matrix D in Σ is either in $\mathcal{M}_n$ (if $\sigma_n > 0$) or in $\mathcal{M}_{n-1}$ (if $\sigma_n = 0$)
5. Since eigenvalues are distinct, Theorem 4.20 $\implies$ eigenvectors are orthogonal set. Compute these eigenvectors in the same order as the eigenvalues
6. Normalise them and use them to make the matrix V, i.e., $V = [\mathbf{v}_1 \cdots \mathbf{v}_n]$
7. To find the $\mathbf{u}_i$, compute, for $i = 1, \ldots, r$,

$$\mathbf{u}_i = \frac{1}{\sigma_i} A\mathbf{v}_i$$

   and ensure that $\|\mathbf{u}_i\| = 1$

4.4.3 Computing the SVD (case where some eigenvalues are =)

1. Compute $A^TA \in \mathcal{M}_n$
2. Compute eigenvalues $\lambda_1, \ldots, \lambda_n$ of A^TA; order them as $\lambda_1 \geq \cdots \geq \lambda_n \geq 0$
3. Compute singular values $\sigma_1 = \sqrt{\lambda_1}, \ldots, \sigma_n = \sqrt{\lambda_n}$, with $r \leq n$ the index of the last positive singular value
4. For eigenvalues that are distinct, proceed as before
5. For eigenvalues with multiplicity > 1, we need to ensure that the resulting eigenvectors are LI *and* orthogonal

Dealing with eigenvalues with multiplicity > 1 When an eigenvalue has (algebraic) multiplicity > 1, e.g., characteristic polynomial contains a factor like $(\lambda - 2)^2$, things can become a little bit more complicated

The proper way to deal with this involves the so-called Jordan Normal Form (another matrix decomposition)

In short: not all square matrices are diagonalisable, but all square matrices admit a JNF

Sometimes, we can find several LI eigenvectors associated to the same eigenvalue. Check this. If not, need to use the following

Definition 4.21 (Generalised eigenvectors)**.** $\mathbf{x} \neq \mathbf{0}$ ***generalized eigenvector*** *of rank m of $A \in \mathcal{M}_n$ corresponding to eigenvalue λ if*

$$(A - \lambda\mathbb{I})^m \mathbf{x} = \mathbf{0}$$

but

$$(A - \lambda\mathbb{I})^{m-1} \mathbf{x} \neq \mathbf{0}$$

Procedure for generalised eigenvectors $A \in \mathcal{M}_n$ and assume λ eigenvalue with algebraic multiplicity k

Find $\mathbf{v}_1$, "classic" eigenvector, i.e., $\mathbf{v}_1 \neq \mathbf{0}$ s.t. $(A - \lambda\mathbb{I})\mathbf{v}_1 = \mathbf{0}$

Find generalised eigenvector $\mathbf{v}_2$ of rank 2 by solving for $\mathbf{v}_2 \neq \mathbf{0}$,

$$(A - \lambda\mathbb{I})\mathbf{v}_2 = \mathbf{v}_1$$

...

Find generalised eigenvector $\mathbf{v}_k$ of rank k by solving for $\mathbf{v}_k \neq \mathbf{0}$,

$$(A - \lambda\mathbb{I})\mathbf{v}_k = \mathbf{v}_{k-1}$$

Then $\{\mathbf{v}_1, \ldots, \mathbf{v}_k\}$ LI

Back to the normal procedure With the LI eigenvectors $\{\mathbf{v}_1, \ldots, \mathbf{v}_k\}$ corresponding to λ

Apply Gram-Schmidt to get orthogonal set

For all eigenvalues with multiplicity > 1, check that you either have LI eigenvectors or do what we just did

When you are done, be back on your merry way to step 6 in the case where eigenvalues are all $\neq$

I am caricaturing a little here: there can be cases that do not work exactly like this, but this is general enough..

4.5 Compressing images

This example is adapted from ... To summarise, we consider an image that, for simplicity, we assume is in shades of grey. Such an image can be stored in a matrix $A \in \mathcal{M}_{mn}$ in which, typically, a value of 0 means the pixel is black and a value of 1 means it is white, with grey scale covering all the range in between. Take the SVD of A. Then the small singular values carry information about the regions with little variation and can perhaps be omitted, whereas the large singular values carry information about more "dynamic" regions of the image. To see this, we use the outer product form of the SVD given by Theorem 4.19 to reconstruct an image from its SVD.

Namely, if we suppose $A \in \mathcal{M}_{mn}$ has r nonzero singular values, then for $k \leq r$, we let

$$A_k = \sigma_1 \mathbf{u}_1 \mathbf{v}_1^T + \cdots + \sigma_k \mathbf{u}_k \mathbf{v}_k^T. \tag{4.3}$$

For $k = r$, we have the usual outer product form given in Theorem 4.19 and we fully recuperate A. Using a partial sum ($k < r$) gives some (but not all) information and the current example illustrates this.

We need two libraries to deal with the image, `bmp` and `pixmap`, which I assume here are installed and loaded. Let us read in the image using `read.bmp` (from the `bmp` library) and transform it to grey scale using `pixmapGrey` (from the `pixmap` library).

```
> orig_image = read.bmp("FIGS/Julien-and-friend.bmp")
> orig_image = pixmapGrey(orig_image)
```

As usual in `R`, the `plot` function is very versatile and adapts to this new type of object, so `plot(my_image)` produces

For context, I "met" this friend in the Natural History Museum of Vienna (the Naturhistorisches Museum Wien). Very nice museum to visit if you are ever in the area. (At the same time, you had better be in the area for a while as there is no shortage of very nice museums to visit in Vienna.) Let us show some information about the image.

```
> orig_image
```

```
Pixmap image
  Type          : pixmapGrey
  Size          : 1000x890
  Resolution    : 1x1
  Bounding box  : 0 0 890 1000
```

The pixelmap (the matrix of greyscale values) is stored in `my_image@grey`, so we set

```
> M = orig_image@grey
```

From now on, we can forget about the image itself and focus on the matrix M.

4.5.1 Doing things "by hand"

4.5.2 Doing things using proper functions

R has, as can be expected from a language originating in statistics, a native function to perform an SVD, which is, very surprisingly, called `svd`. We use this function and create a function to perform an image compression.

```
> compress_image = function(im, n) {
+   M = svd(im@grey)
+   if (n > length(M$d)) {
+     n = length(im$d)
+   }
+   d_tmp = M$d[1:n]
+   u_tmp = M$u[,1:n]
+   v_tmp = M$v[,1:n]
+   out = list()
+   out$img = mat.or.vec(nr = dim(M$u)[1], nc = dim(M$v)[1])
+   for (i in 1:n) {
+     out$img = out$img + d_tmp[i] * u_tmp[,i] %*% t(v_tmp[,i])
+   }
+   if (min(min(out$img)) < 0 ) {
+     out$img = out$img - min(min(out$img))
+   }
+   out$img = out$img / max(max(out$img))
+   out$nb_pixels_original = dim(im@grey)[1] * dim(im@grey)[2]
+   out$nb_pixels_compressed =
+     length(d_tmp) + dim(u_tmp)[1]*dim(u_tmp)[2] +
+     dim(v_tmp)[1]*dim(v_tmp)[2]
+   out$pct_of_original =
+     out$nb_pixels_compressed / out$nb_pixels_original * 100
+   return(out)
+ }
```

Let me explain what this function does. The arguments to the function are the image to process `im` and the number `n` of singular values to use in the compression. The image `im` is assumed to already be in the form of a greyscale pixelmap. We first idiot-proof the code: if the number of SVD to use is larger than the number possible, we set `n` to that maximum value.

Let us use the function with 10 singular values. Note that we need to copy the image and then substitute the result of the function to the pixelmap of the copied image. Indeed, the returned matrix cannot simply be displayed as an image.

```
> compressed_image = orig_image
```

```
> result_tmp = compress_image(orig_image, 10)
> compressed_image@grey = result_tmp$img
```

If you did not know the original image, you might find it hard to recognise much of anything, but knowing it, you can probably recognise many features. And this achieved by keeping 10 singular values and their corresponding singular vectors. The function `compress_image` returns this information as `$pct_of_original`.

Chapter 5

Principal component analysis (PCA)

One of the reasons the SVD is used is for dimensionality reduction, as we have seen for instance in the image compression example. Now let us consider another dimensionality reduction technique, the so-called principal components analysis or PCA for short. PCA is often used as a blackbox technique, here we take a look at the mathematics behind it. PCA is another linear algebraic technique, that helps reduce a complex dataset to a lower dimensional one. It is a non-parametric method that does not assume anything about data distribution (from the statistical point of view).

5.1 Brief "review" of some probability concepts

A proper treatment of *probability* requires to use *measure theory* and is not the object of this course. Here, we present just what is needed to understand the content of this chapter. For instance, a **random variable** X is a *measurable* function $X : \Omega \to E$, where Ω is a set of outcomes (*sample space*) and E is a measurable space and we define the probability as follows:

$$\mathbb{P}(X \in S \subseteq E) = \mathbb{P}(\omega \in \Omega | X(\omega) \in S).$$

However, let us not worry about the detailed specifics here.

Distribution function of a r.v., $F(x) = \mathbb{P}(X \leq x)$, describes the distribution of a r.v.

R.v. can be discrete or continuous or .. other things.

Definition 5.1 (Variance)**.** *Let X be a random variable. The **variance** of X is given by*

$$\mathsf{Var}\ X = E\left[(X - E(X))^2\right]$$

where E is the expected value

Definition 5.2 (Covariance)**.** *Let X, Y be jointly distributed random variables. The **covariance** of X and Y is given by*

$$\mathsf{cov}(X, Y) = E\left[(X - E(X))\,(Y - E(Y))\right]$$

Note that $\mathsf{cov}(X, X) = E\left[(X - E(X))^2\right] = \mathsf{Var}\ X$

In practice: "true law" versus "observation" In statistics: we reason on the *true law* of distributions, but we usually have only access to a sample

We then use **estimators** to .. estimate the value of a parameter, e.g., the mean, variance and covariance

Definition 5.3 (Unbiased estimators of the mean and variance)**.** *Let $x_1, \ldots, x_n$ be data points (the* sample*) and*

$$\bar{x} = \frac{1}{n}\sum_{i=1}^{n} x_i$$

*be the **mean** of the data. An unbiased estimator of the variance of the sample is*

$$\sigma^2 = \frac{1}{n-1}\sum_{i=1}^{n}(x_i - \bar{x})^2$$

Definition 5.4 (Unbiased estimator of the covariance)**.** *Let $(x_1, y_1), \ldots, (x_n, y_n)$ be data points,*

$$\bar{x} = \frac{1}{n}\sum_{i=1}^{n} x_i \text{ and } \bar{y} = \frac{1}{n}\sum_{i=1}^{n} y_i$$

be the means of the data. An estimator of the covariance of the sample is

$$\mathsf{cov}(x, y) = \frac{1}{n}\sum_{i=1}^{n}(x_i - \bar{x})(y_i - \bar{y})$$

What does covariance do? Variance explains how data disperses around the mean, in a 1-D case

Covariance measures the relationship between two dimensions. E.g., height and weight

More than the exact value, the sign is important:

- $\mathsf{cov}(X, Y) > 0$: both dimensions change in the same "direction"; e.g., larger height usually means higher weight
- $\mathsf{cov}(X, Y) < 0$: both dimensions change in reverse directions; e.g., time spent on social media and performance in this class
- $\mathsf{cov}(X, Y) = 0$: the dimensions are independent from one another; e.g., sex/gender and "intelligence"

The covariance matrix Typically, we consider more than 2 variables..

