

Building reproducible analytical pipelines with R

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Welcome!

How using a few ideas from software engineering can help data scientists, analysts and researchers write reliable code

Data scientists, statisticians, analysts, researchers, and many other professionals write *a lot of code*.

Not only do they write a lot of code, but they must also read and review a lot of code as well. They either work in teams and need to review each other's code, or need to be able to reproduce results from past projects, be it for peer review or auditing purposes. And yet, they never, or very rarely, get taught the tools and techniques that would make the process of writing, collaborating, reviewing and reproducing projects possible.

Which is truly unfortunate because software engineers face the same challenges and solved them decades ago.

The aim of this book is to teach you how to use some of the best practices from software engineering and DevOps to make your projects robust, reliable and reproducible. It doesn't matter if you work alone, in a small or in a big team. It doesn't matter if your work gets (peer-)reviewed or audited: the techniques

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presented in this book will make your projects more reliable and save you a lot of frustration!

As someone whose primary job is analysing data, you might think that you are not a developer. It seems as if developers are these genius types that write extremely high-quality code and create these super useful packages. The truth is that you are a developer as well. It's just that your focus is on writing code for your purposes to get your analyses going instead of writing code for others. Or at least, that's what you think. Because in *others*, your team-mates are included. Reviewers and auditors are included. Any people that will read your code are included, and there **will** be people that will read your code. At the very least future you will read your code. By learning how to set up projects and write code in a way that future you will understand and not want to murder you, you will actually work towards improving the quality of your work, naturally.

The book can be read for free on <https://raps-with-r.dev> and you can buy a DRM-free Epub or PDF on Leanpub¹.

You can submit issues, PRs and ask questions on the book's Github repository².

¹<https://leanpub.com/raps-with-r/>

²<https://github.com/b-rodrigues/rap4all>

Preface

In the summer of 2022, a former colleague from my first job asked me if I wanted to help him teach a class at the University of Luxembourg. It was a class for the Master’s of Data Science, and the class was supposed to be taught by non-academics like us. The idea was to teach the students some “real-world” skills from the industry. It was a 40 hours class, and naturally we split them equally between us; my colleague focused on time series statistics but I really didn’t know what I should do. I knew I wanted to teach, I always liked teaching, but I am a public servant in the ministry of higher education and research in Luxembourg. I still code a lot, but I don’t do exciting machine learning anymore, or advanced econometrics like my colleague. Before (re)joining the public service I was a senior data scientist and then manager in one of the big four accounting firms. Before that, and this is where my colleague and I met, I was a research assistant in the research department of the national statistical institute of statistics in Luxembourg, and my colleague is still an applied researcher there.

What could I teach these students? What “skills from the industry” could I possibly share with them? I am an expert in nothing in particular. Actually, I don’t really know anything very deeply, but know at least a little about many different things. There are many self-help books out there that state that it’s better to know a lot about only a few, maybe even only one, topic, than know a lot about many topics. I tend to disagree with this; at least

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in my experience, knowing enough about many different topics always allowed me to communicate effectively with many different people, from researchers focusing on very specific topics that needed my help to assist them in their research, to clients from a wide range of industries that were sharing their problems with me in my consulting years. If I needed to deepen my knowledge on a particular topic before I could intervene, I had the necessary theoretical background to grab a few books and learn the material. Also, I was never afraid of asking questions.

This is reflected in my blogging. As I'm writing these lines (beginning of 2023), I have been blogging for about ten years. Most of my blog posts are me trying to lay out a problem I had at work and how I solved it. Sometimes I do some things for pleasure or curiosity, like the two posts on the video game nethack, or the ones on 19th century newspapers where I learned a lot about NLP. Because I was lucky enough to work with different people from many backgrounds, I always had to solve a very wide range of problems.

But that still didn't really help me to find a topic to teach... but then it dawned on me. Even though in my career I had to help many different people with many different backgrounds and needs, there were two things that everyone always required: traceability and reliability.

Everyone wanted to know how I came to the conclusions that I came to, and most of them even wanted to be able to reproduce my steps as a form of double checking what I did (consultants are expensive, so you better make sure that they're worth their hourly rate!). When I was a manager, I applied the same logic to my teammates. I wanted to be able to understand what they were doing, or at least know that if I needed to review their work deeply, the possibility was there.

So what I had to teach these students of data science was some best practices in software engineering. Most people working with data don't get taught software engineering skills. Courses focus on probability theory, linear algebra, algorithms, and programming but not software engineering. That's because software engineering skills get taught to software engineers. But while statisticians, data scientists, (or whatever we get called these days), are not software engineers, they do write a lot of code. And code that is quite important at that. And yet, most of us do work like pigs (no disrespect to pigs).

For example, how much of the code you write that produces very sensitive and important results, be it in science or in industry, is thoroughly tested? How much of the code you use relies on a single person showing up for work and using some secret knowledge that is undocumented? What if that person ends up under a bus? How much code do you run that no one dares touch anymore because that one person from before did end up under a bus?

How many people do you have to ping when you need to get an update to a quarterly report? How many people do you have to ping to know how Table 3 from that report from 2020 that was quickly put together during the Covid-19 lockdowns was computed? Are all the people involved even working in your company still?

When collaborating with teammates to write a report or scientific paper, do you consider potential risks? (If you're wondering *What risks?* then you're definitely not considering them.)

Are you able to tell anyone, *exactly*, how that number that gets used by the CEO in that one report was made? What if there's an investigation, or some external audit? Would the auditors be able to run the code and understand what is going on with

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as little intervention as possible (ideally none) from you? *But I don't work in an industry that gets audited*, you may think. Well, maybe not, or maybe one day your work will get audited anyways. Maybe it'll get audited internally for whatever reason. Maybe there's a new law that went into force that requires your work, or parts of your work, to be easily traceable.

And if you're a scientist, your work does get audited, or at least it should be in theory. I don't know any scientist (and I know more scientists than the average person, thanks to my background and current job) that is against the idea of open science, open data, reproducibility, and so on. Not one. But in practice, how many papers are truly reproducible? How many scientific results are auditable and traceable?

Lack of traceability and reproducibility can sometimes lead to serious consequences. If you're in the social sciences, you likely know about the *Reinhart and Rogoff* paper. Reinhard and Rogoff are two American economists that published a paper in 2010 that showed that when countries are too much in debt (over 60% of GDP according to the authors) then annual growth decreases by two percent. These papers provided an empirical justification for austerity measures in the aftermath of the 2009 European debt crisis. But there was a serious problem with the Reinhard and Rogoff paper. It's not that they somehow didn't use the *correct* theoretical framework or modelling procedure in their paper. It's not that their assumptions were disputable or too unrealistic. It's that they performed their calculations inside an Excel spreadsheet and did not, and this is not a joke, they did not select every country's real GDP growth to compute the average real GDP growth for high-debt countries:

	B	C	I	J	K	L	M
2			Real GDP growth Debt/GDP				
3			30 or less	30 to 60	60 to 90	90 or above	30 or less
4	Country	Coverage	3.7	3.0	3.5	1.7	5.5
26			1.6	0.3	1.3	-1.8	0.8
27	Minimum		5.4	4.9	10.2	3.6	13.3
28	Maximum						
29							
30	US	1946-2009	n.a.	3.4	3.3	-2.0	n.a.
31	UK	1946-2009	n.a.	2.4	2.5	2.4	n.a.
32	Sweden	1946-2009	3.6	2.9	2.7	n.a.	6.3
33	Spain	1946-2009	1.5	3.4	4.2	n.a.	9.9
34	Portugal	1952-2009	4.8	2.5	0.3	n.a.	7.9
35	New Zealand	1948-2009	2.5	2.9	3.9	-7.9	2.6
36	Netherlands	1956-2009	4.1	2.7	1.1	n.a.	6.4
37	Norway	1947-2009	3.4	5.1	n.a.	n.a.	5.4
38	Japan	1946-2009	7.0	4.0	1.0	0.7	7.0
39	Italy	1951-2009	5.4	2.1	1.8	1.0	5.6
40	Ireland	1948-2009	4.4	4.5	4.0	2.4	2.9
41	Greece	1970-2009	4.0	0.3	2.7	2.9	13.3
42	Germany	1946-2009	3.9	0.9	n.a.	n.a.	3.2
43	France	1949-2009	4.9	2.7	3.0	n.a.	5.2
44	Finland	1946-2009	3.8	2.4	5.5	n.a.	7.0
45	Denmark	1950-2009	3.5	1.7	2.4	n.a.	5.6
46	Canada	1951-2009	1.9	3.6	4.1	n.a.	2.2
47	Belgium	1947-2009	n.a.	4.2	3.1	2.6	n.a.
48	Austria	1948-2009	5.2	3.3	-3.8	n.a.	5.7
49	Australia	1951-2009	3.2	4.9	4.0	n.a.	5.9
50							
51			4.1	2.8	2.8	=AVERAGE(L30:L44)	

Figure 1.: You can see that not all countries are selected...

(source to image, archived link³)

And this is not the only problem with this paper.

The problem is not that this mistake was made. Reinhart and Rogoff are only human and mistakes can happen. What's problematic is that this was picked up and corrected too late. In an ideal world, Reinhart and Rogoff would not have used tools that make mistakes like this almost impossible to find once they're made. Instead, they would have used tools that would have made such a thing not happen in the first place, or, as a second best, making it easier and faster for someone else to find this mistake. And this is not something that is only useful in research, but also in any industry. Being able to trust results,

³<https://archive.is/DTGpC>

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tracing back calculations and auditing are not only concerns of researchers.

So this is what I decided to teach the students: how they could structure their projects in such a way that they could spot problems like that during development, but also make it easy to reproduce and retrace who did what and when. I wrote my course notes into a freely available bookdown that I used for teaching. When I started compiling my notes, I discovered the concept *Reproducible Analytical Pipelines* as developed by the Office for National Statistics (henceforth ONS). I found the name “Reproducible Analytical Pipeline” (henceforth RAP) really perfect for what I was aiming at. The ONS team responsible for evangelising RAPs also published a free ebook in 2019 already. Another big source of inspiration is Software Carpentry to which I was exposed during my PhD years, around 2014-ish if memory serves. While working on a project with some German colleagues from the University of Bonn, the principal investigator made us work using these concepts to manage the project. I was really impressed by it, and these ideas and techniques stayed with me since then.

The bottom line is: the ideas I’m presenting here are nothing new. It’s just that I took some time to compile them and make them accessible and interesting (at least I hope so) for users of the R programming language.

At least my students found the course interesting. But not just students. I tweeted about this course and shared the notes with a wider audience, and this is when I got very positive feedback from people that were not my students. People wanted to buy this as a book and go deeper into the topics laid out. This is when I realised that, as far as I know, there is not a practical book available discussing these topics. So I decided to write one, but I took my time getting started. What finally, really, got me

working on it was when Dmytro Perepolkin reached out to me and suggested I contact several persons to get their inputs and ideas and get started. I followed his advice, and this led to very fruitful discussions with Sébastien Rochette, Miles McBain and Dmytro. Their ideas and inputs definitely improved the quality of this book, so many thanks to them. Also thanks to David Solito, Matan Hakim, Stas Kolenikov, Sam Parmar, Chuck, Matouš Eibich, Jonathan Moore, Alain Vagner and Matthias Meiksnier for proofreading the book and providing valuable feedback and fixes. And thank you, dear reader, for picking this up!

This book is divided into two parts. The first part teaches you what I believe is essential knowledge you should possess in order to write truly reproducible pipelines. This essential knowledge is constituted of:

- Version control with Git and how to manage projects with Github;
- Functional programming;
- Literate programming.

The main idea from part 1 is “don’t repeat yourself”. Git and Github will help us avoid losing code, and losing track of who should do what in a project (even if you’re working alone on a project, you will see that using Git and Github will save you many hours and headaches). Getting familiar with functional and literate programming should improve the quality of our code by avoiding two common sources of mistakes: computing results that rely on the state of our program (and later, the state of the whole hardware we are using) and copy and paste mistakes.

The second part of the book will then build upon this knowledge to introduce several tools that will help us go beyond the benefits of version control and functional and literate programming:

- Dependency management with `{renv}`;

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- Package development with `{fusen}`;
- Unit and assertive testing;
- Build automation with `{targets}`;
- Reproducible environments with Docker;
- Continuous integration and delivery.

While this is not a book for beginners (you really should be familiar with R before reading this), I will not assume that you have any knowledge of the tools presented in part 2. In fact, even if you're already familiar with Git, Github, functional programming and literate programming, I think that you will still learn something useful from reading part 1. But be warned, this book will require you to take the time to read it, and then type on your computer. Type *a lot*.

I hope that you will enjoy reading this book and applying the ideas in your day-to-day, ideas which hopefully should improve the reliability, traceability and reproducibility of your code. You can read this book for free on <https://raps-with-r.dev/>, or if you want you can buy a DRM-free PDF or Epub over at <https://leanpub.com/raps-with-r>.

If you want to get to know me better, read my bio⁴.

If you have feedback, drop me an email at bruno [at] brodrigues [dot] co.

Enjoy!

⁴<https://www.brodrigues.co/about/me/>

1. Introduction

This book will not teach you about machine learning, statistics or visualisation.

The goal is to teach you a set of tools, practices and project management techniques that should make your projects easier to reproduce, replicate and retrace. These tools and techniques can be used right from the start of your project at a minimal cost, such that once you're done with the analysis, you're also done with making the project reproducible. Your projects are going to be reproducible simply because they were engineered, from the start, to be reproducible.

There are two main ideas in this book that you need to keep in mind at all times:

- DRY: Don't Repeat Yourself;
- WIT: Write IT down.

DRY WIT is not only the best type of humour, it is also the best way to write reproducible analytical pipelines.

1.1. Who is this book for?

This book is for anyone that uses raw data to build any type of output based on that raw data. This can be a simple quarterly

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report for example, in which the data is used for tables and graphs, or a scientific article for a peer reviewed journal or even an interactive web application. It doesn't matter, because the process is, at its core, always very similar:

- Get the data;
- Clean the data;
- Write code to analyse the data;
- Put the results into the final product.

This book will already assume some familiarity with programming, and in particular the R programming language. However, if you're comfortable with another programming language like Python, you could still learn a lot from reading this book. The tools presented in this book are specific to R, but there will always be an alternative for the language you prefer using, meaning that you could apply the advice from this book to your needs and preferences.

1.2. What is the aim of this book?

The aim of this book is to make the process of analysing data as reliable, retraceable, and reproducible as possible, and do this by design. This means that once you're done with the analysis, you're done. You don't want to spend time, which you often don't have anyways, to rewrite or refactor an analysis and make it reproducible after the fact. We both know that this is not going to happen. Once an analysis is done, it's time to go to the next analysis. And if you need to rerun an older analysis (for example, because the data got updated), then you'll simply figure it out at that point, right? That's a problem for future you, right? Hopefully, future you will remember every quirk of

1.2. *What is the aim of this book?*

your code and know which script to run at which point in the process, which comments are outdated and can be safely ignored, what features of the data need to be checked (and when they need to be checked), and so on... You better hope future you is a more diligent worker than you!

Going forward, I'm going to refer to a project that is reproducible as a “reproducible analytical pipeline”, or RAP for short. There are only two ways to make such a RAP; either you are lucky enough to have someone on the team whose job is to turn your messy code into a RAP, or you do it yourself. And this second option is very likely the most common. The issue is, as stated above, that most of us simply don't do it. We are always in the rush to get to the results, and don't think about making the process reproducible. This is because we always think that making the process reproducible takes time and this time is better spent working on the analysis itself. But this is a misconception, for two reasons.

The first reason is that employing the techniques that we are going to discuss in this book won't actually take much time. As you will see, they're not really things that you “add on top of the analysis”, but will be part of the analysis itself, and they will also help with managing the project. And some of these techniques will even save you time (especially testing) and headaches.