Definition 5.5. *Suppose p random variables $X_1, \ldots, X_p$. Then the covariance matrix is the symmetric matrix*

$$\begin{pmatrix} \mathsf{cov}(X_1, X_1) & \mathsf{cov}(X_1, X_2) & \cdots & \mathsf{cov}(X_1, X_p) \\ \mathsf{cov}(X_2, X_1) & \mathsf{cov}(X_2, X_2) & \cdots & \mathsf{cov}(X_2, X_p) \\ \vdots & \vdots & & \vdots \\ \mathsf{cov}(X_p, X_1) & \mathsf{cov}(X_p, X_2) & \cdots & \mathsf{cov}(X_p, X_p) \end{pmatrix}$$

i.e., using the properties of covariance,

$$\begin{pmatrix} \mathsf{Var}\ X_1 & \mathsf{cov}(X_1, X_2) & \cdots & \mathsf{cov}(X_1, X_p) \\ \mathsf{cov}(X_1, X_2) & \mathsf{Var}\ X_2 & \cdots & \mathsf{cov}(X_2, X_p) \\ \vdots & \vdots & & \vdots \\ \mathsf{cov}(X_1, X_p) & \mathsf{cov}(X_2, X_p) & \cdots & \mathsf{Var}\ X_p \end{pmatrix}$$

We want to find what carries the most information

For this, we are going to project the information in a new basis in which the first "dimension" will carry most variance, the second dimension will carry a little less, etc.

In order to do so, we need to learn how to change bases

Change of basis

Definition 5.6 (Change of basis matrix)**.** *$\mathcal{B} = \{\mathbf{u}_1, \ldots, \mathbf{u}_n\}$ and $\mathcal{C} = \{\mathbf{v}_1, \ldots, \mathbf{v}_n\}$ bases of vector space V*

*The **change of basis matrix** $P_{\mathcal{C}\leftarrow\mathcal{B}} \in \mathcal{M}_n$,*

$$P_{\mathcal{C}\leftarrow\mathcal{B}} = [[\mathbf{u}_1]_{\mathcal{C}} \cdots [\mathbf{u}_n]_{\mathcal{C}}]$$

has columns the coordinate vectors $[\mathbf{u}_1]_{\mathcal{C}}, \ldots, [\mathbf{u}_n]_{\mathcal{C}}$ of the vectors in $\mathcal{B}$ with respect to $\mathcal{C}$

Theorem 5.7. *$\mathcal{B} = \{\mathbf{u}_1, \ldots, \mathbf{u}_n\}$ and $\mathcal{C} = \{\mathbf{v}_1, \ldots, \mathbf{v}_n\}$ bases of vector space V and $P_{\mathcal{C}\leftarrow\mathcal{B}}$ a change of basis matrix from $\mathcal{B}$ to $\mathcal{C}$*

1. *$\forall \mathbf{x} \in V$, $P_{\mathcal{C}\leftarrow\mathcal{B}}[\mathbf{x}]_{\mathcal{B}} = [\mathbf{x}]_{\mathcal{C}}$*
2. *$P_{\mathcal{C}\leftarrow\mathcal{B}}$ s.t. $\forall \mathbf{x} \in V$, $P_{\mathcal{C}\leftarrow\mathcal{B}}[\mathbf{x}]_{\mathcal{B}} = [\mathbf{x}]_{\mathcal{C}}$ is **unique***
3. *$P_{\mathcal{C}\leftarrow\mathcal{B}}$ invertible and $P^{-1}_{\mathcal{C}\leftarrow\mathcal{B}} = P_{\mathcal{B}\leftarrow\mathcal{C}}$*

Row-reduction method for changing bases

Theorem 5.8. *$\mathcal{B} = \{\mathbf{u}_1, \ldots, \mathbf{u}_n\}$ and $\mathcal{C} = \{\mathbf{v}_1, \ldots, \mathbf{v}_n\}$ bases of vector space V. Let $\mathcal{E}$ be any basis for V,*

$$B = [[\mathbf{u}_1]_{\mathcal{E}}, \ldots, [\mathbf{u}_n]_{\mathcal{E}}] \text{ and } C = [[\mathbf{v}_1]_{\mathcal{E}}, \ldots, [\mathbf{v}_n]_{\mathcal{E}}]$$

and let $[C|B]$ be the augmented matrix constructed using C and B. Then

$$RREF\,([C|B]) = [\mathbb{I}|P_{\mathcal{C}\leftarrow\mathcal{B}}]$$

If working in $\mathbb{R}^n$, this is quite useful with $\mathcal{E}$ the standard basis of $\mathbb{R}^n$ (it does not matter if $\mathcal{B} = \mathcal{E}$)

So the question now becomes

How do we find what new basis to look at our data in?

(Changing the basis does not change the data, just the view you have of it)

(Think of what happens when you do a headstand.. your up becomes down, your right and left switch, but the world does not change, just your view of it)

(Changes of bases are *fundamental* operations in Science)

Setting things up I will use notation (mostly) as in Joliffe's *Principal Component Analysis* (PDF of older version available for free from UofM Libraries)

$\mathbf{x} = (x_1, \ldots, x_p)$ vector of p random variables

We seek a linear function $\mathbf{m}\alpha_1^T\mathbf{x}$ with maximum variance, where $\mathbf{m}\alpha_1 = (\alpha_{11}, \ldots, \alpha_{1p})$, i.e.,

$$\mathbf{m}\alpha_1^T\mathbf{x} = \sum_{j=1}^{p} \alpha_{1j}x_j$$

Then we seek a linear function $\mathbf{m}\alpha_2^T\mathbf{x}$ with maximum variance, uncorrelated to $\mathbf{m}\alpha_1^T\mathbf{x}$

And we continue...

At kth stage, we find a linear function $\mathbf{m}\alpha_k^T\mathbf{x}$ with maximum variance, uncorrelated to $\mathbf{m}\alpha_1^T\mathbf{x}, \ldots, \mathbf{m}\alpha_{k-1}^T\mathbf{x}$

$\mathbf{m}\alpha_i^T\mathbf{x}$ is the ith **principal component** (PC)

Case of known covariance matrix Suppose we know Σ, covariance matrix of $\mathbf{x}$ (i.e., typically: we know $\mathbf{x}$)

Then the kth PC is

$$z_k = \mathbf{m}\alpha_k^T\mathbf{x}$$

where $\mathbf{m}\alpha_k$ is an eigenvector of Σ corresponding to the kth largest eigenvalue λ_k

If, additionally, $\|\mathbf{m}\alpha_k\| = \mathbf{m}\alpha_k^T\mathbf{m}\alpha = 1$, then $\lambda_k = \mathsf{Var}\ z_k$

Why is that? Let us start with

$$\mathbf{m}\alpha_1^T\mathbf{x}$$

We want maximum variance, where $\mathbf{m}\alpha_1 = (\alpha_{11}, \ldots, \alpha_{1p})$, i.e.,

$$\mathbf{m}\alpha_1^T\mathbf{x} = \sum_{j=1}^{p} \alpha_{1j}x_j$$

with the constraint that $\|\mathbf{m}\alpha_1\| = 1$

We have

$$\mathsf{Var}\ \mathbf{m}\alpha_1^T\mathbf{x} = \mathbf{m}\alpha_1^T\Sigma\mathbf{m}\alpha_1$$

Objective We want to maximise $\mathsf{Var}\ \mathbf{m}\alpha_1^T\mathbf{x}$, i.e.,

$$\mathbf{m}\alpha_1^T\Sigma\mathbf{m}\alpha_1$$

under the constraint that $\|\mathbf{m}\alpha_1\| = 1$

$\Longrightarrow$ use **Lagrange multipliers**

Maximisation using Lagrange multipliers

subtitle(A.k.a. super-brief intro to multivariable calculus) We want the max of $f(x_1, \ldots, x_n)$ under the constraint $g(x_1, \ldots, x_n) = k$

1. Solve

$$\begin{aligned} \nabla f(x_1, \ldots, x_n) &= \lambda \nabla g(x_1, \ldots, x_n) \\ g(x_1, \ldots, x_n) &= k \end{aligned}$$

   where $\nabla = (\frac{\partial}{\partial x_1}, \ldots, \frac{\partial}{\partial x_n})$ is the **gradient operator**
2. Plug all solutions into $f(x_1, \ldots, x_n)$ and find maximum values (provided values exist and $\nabla g \neq \mathbf{0}$ there)

λ is the **Lagrange multiplier**

The gradient subtitle(Continuing our super-brief intro to multivariable calculus) $f : \mathbb{R}^n \to \mathbb{R}$ function of several variables, $\nabla = \left(\frac{\partial}{\partial x_1}, \ldots, \frac{\partial}{\partial x_n}\right)$ the gradient operator

Then

$$\nabla f = \left(\frac{\partial}{\partial x_1} f, \ldots, \frac{\partial}{\partial x_n} f\right)$$

So ∇f is a *vector-valued* function, $\nabla f : \mathbb{R}^n \to \mathbb{R}^n$; also written as

$$\nabla f = f_{x_1}(x_1, \ldots, x_n)\mathbf{e}_1 + \cdots f_{x_n}(x_1, \ldots, x_n)\mathbf{e}_n$$

where f_{x_i} is the partial derivative of f with respect to x_i and $\{\mathbf{e}_1, \ldots, \mathbf{e}_n\}$ is the standard basis of $\mathbb{R}^n$

$\mathbf{m}\alpha_1^T \Sigma \mathbf{m}\alpha_1$ and $\|\mathbf{m}\alpha_1\|^2 = \mathbf{m}\alpha_1^T \mathbf{m}\alpha_1$ are functions of $\mathbf{m}\alpha_1 = (\alpha_{11}, \ldots, \alpha_{1p})$

In the notation of the previous slide, we want the max of

$$f(\alpha_{11}, \ldots, \alpha_{1p}) := \mathbf{m}\alpha_1^T \Sigma \mathbf{m}\alpha_1$$

under the constraint that

$$g(\alpha_{11}, \ldots, \alpha_{1p}) := \mathbf{m}\alpha_1^T \mathbf{m}\alpha_1 = 1$$

and with gradient operator

$$\nabla = \left(\frac{\partial}{\partial \alpha_{11}}, \ldots, \frac{\partial}{\partial \alpha_{1p}}\right)$$

Effect of ∇ on g

g is easiest to see:

$$\begin{aligned}\nabla g(\alpha_{11},\ldots,\alpha_{1p}) &= \left(\frac{\partial}{\partial\alpha_{11}},\ldots,\frac{\partial}{\partial\alpha_{1p}}\right)(\alpha_{11},\ldots,\alpha_{1p})\begin{pmatrix}\alpha_{11}\\ \vdots\\ \alpha_{1p}\end{pmatrix}\\ &= \left(\frac{\partial}{\partial\alpha_{11}},\ldots,\frac{\partial}{\partial\alpha_{1p}}\right)\left(\alpha_{11}^2+\cdots+\alpha_{1p}^2\right)\\ &= (2\alpha_{11},\ldots,2\alpha_{1p})\\ &= 2\mathbf{m}\alpha_1\end{aligned}$$

(And that's a general result: $\nabla\|\mathbf{x}\|_2^2 = 2\mathbf{x}$ with $\|\cdot\|_2$ the Euclidean norm)