The second reason is that an analysis is never, ever, a one-shot. Only the most simple things, like pulling out a number from some data base may be a one-shot. And even then, chances are that once you provide that number, you'll be asked to pull out a variation of that number (for example, by disaggregating by one or several variables). Or maybe you'll get asked for an update to that number in six months. So you will learn very quickly to keep that SQL query in a script somewhere to make sure that you provide a number that is consistent. But what about more

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complex analyses? Is keeping the script enough? Keeping the script is already a good start of course. The problem is that very often, there is no script, or not a script for each step of the analysis.

I've seen this play out many times in many different organisations. It's that time of the year again, we have to write a report. 10 people are involved, and just gathering the data is already complicated. Some get their data from Word documents attached to emails, some from a website, some from a report from another department that is a PDF... I remember a story that a senior manager at my previous job used to tell us: once, a client put out a call for a project that involved helping them setting up a PDF scraper. They periodically needed data from another department that came in PDFs. The manager asked what was, at least from our perspective, an obvious question: why can't they send you the underlying data from that PDF in a machine readable format? They had never thought to ask. So my manager went to that department, and talked to the people putting that PDF together. Their answer? "Well, we could send them the data in any format they want, but they've asked us to send the tables in a PDF format".

So the first, and probably most important lesson here is: when starting to build a RAP, make sure that you talk with all the people involved.

1.3. Prerequisites

You should be comfortable with the R programming language. This book will assume that you have been using R for some projects already, and want to improve not only your knowledge

1.4. What actually is reproducibility?

of the language itself, but also how to successfully manage complex projects. Ideally, you should know about packages, how to install them, you should have written some functions already, know about loops and have some basic knowledge of data structures like lists. While this is not a book on visualisation, we will be making some graphs using the `{ggplot2}` package, so if you're familiar with that, that's good. If not, no worries, visualisation, data munging or data analysis is not the point of this book. Chapter 2, *Before we start* should help you gauge how easily you will be able to follow this book.

Ideally, you should also not be afraid of not using Graphical User Interfaces (GUIs). While you can follow along using an IDE like RStudio, I will not be teaching any features from any program with a GUI. This is not to make things harder than they should be (quite the contrary actually) but because interacting graphically with a program is simply not reproducible. So our aim is to write code that can be executed non-interactively by a machine. This is because one necessary condition for a workflow to be reproducible and get referred to as a RAP, is for the workflow to be able to be executed by a machine, automatically, without any human intervention. This is the second lesson of building RAPs: there should be no human intervention needed to get the outputs once the RAP is started. If you achieve this, then your workflow is likely reproducible, or can at least be made reproducible much more easily than if it requires some special manipulation by a human somewhere in the loop.

1.4. What actually is reproducibility?

A reproducible project means that this project can be rerun by anyone at 0 (or very minimal) cost. But there are different

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levels of reproducibility, and I will discuss this in the next section. Let's first discuss some requirements that a project must have to be considered a RAP.

1.4.1. Using open-source tools to build a RAP is a hard requirement

Open source is a hard requirement for reproducibility.

No ifs nor buts. And I'm not only talking about the code you typed for your research paper/report/analysis. I'm talking about the whole ecosystem that you used to type your code and build the workflow.

Is your code open? That's good. Or is it at least available to other people from your organisation, in a way that they could re-execute it if needed? Good.

But is it code written in a proprietary program, like STATA, SAS or MATLAB? Then your project is not reproducible. It doesn't matter if this code is well documented and written and available on a version control system (internally to your company or open to the public). This project is just not reproducible. Why?

Because on a long enough time horizon, there is no way to re-execute your code with the exact same version of the proprietary programming language and on the exact same version of the operating system that was used at the time the project was developed. As I'm writing these lines, MATLAB, for example, is at version R2022b. And buying an older version may not be simple. I'm sure if you contact their sales department they might be able to sell you an older version. Maybe you can even simply re-download older versions that you've already bought

1.4. What actually is reproducibility?

from their website. But maybe it's not that simple. Or maybe they won't offer this option anymore in the future, who knows? In any case, if you google "purchase old version of Matlab" you will see that many researchers and engineers have this need.

Old version of matlab

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on 29 Nov 2018 STAFF MVP on 29 Nov 2018

Haloo after a few years we need to use again an old program written with matlab R12 6.0.0.88. We don't find the installation CD, can we buy again this old version of the program? Thanks best regard

0 Comments

Sign in to comment.

Sign in to answer this question.

Vote | Link

Answers (1)

STAFF MVP on 29 Nov 2018

Have you tried running the old program on a more recent release of MATLAB?

MATLAB 6.0 (R12) is **eighteen years old** (released in November 2000) and I think it highly unlikely you'll be able to get it working on a new operating system. The [Windows system requirements](#) lists several Windows versions on which that release was supported, the **newest** of which was Windows ME which was released in September 2000. Microsoft ended mainstream support for this OS in 2003 and ended extended support in July 2006 according to [Wikipedia](#).

0 Comments

Sign in to comment.

Vote | Link

Figure 1.1.: Wanting to run older versions of analytics software is a recurrent need.

And if you're running old code written for version, say, R2008a, there's no guarantee that it will produce the exact same results on version 2022b. And let's not even mention the toolboxes (if you're not familiar with MATLAB's toolboxes, they're the equivalent of packages or libraries in other programming languages). These evolve as well, and there's no guarantee that you can purchase older versions of said toolboxes. And it's likely that

1. Introduction

newer versions of toolboxes cannot even run on older versions of Matlab.

And let me be clear, what I'm describing here with MATLAB could also be said for any other proprietary programs still commonly (unfortunately) used in research and in statistics (like STATA, SAS or SPSS). And even if some, or even all, of the editors of these proprietary tools provide ways to buy and run older versions of their software, my point is that the fact that you have to rely on them for this is a barrier to reproducibility, and there is no guarantee they will provide the option to purchase older versions forever. Also, who guarantees that the editors of these tools will be around forever? Or, and that's more likely, that they will keep offering a program that you install on your machine instead of shifting to a subscription based model?

For just \$199 a month, you can execute your SAS (or whatever) scripts on the cloud! Worry about data confidentiality? No worries, data gets encrypted and stored safely on our secure servers! Run your analysis from anywhere and don't worry about losing your work if your cat knocks over your coffee on your laptop! And if you purchase the pro licence, for an additional \$100 a month, you can even execute your code in parallel!

Think this is science fiction? Google “SAS cloud” to see SAS’s cloud based offering.

1.4.2. There are hidden dependencies that can hinder the reproducibility of a project

Then there's another problem: let's suppose you've written a nice, thoroughly tested and documented workflow, and made it available on Github (and let's even assume that the data is available for people to freely download, and that the paper is

1.4. What actually is reproducibility?

open access). Or, if you're working in the private sector, you did everything above as well, the only difference being that the workflow is only available to people inside the company instead of being available freely and publicly online.

Let's further assume that you've used R or Python, or any other open source programming language. Could this study/analysis be said to be reproducible? Well, if the analysis ran on a proprietary operating system, then the conclusion is: your project is not reproducible.

This is because the operating system the code runs on can also influence the outputs that your pipeline builds. There are some particularities in operating systems that may make certain things work differently. Admittedly, this is in practice rarely a problem, but it does happen¹, especially if you're working with very high precision floating point arithmetic like you would do in the financial sector for instance.

Thankfully, there is no need to change operating systems to deal with this issue, and we will learn how to use Docker to safeguard against this problem.

1.4.3. The requirements of a RAP

So where does that leave us? Basically, for something to be truly reproducible, it has to respect the following bullet points:

- Source code must obviously be available and thoroughly tested and documented (which is why we will be using Git and Github);

¹<https://github.com/numpy/numpy/issues/9187>

1. Introduction

- All the dependencies must be easy to find and install (we are going to deal with this using dependency management tools);
- To be written with an open source programming language (nocode tools like Excel are by default non-reproducible because they can't be used non-interactively, and which is why we are going to use the R programming language);
- The project needs to be run on an open source operating system (thankfully, we can deal with this without having to install and learn to use a new operating system, thanks to Docker);
- Data and the paper/report need obviously to be accessible as well, if not publicly as is the case for research, then within your company. This means that the concept of “scripts and/or data available upon request” belongs in the trash.

Availability of data and material

Data available upon reasonable request.

Figure 1.2.: A real sentence from a real paper published in *THE LANCET Regional Health*. How about *make the data available and I won't scratch your car*, how's that for a reasonable request?

1.5. Are there different types of reproducibility?

Let's take one step back: we live in the real world, and in the real world, there are some constraints that are outside of our control.

1.5. Are there different types of reproducibility?

These constraints can make it impossible to build a true RAP, so sometimes we need to settle for something that might not be a true RAP, but a second or even third best thing.

In what follows, let's assume this: in the discussion below, code is tested and documented, so let's only discuss the code running the pipeline itself.

The *worst* reproducible pipeline would be something that works, but only on your machine. This can be simply due to the fact that you hardcoded paths that only exist on your laptop. Anyone wanting to rerun the pipeline would need to change the paths. This is something that needs to be documented in a README which we assumed was the case, so there's that. But maybe this pipeline only runs on your laptop because the computational environment that you're using is hard to reproduce. Maybe you use software, even if it's open source software, that is not easy to install (anyone that tried to install R packages on Linux that depend on the `{rJava}` package know what I'm talking about).

So a least worse pipeline would be one that could be run more easily on any similar machine to yours. This could be achieved by not using hardcoded absolute paths, and by providing instructions to set up the environment. For example, in the case of R, this could be as simple as providing a script called something like `install_deps.R` that would be a call to `install.packages()`. It could look like this:

```
install.packages(c("package1",
                   "package2",
                   etc))
```

The issue here is that you need to make sure that the right versions of the packages get installed. If your script uses `ggplot2`

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version 2.2.1, then users should install this version as well, and by running the script above, the latest version of `{ggplot2}` (as of writing, version 3.4.0) will get installed. Maybe that's not a problem, but it can be if your script uses a function from version 2.2.1 that is not available anymore in the latest version (or maybe its name got changed, or maybe it was modified somehow and doesn't provide the exact same result). The more packages the script uses (and the older it is), the higher the likelihood that some package version will not be compatible. There is also the issue of the R version itself. Generally speaking, recent versions of R seem to not be too bad when it comes to running older code written in R. I know this because in 2022 I've run every example that comes bundled with R since version 0.6.0 on the then current version (as of writing) of R, version 4.2.2.

1.5. Are there different types of reproducibility?

Here is the result of this experiment:

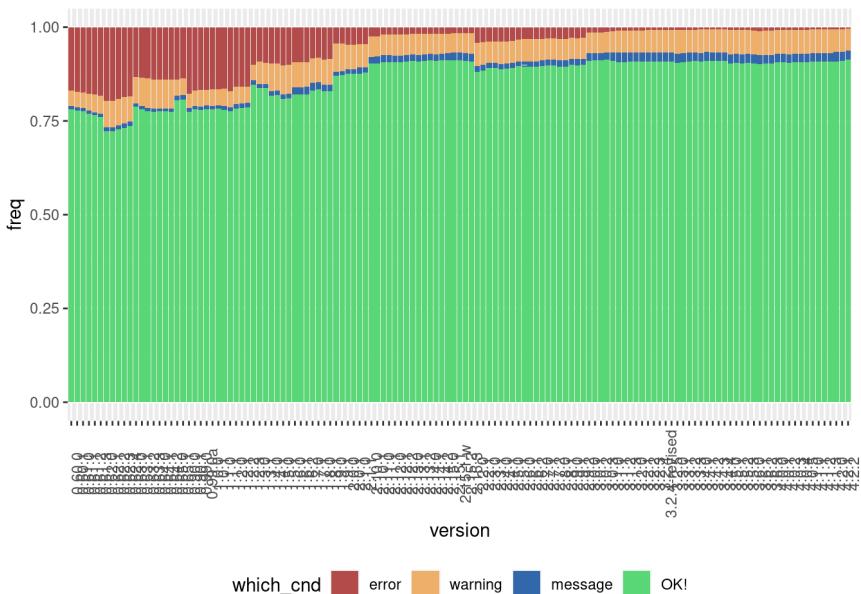


Figure 1.3.: Examples from older versions of R run most of the time successfully on the current version of R

This graph shows the following: for each version of R, starting with R version 0.6.0 (released in 1997), how well the examples that came with a standard installation of R run on the current version of R (version 4.2.2 as of writing). These are the examples from the default packages like `{base}`, `{stats}`, `{stats4}`, and so on. Turns out that more than 75% of the example code from version 0.6.0 still work on the current version of R. A small fraction output a message (which doesn't mean the code doesn't work), some 5% raise a warning, which again doesn't necessarily mean that the code doesn't work, and finally around 20% or so produce errors. As you can see, the closer we get to the current

1. Introduction

release, the fewer errors get raised (if you want to run the code for yourself, check out this Github repository²).

(But something important should be noted: just because some old piece of code runs without error, doesn't mean that the result is exactly the same. There might be cases where the same function returns different results on different versions of R.)

While this is evidence of R itself being quite stable through time, there are studies that show a less rosy picture. In a recent study (Trisovic et al. (2022)³), some researchers tried to rerun up to 9000 R scripts downloaded from the Harvard Dataverse. There were several issues when trying to rerun the scripts, which lead to, and I quote the paper here, “[...] 74% of R files [failing] to complete without error in the initial execution, while 56% failed when code cleaning was applied, showing that many errors can be prevented with good coding practices”.

The take-away message is that counting on the language itself being stable through time as a sufficient condition for reproducibility is not enough. We have to set up the code in a way that it actually is reproducible.

So what does this all mean? This means that reproducibility is on a continuum, and depending on the constraints you face your project can be “not very reproducible” to “totally reproducible”. Let’s consider the following list of anything that can influence how reproducible your project truly is:

- Version of the programming language used;
- Versions of the packages/libraries of said programming language used;
- Operating System, and its version;

²https://github.com/b-rodrigues/code_longevity

³<https://www.nature.com/articles/s41597-022-01143-6>

1.5. Are there different types of reproducibility?

- Versions of the underlying system libraries (which often go hand in hand with OS version, but not necessarily).
- And even the hardware architecture that you run all that software stack on.

So by “reproducibility is on a continuum”, what I mean is that you could set up your project in a way that none, one, two, three, four or all of the preceding items are taken into consideration when making your project reproducible.

This is not a novel, or new idea. Peng (2011) already discussed this concept but named it the *reproducibility spectrum*. In part 2 of this book, I will reintroduce the idea and call it the “reproducibility iceberg”.

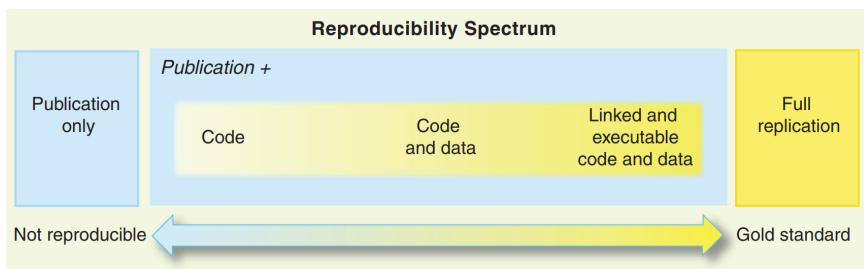


Figure 1.4.: The reproducibility spectrum from Peng’s 2011 paper.

Let me just finish this introduction by discussing the last item on the previous list: hardware architecture. You see, Apple has changed the hardware architecture of their computers recently. Their new computers don’t use Intel based hardware anymore, but instead Apple’s own proprietary architecture (Apple Silicon) based on the ARM specification. And what does that mean concretely? It means that all the binary packages that were built for Intel based Apple computers cannot run on their new computers

1. Introduction

(at least not without a compatibility layer). Which means that if you have a recent M1 or M2 Macbook and need to install old CRAN packages to rerun a project (and we will learn how to do this later in the book), these need to be compiled to work on Apple Silicon first. You cannot even install older versions of R, unless you also compile those from source! Now I have read about a compatibility layer called Rosetta which enables to run binaries compiled for the Intel architecture on the ARM architecture, and maybe this works well with R and CRAN binaries compiled for Intel architecture. Maybe, I don't know. But my point is that you never know what might come in the future, and thus needing to be able to compile from source is important, because compiling from source is what requires the least amount of dependencies that are outside of your control. Relying on binaries is not future-proof (and which is again, another reason why open-source tools are a hard requirement for reproducibility).

And for you Windows users, don't think that the preceding paragraph does not concern you. I think that it is very likely that Microsoft will push in the future for OEM manufacturers to build more ARM based computers. There is already an ARM version of Windows after all, and it has been around for quite some time, and I think that Microsoft will not kill that version any time in the future. This is because ARM is much more energy efficient than other architectures, and any manufacturer can build its own ARM cpus by purchasing a license, which can be quite interesting from a business perspective. For example in the case of Apple Silicon cpus, Apple can now get exactly the cpus they want for their machines and make their software work seamlessly with it (also, further locking in their users to their hardware). I doubt that others will pass the chance to do the same.

Also, something else that might happen is that we might move

1.5. Are there different types of reproducibility?

towards more and more cloud based computing, but I think that this scenario is less likely than the one from before. But who knows. And in that case it is quite likely that the actual code will be running on Linux servers that will likely be ARM based because of energy and licensing costs. Here again, if you want to run your historical code, you'll have to compile old packages and R versions from source.

Ok, so this might seem all incredibly complicated. How on earth are we supposed to manage all these risks and balance the immediate need for results with the future need of rerunning an old project? And what if rerunning this old project is not even needed in the future?

This is where this book will help you. By employing the techniques discussed in this book, not only will it be very easy and quick to set up a project from the ground up that is truly reproducible, the very fact of building the project this way will also ensure that you avoid mistakes and producing results that are wrong. It will be easier and faster to iterate and improve your code, to collaborate, and ultimately to trust the results of your pipelines. So even if no one will rerun that code ever again, you will still benefit from the best practices presented in this book. Let's dive in!

Part I.

Part 1: Don't Repeat Yourself

The first idea we are going to focus on is Don't Repeat Yourself. Simply by avoiding having to repeat yourself, you will naturally implement best practices to make your pipelines reproducible.

Introduction

Part 1 will focus on teaching you the fundamental ingredients to reproducibility. By fundamental ingredients I mean those tools that you absolutely need to have in your toolbox before even attempting to make a project reproducible. These tools are so important that a good chunk of this book is dedicated to them:

- Version control;
- Functional programming;
- Literate programming.

You might already be familiar with these topics, and maybe already use them in your day to day. If that's the case, you still might want to at least skim part 1 before tackling part 2 of the book, which will focus on another set of tools to actually build reproducible analytical pipelines (RAPs).

So this means that part 1 will not teach you how to build reproducible pipelines. But I cannot immediately start teaching you how to build reproducible analytical pipelines without first making sure that you understand the core concepts laid out above. To help you understand these concepts, we will start by analysing some data together. We are going to download, clean and plot some data, and we will achieve this by writing two scripts. These scripts will be written in a very typical non-“software engineering” way, as to mimic how analysts, data scientists or researchers without any formal training in computer

science would perform such an analysis. This does not mean that the quality of the analysis will be low. But it means that, typically, these programmers have delivering results fast, and by any means necessary, as their top priority. My goal with this book is to show you, and hopefully convince you, that by adopting certain simple ideas from software engineering it is possible to deliver just as fast as before, but in a more consistent and robust way.

2. Before we start

This is not an introductory book, so before tackling the topics presented here, make sure that you are familiar with the different topics presented below. If you read this chapter and everything is obvious or known to you, then you should have no trouble following along. If instead what you read here is cryptic, then take some time to improve your understanding of these topics first.

2.1. Essential knowledge

It's important to know the parts that constitute R. Let's make something clear: R is not RStudio, or whatever interface you are using to interact with R. R is a domain-specific interpreted programming language. R is domain-specific because its primary use is in performing statistics. Interpreted, because results get returned immediately when you execute a script in the console. In other words, when you write `1+1` in the console, you get back `2` immediately. There are programming languages, called *compiled* programming languages, that require code to be compiled into binaries before execution. C is such a language. The fact that R is interpreted makes interactive exploratory data analysis easy, but also introduces certain negative aspects. I will discuss these in detail in the book. R's console is an example of a REPL – *Read-Eval-Print-Loop* – environment. Code gets *read*,

2. Before we start

evaluated, printed and the read state gets returned, starting the *loop* over.

To make working with R easier, you should not write code in the console and execute it, but instead write it in a text file. You can keep these text files, update and share them with collaborators. Such text files are called scripts. You *could* write these scripts using the most basic text editor included in your operating system (that would be Notepad.exe on Windows for example), but you should instead use a text editor made specifically to make programming easier. Popular choices among R users include RStudio, Visual Studio Code, or maybe something more exotic like Emacs combined with ESS (my personal choice). Whatever text editor you choose, take time to configure it and learn how to use it. You will spend many, many, many hours inside that text editor. The code you write in that text editor is what's going to feed you and your family. Learn your chosen text editor's keyboard shortcuts and other advanced features. This initial investment will pay for itself many times over. Also, you need to know what an actual text file is. A document written in Word (with the .docx extension) is not a text file. It looks like text, but is not. The .docx format is a much more complex format with many layers of abstraction. “True” plain text files can be opened with the simplest text editor included in your operating system. I've had students trying to create text files with word processors like MS Word and then being confused when things would not work.

As stated before, R is a domain-specific programming language mainly used for doing statistics, or whatever modernized term you may prefer like “*data science*”. Its base capabilities can be extended by installing packages. For example, a base installation of R provides you with useful functions like `mean()` or `sd()`, to compute the average or standard deviation of a

vector of numbers, or `rnorm()` to compute random variates from a Gaussian (Normal) distribution. However, there is no function available to train a random forest. If you need to train a random forest you need to install a package using the `install.packages("randomForest")` command. This installs the `{randomForest}` package (in the rest of the book, I will surround package names with curly braces). The collection of packages installed is called a “library”. Packages get downloaded from CRAN, the *Comprehensive R Archive Network*. There is no doubt in my mind that the reason R became so popular is because it is quite easy to write packages for it; and this is something that we will learn as well! Some packages are written with other programming languages, very often Fortran or C++. The code included in these packages is then compiled and can be executed by R using a user-facing function. For example, if you dig into the source code of the `{randomForest}` package, you will find C and Fortran code. This is important to know, because sometimes R packages need to be compiled by `install.packages()`, and this compilation can sometimes fail (especially on Linux, but more on that later in the book).

When you use R, you will load data sets, create plots, train models, etc. These data sets, plots, models, are all *objects* and they get saved in the global environment. To see a list of objects currently available in the global environment, type `ls()` in the R console. When you quit R, you get asked to save the *workspace*: this will save the current state of the global environment and load it next time you start R. I highly recommend for you to not save the workspace. If you are using RStudio you can change this behaviour in the global options (under *Workspace*, set *Save workspace to .RData on exit* to *Never*). Other editors might have a similar option. Saving and loading the workspace makes it impossible to start with a fresh R session (unless you start R with the `--vanilla` flag), which can cause issues that are

2. Before we start

difficult to pinpoint.

You should also be comfortable with paths and your computer’s file system. *Comfortable* means having no problems finding where a file gets downloaded for example, or being able to navigate to any folder, either through a GUI file browser or through a terminal (if you’re familiar with navigating your computer using the terminal, you will have an easier time with this book than if you didn’t). I also highly recommend that you strive to use relative paths in your scripts, and not absolute paths. In other words: don’t start your scripts with a line such as:

```
setwd("H:/Username/Projects/housing_regression/")
```

but instead, use “Projects” if you’re using RStudio, or similar features from your preferred IDE. This way, you can use relative paths instead. This makes collaboration much easier. Using “Projects” in RStudio, if you need to load data, you can simply write:

```
dataset <- read.csv("data.csv")
```

and don’t need to set working directories using `setwd()`, which obviously will not exist on your collaborators computer.

There is also the `{here}` package that makes using relative paths easier, but I won’t discuss it in this book. If you’re interested you can read this post¹.

You should be familiar with writing functions. This book has a whole chapter on functional programming, and I will teach you how to write functions, but if you’re already familiar with this, then it will make going through that chapter easier.

¹https://github.com/jennybc/here_here

2.1. Essential knowledge

Finally, you should know how to ask for help. If you need help with this book, feel free to open an issue on the book’s Github repo here², or open a thread on the book’s Leanpub forum (if you bought a copy) over here³. Just like for this book, if you have an issue with an R package, look for its repository: many packages’ source code is hosted on Github (but not always). You can also try to reach out to the author, or open a thread on Stackoverflow. Whatever you do, make sure that you do your homework first:

- Read the documentation. Maybe you’re using the tool wrong.
- Take note of the error message. Error messages can be cryptic sometimes, but as you gain in experience, you will learn to decrypt them.
- Write down the simplest script possible that reproduces the issue you’re facing. This is called an MRE, “Minimal Reproducible Example”. If you need to open a thread asking for help, post this MRE, this will make helping you much easier. For general advice on how to write an MRE, you can read this classic blog post⁴.

Finally, keep in mind the following saying from my father, a mason (the ones that lay bricks, not the ones meeting in secrecy to govern the world):

The tools are always right. If you’re using a tool and it’s not behaving as expected, it is much more likely that your expectations are wrong. Take this opportunity to review your knowledge of the tool.

²<https://github.com/b-rodrigues/rap4all>

³<https://community.learnpub.com/c/raps-with-r/>

⁴<https://jonskeet.uk/csharp/complete.html>

3. Project start

In this chapter, we are going to work together on a very simple project. This project will stay with us until the end of the book. As we will go deeper into the book together, you will rewrite that project by implementing the techniques I will teach you. By the end of the book you will have built a reproducible analytical pipeline. To get things going, we are going to keep it simple; our goal here is to get an analysis done, that's it. We won't focus on reproducibility. We are going to download some data, and analyse it, that's it.

3.1. Housing in Luxembourg

We are going to download data about house prices in Luxembourg. Luxembourg is a little Western European country the author hails from that looks like a shoe and is about the size of .98 Rhode Islands. Did you know that Luxembourg is a constitutional monarchy, and not a kingdom like Belgium, but a Grand-Duchy, and actually the last Grand-Duchy in the World? Also, what you should know to understand what we will be doing is that the country of Luxembourg is divided into Cantons, and each Cantons into Communes. If Luxembourg was the USA, Cantons would be States and Communes would be Counties (or Parishes or Boroughs). What's confusing is that "Luxembourg" is also the name of a Canton, and of a Commune, which also has

3. Project start

the status of a city and is the capital of the country. So Luxembourg the country, is divided into Cantons, one of which is called Luxembourg as well, cantons are divided into communes, and inside the canton of Luxembourg, there's the commune of Luxembourg which is also the city of Luxembourg, sometimes called Luxembourg-City, which is the capital of the country.

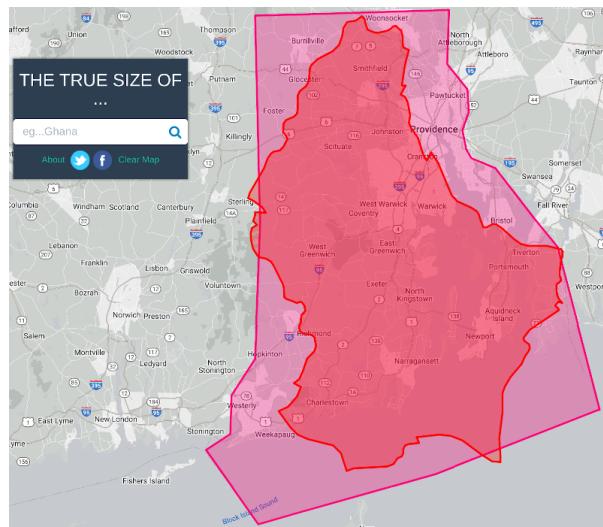


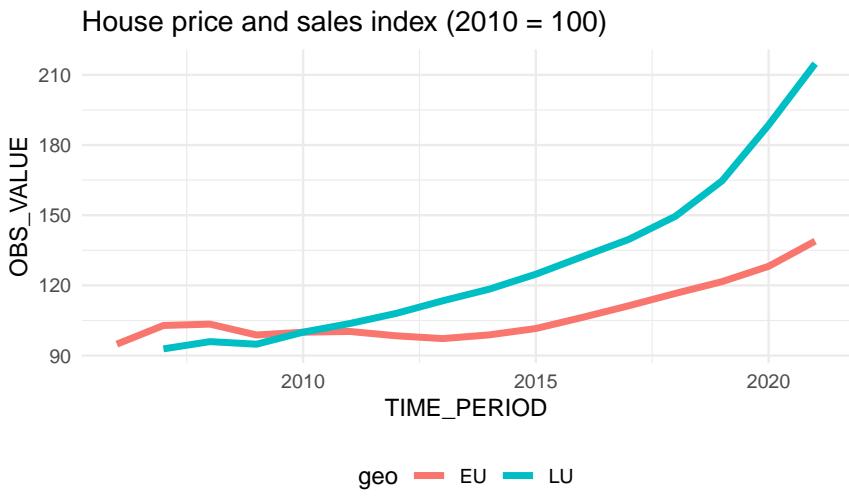
Figure 3.1.: Luxembourg is about as big as the US State of Rhode Island.

What you should also know is that the population is about 645,000 as of writing (January 2023), half of which are foreigners. Around 400,000 persons work in Luxembourg, of which half do not live in Luxembourg; so every morning from Monday to Friday, 200,000 people enter the country to work and then leave in the evening to go back to either Belgium, France or Germany, the neighbouring countries. As you can imagine, this puts enormous pressure on the transportation system and on the roads,

3.1. Housing in Luxembourg

but also on the housing market; everyone wants to live in Luxembourg to avoid the horrible daily commute, and everyone wants to live either in the capital city, or in the second largest urban area in the south, in a city called Esch-sur-Alzette.

The plot below shows the value of the House Price Index over time for Luxembourg and the European Union:



If you want to download the data, click [here](#)¹.

Let us paste the definition of the HPI in here (taken from the HPI's metadata² page):

The House Price Index (HPI) measures inflation in the residential property market. The HPI captures price changes of all types of dwellings purchased by households (flats, detached houses, terraced houses, etc.). Only transacted dwellings are considered,

¹<https://is.gd/AET0ir>

²<https://archive.is/OrQwA>, archived link for posterity.

3. Project start

self-build dwellings are excluded. The land component of the dwelling is included.

So from the plot, we can see that the price of dwellings more than doubled between 2010 and 2021; the value of the index is 214.81 in 2021 for Luxembourg, and 138.92 for the European Union as a whole.

There is a lot of heterogeneity though; the capital and the communes right next to the capital are much more expensive than communes from the less densely populated north, for example. The south of the country is also more expensive than the north, but not as much as the capital and surrounding communes. Not only is price driven by demand, but also by scarcity; in 2021, 0.5% of residents owned 50% of the buildable land for housing purposes (Source: *Observatoire de l'Habitat, Note 29*, archived download link³).

Our project will be quite simple; we are going to download some data, supplied as an Excel file, compiled by the Housing Observatory (*Observatoire de l'Habitat*, a service from the Ministry of Housing, which monitors the evolution of prices in the housing market, among other useful services like the identification of vacant lots). The advantage of their data when compared to Eurostat's data is that the data is disaggregated by commune. The disadvantage is that they only supply nominal prices, and no index (and the data is trapped inside Excel and not ready for analysis with R). Nominal prices are the prices that you read on price tags in shops. The problem with nominal prices is that it is difficult to compare them through time. Ask yourself the following question: would you prefer to have had 500€ (or USDs) in 2003 or in 2023? You probably would have preferred them in 2003, as you could purchase a lot more with \$500 then than now.

³<https://archive.org/download/note-29/note-29.pdf>

3.1. Housing in Luxembourg

In fact, according to a random inflation calculator I googled, to match the purchasing power of \$500 in 2003, you'd need to have \$793 in 2023 (and I'd say that we find very similar values for €). But it doesn't really matter if that calculation is 100% correct: what matters is that the value of money changes, and comparisons through time are difficult, hence why an index is quite useful. So we are going to convert these nominal prices to real prices. Real prices take inflation into account and so allow us to compare prices through time.