Effect of ∇ on f

Expand (write $\Sigma = [s_{ij}]$ and do not exploit symmetry)

$$\begin{aligned}\mathbf{m}\alpha_1^T\Sigma\mathbf{m}\alpha_1 &= (\alpha_{11},\ldots,\alpha_{1p})\begin{pmatrix}s_{11} & s_{12} & \cdots & s_{1p}\\ s_{21} & s_{22} & \cdots & s_{2p}\\ \vdots & \vdots & & \vdots\\ s_{p1} & s_{p2} & & s_{pp}\end{pmatrix}\begin{pmatrix}\alpha_{11}\\ \alpha_{12}\\ \vdots\\ \alpha_{1p}\end{pmatrix}\\ &= (\alpha_{11},\ldots,\alpha_{1p})\begin{pmatrix}s_{11}\alpha_{11}+s_{12}\alpha_{12}+\cdots+s_{1p}\alpha_{1p}\\ s_{21}\alpha_{11}+s_{22}\alpha_{12}+\cdots+s_{2p}\alpha_{1p}\\ \vdots\\ s_{p1}\alpha_{11}+s_{p2}\alpha_{12}+\cdots+s_{pp}\alpha_{1p}\end{pmatrix}\\ &= (s_{11}\alpha_{11}+s_{12}\alpha_{12}+\cdots+s_{1p}\alpha_{1p})\alpha_{11}\\ &\quad+(s_{21}\alpha_{11}+s_{22}\alpha_{12}+\cdots+s_{2p}\alpha_{1p})\alpha_{12}\\ &\quad\vdots\\ &\quad+(s_{p1}\alpha_{11}+s_{p2}\alpha_{12}+\cdots+s_{pp}\alpha_{1p})\alpha_{1p}\end{aligned}$$

We have

$$\begin{aligned}\mathbf{m}\alpha_1^T\Sigma\mathbf{m}\alpha_1 &= (s_{11}\alpha_{11}+s_{12}\alpha_{12}+\cdots+s_{1p}\alpha_{1p})\alpha_{11}\\ &\quad+(s_{21}\alpha_{11}+s_{22}\alpha_{12}+\cdots+s_{2p}\alpha_{1p})\alpha_{12}\\ &\quad\vdots\\ &\quad+(s_{p1}\alpha_{11}+s_{p2}\alpha_{12}+\cdots+s_{pp}\alpha_{1p})\alpha_{1p}\end{aligned}$$

So

$$\begin{aligned}\frac{\partial}{\partial\alpha_{11}}\mathbf{m}\alpha_1^T\Sigma\mathbf{m}\alpha_1 &= (s_{11}\alpha_{11}+s_{12}\alpha_{12}+\cdots+s_{1p}\alpha_{1p})+s_{11}\alpha_{11}\\ &\quad+s_{21}\alpha_{12}\\ &\quad\vdots\\ &\quad+s_{p1}\alpha_{1p}\\ &= s_{11}\alpha_{11}+s_{12}\alpha_{12}+\cdots+s_{1p}\alpha_{1p}\\ &\quad+s_{11}\alpha_{11}+s_{21}\alpha_{12}+\cdots+s_{p1}\alpha_{1p}\\ &= 2(s_{11}\alpha_{11}+s_{12}\alpha_{12}+\cdots+s_{1p}\alpha_{1p})\end{aligned}$$

(last equality stems from symmetry of Σ)

In general, for $i=1,\ldots,p$,

$$\begin{aligned}\frac{\partial}{\partial\alpha_{1i}}\mathbf{m}\alpha_1^T\Sigma\mathbf{m}\alpha_1 &= s_{i1}\alpha_{11}+s_{i2}\alpha_{12}+\cdots+s_{ip}\alpha_{1p}\\ &\quad+s_{i1}\alpha_{11}+s_{2i}\alpha_{12}+\cdots+s_{pi}\alpha_{1p}\\ &= 2(s_{i1}\alpha_{11}+s_{i2}\alpha_{12}+\cdots+s_{ip}\alpha_{1p})\end{aligned}$$

(because of symmetry of Σ)

As a consequence,

$$\nabla\mathbf{m}\alpha_1^T\Sigma\mathbf{m}\alpha_1 = 2\Sigma\mathbf{m}\alpha_1$$

So solving

$$\nabla f(x_1,\ldots,x_n) = \lambda\nabla g(x_1,\ldots,x_n)$$

means solving

$$2\Sigma\mathbf{m}\alpha_1 = \lambda 2\mathbf{m}\alpha_1$$

i.e.,

$$\Sigma\mathbf{m}\alpha_1 = \lambda\mathbf{m}\alpha_1$$

$\Longrightarrow$ $(\lambda,\mathbf{m}\alpha_1)$ eigenpair of Σ, with $\mathbf{m}\alpha_1$ having unit length

Picking the right eigenvalue

$(\lambda,\mathbf{m}\alpha_1)$ eigenpair of Σ, with $\mathbf{m}\alpha_1$ having unit length

But which λ to choose?

Recall that we want $\mathsf{Var}\ \mathbf{m}\alpha_1^T\mathbf{x} = \mathbf{m}\alpha_1^T\Sigma\mathbf{m}\alpha_1$ maximal

We have

$$\mathsf{Var}\ \mathbf{m}\alpha_1^T\mathbf{x} = \mathbf{m}\alpha_1^T\Sigma\mathbf{m}\alpha_1 = \mathbf{m}\alpha_1^T(\Sigma\mathbf{m}\alpha_1) = \mathbf{m}\alpha_1^T(\lambda\mathbf{m}\alpha_1) = \lambda(\mathbf{m}\alpha_1^T\mathbf{m}\alpha_1) = \lambda$$

$\Longrightarrow$ we pick $\lambda=\lambda_1$, the largest eigenvalue (covariance matrix symmetric so eigenvalues real)

What we have this far.. The first principal component is $\mathbf{m}\alpha_1^T\mathbf{x}$ and has variance λ_1, where λ_1 the largest eigenvalue of Σ and $\mathbf{m}\alpha_1$ an associated eigenvector with $\|\mathbf{m}\alpha_1\| = 1$

We want the second principal component to be *uncorrelated* with $\mathbf{m}\alpha_1^T\mathbf{x}$ and to have maximum variance $\mathsf{Var}\ \mathbf{m}\alpha_2^T\mathbf{x} = \mathbf{m}\alpha_2^T\Sigma\mathbf{m}\alpha_2$, under the constraint that $\|\mathbf{m}\alpha_2\| = 1$

$\mathbf{m}\alpha_2^T\mathbf{x}$ uncorrelated to $\mathbf{m}\alpha_1^T\mathbf{x}$ if $\mathsf{cov}(\mathbf{m}\alpha_1^T\mathbf{x}, \mathbf{m}\alpha_2^T\mathbf{x}) = 0$

We have

$$\begin{aligned}\mathsf{cov}(\mathbf{m}\alpha_1^T\mathbf{x}, \mathbf{m}\alpha_2^T\mathbf{x}) &= \mathbf{m}\alpha_1^T\Sigma\mathbf{m}\alpha_2 \\ &= \mathbf{m}\alpha_2^T\Sigma^T\mathbf{m}\alpha_1 \\ &= \mathbf{m}\alpha_2^T\Sigma\mathbf{m}\alpha_1 \quad [\Sigma \text{ symmetric}] \\ &= \mathbf{m}\alpha_2^T(\lambda_1\mathbf{m}\alpha_1) \\ &= \lambda\mathbf{m}\alpha_2^T\mathbf{m}\alpha_1\end{aligned}$$

So $\mathbf{m}\alpha_2^T\mathbf{x}$ uncorrelated to $\mathbf{m}\alpha_1^T\mathbf{x}$ if $\mathbf{m}\alpha_1 \perp \mathbf{m}\alpha_2$

This is beginning to sound a lot like Gram-Schmidt, no?

In short Take whatever covariance matrix is available to you (known Σ or sample S_X) – assume sample from now on for simplicity

For $i = 1, \ldots, p$, the ith principal component is

$$z_i = \mathbf{v}_i^T\mathbf{x}$$

where $\mathbf{v}_i$ eigenvector of S_X associated to the ith largest eigenvalue λ_i

If $\mathbf{v}_i$ is normalised, then $\lambda_i = \mathsf{Var}\ z_k$

Covariance matrix Σ the covariance matrix of the random variable, S_X the sample covariance matrix

$X \in \mathcal{M}_{mp}$ the data, then the (sample) covariance matrix S_X takes the form

$$S_X = \frac{1}{n-1}X^TX$$

where the data is centred!

Sometimes you will see $S_X = 1/(n-1)XX^T$. This is for matrices with observations in columns and variables in rows. Just remember that you want the covariance matrix to have size the number of variables, not observations, this will give you the order in which to take the product

5.1.1 Hockey players (eh!)

Let us consider a very Canadian example, although it involves players from all over the world. The height and weight of hockey players who participated in IIHF world championship games during the period 2001-2016 can be found online (here), as part of a study.

We download the data

```
> data = read.csv("https://figshare.com/ndownloader/files/5303173")
```

and take a quick peek (using `kable` and `head`), focusing on the first few columns.

year	country	no	name	position	side	height	weight	birth
2001	RUS	10	tverdovsky oleg	D	L	185	84	1976-05-18
2001	RUS	2	vichnevsky vitali	D	L	188	86	1980-03-18
2001	RUS	26	petrochinin evgeni	D	L	182	95	1976-02-07
2001	RUS	28	zhdan alexander	D	R	178	85	1971-08-28
2001	RUS	32	orekhovsky oleg	D	R	175	88	1977-11-03
2001	RUS	4	zhukov sergei	D	L	193	93	1975-11-23

There is also information about players' club, age, age cohort and BMI, but we will not be using any of these for sure. The table contains 6292 rows. However, the author of the study was interested in the evolution of weights, so it is likely that the same person will be in the dataset several times. Let us check if this is indeed the case. The command `any` returns true if any of the entries in the vector it is passed as an argument is true and `duplicated` is true if an entry is present more than once in its argument.

```
> any(duplicated(data$name))
```

```
[1] TRUE
```

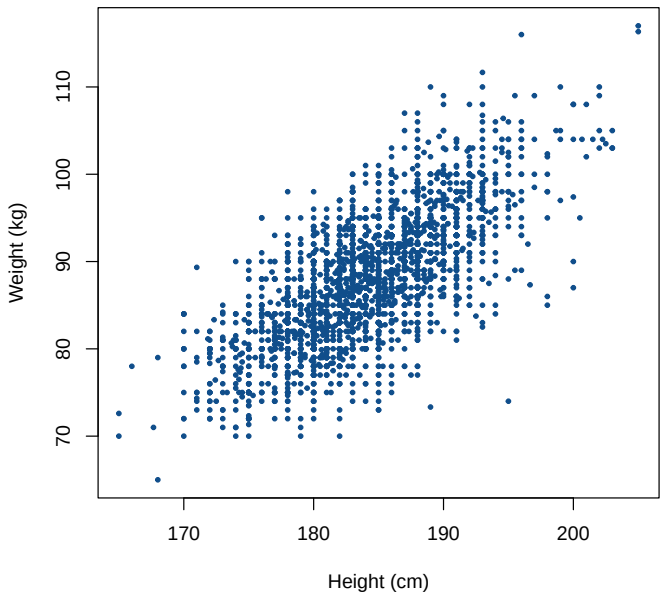
So, indeed, there are players present several times. We are not interested in the evolution of weights, so let us simplify things: if we have more than one record for someone, let us take their height and weight as the average of the heights and weights recorded for them. We keep only three characteristics for a player: their country, height and weight. (We do keep their name as well.) It could be worth checking if there is any case of a player playing for two different countries, which would require to decide on a mechanism to attribute a country to them. However, in this illustrative example, we choose to ignore this possibility.

```
> data_simplified = data.frame(name = unique(data$name))
> c = c()
> w = c()
> h = c()
> for (n in data_simplified$name) {
+     tmp = data[which(data$name == n),]
+     c = c(c, tmp$country[1])
+     h = c(h, mean(tmp$height))
+     w = c(w, mean(tmp$weight))
+ }
> data_simplified$country = c
> data_simplified$weight = w
> data_simplified$height = h
> data = data_simplified
```

The resulting table looks like this

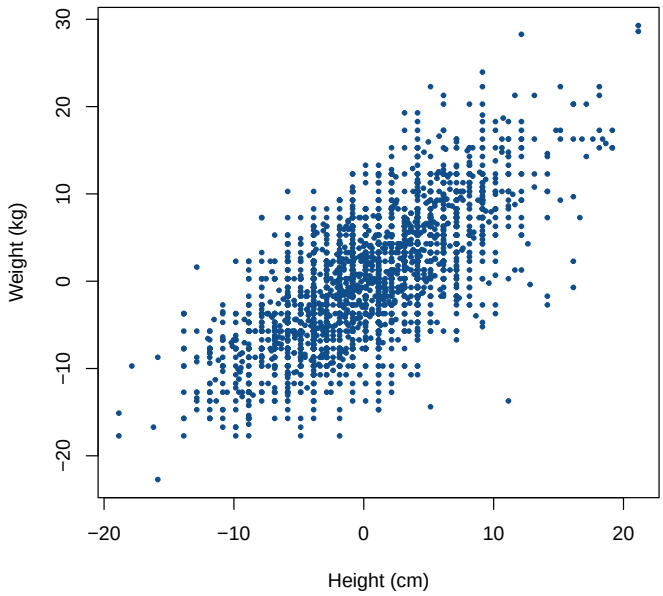
name	country	weight	height
tverdovsky oleg	RUS	84.0	185.0
vichnevsky vitali	RUS	86.0	188.0
petrochinin evgeni	RUS	95.0	182.0
zhdan alexander	RUS	85.5	178.5
orekhovsky oleg	RUS	88.0	175.0
zhukov sergei	RUS	92.5	193.0

Let us plot the height and weight data as it stands after this preprocessing step.



The mean height of players in the data is 183.9 centimetres, their mean weight is 87.72 kilograms. Let us centre the data:

```
> data$weight.c = data$weight-mean(data$weight)
> data$height.c = data$height-mean(data$height)
```



If you do not pay attention to the axes, you can see no difference between the two figures. Although this is a change of basis, this is a rather simple one. Let us now compute the covariance of the data.

```
> cov(data$height, data$weight)
```

```
[1] 26.63506
```

(Note that using the centred data would have given exactly the same result.) So there is a positive linear relationship between the two variables (duh!). Let us now compute the sample covariance matrix, using the centred data.

```
> X = as.matrix(data[,c("height.c", "weight.c")])
> S = 1/(dim(X)[1]-1)*t(X) %*% X
```

The result is a 2×2 matrix,

```
> S
```

```
          height.c weight.c
height.c 29.66176 26.63506
weight.c 26.63506 47.81112
```

One important remark here: the sample covariance matrix, when computed using this method, *requires* the data to be centred. If you do not centre the data prior to computing that matrix, this is what you find.

```
> X2 = as.matrix(data[,c("height", "weight")])
> S2 = 1/(dim(X)[1]-1)*t(X2) %*% X2
> S2
```

```
         height    weight
height 33844.33 16158.902
weight 16158.90  7744.176
```

Let us now compute the principal components. For this, we need eigenvalues and eigenvectors.

```
> ev = eigen(S)
> ev
```

```
eigen() decomposition
$values
[1] 66.87496 10.59793

$vectors
          [,1]       [,2]
[1,] 0.5820222 -0.8131729
[2,] 0.8131729  0.5820222
```

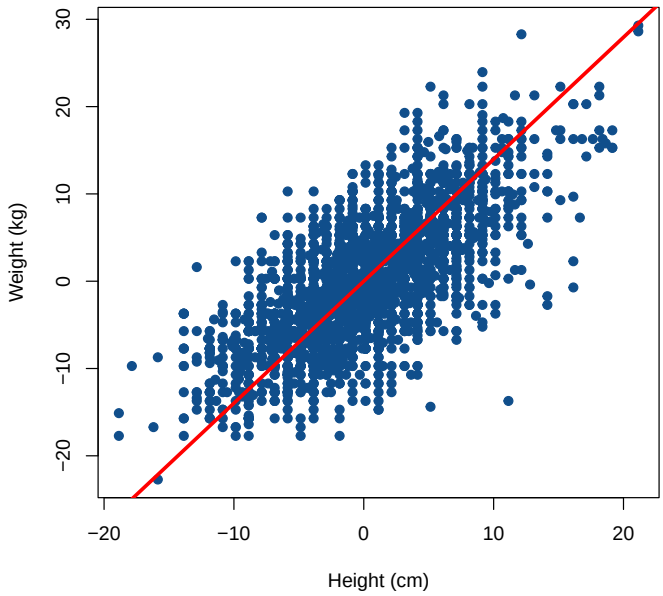
For matrices with only real eigenvalues, `eigen` returns eigenvalues sorted in decreasing order. If we needed to ensure that eigenvalues (and their corresponding eigenvectors) are ordered as we want them to be, we would for instance proceed as follows.

```
> idx_order = order(ev$values, decreasing = TRUE)
> ev$values = ev$values[idx_order]
> ev$vectors = ev$vectors[, idx_order]
```

Let us normalise the first eigenvector. This way, we now that the variance of the first principal component is the corresponding eigenvalue.

```
> ev$vectors[,1] = ev$vectors[,1] / sqrt(sum(ev$vectors[,1]^2))
```

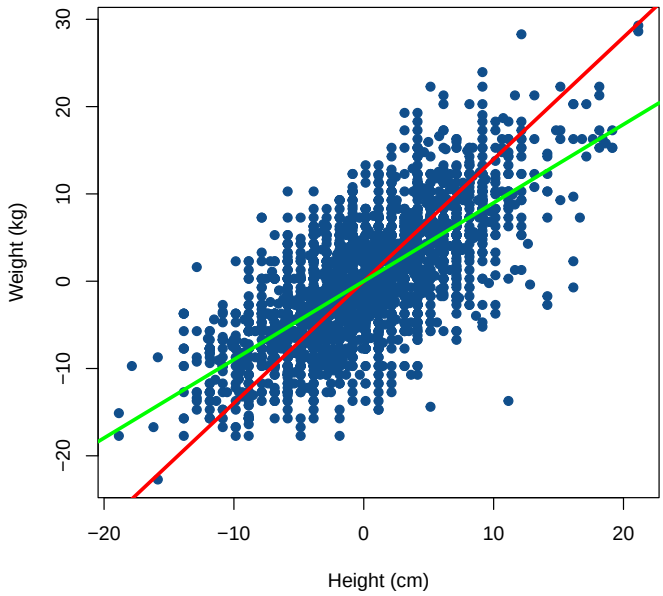
Let us plot this first eigenvector (well, the line carrying this first eigenvector). To use the function 'abline', we need to give the coefficients of the line in the form of (intercept,slope). Intercept is easy, as the line goes through the origin (by construction and because we have centred the data). The slope is also quite simple..



I will let you in a little "secret": least squares are used so often in Stats that 'R' has a very simple function that does that very well. The function is 'lm' (linear models) and you can use it as follows.

```
> z <- lm(weight.c ~ 0 + height.c, data = data)
```

This essentially says "fit a linear model with `weight.c` function of `height.c` and store the result in `z`". You can then use this result in a variety of contexts. First of all, this is what the result looks like (in green), in comparison to the one we found.



Why, you may ask, are the two results so different?

Let us rotate the data so that the red line becomes the red axis. To do that, we use a rotation matrix,

$$R_\theta = \begin{pmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{pmatrix}.$$

To find the angle θ, recall that $\tan\theta$ is equal to opposite length over adjacent length, i.e.,

$$\tan\theta = \frac{\texttt{ev\$vectors}[2,1]}{\texttt{ev\$vectors}[1,1]}$$

So we just use the arctan of this. (Note that angles are in radians.)

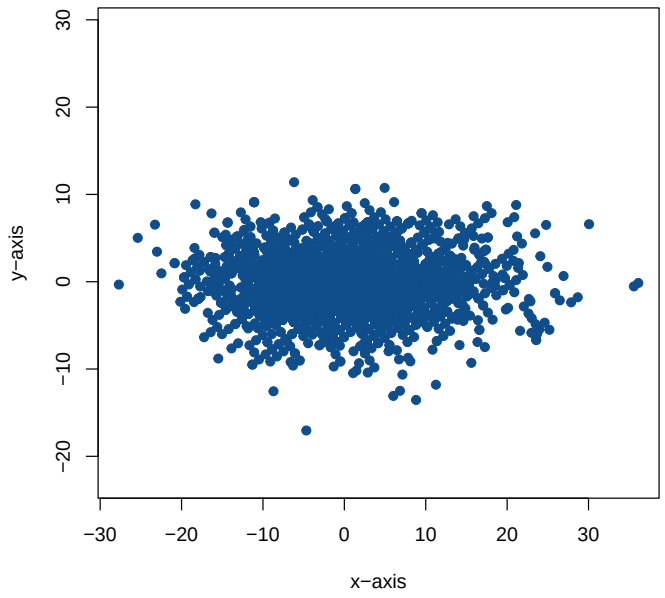
```
> theta = atan(ev$vectors[2,1]/ev$vectors[1,1])
> R_theta = matrix(c(cos(theta), -sin(theta),
+                    sin(theta), cos(theta)),
+                  nr = 2, byrow = TRUE)
```

And now we rotate the points. (In this case, we think of the points as vectors, of course.)

```
> tmp_in = matrix(c(data$weight.c, data$height.c),
+                 nc = 2)
> tmp_out = c()
> for (i in 1:dim(tmp_in)[1]) {
+     tmp_out = rbind(tmp_out,
```

```
+                       t(R_theta %*% tmp_in[i,]))
+ }
> data$weight.c_r = tmp_out[,1]
> data$height.c_r = tmp_out[,2]
```

This change of basis has recast the data in a way where the first axis (the x-axis) is the dimension along which there is the highest variance. To see this, we need to plot the data with the same range as was used before.



It is of course possible to do the same thing with existing R functions.

```
> if (!require("pracma")) {
+     install.packages("pracma")
+ }
> GS = pracma::gramSchmidt(A = ev$vectors)
```

Now recall we saw a theorem that told us how to construct a new basis.

```
> A=matrix(c(GS$Q,1,0,0,1), nr = 2)
> pracma::rref(A)
```

```
     [,1] [,2]       [,3]      [,4]
[1,]    1    0  0.5820222 0.8131729
[2,]    0    1 -0.8131729 0.5820222
```

```
> P = pracma::rref(A)[,c(3,4)]
> X.new = X %*% t(P)
```

5.1.2 Example of a PCA problem

We collect a bunch of information about a bunch of people.. for instance this data from Loughborough University

> This dataset contains the height, weight and 4 fingerprint measurements (length, width, area and circumference), collected from 200 participants.

What best describes a participant?

Each participant is associated to 11 variables. Variables have different natures.

- "Participant Number": $\in \mathbb{N}$ (not interesting)
- "Gender": categorical
- "Age": $\in \mathbb{N}$
- "Dominant Hand": categorical
- "Height (cm) (average of 3 measurements)": $\in \mathbb{R}$
- "Weight (kg) (average of 3 measurements)": $\in \mathbb{R}$
- "Fingertip Temperature (°C)": $\in \mathbb{R}$
- "Fingerprint Height (mm)": $\in \mathbb{R}$
- "Fingerprint Width (mm)": $\in \mathbb{R}$
- "Fingerprint Area (mm2)": $\in \mathbb{R}$
- "Fingerprint Circumference (mm)": $\in \mathbb{R}$

Each participant is a row in the matrix (an *observation*). Each variable is a column. So we have an 200×10 matrix (we discard the "Participant number" column).