So to summarise; our goal is to:

- Get data trapped inside an Excel file into a neat data frame;
- Convert nominal to real prices using a simple method;
- Make some tables and plots and call it a day (for now).

We are going to start in the most basic way possible; we are simply going to write a script and deal with each step separately.

3. Project start

3.2. Saving trapped data from Excel

Getting data from Excel into a tidy data frame can be very tricky. This is because very often, Excel is used as some kind of dashboard or presentation tool. So data is made human-readable, in contrast to machine-readable. Let us quickly discuss this topic as it is essential to grasp the difference between the two (and in our experience, a lot of collective pain inflicted to statisticians and researchers could have been avoided if this concept was more well-known). The picture below shows an Excel file made for human consumption:

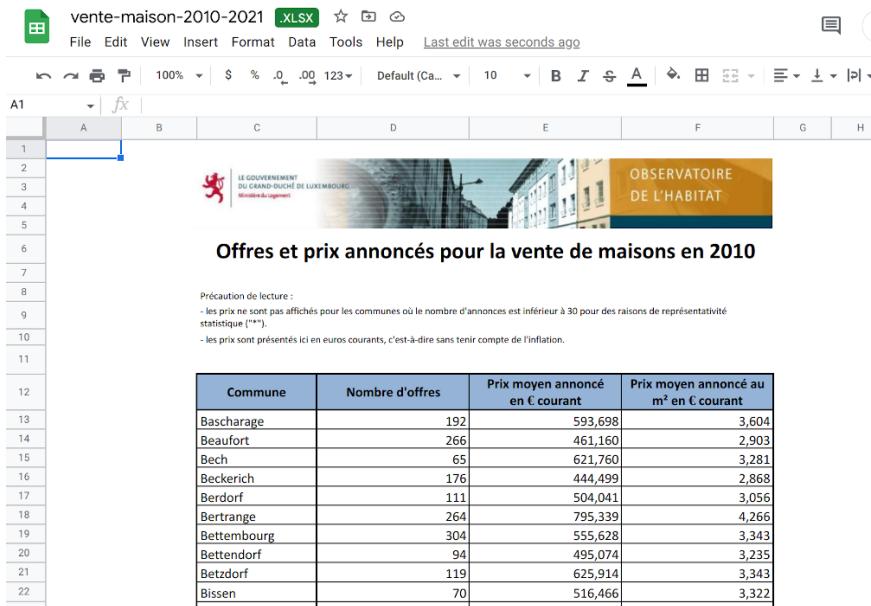


Figure 3.2.: An Excel file meant for human eyes.

So why is this file not machine-readable? Here are some issues:

3.2. Saving trapped data from Excel

- The table does not start in the top-left corner of the spreadsheet, which is where most importing tools expect it to be;
- The spreadsheet starts with a header that contains an image and some text;
- Numbers are text and use “,” as the thousands separator;
- You don’t see it in the screenshot, but each year is in a separate sheet.

That being said, this Excel file is still very tame, and going from this Excel to a tidy data frame will not be too difficult. In fact, we suspect that whoever made this Excel file is well aware of the contradicting requirements of human and machine-readable formatting of data, and strove to find a compromise. Because more often than not, getting human-readable data into a machine-readable format is a nightmare. We could call data like this *machine-friendly* data.

If you want to follow along, you can download the Excel file here⁴ (downloaded on January 2023 from the luxembourgish open data portal⁵). But you don’t need to follow along with code, because I will link the completed scripts for you to download later.

Each sheet contains a dataset with the following columns:

- *Commune*: the commune (the smallest administrative division of territory);
- *Nombre d’offres*: the total number of selling offers;
- *Prix moyen annoncé en Euros courants*: Average selling price in nominal Euros;
- *Prix moyen annoncé au m² en Euros courants*: Average selling price in square meters in nominal Euros.

⁴<https://is.gd/1vvBAc>

⁵<https://data.public.lu/en/datasets/prix-annonces-des-logements-par-commune/>

3. Project start

For ease of presentation, I'm going to show you each step of the analysis here separately, but I'll be putting everything together in a single script once I'm done explaining each step. So first, let's load some packages:

```
library(dplyr)
library(purrr)
library(readxl)
library(stringr)
library(janitor)
```

Even though this book is not about analysing data per se, let me just briefly explain what these packages do, in case you're not familiar with them. The `{dplyr}` package provides many functions for data manipulation, for example aggregating group-wise. `{purrr}` is a package for functional programming, a programming paradigm that I'll introduce later in the book, `{readxl}` reads in Excel workbooks, `{stringr}` is a package for manipulating strings, and finally `{janitor}` (Firke 2023) provides some very nice functions, to perform some common tasks like easily rename every column of a data frame in snake case.

Next, the code below downloads the data, and puts it in a data frame:

```
# The url below points to an Excel file
# hosted on the book's github repository
url <- "https://is.gd/1vvBAc"

raw_data <- tempfile(fileext = ".xlsx")

download.file(url, raw_data,
              method = "auto",
```

3.2. Saving trapped data from Excel

```
mode = "wb")  
  
sheets <- excel_sheets(raw_data)  
  
read_clean <- function(..., sheet){  
  read_excel(..., sheet = sheet) |>  
  mutate(year = sheet)  
}  
  
raw_data <- map(  
  sheets,  
  ~read_clean(raw_data,  
              skip = 10,  
              sheet = .))  
  ) |>  
bind_rows() |>  
clean_names()  
  
raw_data <- raw_data |>  
rename(  
  locality = commune,  
  n_offers = nombre_doffres,  
  average_price_nominal_euros =  
    ↵ prix_moyen_annonce_en_courant,  
  average_price_m2_nominal_euros =  
    ↵ prix_moyen_annonce_au_m2_en_courant,  
  average_price_m2_nominal_euros =  
    ↵ prix_moyen_annonce_au_m2_en_courant  
) |>  
mutate(locality = str_trim(locality)) |>  
select(year, locality, n_offers,  
  ↵ starts_with("average"))
```

3. Project start

If you are familiar with the `{tidyverse}` (Wickham et al. 2019) the above code should be quite easy to follow. We start by downloading the raw Excel file and saving the sheet names into a variable. We then use a function called `read_clean()`, which takes the path to the Excel file and the sheet names as an argument to read the required sheet into a data frame. We use `skip = 10` to skip the first 10 lines in each Excel sheet because the first 10 lines contain a header. The last thing this function does is add a new column called `year` which contains the year of the data. We're lucky because the sheet names are the years: "2010", "2011" and so on. We then map this function to the list of sheet names, thus reading in all the data from all the sheets into one list of data frames. We then use `bind_rows()`, to bind each data frame into a single data frame, by row. Finally, we rename the columns (by translating their names from French to English) and only select the required columns. If you don't understand each step of what is going on, don't worry too much about it; this book is not about learning how to use R.

Running this code results in a neat data set:

```
raw_data

# A tibble: 1,343 x 5
  year   locality     n_offers
  <chr>  <chr>        <dbl> <chr>
1 2010   Bascharage    192  593698.31000000006
2 2010   Beaufort      266  461160.29
3 2010   Bech          65   621760.22
4 2010   Beckerich    176  444498.68
5 2010   Berdorf       111  504040.85
6 2010   Bertrange     264  795338.87
7 2010   Bettembourg   304  555628.29
```

3.2. Saving trapped data from Excel

```
8 2010 Bettendorf         94 495074.38
9 2010 Betzdorf          119 625914.47
10 2010 Bissen            70 516465.57
# i 1,333 more rows
# i 1 more variable: average_price_m2_nominal_euros
<chr>
```

But there's a problem: columns that should be of type numeric are of type character instead (`average_price_nominal_euros` and `average_price_m2_nominal_euros`). There's also another issue, which you would eventually catch as you'll explore the data: the naming of the communes is not consistent. Let's take a look:

```
raw_data |>
  filter(grepl("Luxembourg", locality)) |>
  count(locality)

# A tibble: 2 x 2
  locality           n
  <chr>              <int>
1 Luxembourg          9
2 Luxembourg-Ville   2
```

We can see that the city of Luxembourg is spelled in two different ways. It's the same with another commune, Pétange:

```
raw_data |>
  filter(grepl("P.tange", locality)) |>
  count(locality)

# A tibble: 2 x 2
  locality       n
  <chr>          <int>
1 Pétange        1
2 Pétange-Ville 1
```

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```
<chr>    <int>
1 Petange      9
2 Pétange      2
```

So sometimes it is spelled correctly, with an “é”, sometimes not.
Let’s write some code to correct both these issues:

```
raw_data <- raw_data |>
  mutate(
    locality = ifelse(grepl("Luxembourg-Ville",
      ↵ locality),
      "Luxembourg",
      locality),
    locality = ifelse(grepl("P.tange",
      ↵ locality),
      "Pétange",
      locality)
  ) |>
  mutate(across(starts_with("average"),
    as.numeric))
```

Warning: There were 2 warnings in `mutate()``.

The first warning was:

i In argument: `across(starts_with("average"),
 as.numeric)`.

Caused by warning:

! NAs introduced by coercion
i Run `dplyr::last_dplyr_warnings()` to see the 1
remaining
warning.

Now this is interesting – converting the `average` columns to numeric resulted in some `NA` values. Let’s see what happened:

3.2. Saving trapped data from Excel

```
raw_data |>
  filter(is.na(average_price_nominal_euros))

# A tibble: 290 x 5
  year   locality           n_offers
  <chr>  <chr>                <dbl>
  average_price_nomina~1
  <dbl>
  <dbl>
  1 2010   Consthum            29
  NA
  2 2010   Esch-sur-Sûre       7
  NA
  3 2010   Heiderscheid       29
  NA
  4 2010   Hoscheid            26
  NA
  5 2010   Saeul               14
  NA
  6 2010   <NA>                NA
  NA
  7 2010   <NA>                NA
  NA
  8 2010   Total d'offres      19278
  NA
  9 2010   <NA>                NA
  NA
  10 2010  Source : Ministère~ NA
  NA
# i 280 more rows
# i abbreviated name: 1: average_price_nominal_euros
# i 1 more variable: average_price_m2_nominal_euros
<dbl>
```

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It turns out that there are no prices for certain communes, but that we also have some rows with garbage in there. Let's go back to the raw data to see what this is about:

Commune	Nombre d'offres	Prix moyen annoncé en € courant	Prix moyen annoncé au m ² en € courant
Consthum	29	*	*
Esch-sur-Sûre	7	*	*
Heiderscheid	29	*	*
Hoscheid	26	*	*
Saeul	14	*	*
Moyenne nationale		569,216	3,251
Total d'offres	19,278		

Source : Ministère du Logement - Observatoire de l'Habitat (base prix 2010).

Figure 3.3.: Always look at your data.

So it turns out that there are some rows that we need to remove. We can start by removing rows where `locality` is missing. Then we have a row where `locality` is equal to “Total d’offres”. This is simply the total of every offer from every commune. We could keep that in a separate data frame, or even remove it. The very last row states the source of the data and we can also remove it. Finally, in the screenshot above, we see another row that we don’t see in our filtered data frame: one where `n_offers` is missing. This row gives the national average for columns `average_price_nominal_euros` and `average_price_m2_nominal_euros`. What we are going to do is create two datasets: one with data on communes, and the other on national prices. Let’s first remove the rows stating the sources:

3.2. Saving trapped data from Excel

```
raw_data <- raw_data |>  
  filter(!grepl("Source", locality))
```

Let's now only keep the communes in our data:

```
commune_level_data <- raw_data |>  
  filter(!grepl("nationale|offres", locality),  
         !is.na(locality))
```

And let's create a dataset with the national data as well:

```
country_level <- raw_data |>  
  filter(grepl("nationale", locality)) |>  
  select(-n_offers)  
  
offers_country <- raw_data |>  
  filter(grepl("Total d.offres", locality)) |>  
  select(year, n_offers)  
  
country_level_data <- full_join(country_level,  
  ↪  offers_country) |>  
  select(year, locality, n_offers, everything())  
  ↪  |>  
  mutate(locality = "Grand-Duchy of Luxembourg")
```

Joining with `by = join_by(year)`

Now the data looks clean, and we can start the actual analysis... or can we? Before proceeding, it would be nice to make sure that we got every commune in there. For this, we need a list of communes from Luxembourg. Thankfully, Wikipedia has such

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a list⁶.

Let's scrape and save this list:

```
current_communes <- "https://w.wiki/6nPu" |>  
  rvest::read_html() |>  
  rvest::html_table() |>  
  purrr::pluck(1) |>  
  janitor::clean_names()
```

We scrape the table from the Wikipedia page using `{rvest}`. `rvest::html_table()` returns a list of tables from the Wikipedia table, and then we use `purrr::pluck()` to keep the first table from the website, which is what we need (I made the calls to the packages explicit, because you might not be familiar with these packages). `janitor::clean_names()` transforms column names written for human eyes into machine-friendly names (for example `Growth rate in %` would be transformed to `growth_rate_in_percent`).

Let's see if we have all the communes in our data:

```
setdiff(unique(commune_level_data$locality),  
        current_communes$commune)
```

```
[1] "Bascharage"           "Boevange-sur-Attert"  
[3] "Burmerange"          "Clémency"  
[5] "Consthum"             "Ermsdorf"  
[7] "Erpeldange"           "Eschweiler"  
[9] "Heiderscheid"         "Heinerscheid"  
[11] "Hobscheid"            "Hoscheid"  
[13] "Hosingen"              "Luxembourg"
```

⁶<https://w.wiki/6nPu>

3.2. Saving trapped data from Excel

```
[15] "Medernach"           "Mompach"  
[17] "Munshausen"         "Neunhausen"  
[19] "Redange-sur-Attert" "Rosport"  
[21] "Septfontaines"       "Tuntange"  
[23] "Wellenstein"        "Kaerjeng"
```

We see many communes that are in our `commune_level_data`, but not in `current_communes`. There's one obvious reason: differences in spelling, for example, “Kaerjeng” in our data, but “Käerjeng” in the table from Wikipedia. But there's also a less obvious reason; since 2010, several communes have merged into new ones. So there are communes that are in our data in 2010 and 2011, but disappear from 2012 onwards. So we need to do several things: first, get a list of all existing communes from 2010 onwards, and then, harmonise spelling. Here again, we can use a list from Wikipedia:

```
former_communes <- "https://w.wiki/_wFe7" |>  
rvest::read_html() |>  
rvest::html_table() |>  
purrr::pluck(3) |>  
janitor::clean_names() |>  
dplyr::filter(year_dissolved > 2009)  
  
former_communes
```

```
# A tibble: 20 x 3  
  name          year_dissolved reason  
  <chr>           <int> <chr>  
1 Bascharage            2011 merged to form  
Käerje~  
2 Boevange-sur-Attert      2018 merged to form  
Helper~
```

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3 Burmerange	2011 merged into
Schengen	
4 Clemency	2011 merged to form
Käerje~	
5 Consthum	2011 merged to form
Parc H~	
6 Ermsdorf	2011 merged to form
Vallée~	
7 Eschweiler	2015 merged into
Wiltz	
8 Heiderscheid	2011 merged into
Esch-sur-~	
9 Heinerscheid	2011 merged into
Clervaux	
10 Hobscheid	2018 merged to form
Habscht	
11 Hoscheid	2011 merged to form
Parc H~	
12 Hosingen	2011 merged to form
Parc H~	
13 Mompach	2018 merged to form
Rospor~	
14 Medernach	2011 merged to form
Vallée~	
15 Munshausen	2011 merged into
Clervaux	
16 Neunhausen	2011 merged into
Esch-sur-~	
17 Rosport	2018 merged to form
Rospor~	
18 Septfontaines	2018 merged to form
Habscht	

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19 Tuntange	2018 merged to form
Helper~	
20 Wellenstein	2011 merged into
Schengen	

As you can see, since 2010 many communes have merged to form new ones. We can now combine the list of current and former communes, as well as harmonise their names:

```
communes <- unique(c(former_communes$name,
                      current_communes$commune))
# we need to rename some communes

# Different spelling of these communes between
# wikipedia and the data

communes[which(communes == "Clemency")] <-
  "Clémency"
communes[which(communes == "Redange")] <-
  "Redange-sur-Attert"
communes[which(communes ==
  "Erpeldange-sur-Sûre")] <- "Erpeldange"
communes[which(communes == "Luxembourg-City")]
  <- "Luxembourg"
communes[which(communes == "Käerjeng")] <-
  "Kaerjeng"
communes[which(communes == "Petange")] <-
  "Pétange"
```

Let's run our test again:

```
setdiff(unique(commune_level_data$locality),
        communes)
```

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```
character(0)
```

Great! When we compare the communes that are in our data with every commune that has existed since 2010, we don't have any commune that is unaccounted for. So are we done with cleaning the data? Yes, we can now start with analysing the data. Take a look here⁷ to see the finalised script. Also read some of the comments that I've added. This is a typical R script, and at first glance, one might wonder what is wrong with it. Actually, not much, but the problem if you leave this script as it is, is that it is very likely that we will have problems rerunning it in the future. As it turns out, this script is not reproducible. But we will discuss this in much more detail later on. For now, let's analyse our cleaned data.