Appendix A

Review/presentation of some required concepts

In this course, we rely on notions you acquired in first year Linear Algebra. So let us (briefly) go over material in these courses. I also add (for some of you) a few things that will be handy and establish some terminology that we use throughout the course. Some of the results in this appendix will be studied and proved in class, others you can just admit.

A.1 Sets

A.1.1 Sets and elements

Sets are some of the most elementary structures used in mathematics. They are also extremely useful in programming languages.

Definition A.1 (Set)**.** *A **set** X is a collection of **elements**.*

We write $x \in X$ or $x \notin X$ to indicate that the element x belongs to the set X or does not belong to the set X, respectively.

Definition A.2 (Subset)**.** *Let X be a set. The set S is a **subset** of X, which is denoted $S \subseteq X$, if all its elements belong to X. We say that the subset S is a **proper subset** of X and write $S \subsetneq X$, if it is a subset of X and not equal to X.*

Let A and B two sets. U the universal set ($A \subseteq U$ and $B \subseteq U$).

Definition A.3. *Union of A and B $A \cup B = \{x : x \in A \text{ or } x \in B\}$ set consisting of elements belonging to A or B*

Definition A.4 (Intersection of A and B)**.** $A \cap B = \{x : x \in A \text{ and } x \in B\}$ *set containing those elements belonging to both A and B*

Definition A.5 (Empty set)**.** *The empty set $\emptyset$ contains no element.*

Definition A.6 (Disjoints sets)**.** *If $A \cap B = \emptyset$, then A and B are disjoints sets. (A and B have no elements in common).*

Definition A.7 (Complement of A)**.** $\bar{A} = \{x : x \in U \text{ and } x \notin A\}$ *set consisting of all elements of U not belonging to A.*

Definition A.8 (Difference)**.** $A \backslash B = \{x : x \in A \text{ and } x \notin B\}$ *set containing those elements of A that do not belong to B*

Definition A.9 (Partition)**.** *Let A be a non-empty set. A partition of A is the set $\{A_1, A_2, \ldots, A_n\}$ such that*

- $\forall i \in \{1, \ldots, n\}$, $A_i \neq \emptyset$ *and* $A_i \subset A$ *(non-empty and subset of A)*
- *If* $A_i \neq A_j$ *then* $A_i \cap A_j = \emptyset$ *(every two subsets are disjoint)*
- $A_1 \cup A_2 \cup \cdots \cup A_n = A$

A.1.2 Quantifiers

A shorthand notation for "for all elements x belonging to X" is $\forall x \in X$. For example, if $X = \mathbb{R}$, the *field* of real numbers, then $\forall x \in \mathbb{R}$ means "for all real numbers x".

A shorthand notation for "there exists an element x in the set X" is $\exists x \in X$. $\forall$ and $\exists$ are **quantifiers**.

A.1.3 Intersection and union of sets

Let X and Y be two sets.

Definition A.10 (Intersection)**.** *The* ***intersection*** $X \cap Y$ *of X and Y is the set of elements that belong to X* ***and*** *to Y,*

$$X \cap Y = \{x : x \in X \ \textbf{\textit{and}} \ x \in Y\}.$$

Definition A.11 (Union)**.** *The* ***union*** $X \cup Y$ *of X and Y is the set of elements that belong to X* ***or*** *to Y,*

$$X \cup Y = \{x : x \in X \ \textbf{\textit{or}} \ x \in Y\}.$$

In mathematics, or=and/or in common parlance and I tend to get angry when the latter formulation is used. If you want to specify that elements should belong to one of the sets but not to both, the notion of **exclusive or** (xor) also exists, which is defined as

$$(X \cup Y) \setminus (X \cap Y).$$

A.2 Just enough logic to get by

A **proposition** is an assertion (or statement) whose truth value (true or false) can be asserted. For example, a theorem is a proposition that has been shown to be true. "The sky is blue" is also a proposition. Let A be a proposition. We generally write

$$A$$

to mean that A is true, and

$$\textbf{not } A$$

to mean that A is false. **not** A is the **negation** of A (or **not** A is the negative of A).

Let A, B be propositions. Then

- $A \Rightarrow B$ (read A implies B) means that whenever A is true, then so is B.
- $A \Leftrightarrow B$, also denoted A if and only if B (A iff B for short), means that $A \Rightarrow B$ **and** $B \Rightarrow A$
  We also say that A and B are **equivalent**.

Let A and B be propositions. Then

$$(A \Rightarrow B) \Leftrightarrow (\textbf{not } B \Rightarrow \textbf{not } A).$$

Necessary or sufficient conditions Suppose we want to establish whether a given statement P is true, depending on the truth value of a statement H. Then we say that

- H is a **necessary condition** if $P \Rightarrow H$
  (It is necessary that H be true for P to be true; so whenever P is true, so is H)
- H is a **sufficient condition** if $H \Rightarrow P$
  (It suffices for H to be true for P to also be true)
- H is a **necessary and sufficient condition** if $H \Leftrightarrow P$, i.e., H and P are equivalent

Playing with quantifiers For the quantifiers $\forall$ (for all) and $\exists$ (there exists),

$$\exists \text{ is the contraposite of } \forall$$

Therefore, for example, the contraposite of

$$\forall x \in X, \exists y \in Y$$

is

$$\exists x \in X, \forall y \in Y$$

A.3 Vectors and vector spaces

A.3.1 Vectors

A **vector** $\mathbf{v}$ is an ordered n-tuple of real or complex numbers

Denote $\mathbb{F} = \mathbb{R}$ or $\mathbb{C}$ (real or complex numbers). For $v_1, \ldots, v_n \in \mathbb{F}$,

$$\mathbf{v} = (v_1, \ldots, v_n) \in \mathbb{F}^n$$

is a vector. $v_1, \ldots, v_n$ are the **components** of $\mathbf{v}$

If unambiguous, we write v. Otherwise, $\mathbf{v}$ or $\vec{v}$

A.3.2 Vector space

Definition A.12 (Vector space)**.** *A **vector space** over $\mathbb{F}$ is a set V together with two binary operations, **vector addition**, denoted $+$, and **scalar multiplication**, that satisfy the relations:*

1. $\forall \mathbf{u}, \mathbf{v}, \mathbf{w} \in V$, $\mathbf{u} + (\mathbf{v} + \mathbf{w}) = (\mathbf{u} + \mathbf{v}) + \mathbf{w}$
2. $\forall \mathbf{v}, \mathbf{w} \in V$, $\mathbf{v} + \mathbf{w} = \mathbf{w} + \mathbf{v}$
3. $\exists \mathbf{0} \in V$, *the zero vector, such that* $\mathbf{v} + \mathbf{0} = \mathbf{v}$ *for all* $\mathbf{v} \in V$
4. $\forall \mathbf{v} \in V$, *there exists an element* $\mathbf{w} \in V$, *the additive inverse of* $\mathbf{v}$, *such that* $\mathbf{v} + \mathbf{w} = \mathbf{0}$
5. $\forall \alpha \in \mathbb{R}$ *and* $\forall \mathbf{v}, \mathbf{w} \in V$, $\alpha(\mathbf{v} + \mathbf{w}) = \alpha\mathbf{v} + \alpha\mathbf{w}$
6. $\forall \alpha, \beta \in \mathbb{R}$ *and* $\forall \mathbf{v} \in V$, $(\alpha + \beta)\mathbf{v} = \alpha\mathbf{v} + \beta\mathbf{v}$
7. $\forall \alpha, \beta \in \mathbb{R}$ *and* $\forall \mathbf{v} \in V$, $\alpha(\beta\mathbf{v}) = (\alpha\beta)\mathbf{v}$
8. $\forall \mathbf{v} \in V$, $1\mathbf{v} = \mathbf{v}$

A.3.3 Norms

Definition A.13 (Norm)**.** *Let V be a vector space over $\mathbb{F}$, and $\mathbf{v} \in V$ be a vector. The **norm** of $\mathbf{v}$, denoted $\|\mathbf{v}\|$, is a function from V to $\mathbb{R}_+$ that has the following properties:*

1. *For all $\mathbf{v} \in V$, $\|\mathbf{v}\| \geq 0$ with $\|\mathbf{v}\| = 0$ iff $\mathbf{v} = \mathbf{0}$.*
2. *For all $\alpha \in \mathbb{F}$ and all $\mathbf{v} \in V$, $\|\alpha\mathbf{v}\| = |\alpha| \, \|\mathbf{v}\|$.*
3. *For all $\mathbf{u}, \mathbf{v} \in V$, $\|\mathbf{u} + \mathbf{v}\| \leq \|\mathbf{u}\| + \|\mathbf{v}\|$.*

Let V be a vector space (for example, $\mathbb{R}^2$ or $\mathbb{R}^3$)

The **zero element** (or **zero vector**) is the vector $\mathbf{0} = (0, \ldots, 0)$

The **additive inverse** of $\mathbf{v} = (v_1, \ldots, v_n)$ is $-\mathbf{v} = (-v_1, \ldots, -v_n)$

For $\mathbf{v} = (v_1, \ldots, v_n) \in V$, the length (or Euclidean norm) of $\mathbf{v}$ is the **scalar**

$$\|\mathbf{v}\| = \sqrt{v_1^2 + \cdots + v_n^2}$$

To **normalize** the vector $\mathbf{v}$ consists in considering $\tilde{\mathbf{v}} = \mathbf{v}/\|\mathbf{v}\|$, i.e., the vector in the same direction as $\mathbf{v}$ that has unit length

A.3.4 Standard basis vectors

Vectors $\mathbf{i} = (1, 0, 0)$, $\mathbf{j} = (0, 1, 0)$ and $\mathbf{k} = (0, 0, 1)$ are the **standard basis vectors** of $\mathbb{R}^3$. A vector $\mathbf{v} = (v_1, v_2, v_3)$ can then be written as the linear combination of $\mathbf{i}, \mathbf{j}, \mathbf{k}$,

$$\mathbf{v} = v_1\mathbf{i} + v_2\mathbf{j} + v_3\mathbf{k}.$$

That representation is unique (in the basis $\{\mathbf{i}, \mathbf{j}, \mathbf{k}\}$). For V $(\mathbb{R}^n)$, the standard basis vectors are usually denoted $\mathbf{e}_1, \ldots, \mathbf{e}_n$, with

$$\mathbf{e}_k = (\underbrace{0, \ldots, 0}_{k-1}, 1, \underbrace{0, \ldots, 0}_{n-k+1}).$$

A.3.5 Dot product

Definition A.14 (Dot product)**.** *Let* $\mathbf{a} = (a_1, \ldots, a_n) \in \mathbb{R}^n$, $\mathbf{b} = (b_1, \ldots, b_n) \in \mathbb{R}^n$. *The* ***dot product*** *of* $\mathbf{a}$ *and* $\mathbf{b}$ *is the* ***scalar***

$$\mathbf{a} \bullet \mathbf{b} = \sum_{i=1}^{n} a_i b_i = a_1 b_1 + \cdots + a_n b_n$$

The dot product is a special case of **inner product**.

Theorem A.15 (Properties of the dot product)**.** *For* $\mathbf{a}, \mathbf{b}, \mathbf{c} \in \mathbb{R}^n$ *and* $\alpha \in \mathbb{R}$,

- $\mathbf{a} \bullet \mathbf{a} = \|\mathbf{a}\|^2$ *(so* $\mathbf{a} \bullet \mathbf{a} \geq 0$*, with* $\mathbf{a} \bullet \mathbf{a} = 0 \iff \mathbf{a} = \mathbf{0}$*)*
- $\mathbf{a} \bullet \mathbf{b} = \mathbf{b} \bullet \mathbf{a}$ *(*$\bullet$ *is commutative)*
- $\mathbf{a} \bullet (\mathbf{b} + \mathbf{c}) = \mathbf{a} \bullet \mathbf{b} + \mathbf{a} \bullet \mathbf{c}$ *(*$\bullet$ *distributive over* $+$*)*
- $(\alpha\mathbf{a}) \bullet \mathbf{b} = \alpha(\mathbf{a} \bullet \mathbf{b}) = \mathbf{a} \bullet (\alpha\mathbf{b})$
- $\mathbf{0} \bullet \mathbf{a} = 0$

A.3.6 Some results stemming from the dot product

Theorem A.16. *If* θ *is the angle between the vectors* $\mathbf{a}$ *and* $\mathbf{b}$*, then*

$$\mathbf{a} \bullet \mathbf{b} = \|\mathbf{a}\| \, \|\mathbf{b}\| \, \cos\theta$$

Corollary A.17 (Cauchy-Schwarz inequality)**.** *For any two vectors* $\mathbf{a}$ *and* $\mathbf{b}$*, we have*

$$|\mathbf{a} \bullet \mathbf{b}| \leq \|\mathbf{a}\| \, \|\mathbf{b}\|$$

with equality if and only if $\mathbf{a}$ *is a scalar multiple of* $\mathbf{b}$*, or one of them is* $\mathbf{0}$*.*

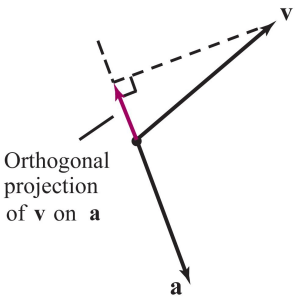
Theorem A.18. $\mathbf{a}$ *and* $\mathbf{b}$ *are orthogonal if and only if* $\mathbf{a} \bullet \mathbf{b} = 0$*.*

A.3.7 Scalar and vector projections

Let $\mathbf{a}, \mathbf{v}$ be vectors.

The **scalar projection** of $\mathbf{v}$ onto $\mathbf{a}$ (or **component** of $\mathbf{v}$ along $\mathbf{a}$) is given by

$$\text{comp}_{\mathbf{a}}\mathbf{v} = \frac{\mathbf{a} \bullet \mathbf{v}}{\|\mathbf{a}\|} \tag{A.1}$$



The **vector projection** (or **orthogonal projection**) of $\mathbf{v}$ onto $\mathbf{a}$ is given by

$$\text{proj}_{\mathbf{a}}\mathbf{v} = \left(\frac{\mathbf{a} \bullet \mathbf{v}}{\|\mathbf{a}\|}\right)\frac{\mathbf{a}}{\|\mathbf{a}\|} = \frac{\mathbf{a} \bullet \mathbf{v}}{\|\mathbf{a}\|^2}\mathbf{a} \tag{A.2}$$

A.4 Complex numbers

Definition A.19 (Complex numbers)**.** *A **complex number** is an ordered pair (a, b), where $a, b \in \mathbb{R}$. Usually written $a + ib$ or $a + bi$, where $i^2 = -1$ (i.e., $i = \sqrt{-1}$). The set of all complex numbers is denoted $\mathbb{C}$,*

$$\mathbb{C} = \{a + ib : a, b \in \mathbb{R}\}.$$

Definition A.20 (Addition and multiplication on $\mathbb{C}$)**.** *Letting $a + ib$ and $c + id \in \mathbb{C}$, addition on $\mathbb{C}$ is defined by*

$$(a + ib) + (c + id) = (a + c) + i(b + d)$$

and multiplication on $\mathbb{C}$ is defined by

$$(a + ib)(c + id) = (ac - bd) + i(ad + bc).$$

Note that the latter is easy to obtain using regular multiplication and the fact that $i^2 = -1$.

Proposition A.21. *1. $\forall \alpha, \beta, \gamma \in \mathbb{C}$,*

2. $\alpha + \beta = \beta + \alpha$ and $\alpha\beta = \beta\alpha$ ***[commutativity]***

3. $(\alpha + \beta) + \gamma = \alpha + (\beta + \gamma)$ and $(\alpha\beta)\gamma = \alpha(\beta\gamma)$ ***[associativity]***

4. $\gamma + 0 = \gamma$ and $\gamma 1 = \gamma$ ***[identities]***

5. $\forall \alpha \in \mathbb{C}$, $\exists \beta \in \mathbb{C}$ unique s.t. $\alpha + \beta = 0$ ***[additive inverse]***

6. $\forall \alpha \neq 0 \in \mathbb{C}$, $\exists \beta \in \mathbb{C}$ unique s.t. $\alpha\beta = 1$ ***[multiplicative inverse]***

7. $\gamma(\alpha + \beta) = \gamma\alpha + \gamma\beta$ ***[distributivity]***

Additive & multiplicative inverse, subtraction, division

Definition A.22. *Let $\alpha, \beta \in \mathbb{C}$*

- *$-\alpha$ is the **additive inverse** of α, i.e., the unique number in $\mathbb{C}$ s.t. $\alpha + (-\alpha) = 0$*
- ***Subtraction** on $\mathbb{C}$:*

$$\beta - \alpha = \beta + (-\alpha)$$

- *For $\alpha \neq 0$, $1/\alpha$ is the **multiplicative inverse** of α, i.e., the unique number in $\mathbb{C}$ s.t.*
$$\alpha(1/\alpha) = 1$$
- ***Division** on $\mathbb{C}$:*
$$\beta/\alpha = \beta(1/\alpha)$$

Definition A.23 (Real and imaginary parts)**.** *Let $z = a + ib$. Then $\Re(z) = a$ is **real part** and $\Im(z) = b$ is **imaginary part** of z.*

Definition A.24 (Conjugate and Modulus)**.** *Let $z = a + ib \in \mathbb{C}$. Then*
- *The **complex conjugate** of z is*
$$\bar{z} = a - ib.$$
- *The **modulus** (or **absolute value**) of z is*
$$|z| = \sqrt{a^2 + b^2} \geq 0.$$

Property A.25 (Properties of complex numbers)**.** *Let $w, z \in \mathbb{C}$, then*
- $z + \bar{z} = 2\Re z$
- $z - \bar{z} = 2i\Im z$
- $z\bar{z} = |z|^2$
- $\overline{w + z} = \bar{w} + \bar{z}$ *and* $\overline{wz} = \bar{w}\bar{z}$
- $\bar{\bar{z}} = z$
- $|\Re z| \leq |z|$ *and* $|\Im z| \leq |z|$
- $|\bar{z}| = |z|$
- $|wz| = |w|\,|z|$
- $|w + z| \leq |w| + |z|$ ***[triangle inequality]***

A.4.1 Solving quadratic equations

The interest of complex numbers is easily illustrated as follows. Consider the polynomial

$$P(x) = a_0 + a_1 x + a_2 x^2, \tag{A.3}$$

where $x, a_0, a_1, a_2 \in \mathbb{R}$. Letting

$$\Delta = a_1^2 - 4a_0 a_2,$$

we know from high school mathematics that if $\Delta > 0$, then

$$P(x) = 0$$

has two distinct *real* solutions,

$$x_1 = \frac{-a_1 - \sqrt{\Delta}}{2a_2} \quad \text{and} \quad x_2 = \frac{-a_1 + \sqrt{\Delta}}{2a_2},$$

while if $\Delta = 0$, then there is a (multiplicity 2) unique *real* solution

$$x_1 = \frac{-a_1}{2a_2}.$$

Finally, if $\Delta < 0$, then there is no (real) solution. Now suppose that instead of seeking real roots, we allow roots to be complex numbers. For this, consider again the polynomial (A.3). If instead of seeking $x \in \mathbb{R}$, we seek $x \in \mathbb{C}$, then the situation is the same, except when $\Delta < 0$. In the latter case, note that

$$\sqrt{\Delta} = \sqrt{(-1)(-\Delta)} = \sqrt{-1}\sqrt{-\Delta} = i\sqrt{-\Delta}.$$

As a consequence, when $\Delta < 0$, $-\Delta > 0$ and the square root is the usual one. To summarize, consider the polynomial (A.3). Letting

$$\Delta = a_1^2 - 4a_0a_2,$$

then

$$P(x) = 0$$

has two solutions,

$$x_{1,2} = \frac{-a_1 \pm \sqrt{\Delta}}{2a_2},$$

where, if $\Delta < 0$, $x_1, x_2 \in \mathbb{C}$ and take the form

$$x_{1,2} = \frac{-a_1 \pm i\sqrt{-\Delta}}{2a_2}.$$

A.4.2 Why this matters

Recall that the *eigenpairs* of the matrix

$$A = \begin{pmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{pmatrix}, \tag{A.4}$$

are the λ and $\mathbf{v} \neq \mathbf{0}$ solutions to

$$A\mathbf{v} = \lambda\mathbf{v}.$$

We come back to this later in Section A.7.1, but let us recall how one treats this problem. Finding λ and $\mathbf{v} \neq \mathbf{0}$ such that $A\mathbf{v} = \lambda\mathbf{v}$ is equivalent, of course, to finding λ and $\mathbf{v} \neq 0$ such that

$$(A - \lambda\mathbb{I})\mathbf{v} = \mathbf{0}. \tag{A.5}$$

Since we seek nonzero $\mathbf{v}$, we must invoke the contraposite of Theorem A.62 and in particular, the following:

$$A\mathbf{v} = \mathbf{0} \text{ has infinitely many solutions } \iff \det(A) = 0.$$

(Note that the contrapositive of the statement "$A\mathbf{v} = \mathbf{0}$ has the unique solution $\mathbf{v} = \mathbf{0}$" in Theorem A.62 is "$A\mathbf{v} = \mathbf{0}$ has either no or infinitely many solutions". However, we know that $\mathbf{v} = \mathbf{0}$ is *always* solution to the homogeneous linear system $A\mathbf{v} = \mathbf{0}$ and as a consequence, the contraposite just states there are infinitely many solutions.)

As a consequence, we find the eigenvalues λ by solving $\det(A - \lambda\mathbb{I}) = 0$, i.e., finding the λ solutions to

$$|A - \lambda\mathbb{I}| = \begin{vmatrix} a_{11} - \lambda & a_{12} \\ a_{21} & a_{22} - \lambda \end{vmatrix} = (a_{11} - \lambda)(a_{22} - \lambda) - a_{12}a_{21} = 0.$$

Simplifying the latter polynomial,

$$\lambda^2 - (a_{11} + a_{22})\lambda + a_{11}a_{22} - a_{12}a_{21} = 0.$$

Let

$$P(\lambda) = \lambda^2 - (a_{11} + a_{22})\lambda + a_{11}a_{22} - a_{12}a_{21}$$

From previous discussion, letting

$$\begin{aligned} \Delta &= (a_{11} + a_{22})^2 - 4(a_{11}a_{22} - a_{12}a_{21}) \\ &= a_{11}^2 + a_{22}^2 + 2a_{11}a_{22} - 4a_{11}a_{22} + 4a_{12}a_{21} \\ &= a_{11}^2 + a_{22}^2 - 2a_{11}a_{22} + 4a_{12}a_{21} \\ &= (a_{11} - a_{22})^2 + 4a_{12}a_{21}, \end{aligned}$$

we have two (potentially equal) solutions to $P(\lambda) = 0$

$$x_{1,2} = \frac{a_{11} + a_{22} \pm \sqrt{\Delta}}{2}$$

that are complex if $\Delta < 0$.