3.3. Analysing the data

We are now going to analyse the data. The first thing we are going to do is compute a Laspeyeres price index. This price index allows us to make comparisons through time; for example, the index at year 2012 measures how much more expensive (or cheaper) housing became relative to the base year (2010). However, since we only have one 'good' (housing), this index becomes quite simple to compute: it is nothing but the prices at year t divided by the prices in 2010 (if we had a basket of goods, we would need to use the Laspeyeres index formula to compute the index at all periods).

For this section, I will perform a rather simple analysis. I will immediately show you the R script: take a look at it here⁸. For

⁷<https://is.gd/7PhUjd>

⁸<https://is.gd/qCJEbi>

3.4. Your project is not done

the analysis I selected 5 communes and plotted the evolution of prices compared to the national average.

This analysis might seem trivially simple, but it contains all the needed ingredients to illustrate everything else that I'm going to teach you in this book.

Most analyses would stop here: after all, we have what we need; our goal was to get the plots for the 5 communes of Luxembourg, Esch-sur-Alzette, Mamer, Schengen (which gave its name to the Schengen Area⁹) and Wincrange. However, let's ask ourselves the following important questions:

- How easy would it be for someone else to rerun the analysis?
- How easy would it be to update the analysis once new data gets published?
- How easy would it be to reuse this code for other projects?
- What guarantee do we have that if the scripts get run in 5 years, with the same input data, we get the same output?

Let's answer these questions one by one.

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3.4.1. How easy would it be for someone else to rerun the analysis?

The analysis is composed of two R scripts, one to prepare the data, and another to actually run the analysis proper. Performing the analysis might seem quite easy, because each script contains comments as to what is going on, and the code is not

⁹https://en.wikipedia.org/wiki/Schengen_Area

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that complicated. However, we are missing any project-level documentation that would provide clear instructions as to how to run the analysis. This might seem simple for us who wrote these scripts, but we are familiar with R, and this is still fresh in our brains. Should someone less familiar with R have to run the script, there is no clue for them as to how they should do it. And of course, should the analysis be more complex (suppose it's composed of dozens of scripts), this gets even worse. It might not even be easy for you to remember how to run this in 5 months!

And what about the required dependencies? Many packages were used in the analysis. How should these get installed? Ideally, the same versions of the packages you used and the same version of R should get used by that person to rerun the analysis.

All of this still needs to be documented, but listing the packages that were used for an analysis and their versions takes quite some time. Thankfully, in part 2, we will learn about the `{renv}` package to deal with this in a couple lines of code.

3.4.2. How easy would it be to update the project?

If new data gets published, all the points discussed previously are still valid, plus you need to make sure that the updated data is still close enough to the previous data such that it can pass through the data cleaning steps you wrote. You should also make sure that the update did not introduce a mistake in past data, or at least alert you if that is the case. Sometimes, when new years get added, data for previous years also get corrected, so it would be nice to make sure that you know this. Also, in

3.4. Your project is not done

the specific case of our data, communes might get fused into a new one, or maybe even divided into smaller communes (even though this has not happened in a long time, it is not entirely out of the question).

In summary, what is missing from the current project are enough tests to make sure that an update to the data can happen smoothly.

3.4.3. How easy would it be to reuse this code for another project?

Said plainly, not very easy. With code in this state you have no choice but to copy and paste it into a new script and change it adequately. For re-usability, nothing beats structuring your code into functions and ideally you would even package them. We are going to learn just that in future chapters of this book.

But sometimes you might not be interested in reusing code for another project: however, even if that's the case, structuring your code into functions and packaging them makes it easy to reuse code even inside the same project. Look at the last part of the `analysis.R` script: we copied and pasted the same code 5 times and only slightly changed it. We are going to learn how not to repeat ourselves by using functions and you will immediately see the benefits of writing functions, even when simply reusing them inside the same project.

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3.4.4. What guarantee do we have that the output is stable through time?

Now this might seem weird: after all, if we start from the same dataset, does it matter *when* we run the scripts? We should be getting the same result if we build the project today, in 5 months or in 5 years. Well, not necessarily. While it is true that R is quite stable, this cannot necessarily be said of the packages that we use. There is no guarantee that the authors of the packages will not change the package's functions to work differently, or take arguments in a different order, or even that the packages will all be available at all in 5 years. And even if the packages are still available and function the same, bugs in the packages might get corrected which could alter the result. This might seem like a non-problem; after all, if bugs get corrected, shouldn't you be happy to update your results as well? But this depends on what it is we're talking about. Sometimes it is necessary to reproduce results exactly as they were, even if they were wrong, for example in the context of an audit.

So we also need a way to somehow snapshot and freeze the computational environment that was used to create the project originally.

3.5. Conclusion

We now have a basic analysis that has all we need to get started. In the coming chapters, we are going to learn about topics that will make it easy to write code that is more robust, better documented and tested, and most importantly easy to rerun (and thus to reproduce the results). The first step will actually not involve having to start rewriting our scripts though; next, we

3.5. Conclusion

are going to learn about Git, a tool that will make our life easier by versioning our code.

4. Version control with Git

Modern software development would be impossible without version control systems, and the same goes for building analytical pipelines that are reproducible and robust. It doesn't really matter what the output of the pipeline is: a simple graph, a report with a statistical analysis, a scientific publication, a trained machine learning model that you want to hook to an API... if the code to the project is not versioned, you incur major risks and the pipeline is not reproducible.

But what is version control anyway?

Version control tools make it easy to keep track of the changes that were made to text files (like R scripts). Any change made to any file of a project is catalogued, making it possible to trace back how the file changed, who made the changes, and when these changes were made. Using version control it is also quite easy to collaborate on a project by forcing team members to deal explicitly with the potential conflicts that might arise when the same file got changed by different people at the same time. Should your computer get lost, stolen, or explode, your projects are safely backed up on a server: this is because version control tools make use of a server which keeps track of all the changes (and in some cases, this *server* is actually your team-mates' computers!)

Version control tools also make it easy to experiment with new ideas. You can start new *branches* which essentially make a

4. Version control with Git

copy of your current project. In this new branch, you can safely experiment with new features, and if the experiments are not conclusive, you can simply discard this branch: the *original* copy of your project will remain untouched. We will also use branches to implement features, fix bugs quickly, and manage the project in a paradigm called *trunk-based development*.

There are several version control tools out there, but Git is undoubtedly the most popular one. You might have heard of Github; this is a service that hosts repositories for your projects, and provides other project management tools such as an issue tracker, project wiki, feature requests... and also very importantly continuous integration. Don't worry if this all sounds very abstract: by the end of the next chapter you will have all the basic knowledge to use Git and Github.com for your projects.

Git is a tool that you must install on your computer to get started. Once Git is installed, you can immediately start using it; you don't need to open an account on Github (or a similar service), but it is recommended to make collaboration easier (it is possible to collaborate with several people using Git without a service like Github, by setting up a bare repository on a server or on a network drive you control, but this is outside the scope of this book).

You should know that Github offers private repositories for free, so if you don't want your work to be accessible to the public, that is possible. Only people that you invite to your private repositories will be able to see the code and collaborate with you. It is also possible that your work place has set up a self-hosted Git platform, ask your IT department! Usually these self-hosted platforms are Gitea or Gitlab instances. Gitea, Gitlab, Bitbucket, Codeberg, these are all similar services to Github. All have their advantages and disadvantages.

The advantages of Github are twofold:

- It has a very large community of users;
- Its continuous integration service is incredibly useful, and free for up to 2000 minutes a month.

Disadvantages are:

- It has been bought by Microsoft in 2018;
- It is not possible to self-host an instance of Github (not for free at least).

The fact it is owned by Microsoft may not seem like an issue, but Microsoft's track record of previous acquisitions is open to question (Nokia, Skype), and the recent discussions about using source code hosted on Github to train machine learning models (Copilot)¹ can make one uneasy about relying too much on Github.

So while we are going to use Github to host our projects in the remainder of this book, almost everything you are going to learn will be easily transferable to another code hosting platform such as Gitlab or Bitbucket, should you want to switch (or if your workplace has a self-hosted instance from one of Github's competitors). Installing and configuring Git will be exactly the same regardless of the hosting service we use, and all the commands we will use to actually interact with our repositories will be the same as well. So why did I write *almost everything* is the same across any of the code hosting platforms? Well, the two advantages I cited above really give Github an edge; many developers, researchers and data scientists have a Github account already and so if one day you need to collaborate with people, chances are they have an account on Github and not on another code hosting platform.

¹<https://is.gd/rQgCj8>

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But what really sets up Github.com apart is Github Actions, Github's continuous integration service. Github Actions is literally a computer in the cloud that you can use to run a set of actions each time you interact with the repository (or at defined moments as well). For example, it would be possible to run automated tests each time a collaborator uploads some changes to the project. This way, we can make sure that no change introduced a bug. Or take this book; each time I write and push a new section or chapter to Github, the website, PDF and Epub of this book get re-generated and updated automatically. Each Github account gets 2000 minutes a month of free computing time, which is really a lot. In part 2, we will make use of Github Actions to run our RAP in the cloud, by simply pushing updates to our code on Github.

By the way, if you're using a cloud service like Dropbox, Onedrive, and the like, DO NOT put projects tracked by Git in them! I really need to stress this: do not track projects with both something like Dropbox and Git. This is because Dropbox and similar services do not deal gracefully with conflicts: if two collaborators change the same file, Dropbox makes two copies of the files. One of the collaborators then has to manually deal with the conflict. The issue is that inside a project that is being tracked by Git, there is a hidden folder with many files that get used for synching the project and making sure that everything runs smoothly. If you put a Git-enabled project inside a Dropbox folder, these files will get accessed simultaneously by different people, and Dropbox will start making copies of these because of conflicts. This really messes up the project and can lead to data loss. Let Git handle the tracking and the collaborating for you. It might seem more complex than a service like Dropbox, and it is, but it is immensely more powerful, and what steep learning curve it might have, it more than makes up for it with the many features it makes available

4.1. Installing Git and opening a Github account

at your fingertips. Unlike Dropbox (or similar services), Git deals with conflicts not on a per-file basis, but on a per-line basis. So if two collaborators change the same file, but different lines of this same file, there will be no conflict: Git will handle the merge on its own.

Finally, before starting, there is something important that you need to understand, and people sometimes get confused by it: if a repository is public, this does not mean that anyone can make changes to the code. What this means is that anyone can fork the repository (essentially making a copy of the repository to their Github account) and then *suggest* some changes in a so-called pull request. The maintainer and owner of the original project can then accept these edits or not.

In the remainder of this chapter, you are going to learn how to set up Git on your machine, open a Github account and start using it right away. Then, I'm going to discuss several scenarios:

- how to collaborate, as a team, on a project;
- how to contribute to someone else's project.

4.1. Installing Git and opening a Github account

Git is a program that you install on your computer. If you're running a Linux distribution, chances are Git is already installed. Try to run the following command in a terminal to see if this is the case:

```
which git
```

4. Version control with Git

If a path like `/usr/bin/git` gets shown, congratulations, you can skip the rest of this paragraph. If something like:

```
/usr/bin/which: no git in  
↳ (/home/username/.local/bin:  
↳ /home/username/bin:etc...)
```

gets shown instead, then this means that Git is not installed on your system. To install Git, use your distribution's package manager, as it is very likely that Git is packaged for your system. On Ubuntu, arguably the most popular Linux distribution, this means running:

```
sudo apt-get update  
sudo apt-get install git
```

If you're using Ubuntu, you may use `apt` instead of `apt-get`. Both commands are basically interchangeable, use whatever you're used to. I've first used Ubuntu in 2008, and even though I don't use it anymore as my daily Linux distro (that honor goes to openSUSE), I still use `apt-get` out of habit.

On macOS and Windows, follow the instructions from the Git Book². It should be as easy as running an installer for any program.

Depending on your operating system, a graphical user interface might have been installed with Git, making it possible to interact with Git outside of the command line. It is also possible to use Git from within RStudio and many other editors have interfaces to Git as well. We are not going to use any graphical user interface, however. This is because there is no common, universal graphical user interface; they all work slightly differently.

²<https://is.gd/9HZqW4>

4.1. Installing Git and opening a Github account

The only universal is the command line. Also, learning how to use Git via the command line will make it easier the day you will need to use it from a server, which will very likely happen. It also makes my job easier: it is simpler to tell you which commands to run and explain them to you than littering the book with dozens upon dozens of screenshots that might get outdated as soon as a new version of the interface gets released.

Don't worry, using the command line is not as hard as it sounds.

If you don't already have a Github account, now is the time to create one. Just go over to <https://github.com/> and simply follow the instructions and select the free tier to open your account.

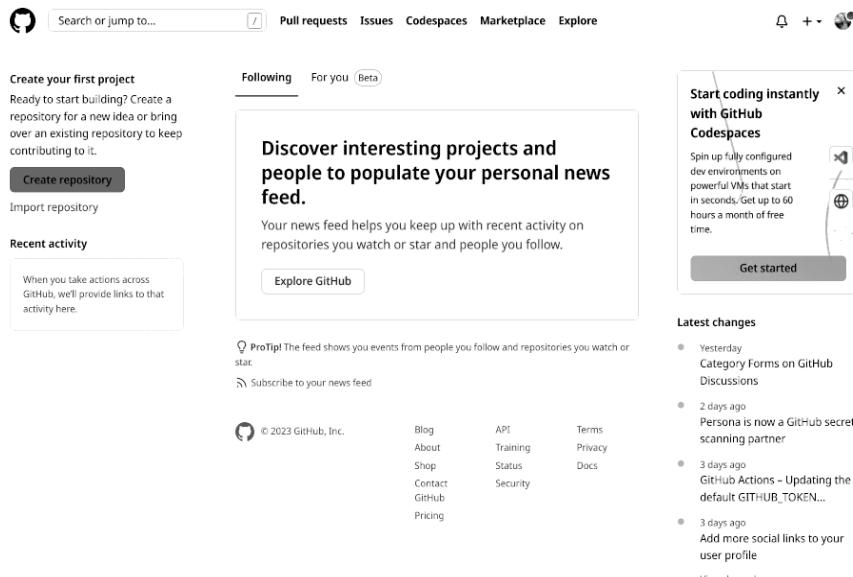


Figure 4.1.: This is your Github dashboard.

4. Version control with Git

In the next section, we are going to learn some basic Git commands by versioning the two scripts that we wrote before.