Example: $\begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}$

A.5 Linear systems and matrices

A.5.1 Linear systems

Definition A.26 (Linear system)**.** *A **linear system** of m equations in n unknowns takes the form*

$$\begin{array}{ccccccccc} a_{11}x_1 & + & a_{12}x_2 & + & \cdots & + & a_{1n}x_n & = & b_1 \\ a_{21}x_1 & + & a_{22}x_2 & + & \cdots & + & a_{2n}x_n & = & b_2 \\ \vdots & & \vdots & & \vdots & & \vdots & & \vdots \\ a_{m1}x_1 & + & a_{m2}x_2 & + & \cdots & + & a_{mn}x_n & = & b_n \end{array} \tag{A.6}$$

The a_{ij}, x_j and b_j could be in $\mathbb{R}$ or $\mathbb{C}$, although here we typically assume they are in $\mathbb{R}$

The aim is to find $x_1, x_2, \ldots, x_n$ that satisfy all equations simultaneously

Theorem A.27 (Nature of solutions to a linear system)**.** *A linear system can have*

- *no solution*
- *a unique solution*
- *infinitely many solutions*

Operations on linear systems You learned to manipulate linear systems using

- Gaussian elimination
- Gauss-Jordan elimination

with the aim to put the system in **row echelon form** (REF) or **reduced row echelon form** (RREF)

Matrices and linear systems Writing

$$A = \begin{pmatrix} a_{11} & a_{12} & \cdots & a_{1n} \\ a_{21} & a_{22} & \cdots & a_{2n} \\ \vdots & \vdots & & \vdots \\ a_{m1} & a_{m2} & \cdots & a_{mn} \end{pmatrix}, \quad \mathbf{x} = \begin{pmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{pmatrix} \quad \text{and} \quad \mathbf{b} = \begin{pmatrix} b_1 \\ b_2 \\ \vdots \\ b_n \end{pmatrix}$$

where A is an $m \times n$ **matrix**, $\mathbf{x}$ and $\mathbf{b}$ are n (column) **vectors** (or $n \times 1$ matrices), then the linear system in the previous slide takes the form

$$A\mathbf{x} = \mathbf{b}$$

Notation for vectors We usually assume vectors are column vectors and thus write, e.g.,

$$\mathbf{x} = \begin{pmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{pmatrix} = (x_1, x_2, \ldots, x_n)^T$$

Here, ^{T} is the **transpose operator** (more on this soon)

Consider the system

$$A\mathbf{x} = \mathbf{b}$$

If $\mathbf{b} = \mathbf{0}$, the system is **homogeneous** and always has the solution $\mathbf{x} = 0$ and so the "no solution" option in Theorem A.27 goes away

A.6 Matrix arithmetic

Definition A.28 (Matrix)**.** *An m-by-n or $m \times n$ matrix is a rectangular array of elements of $\mathbb{R}$ or $\mathbb{C}$ with m rows and n columns,*

$$A = [a_{ij}] = \begin{pmatrix} a_{11} & \cdots & a_{1n} \\ \vdots & & \vdots \\ a_{m1} & \cdots & a_{mn} \end{pmatrix}$$

We always list indices as "row,column"

We denote $\mathcal{M}_{mn}(\mathbb{F})$ or $\mathbb{F}^{mn}$ the set of $m \times n$ matrices with entries in $\mathbb{F} = \{\mathbb{R}, \mathbb{C}\}$. Often, we omit $\mathbb{F}$ in $\mathcal{M}_{mn}$ if the nature of $\mathbb{F}$ is not important

When $m = n$, we usually write $\mathcal{M}_n$

Basic matrix arithmetic Let $A \in \mathcal{M}_{mn}, B \in \mathcal{M}_{mn}$ be matrices (of the same size) and $c \in \mathbb{F} = \{\mathbb{R}, \mathbb{C}\}$ be a scalar

- **Scalar multiplication**
$$cA = [ca_{ij}]$$
- **Addition**
$$A + B = [a_{ij} + b_{ij}]$$
- **Subtraction** (addition of $-B = (-1)B$ to A)
$$A - B = A + (-1)B = [a_{ij} + (-1)b_{ij}] = [a_{ij} - b_{ij}]$$
- **Transposition** of A gives a matrix $A^T = \mathcal{M}_{nm}$ with
$$A^T = [a_{ji}], \quad j = 1, \ldots, n, \quad i = 1, \ldots, m$$

Matrix multiplication The (matrix) **product** of A and B, AB, requires the "inner dimensions" to match, i.e., the number of columns in A must equal the number of rows in B

Suppose that is the case, i.e., let $A \in \mathcal{M}_{mn}$, $B \in \mathcal{M}_{np}$. Then the i, j entry in $C := AB$ takes the form
$$c_{ij} = \sum_{k=1}^{n} a_{ik} b_{kj}$$

Recall that the matrix product is not commutative, i.e., in general, $AB \neq BA$ (when both those products are defined, i.e., when $A, B \in \mathcal{M}_n$)

Special matrices

Definition A.29 (Zero and identity matrices)**.** *The **zero** matrix is the matrix 0_{mn} whose entries are all zero. The **identity** matrix is a square $n \times n$ matrix $\mathbb{I}_n$ with all entries on the main diagonal equal to one and all off diagonal entries equal to zero*

A.6.1 Symmetric matrices

Symmetric matrices occur quite frequently in this course, so let us go over some of their properties in some detail. First, recall that a symmetric matrix is defined as follows.

Definition A.30 (Symmetric matrix)**.** *A square matrix $A \in \mathcal{M}_n$ is **symmetric** if $\forall i, j = 1, \ldots, n$, $a_{ij} = a_{ji}$. In other words, $A \in \mathcal{M}_n$ is symmetric if $A = A^T$.*

Theorem A.31. *1. If $A \in \mathcal{M}_n$, then $A + A^T$ is symmetric.*

2. If $A \in \mathcal{M}_{mn}$, then $AA^T \in \mathcal{M}_m$ and $A^T A \in \mathcal{M}_n$ are symmetric.

Proof. 1. The statement is true if $A + A^T = (A + A^T)^T$. We have

$$(A + A^T)^T = A^T + (A^T)^T = A^T + A = A + A^T,$$

so the property is true.
2. AA^T is symmetric if $AA^T = (AA^T)^T$. We have

$$(AA^T)^T = (A^T)^T A^T = AA^T$$

and the property is true. Similarly, $(A^T A)^T = A^T (A^T)^T = A^T A$ and thus both AA^T and $A^T A$ are symmetric. □

Real symmetric matrices have a spectrum (set of eigenvalues) that has very specific properties.

Theorem A.32. *Let $A \in \mathcal{M}_n(\mathbb{R})$ be symmetric. Then all eigenvalues of A are real.*

Proof. Let $A \in \mathcal{M}_n(\mathbb{R})$ be symmetric and assume $(\lambda, \mathbf{v})$ is an eigenpair of A, i.e, $A\mathbf{v} = \lambda\mathbf{v}$ and $\mathbf{v} \neq \mathbf{0}$. Taking the complex conjugate, $\overline{A\mathbf{v}} = \overline{\lambda\mathbf{v}}$. Recall that $z \in \mathbb{C}$ is such that $z = \bar{z} \iff z \in \mathbb{R}$. So, since $A \in \mathcal{M}_n(\mathbb{R})$, $\overline{A} = A$ (consider the matrix entry by entry). Therefore,

$$A\bar{\mathbf{v}} = \overline{A}\bar{\mathbf{v}} = \overline{A\mathbf{v}} = \overline{\lambda\mathbf{v}} = \bar{\lambda}\bar{\mathbf{v}},$$

i.e., if $(\lambda, \mathbf{v})$ is an eigenpair, then $(\bar{\lambda}, \bar{\mathbf{v}})$ is also an eigenpair.

Still assuming that $A \in \mathcal{M}_n(\mathbb{R})$ is symmetric and $(\lambda, \mathbf{v})$ is an eigenpair of A, using what we just proved (that $(\bar{\lambda}, \bar{\mathbf{v}})$ also eigenpair), take transposes:

$$\begin{aligned} A\bar{\mathbf{v}} = \bar{\lambda}\bar{\mathbf{v}} &\iff (A\bar{\mathbf{v}})^T = (\bar{\lambda}\bar{\mathbf{v}})^T \\ &\iff \bar{\mathbf{v}}^T A^T = \bar{\lambda}\bar{\mathbf{v}}^T \\ &\iff \bar{\mathbf{v}}^T A = \bar{\lambda}\bar{\mathbf{v}}^T. \end{aligned}$$

Let us now compute $\lambda(\bar{\mathbf{v}} \bullet \mathbf{v})$. We have

$$\begin{aligned} \lambda(\bar{\mathbf{v}} \bullet \mathbf{v}) &= \lambda\bar{\mathbf{v}}^T\mathbf{v} = \bar{\mathbf{v}}^T(\lambda\mathbf{v}) \\ &= \bar{\mathbf{v}}^T(A\mathbf{v}) = (\bar{\mathbf{v}}^T A)\mathbf{v} \\ &= (\bar{\lambda}\bar{\mathbf{v}}^T)\mathbf{v} = \bar{\lambda}(\bar{\mathbf{v}} \bullet \mathbf{v}) \iff (\lambda - \bar{\lambda})(\bar{\mathbf{v}} \bullet \mathbf{v}) = 0. \end{aligned}$$

We have shown

$$(\lambda - \bar{\lambda})(\bar{\mathbf{v}} \bullet \mathbf{v}) = 0.$$

Let

$$\mathbf{v} = \begin{pmatrix} a_1 + ib_1 \\ \vdots \\ a_n + ib_n \end{pmatrix}.$$

Then

$$\bar{\mathbf{v}} = \begin{pmatrix} a_1 - ib_1 \\ \vdots \\ a_n - ib_n \end{pmatrix}.$$

So

$$\bar{\mathbf{v}} \bullet \mathbf{v} = (a_1^2 + b_1^2) + \cdots + (a_n^2 + b_n^2).$$

But $\mathbf{v}$, as an eigenvector, is $\neq \mathbf{0}$, so $\bar{\mathbf{v}} \bullet \mathbf{v} \neq 0$ and finally,

$$(\lambda - \bar{\lambda})(\bar{\mathbf{v}} \bullet \mathbf{v}) = 0 \iff \lambda - \bar{\lambda} = 0 \iff \lambda = \bar{\lambda} \iff \lambda \in \mathbb{R}.$$

The result is proved. □

By Theorem A.31, any matrix $A \in \mathcal{M}_{mn}$ gives rise to a symmetric matrix when it is multiplied to its transpose. A symmetric matrix generated this way enjoys even "better" spectrum properties.

Theorem A.33. *Let $A \in \mathcal{M}_{mn}(\mathbb{R})$. Then the eigenvalues of A^TA (and AA^T) are real* and nonnegative.

Proof. Let $A \in \mathcal{M}_{mn}(\mathbb{R})$. By Theorem A.31, A^TA is symmetric. It is also real, as the product of two real matrices. As a consequence, from Theorem A.32, A^TA has real eigenvalues.