4.2. Git superbasics

We are going to use the two scripts that we wrote in the previous section. If you want to follow along, create a folder called `housing` and put the two scripts we developed before in there:

- `save_data.R`: <https://is.gd/7PhUjd>
- `analysis.R`: <https://is.gd/qCJEbi>

Open the folder that contains the two scripts in a file explorer. On most Linux desktop environments you should be able to right-click inside that folder anywhere on a blank space and select an option titled something like “Open Terminal here”. If you’re using Windows, you can pretty much do the same but look instead for the option titled “Open Git Bash here”. On macOS, you need to first activate this option. Simply google for “open terminal at folder macOS” and follow the instructions. It is also possible to drag and drop a folder into a terminal which will then open the correct path in the terminal. Another option, of course, is to simply open a terminal and navigate to the correct folder using `cd` (change directory, this should work the same on Windows, macOS and Linux):

```
cd /home/user/housing/
```

Make sure that you are in the right folder by listing the contents of the folder:

```
ls
```

From now on, make sure to type the commands you see in the terminal (on Linux and macOS) or in the Git Bash terminal on Windows. To distinguish the terminal from the R command line prompt, the prompt of a terminal (or Git Bash terminal on Windows) will start with `owner@localhost`. `owner` is the username of the project manager in our examples from now on, and the computer `owner` used by this project manager is called `localhost` (this prompt can look different on your machine, sometimes the full path to the current working directory is listed instead). So here is what happens when `owner` runs `ls` on the root directory of the project:

```
owner@localhost $ ls  
analysis.R save_data.R
```

(On Linux you could also try `ll` which is often available. It is an alias for `ls -l` which provides a more detailed view. There's also `ls -la` which also lists hidden files.)

Make sure that you see the two scripts being listed when running `ls`. If not, this means that you are in the wrong directory, so make sure that you open the terminal in the correct folder.

It's now time to start tracking these files using Git. In the same terminal in which we ran `ls`, run now the following `git` command:

```
owner@localhost $ git init
```

4. Version control with Git

```
hint: Using 'master' as the name for the initial
     ↵ branch.
hint: This default branch name is subject to
     ↵ change.
hint: To configure the initial branch name to
     ↵ use in all of your
hint: new repositories, which will suppress this
     ↵ warning, call:
hint:
hint:   git config --global init.defaultBranch
     ↵ <name>
hint:
hint: Names commonly chosen instead of 'master'
     ↵ are 'main',
hint: 'trunk' and 'development'. The
     ↵ just-created branch can be
hint: renamed via this command:
hint:
hint:   git branch -m <name>
Initialized empty Git repository in
     ↵ /home/user/housing/.git/
```

Take some time to read the hints. Many `git` commands give you hints and it's always a good idea to read them. This hint here tells us that the default branch name is “master” and that this is subject to change. Think of a branch as a *version* of your code. The “master” branch will hold the default version of your code. But you could create a branch called “dev” that would contain a version of the code with features that are still in development. There is nothing special about the default, “master” branch, and it could have been called anything else. For example, if you create a repository on Github first, instead of creating it on your computer, the default branch will be called “main”. You need to

pay attention to this, because when we will start interacting with our Github repository, we need to make sure that we have the right branch name in mind. Also, note that because the “master” branch is the most important branch, it gets sometimes referred to as the “trunk”. Some teams that use trunk-based development (which I will discuss in the next chapter) even name this branch “trunk”.

Let’s now run this other git command:

```
owner@localhost $ git status

On branch master

No commits yet

Untracked files:
  (use "git add <file>..." to include in what
   ↵ will be committed)
    analysis.R
    save_data.R

nothing added to commit but untracked files
  ↵ present (use "git add" to track)
```

Git tells us quite clearly that it sees two files, but that they’re currently not being tracked. So if we would modify them, Git would not keep track of the changes. So it’s a good idea to just do what Git tells us to do: let’s *add* them so that Git can track them:

```
owner@localhost $ git add
```

4. Version control with Git

```
Nothing specified, nothing added.  
hint: Maybe you wanted to say 'git add .'?  
hint: Turn this message off by running  
hint: "git config advice.addEmptyPathspec false"
```

Shoot, simply running `git add` does not do us any good. We need to specify which files we want to add. We can name them one by one, for example `git add file1.R file2.txt`, but if we simply want to track all the files in the folder, we can simply use the `.` placeholder:

```
owner@localhost $ git add .
```

No message this time... is that a good thing? Let's run `git status` and see what's going on:

```
owner@localhost $ git status
```

```
On branch master
```

```
No commits yet
```

```
Changes to be committed:
```

```
(use "git rm --cached <file>..." to unstage)  
    new file:   analysis.R  
    new file:   save_data.R
```

Nice! Our two files are being tracked now, so we can commit the changes. *Committing* means that we are happy with our work, and we can snapshot it. These snapshots then get uploaded to Github by pushing them. This way, the changes will be available for our coworkers for them to pull. I'll explain what this means

later, so don't worry if this is confusing, it won't be by the end of the chapter. Also, you should know that there is a special file, called `.gitignore`, that allows you to list files or folders that you want Git to ignore. This can be useful in cases where you are working with sensitive data and don't want it to be uploaded to Github. We will not use the `.gitignore` file just yet, but will do so in part two of the book. So for now, just remember that this is an option.

We are now ready to commit our files. Each commit must have a commit message, and we can write this message as an option to the `git commit` command:

```
owner@localhost $ git commit -m "Project start"
```

The `-m` option is there to specify the message for the commit. Before pushing the commit, let's run `git status` again:

```
owner@localhost $ git status
```

```
On branch master
nothing to commit, working tree clean
```

This means that every change is accounted for in a commit. So if we were to push now, we could then set our computer on fire: every change would be safely backed up on Github.com. We can also choose to not push yet, and keep working and committing. For example, we could commit 5 times and just push once: all of the 5 commits would be pushed to Github.com.

Let's do just that by changing one file. Open `analysis.R` in any editor and simply change the start of the script by adding one line. So go from:

4. Version control with Git

```
library(dplyr)
library(ggplot2)
library(purrr)
library(tidyr)
```

To:

```
# This script analyses housing data for
↪ Luxembourg

library(dplyr)
library(ggplot2)
library(purrr)
library(tidyr)
```

and now run `git status` again:

```
owner@localhost $ git status

On branch master
Changes not staged for commit:
  (use "git add <file>..." to update what will
   ↪ be committed)
  (use "git restore <file>..." to discard
   ↪ changes in working directory)
    modified:   analysis.R

no changes added to commit (use "git add" and/or
   ↪ "git commit -a")
```

Because the file is being tracked, Git can now tell us that something changed and that we did not commit this change. So if

our computer would self-combust, these changes would get lost forever. Better commit them and push them to Github.com as soon as possible!

Remember, first, we need to add these changes to a commit using `git add .`:

```
owner@localhost $ git add .
```

(You can run `git status` at this point to check if the file was correctly added to be committed.)

Then, we need to commit the changes and add a nice commit message:

```
owner@localhost $ git commit -m "Added a comment  
↪ to analysis.R"
```

Try to keep commit messages as short and as explicit as possible. This is not always easy, but it really pays off to strive for short, clear messages. Also, ideally, you would want to keep commits as small as possible, ideally one commit per change. For example, if you're adding and amending comments in scripts, once you're done with that make this a commit. Then, maybe clean up some code. That's another, separate commit. This makes rolling back changes or reviewing them much easier. This will be crucial later on when we will use trunk-based development to collaborate with our teammates on a project. It is generally not a good idea to code all day and then only push one single big fat commit at the end of the day, but that is what happens very often...

By the way, even if our changes are still not on Github.com, we can still roll back to previous commits. For example, suppose that I delete the file accidentally by running `rm analysis.R`:

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```
owner@localhost $ rm analysis.R
```

Let's run `git status` and look for the changes (it's a line starting with the word `deleted`):

```
On branch master
Changes not staged for commit:
  (use "git add/rm <file>..." to update what
   ↵ will be committed)
  (use "git restore <file>..." to discard
   ↵ changes in working directory)
    deleted:    analysis.R

no changes added to commit (use "git add" and/or
   ↵ "git commit -a")
```

Yep, `analysis.R` is gone. And deleting on the console usually means that the file is gone forever. Well technically no, there are still ways to recover deleted files using certain tools, but since we were using Git we can use it to recover the files! Because we did not commit the deletion of the file, we can simple tell Git to ignore our changes. A simple way to achieve this is to stash the changes, and then *drop* (or delete) the stash:

```
owner@localhost $ git stash
```

```
Saved working directory and index state WIP on
  ↵ master: \
    ab43b4b Added a comment to analysis.R
```

So the deletion was stashed away, (so in case we want it back we could get it back with `git stash pop`) and our project was

rolled back to the previous commit. Simply take a look at the files:

```
owner@localhost $ ls  
  
analysis.R save_data.R
```

There it is! You can get rid of the stash with `git stash drop`. But what if we had deleted the file and committed the change? In this scenario, we could not use `git stash`, but we would need to revert to a commit. Let's try, first let me remove the file:

```
owner@localhost $ rm analysis.R
```

and check the status with `git status`:

```
On branch master  
Changes not staged for commit:  
  (use "git add/rm <file>..." to update what  
   ↳ will be committed)  
  (use "git restore <file>..." to discard  
   ↳ changes in working directory)  
    deleted:    analysis.R  
  
no changes added to commit (use "git add" and/or  
  ↳ "git commit -a")
```

Let's add these changes and commit them:

```
owner@localhost $ git add .
```

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```
owner@localhost $ git commit -m "Removed  
↳ analysis.R"
```

```
[master 8e51867] Removed analysis.R  
1 file changed, 131 deletions(-)  
delete mode 100644 analysis.R
```

What's the status now?

```
owner@localhost $ git status
```

```
On branch master  
nothing to commit, working tree clean
```

Now, we've done it! `git stash` won't be of any help now. So how to recover our file? For this, we need to know to which commit we want to roll back. Each commit not only has a message, but also an unique identifier that you can access with `git log`:

```
owner@localhost $ git log
```

```
commit 8e51867dc5ae89e5f2ab2798be8920e703f73455  
↳ (HEAD -> master)  
Author: User <owner@mailbox.com>  
Date:   Sun Feb 5 17:54:30 2023 +0100  
  
       Removed analysis.R
```

```
commit ab43b4b1069cd987685253632827f19d7a402b27
```

```
Author: User <owner@mailbox.com>
Date:   Sun Feb 5 17:41:52 2023 +0100
```

Added a comment to analysis.R

```
commit df2beecba0101304f1b56e300a3cd713ce7366e5
Author: User <owner@mailbox.com>
Date:   Sun Feb 5 17:32:26 2023 +0100
```

Project start

The first one from the top is the last commit we've made. We would like to go back to the one with the message "Added a comment to analysis.R". See the very long string of characters after "commit"? That's the commit's unique identifier, called hash. You need to copy it (or only like the first 10 or so characters, that's enough as well). By the way, depending on your terminal and operating system, `git log` may open `less` to view the log. `less` is a program that makes it easy to view long documents. Quit it by simply pressing `q` on your keyboard. We are now ready to revert to the right commit with the following command:

```
owner@localhost $ git revert
~ ab43b4b1069cd98768..HEAD
```

and we're done! Check that all is right by running `ls` to see that the file magically returned, and `git log` to read the log of what happened:

```
owner@localhost $ git log
```

4. Version control with Git

```
commit b7f82ee119df52550e9ca1a8da2d81281e6aac58
 ↵  (HEAD -> master)
```

```
Author: User <owner@mailbox.com>
```

```
Date: Sun Feb 5 18:03:37 2023 +0100
```

```
Revert "Removed analysis.R"
```

```
This reverts commit
```

```
↪  8e51867dc5ae89e5f2ab2798be8920e703f73455.
```

```
commit 8e51867dc5ae89e5f2ab2798be8920e703f73455
```

```
↪  (HEAD -> master)
```

```
Author: User <owner@mailbox.com>
```

```
Date: Sun Feb 5 17:54:30 2023 +0100
```

```
Removed analysis.R
```

```
commit ab43b4b1069cd987685253632827f19d7a402b27
```

```
Author: User <owner@mailbox.com>
```

```
Date: Sun Feb 5 17:41:52 2023 +0100
```

```
Added a comment to analysis.R
```

```
commit df2beecba0101304f1b56e300a3cd713ce7366e5
```

```
Author: User <owner@mailbox.com>
```

```
Date: Sun Feb 5 17:32:26 2023 +0100
```

```
Project start
```

Using a range of commits in `git revert` reverts all the commits from the starting commit (not included) to the last commit. In this example, because only the commit starting with `8e51867dc5` was included in that range, only this commit was

reverted. You could have achieved the same result with `git revert 8e51867dc5`.

This small example illustrates how useful Git is, even without using Github, and even if working alone on a project. At the very least it offers you a way to simply walk back changes and gives you a nice timeline of your project. Maybe this does not impress you much, because we live in a world where cloud services like Dropbox made things like this very accessible. But where Git (with the help of a service like Github) really shines is when collaboration is needed. Git and code hosting services like Github make it possible to collaborate at very large scale: thousands of developers contribute to the Linux kernel, arguably the most successful open-source project ever, powering most of today's smartphones, servers, supercomputers and embedded computers,³ and you can use these tools to collaborate at a smaller scale very efficiently as well.

4.3. Git and Github

So we got some work done on our machine and made some commits. We are now ready to push these commits to Github. “Pushing” means essentially uploading these changes to Github. This makes them available to your coworkers if you’re pushing to a private repository, or makes them available to the world if you’re pushing to a public repository.

Before pushing anything to Github though, we need to create a new repository. This repository will contain the code for our project, as well as all the changes that Git has been tracking on

³<https://www.zdnet.com/article/who-writes-linux-almost-10000-developers/>

4. Version control with Git

our machine. So if, for example, a new team member joins, he or she will be able to clone the repository to his or her computer and have access to every change, every commit message and every single bit of history of the project. If it's a public repository, anyone will be able to clone the repository and contribute code to it. We are going to walk you through some examples of how to collaborate with Git using Github in the remainder of this chapter.

So, let's first go back to <https://github.com/> and create a new repository:

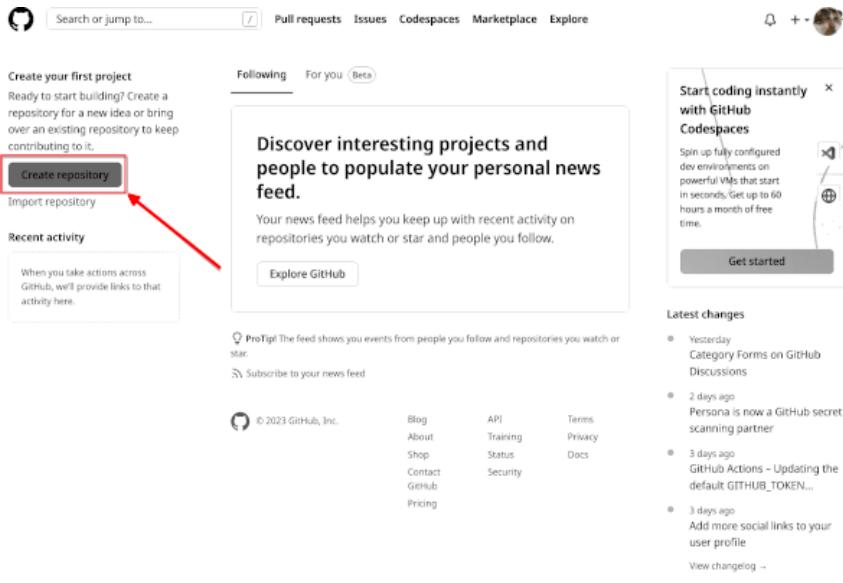


Figure 4.2.: Creating a new repository from your dashboard.

You will then land on this page:

Create a new repository

A repository contains all project files, including the revision history. Already have a project repository elsewhere?
Import a repository.

Owner * Repository name *

 rap4all ✓ / ✓

Great repository name! housing is available. honorable. Need inspiration? How about urban-rotary-phone?

Description (optional)

 **Public**
Anyone on the internet can see this repository. You choose who can commit.

 **Private**
You choose who can see and commit to this repository.

Initialize this repository with:
Skip this step if you're importing an existing repository.

Add a README file
This is where you can write a long description for your project. Learn more.

Add .gitignore
Choose which files not to track from a list of templates. Learn more.

Choose a license
A license tells others what they can and can't do with your code. Learn more.

① You are creating a public repository in your personal account.

Figure 4.3.: Name your repository and choose whether it's a public or private repository.

Name your repository (1), and choose whether it should be open to the world or if it should be private and only accessible to your coworkers (2). We are going to make it a public repository, but

4. Version control with Git

you could make it private and follow along, this would change nothing in what we're going to learn.

Click on *Create repository* (3). You then land on this page:

The screenshot shows a GitHub repository page for 'rap4all / housing'. The top navigation bar includes 'Pin', 'Unwatch 1', 'Fork', 'Code', 'Issues', 'Pull requests', 'Actions', 'Projects', 'Wiki', 'Security', 'Insights', and 'Settings'. Below the navigation, there's a section titled 'Quick setup — if you've done this kind of thing before' with options for 'HTTPS' or 'SSH' and a URL 'https://github.com/rap4all/housing.git'. A note says 'Get started by creating a new file or uploading an existing file. We recommend every repository include a README, LICENSE, and .gitignore.' Below this, there are three sections: '...or create a new repository on the command line' with a code snippet, '...or push an existing repository from the command line' with another code snippet, and '...or import code from another repository' with a note about initializing from Subversion, Mercurial, or TFS and a 'Import code' button.

```
echo "# housing" >> README.md
git init
git add README.md
git commit -m "first commit"
git branch -M main
git remote add origin https://github.com/rap4all/housing.git
git push -u origin main
```

```
git remote add origin https://github.com/rap4all/housing.git
git branch -M main
git push -u origin main
```

Figure 4.4.: Some instructions to get you started.

We get some instructions on how to actually get started with our project. The first thing you need to do though is to click on “SSH”:

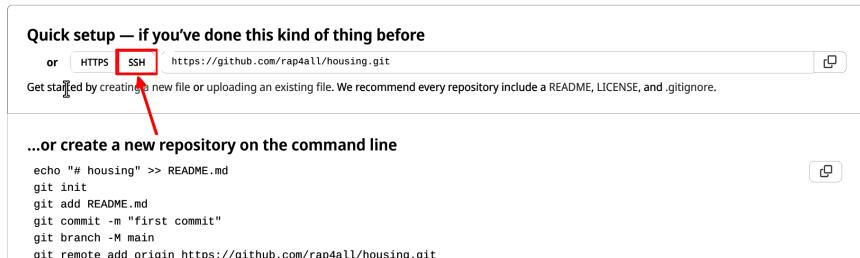


Figure 4.5.: Make sure to select ‘SSH’.

This will change the links in the instructions from `https` to `ssh`. I will explain why this is important in a couple of paragraphs. For now, let’s read the instructions. Since we have already started working, we need to follow the instructions titled “...or push an existing repository from the command line”. Let’s review these commands. This is what Github suggests we run:

```
git remote add origin
  ↳ git@github.com:rap4all/housing.git
git branch -M main
git push -u origin main
```

What’s really important is the first command and last command. The first command adds a remote (referred to as *origin*) that points to our repository. If you’re following along, you should copy the link from your repository here. It would look exactly the same, but the user name `rap4all` would be replaced by your Github username. So now, every time I push, my changes will

4. Version control with Git

get uploaded to Github. The second line renames the branch from “master” to “main”. You are of course free to do so. I don’t like changing the defaults from Git, so I will keep using the name “master”. The last command pushes our changes to the “main” branch (but we need to change “main” to “master”).

Let’s do just that:

```
owner@localhost $ git remote add origin
    ↵ git@github.com:rap4all/housing.git
```

This produces no output. We’re now ready to push:

```
owner@localhost $ git push -u origin master
```

and it fails:

```
ERROR: Permission to rap4all/housing.git denied
    ↵ to b-rodrigues.
fatal: Could not read from remote repository.
```

```
Please make sure you have the correct access
    ↵ rights
and the repository exists.
```

The reason is quite simple: Github has absolutely no idea who we are! Remember, if the repository is public, anyone can clone it. But that doesn’t mean that anyone can simply push code to the repo! This means that we need a way to tell Github that we are the owner of the repository. For this, we need a way to log in securely, and we will do so using a public/private RSA encryption key pair. The idea is quite simple; we are going to generate two files on our computer. These two files form a

public/private key pair. We are going to upload the public key to Github; and every time we want to interact with Github, Github will check the public key against the private key that we keep on our machine (never, ever, send the private key to anyone). If they match, Github knows that we are who we claim to be and will let us push to the repository. This is why we switched from `https` to `ssh` before. `https` would allow us to log in by typing a password each time we push (but actually, not anymore, since password login was turned off some years ago). It is much easier to not have to log in manually and let our key pair do the job for us.

Let's generate a public/private RSA key pair. Open a terminal on Linux or macOS, or Git Bash on Windows and run the following command:

```
owner@localhost $ ssh-keygen
```

The following lines will appear in your terminal:

```
Generating public/private rsa key pair.  
Enter file in which to save the key  
→ (/home/user/.ssh/id_rsa):
```

Simply leave this empty and press enter. This next message now appears:

```
Enter passphrase (empty for no passphrase):
```

Leave it empty as well. Entering a passphrase is not really needed, since the ssh key pair itself will deal with the login. In some situations, a passphrase might be useful if you're worried that someone might get physical access to your machine and

4. Version control with Git

push code by impersonating you. But if you work with such sensitive data and code that this is a real worry, maybe don't use Github?

So once you pressed enter, you get asked to confirm the passphrase:

Enter same passphrase again:

Here again, simply leave it empty and press enter on your keyboard. Once this is done, you should see this:

```
Your identification has been saved in
↳ /home/user/.ssh/id_rsa
Your public key has been saved in
↳ /home/user/.ssh/id_rsa.pub
The key fingerprint is:
SHA256:tPZnR7qdN06mV53Mc36F3mASIyD55ktQJFBAVqJXNQw
↳ owner@localhost
The key's randomart image is:
+---[RSA 3072]----+
|    *=E*=.      |
|    o o.o... .   |
|    . .  o.  o   |
|    .  ..o.  .  o |
|           +S     o.+.| 
|           .o.    o.o*|
|           . o.  + +=*|
|           . o  +++=|
|           ..=oo |
+---[SHA256]----+
```

If now you go to the specified path on the first line (so in our case `/home/user/.ssh/`) you should see two files, `id_rsa` and

4.3. Git and Github

`id_rsa.pub`, the private and public keys respectively. We're almost done: what you need to do now is copy the contents of the `id_rsa.pub` file to Github.

Go to your profile settings:

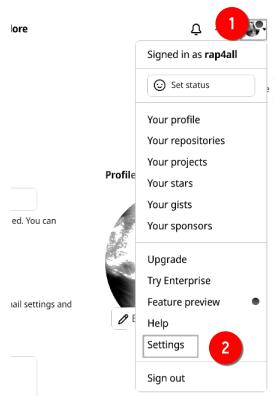


Figure 4.6.: Click on your user profile's image in the top-right corner.

And then click on “SSH and GPG keys”:

4. Version control with Git

The screenshot shows the GitHub user settings interface. On the left, there's a sidebar with various account management options like Public profile, Account, Appearance, Accessibility, Notifications, Access, Billing and plans, Emails, Password and authentication, Sessions, SSH and GPG keys (which has a red circle with '1' over it), Organizations, and Moderation. The main content area is titled 'SSH keys' and displays a message: 'There are no SSH keys associated with your account.' It includes a link to 'Learn how to generate' and a button to 'New SSH key'. Below this is the 'GPG keys' section, which also says 'There are no GPG keys associated with your account.' It has a link to 'Learn how to generate' and a button to 'New GPG key'. At the bottom, there's a 'Vigilant mode' section with a checkbox for 'Flag unsigned commits as unverified' and a note about including unsigned commits from other accounts. A link to 'Learn about vigilant mode' is provided.

Figure 4.7.: Go to your user settings and choose ‘SSH and GPG keys’.

and then click on “New SSH key”. Name this key (it’s a good idea to write something that makes recognizing the computer that generated the key easy) and paste the contents of `id_rsa.pub` in the text box and click on “add SSH key”:

This screenshot shows the 'SSH keys / Add new' form. It has fields for 'Title' (set to 'work_laptop' with a red circle '1' over it), 'Key type' (set to 'Authentication Key'), and a large 'Key' text area containing the public key content. The key content starts with 'ssh-rsa' and a long string of characters. At the bottom, there's a 'Add SSH key' button with a red circle '3' over it.

Figure 4.8.: Copy the contents of the public key here.

We can now go back to our terminal and try to push again:

```
owner@localhost $ git push -u origin master
```

The following message gets printed:

```
The authenticity of host 'github.com
  ↵ (140.82.121.3)' can't be established.
ED25519 key fingerprint is
  ↵ SHA256:+DiY3wvvV6TuJJhbpZisF/
  ↵ zLDAOzPMSvHdkr4UvC0qU.
This key is not known by any other names
Are you sure you want to continue connecting
  ↵ (yes/no/[fingerprint])?
```

Type `yes` and then you should see the following:

```
Enumerating objects: 10, done.
Counting objects: 100% (10/10), done.
Delta compression using up to 4 threads
Compressing objects: 100% (9/9), done.
Writing objects: 100% (10/10), 2.77 KiB | 2.77
  ↵ MiB/s, done.
Total 10 (delta 2), reused 0 (delta 0),
  ↵ pack-reused 0
remote: Resolving deltas: 100% (2/2), done.
To github.com:rap4all/housing.git
 * [new branch]      master -> master
Branch 'master' set up to track remote branch
  ↵ 'master' from 'origin'.
```

And we're done! Our commits are now safely backed up on Github. If we go to our repository's main page, we should see the following:

4. Version control with Git

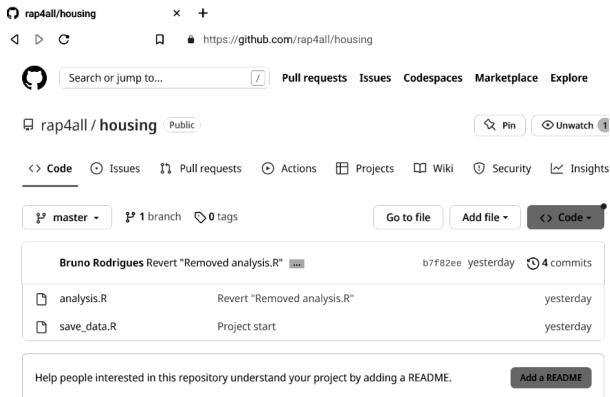


Figure 4.9.: Finally!

4.4. Getting to know Github

We have succeeded in installing Git and making it work with our Github account. If you use another machine for development, you will need to generate another RSA key pair on that machine and add the public key to Github. If you use another code hosting platform, you can use the same RSA key pair, but will need to add the public key to this other code hosting platform. You can even use the same key pair as a passwordless authentication method for ssh (for example to log into a server, but this is outside the scope of this book). Before continuing we are going to take a little tour of Github.

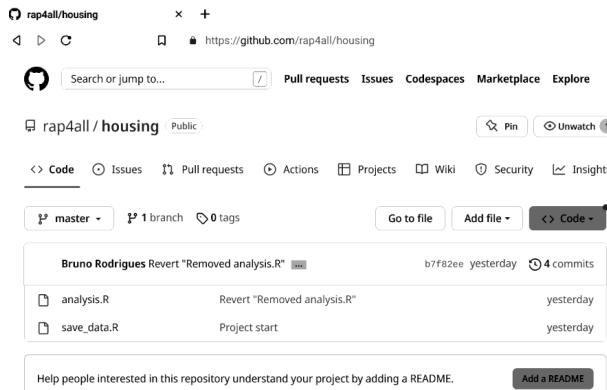


Figure 4.10.: You repository's landing page.

4. Version control with Git

Once you're on your repository's landing page you see the same files and folders as in the root directory of the project on your computer. In our case here, we see our two files. Github suggests that we add a README file; we are going to ignore this for now. Take a closer look at the menu at the top, below your repository's name:

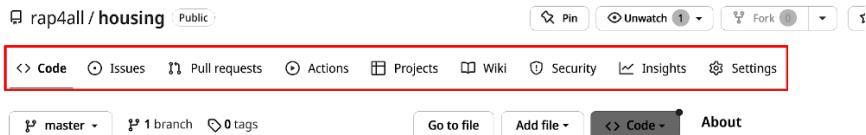


Figure 4.11.: Several options to choose from.

Most important for our needs is the “Issues”, “Pull requests”, “Actions” and “Settings” tab.

In the next chapter we are going to learn about pull requests which are essential for collaborating using Git and Github.com. We will learn about the “Actions” tab in the second part of the book.

So let's start with “Settings”.

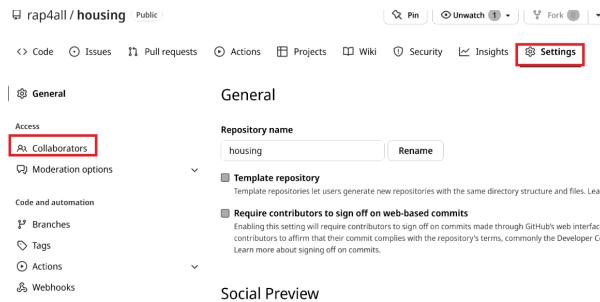


Figure 4.12.: Choose the ‘Settings’ tab.

4.4. Getting to know Github

There are many options that you can choose from, but what's important for our purposes is the “Collaborators” option. This is where you can invite people to contribute to the repository. People that are invited in this way can directly push to the repository. Let's invite the author of this book:

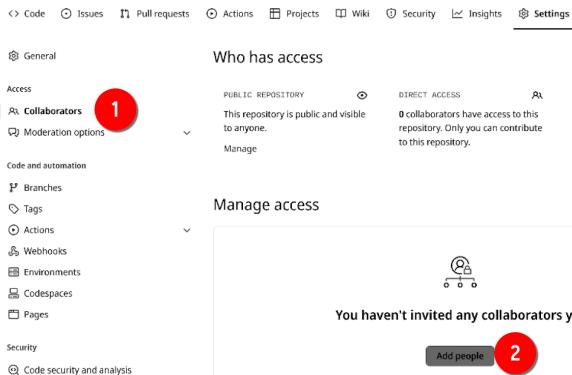


Figure 4.13.: Follow along to add a collaborator.

Start by typing the person's Github username. You can also invite collaborators by providing their email addresses.

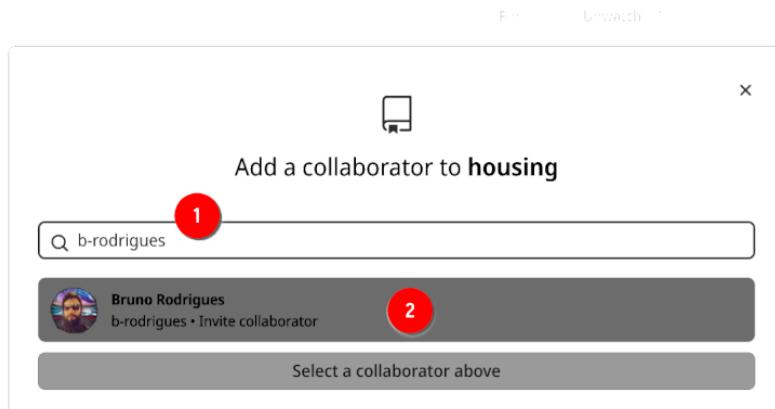


Figure 4.14.: Look for your collaborators.

4. Version control with Git

Then click on the user's profile and he or she should get an invitation by email.

This is what it looks like from the perspective of Bruno's account now:



Figure 4.15.: Bruno can now push as if he owned the repository.

It's important to understand the distinction between inviting someone to contribute to the repository and have someone from outside the project contribute. We are going to explore these two scenarios in the next section, but before that, let's see what the "Issues" tab is about.

If the repository is public, anyone can open an issue to either submit a bug, or suggest some ideas, and if the repository is private, only invited collaborators can do this.