Let then $(\lambda, \mathbf{v})$ be an eigenpair of A^TA, with $\mathbf{v}$ chosen so that $\|\mathbf{v}\| = 1$. Norms are functions $V \to \mathbb{R}_+$ (see Section A.3.3), so $\|A\mathbf{v}\|$ and $\|A\mathbf{v}\|^2$ are ≥ 0 and thus

$$\begin{aligned} 0 \leq \|A\mathbf{v}\|^2 &= (A\mathbf{v}) \bullet (A\mathbf{v}) = (A\mathbf{v})^T(A\mathbf{v}) \\ &= \mathbf{v}^T A^T A\mathbf{v} = \mathbf{v}^T(A^TA\mathbf{v}) = \mathbf{v}^T(\lambda\mathbf{v}) \\ &= \lambda(\mathbf{v}^T\mathbf{v}) = \lambda(\mathbf{v} \bullet \mathbf{v}) = \lambda\|\mathbf{v}\|^2 \\ &= \lambda, \end{aligned}$$

proving the result. □

A.6.2 Determinants

Definition A.34 (Determinant)**.** *Let $A \in \mathcal{M}_n$ with $n \geq 2$. The **determinant** of A is the* scalar

$$\det(A) = |A| = \sum_{j=1}^{n} a_{ij}C_{ij}$$

*where $C_{ij} = (-1)^{i+j}\det(A_{ij})$ is the (i,j)-**cofactor** of A and A_{ij} is the submatrix of A from which the ith row and jth column have been removed*

This is a cofactor expansion along the ith row

This is a recursive formula: it gives result in terms of n $\mathcal{M}_{n-1}$ matrices, to which it must in turn be applied, all the way down to

$$\det \begin{pmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{pmatrix} = a_{11}a_{22} - a_{12}a_{21}$$

Two special matrices and their determinants

Definition A.35. *$A \in \mathcal{M}_n$ is **upper triangular** if $a_{ij} = 0$ when $i > j$, **lower triangular** if $a_{ij} = 0$ when $j > i$, **triangular** if it is* either *upper or lower triangular and **diagonal** if it is* both *upper and lower triangular*

When A diagonal, we often write $A = \mathsf{diag}\ (a_{11}, a_{22}, \ldots, a_{nn})$

Theorem A.36. *Let $A \in \mathcal{M}_n$ be triangular or diagonal. Then*

$$\det(A) = \prod_{i=1}^{n} a_{ii} = a_{11}a_{22} \cdots a_{nn}$$

Inversion/Singularity

Definition A.37 (Matrix inverse)**.** *$A \in \mathcal{M}_n$ is **invertible** (or **nonsingular**) if $\exists A^{-1} \in \mathcal{M}_n$ s.t.*

$$AA^{-1} = A^{-1}A = \mathbb{I}$$

*A^{-1} is the **inverse** of A. If A^{-1} does not exist, A is **singular***

Theorem A.38. *Let $A \in \mathcal{M}_n$, $\mathbf{x}, \mathbf{b} \in \mathbb{F}^n$. Then*

- *A invertible $\iff$ $\det(A) \neq 0$*
- *If A invertible, A^{-1} is unique*
- *If A invertible, then $A\mathbf{x} = \mathbf{b}$ has the unique solution $\mathbf{x} = A^{-1}\mathbf{b}$*

Revisiting matrix arithmetic With addition, subtraction, scalar multiplication, multiplication, transposition and inversion, you can perform arithmetic on matrices essentially as on scalar, if you bear in mind a few rules

- The sizes have to be compatible
- The order is important since matrix multiplication is not commutative
- Transposition and inversion change the order of products:

$$(AB)^T = B^T A^T \text{ and } (AB)^{-1} = B^{-1}A^{-1}$$

A.7 Diagonalisation

A.7.1 Eigenvalues / Eigenvectors / Eigenpairs

Definition A.39. *Let $A \in \mathcal{M}_n$. A vector $\mathbf{x} \in \mathbb{F}^n$ such that $\mathbf{x} \neq \mathbf{0}$ is an **eigenvector** of A if $\exists \lambda \in \mathbb{F}$ called an **eigenvalue**, s.t.*

$$A\mathbf{x} = \lambda\mathbf{x}$$

*A couple $(\lambda, \mathbf{x})$ with $\mathbf{x} \neq \mathbf{0}$ s.t. $A\mathbf{x} = \lambda\mathbf{x}$ is an **eigenpair***

If $(\lambda, \mathbf{x})$ eigenpair, then for $c \neq 0$, $(\lambda, c\mathbf{x})$ also eigenpair since $A(c\mathbf{x}) = cA\mathbf{x} = c\lambda\mathbf{x}$ and dividing both sides by c..

Definition A.40 (Similarity)**.** *$A, B \in \mathcal{M}_n$ are **similar** ($A \sim B$) if $\exists P \in \mathcal{M}_n$ invertible s.t.*

$$P^{-1}AP = B$$

Theorem A.41 ($\sim$ is an equivalence relation)**.** *$A, B, C \in \mathcal{M}_n$, then*

- $A \sim A$ *($\sim$ **reflexive**)*
- $A \sim B \implies B \sim A$ *($\sim$ **symmetric**)*
- *$A \sim B$ and $B \sim C \implies A \sim C$* *($\sim$ **transitive**)*

Theorem A.42. *$A, B \in \mathcal{M}_n$ with $A \sim B$. Then*

- $\det\ A = \det\ B$
- *A invertible $\iff$ B invertible*
- *A and B have the same eigenvalues*

A.7.2 Diagonalisation

Definition A.43 (Diagonalisability)**.** *$A \in \mathcal{M}_n$ is **diagonalisable** if $\exists D \in \mathcal{M}_n$ diagonal s.t. $A \sim D$*

In other words, $A \in \mathcal{M}_n$ is diagonalisable if there exists a diagonal matrix $D \in \mathcal{M}_n$ and a nonsingular matrix $P \in \mathcal{M}_n$ s.t. $P^{-1}AP = D$

Could of course write $PAP^{-1} = D$ since P invertible, but $P^{-1}AP$ makes more sense for computations

Theorem A.44. *$A \in \mathcal{M}_n$ diagonalisable $\iff$ A has n linearly independent eigenvectors*

Corollary A.45 (Sufficient condition for diagonalisability)**.** *$A \in \mathcal{M}_n$ has all its eigenvalues distinct $\implies$ A diagonalisable*

For $P^{-1}AP = D$: in P, put the linearly independent eigenvectors as columns and in D, the corresponding eigenvalues

A.8 Linear independence/Bases/Dimension

Linear combination and span

Definition A.46 (Linear combination)**.** *Let V be a vector space. A **linear combination** of a set $\{\mathbf{v}_1, \ldots, \mathbf{v}_k\}$ of vectors in V is a* vector

$$c_1\mathbf{v}_1 + \cdots + c_k\mathbf{v}_k$$

where $c_1, \ldots, c_k \in \mathbb{F}$

Definition A.47 (Span)**.** *The set of all linear combinations of a set of vectors $\mathbf{v}_1, \ldots, \mathbf{v}_k$ is the **span** of $\{\mathbf{v}_1, \ldots, \mathbf{v}_k\}$,*

$$\mathsf{span}\ (\mathbf{v}_1, \ldots, \mathbf{v}_k) = \{c_1\mathbf{v}_1 + \cdots + c_k\mathbf{v}_k : c_1, \ldots, c_k \in \mathbb{F}\}$$

Finite/infinite-dimensional vector spaces

Theorem A.48. *The span of a set of vectors in V is the smallest subspace of V containing all the vectors in the set*

Definition A.49 (Set of vectors spanning a space)**.** *If* $\mathsf{span}\ (\mathbf{v}_1, \ldots, \mathbf{v}_k) = V$*, we say $\mathbf{v}_1, \ldots, \mathbf{v}_k$ **spans** V*

Definition A.50 (Dimension of a vector space)**.** *A vector space V is **finite-dimensional** if some set of vectors in it spans V. A vector space V is **infinite-dimensional** if it is not finite-dimensional*

Definition A.51 (Linear independence/Linear dependence)**.** *A set $\{\mathbf{v}_1, \ldots, \mathbf{v}_k\}$ of vectors in a vector space V is **linearly independent** if*

$$(c_1\mathbf{v}_1 + \cdots + c_k\mathbf{v}_k = 0) \Leftrightarrow (c_1 = \cdots = c_k = 0)\,,$$

*where $c_1, \ldots, c_k \in \mathbb{F}$. A set of vectors is **linearly dependent** if it is not linearly independent.*

If linearly dependent, assume w.l.o.g. that $c_1 \neq 0$, then

$$\mathbf{v}_1 = -\frac{c_2}{c_1}\mathbf{v}_2 - \cdots - \frac{c_k}{c_1}\mathbf{v}_k$$

i.e., $\mathbf{v}_1$ is a linear combination of the other vectors in the set.

Theorem A.52. *Let V be a finite-dimensional vector space. Then the **cardinal** (number of elements) of every linearly independent set of vectors is less than or equal to the number of elements in every spanning set of vectors.*

E.g., in $\mathbb{R}^3$, a set with 4 or more vectors is automatically linearly dependent.

Definition A.53 (Basis)**.** *Let V be a vector space. A **basis** of V is a set of vectors in V that is both linearly independent and spanning.*

Theorem A.54 (Criterion for a basis)**.** *A set $\{\mathbf{v}_1, \ldots, \mathbf{v}_k\}$ of vectors in a vector space V is a basis of $V \iff \forall \mathbf{v} \in V$, $\mathbf{v}$ can be written uniquely in the form*

$$\mathbf{v} = c_1\mathbf{v}_1 + \cdots + c_k\mathbf{v}_k,$$

where $c_1, \ldots, c_k \in \mathbb{F}$.

Plus/Minus Theorem

Theorem A.55 (Plus/Minus Theorem)**.** *S a nonempty set of vectors in vector space V*

- *If S is linearly independent and $V \ni \mathbf{v} \notin \mathsf{span}\ (S)$, then $S \cup \{\mathbf{v}\}$ is linearly independent*
- *If $\mathbf{v} \in S$ is linear combination of other vectors in S, then $\mathsf{span}\ (S) = \mathsf{span}\ (S - \{\mathbf{v}\})$*

More on bases

Theorem A.56 (Basis of finite-dimensional vector space)**.** *Every finite-dimensional vector space has a basis*

Theorem A.57. *Any two bases of a finite-dimensional vector space have the same number of vectors*

Definition A.58 (Dimension)**.** *The **dimension** $\dim V$ of a finite-dimensional vector space V is the number of vectors in any basis of the vector space*

Theorem A.59 (Dimension of a subspace)**.** *Let V be a finite-dimensional vector space and $U \subset V$ be a subspace of V. Then $\dim U \leq \dim V$*

Constructing bases

Theorem A.60. *Let V be a finite-dimensional vector space. Then every linearly independent set of vectors in V with $\dim V$ elements is a basis of V*

Theorem A.61. *Let V be a finite-dimensional vector space. Then every spanning set of vectors in V with $\dim V$ elements is a basis of V*

A.9 Linear algebra in a nutshell

To finish, here is the "expanding result" that you kept adding to in your first Linear Algebra course. Of course, it can still be expanded... As a "TFAE statement", either all statements in the list are true simultaneously, or (exclusively) they are all false.

Theorem A.62. *Let $A \in \mathcal{M}_n$. The following statements are equivalent (TFAE):*

1. *The matrix A is invertible (or nonsingular).*
2. *$\forall \mathbf{b} \in \mathbb{F}^n$, $A\mathbf{x} = \mathbf{b}$ has a unique solution ($\mathbf{x} = A^{-1}\mathbf{b}$).*
3. *The only solution to $A\mathbf{x} = \mathbf{0}$ is the trivial solution $\mathbf{x} = \mathbf{0}$.*
4. *$RREF(A) = \mathbb{I}_n$.*
5. *The matrix A is equal to a product of elementary matrices.*
6. *$\forall \mathbf{b} \in \mathbb{F}^n$, $A\mathbf{x} = \mathbf{b}$ has a solution.*
7. *There is a matrix $B \in \mathcal{M}_n$ such that $AB = \mathbb{I}_n$.*
8. *There is an invertible matrix $B \in \mathcal{M}_n$ such that $AB = \mathbb{I}_n$.*
9. *$\det(A) \neq 0$.*
10. *0 is not an eigenvalue of A.*

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