4.4. Getting to know Github

Let's open an issue to illustrate how this works:

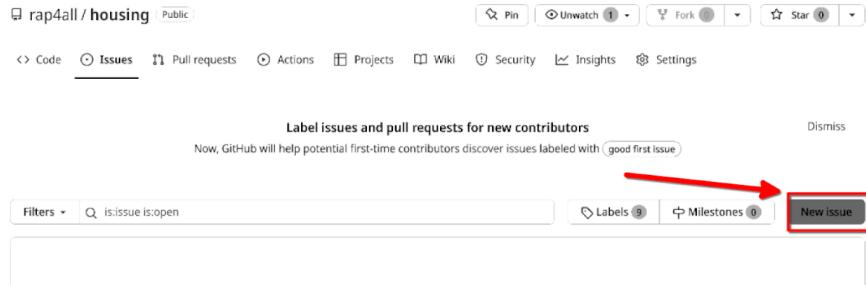


Figure 4.16.: Click on ‘New issue’ in the ‘Issues’ tab of your project.

You will land on this interface:

A screenshot of the GitHub 'New issue' creation interface. It features a title input field, a rich text editor with a toolbar, and a comment input field. On the right, there are sections for Assignees (set to 'No one—assign yourself'), Labels (set to 'None yet'), Projects (set to 'None yet'), Milestone (set to 'No milestone'), Development (described as 'Shows branches and pull requests linked to this issue'), and Helpful resources (linking to 'GitHub Community Guidelines').

Figure 4.17.: Write what the issue’s about here.

4. Version control with Git

Give a nice title to the issue (1), add a thorough description (2), (optionally) assign it to someone (3) and (optionally) add a label to it (4), finally click on “Submit new issue” (5) to submit the issue:

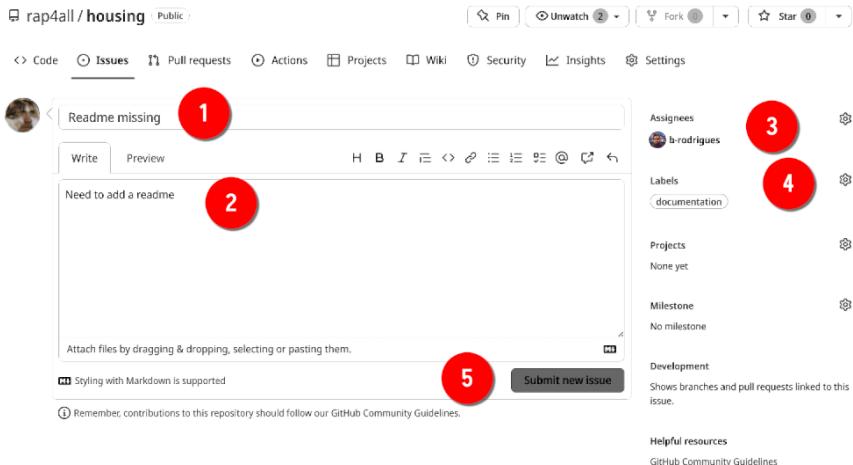


Figure 4.18.: Try to provide as many details as possible.

Sometimes issues don't need to be very long, and act more as reminders than anything else. For example here, the owner of the repository didn't have the time to add a Readme, but didn't want to forget to add one later on. The author assigned the issue to Bruno: so it'll be Bruno's job to add the Readme. Issue-driven project management is a very valid strategy when working asynchronously and in a decentralized fashion.

If you encountered a bug and want to open an issue, it is very important that you provide a minimal, reproducible example (MRE). MREs are snippets of code that can be run very easily by someone other than yourself and which produce the bug reliably. Interestingly, if you understand what makes an MRE minimal

and reproducible, you understand what will make our pipelines reproducible as well. So what's important for an MRE?

First, the code needs to be self-contained. For example, if some data is required you need to provide the data. If the data is sensitive, you need to think about the bug in greater detail: is the bug due to the structure of the data, or does the bug manifest itself on any kind of data? If that's the case, use some of the built-in datasets to R (`iris`, `mtcars`, etc) for your MRE.

Does your MRE require extra packages to run? Then make this as clear as possible, and not only provide the package names, but also their versions (it is a good idea to copy and paste the output of `sessionInfo()` at the end of the issue).

Finally, does your example depend on some object defined in the global state? If yes, you also need to provide the code to create this object.

The bar you need to set for an MRE is as follows: bar needed package dependencies that may need to be installed beforehand, people that try to help you should be able to run your script by simply copy-and-pasting it into an R console. Any other manipulation that you require from them is unacceptable: remember that in open source development, developers very often work during their free time, and don't owe you tech support! And even if they did, it is always a good idea to make it as easy as possible for them to help you, because it simply increases the likelihood that they will actually help.

Also, writing an MRE can usually make you actually debug the code yourself. Just like in rubber duck debugging⁴, the fact of simply trying to explain the problem can lead to finding what's

⁴https://en.wikipedia.org/wiki/Rubber_duck_debugging

4. Version control with Git

wrong. But by writing an MRE, you're also reducing the problem into its most basic parts, and removing everything unnecessary. By doing so, you might realize that what you thought was a bug of the library was maybe rather a problem between the keyboard and the chair.

So don't underestimate the usefulness of creating high-quality MREs for your issues! One package that can assist you with this is {reprex} (read about it here⁵).

4.5. Conclusion

You should now have your first repository and know the very basics of using Git and Github.com. If you did not understand everything, take some time to rerun the commands from above. Maybe add some more files to your repo, remove them, try to revert certain commits, etc. Create a new repo and try to push some files or scripts to it. Really take the time to understand what is going on and how to use these tools, because they are essential for reproducibility.

⁵<https://reprex.tidyverse.org/>

5. Collaborating using Trunk-based development

As already mentioned several times, there are two ways of collaborating with Git (and Github): either as a team, or as an external dev (external, as in, not part of the development team of a given project). External contributors can only contribute code to public repositories, and the project owners can either accept or refuse the patches.

We are going to learn about these two ways of collaborating. Let's first focus on collaboration within a team.

5.1. Collaborating as a team

5.1.1. TBD basics

Remember the issue we opened and assigned to Bruno? Bruno will now take care of this issue by adding a Readme file. This will also be the opportunity to introduce trunk-based development. The idea of trunk-based development is simple; team members should work on separate branches to add features or fix bugs, and then merge their branch to the “trunk” (in our case the

5. Collaborating using Trunk-based development

master branch) to add their changes back to the main codebase. And this process should happen quickly, ideally every day, or as soon as some code is ready. When a lot of work accumulates in a branch for several days or weeks, merging it back to the master branch can be very painful. So by working in short-lived branches, if conflicts arise, they can be dealt with quickly. This also makes code review much easier, because the reviewer only needs to review little bits of code at a time. If instead long-lived branches with a lot of code changes get merged, reviewing all the changes and solving the conflicts that could arise would be a lot of work. To avoid this, it is best to merge every day or each time a piece of code is added, and, **very importantly**, this code does not break the whole project (we will be using unit tests for this later).

So in summary: to avoid a lot of pain by merging branches that moved away too much from the trunk, we will create branches, add our code, and merge them to the trunk as soon as possible. *As soon as possible* can mean several things, but usually this means *as soon as a feature was added, a bug was fixed, or as soon as we added some code that does not break the whole project, even if the feature we wanted to add is not done yet*. The philosophy is that if merging fails, it should fail as early as possible. Early failures are easy to deal with.

Our aim should be to provide a functioning project to anyone cloning the master branch anytime (but still offer a simple way to install a point release of the project).

So, back to our issue. First, Bruno needs to clone the repository:

```
bruno@computer $ git clone
  ↵ git@github.com:rap4all/housing.git
```

5.1. Collaborating as a team

To add the feature, Bruno will now create a new branch by using the `git checkout` command with the `-b` flag:

```
bruno@computer $ git checkout -b "add_readme"
```

The project automatically switches to the new branch:

```
Switched to a new branch 'add_readme'
```

We can also run `git status` to double-check:

```
bruno@computer $ git status
```

```
On branch add_readme
nothing to commit, working tree clean
```

Bruno adds a file called `README.md` and adds the following text to it:

```
# Housing data for Luxembourg
```

```
These scripts for the R programming language
download nominal
housing prices from the *Observatoire de l'Habitat*
and
tidy them up into a flat data frame.
```

- `save_data.R`: downloads, cleans, and creates data frames from the data
- `analysis.R`: creates plots of the data

Let's save this and run `git status` to see what happened:

5. Collaborating using Trunk-based development

```
bruno@computer $ git status
```

Git tells Bruno that the README.md file is not being tracked:

```
On branch add_readme
Untracked files:
  (use "git add <file>..." to include in what
   ↵ will be committed)
    README.md

nothing added to commit but untracked files
  ↵ present (use "git add" to track)
```

So next Bruno is going to track it and push the changes. Also, Bruno is going to use a neat trick when pushing: because Bruno is working on fixing an issue, it would be great if he could close it as he pushes the fix. This is possible by referencing the issue number in the commit message:

```
bruno@computer $ git add .
bruno@computer $ git commit -m "fixed #1"
```

#1 refers to the number of the issue (it's the first issue that was opened in the repository). So by referencing this issue with its number in the commit message and pushing, the issue gets automatically closed when Bruno pushes:

```
bruno@computer $ git push origin add_readme
```

As you can see from the command above, Bruno pushes to “add_readme”, the branch he opened to solve the issue, not “master”. If he tried to push to “master” a message saying that

5.1. Collaborating as a team

“master” is up-to-date would get printed. Let’s see the output of pushing to “add_readme”:

```
Enumerating objects: 4, done.
Counting objects: 100% (4/4), done.
Delta compression using up to 12 threads
Compressing objects: 100% (3/3), done.
Writing objects: 100% (3/3), 501 bytes | 501.00
    ↘ KiB/s, done.
Total 3 (delta 0), reused 0 (delta 0),
    ↘ pack-reused 0
remote:
remote: Create a pull request for 'add_readme'
    ↘ on GitHub by visiting:
remote:     https://github.com/rap4all/housing/
    ↘ pull/new/add_readme
remote:
To github.com:rap4all/housing.git
 * [new branch]      add_readme -> add_readme
```

Git tells us that Bruno now needs to create a pull request. What is that? Well, if we want to merge our branch back into the trunk, we need to do so by using a pull request. Let’s see what Bruno sees on Github:

5. Collaborating using Trunk-based development

The screenshot shows a GitHub repository page for 'rap4all / housing'. At the top, there's a search bar and navigation links for Pulls, Issues, Codespaces, Marketplace, and Explore. Below the header, there are buttons for Unwatch, Fork, Star, and Insights. The main content area shows a message: 'add_readme had recent pushes less than a minute ago'. It includes a 'Compare & pull request' button. A dropdown menu shows 'master' is selected. Below this, a commit by 'Bruno Rodrigues' is listed: 'Revert "Removed analysis.R"' made 5 days ago. There are also two other commits: 'analysis.R' and 'save_data.R', both made 5 days ago. A note at the bottom encourages adding a README. On the right side, there are sections for 'About' (no description, website, or topics provided), '0 stars', '0 forks', 'Releases' (no releases published), 'Packages' (no packages published), and 'Languages' (R 100.0%).

Figure 5.1.: Bruno sees that the ‘add_readme’ branch has been recently updated.

Bruno can now decide to continue working on this branch, or, since the purpose of this branch was only to add the Readme file, decide instead to do a pull request.

By clicking on the “Compare & pull request” button Bruno now sees this:

5.1. Collaborating as a team

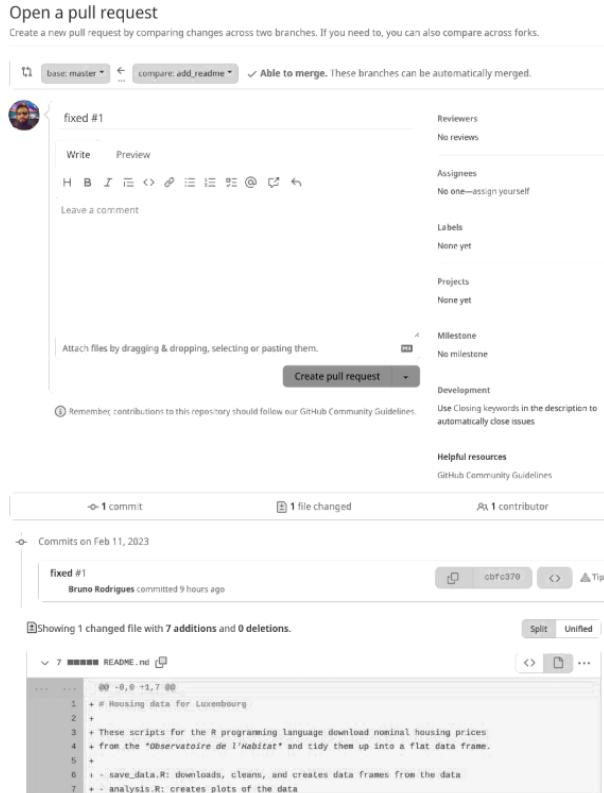


Figure 5.2.: This screen makes it easy to see what changed.

Bruno can leave a comment, and see what changed (in this case, a single file was added) and most importantly, add a reviewer if needed:

5. Collaborating using Trunk-based development

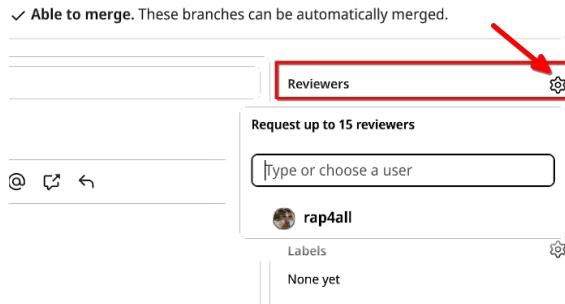


Figure 5.3.: Let boss decide if this is good enough.

This is what Bruno sees now:

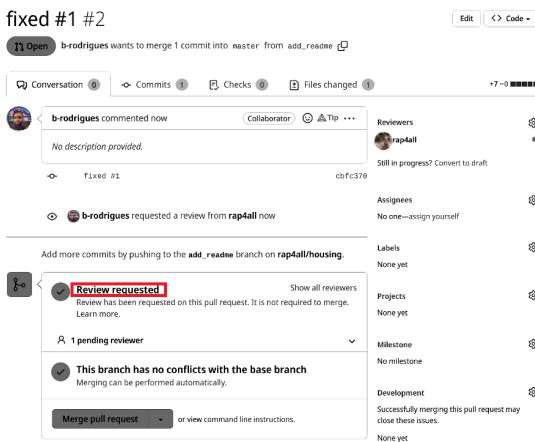


Figure 5.4.: Github tells us that this branch can safely be merged.

Bruno requested the review, but Github tells us that the branch can safely be merged. This is because we added a file and did not touch anything else, and no one else worked on the project while Bruno was working. So there are no risks of conflicts arising.

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Let's see what the owner now sees. The project owner should have gotten a notification to review the pull request:



Figure 5.5.: The owner was notified to review the pull request.

By clicking on the notification, the owner gets taken to this view:

5. Collaborating using Trunk-based development

fixed #1 #2

The screenshot shows a GitHub pull request page for a repository named 'add_readme'. The pull request has been merged, indicated by the 'fixed #1' status and the commit hash 'cbfc370'. The review section shows a comment from 'b-rodrigues' stating 'No description provided.' A review request was made from 'rap4all' 4 minutes ago. The right sidebar provides details about the pull request, including:

- Reviewers:** rap4all
- Assignees:** No one—assign yourself
- Labels:** None yet
- Projects:** None yet
- Milestone:** No milestone
- Development:** Successfully merging this pull request will close these issues.
- Notifications:** You're receiving notification watching this repository.
- Participants:** 1 participant (b-rodrigues)

The main content area displays the pull request details, including the commit message 'fixed #1' and the commit hash 'cbfc370'. It also lists pending reviews and merge rules:

- Review requested:** Review has been requested on this pull request. It is not required to merge. Learn more.
- 1 pending reviewer:** (pending review from rap4all)
- Require approval from specific reviewers before merging:** Branch protection rules ensure specific people approve pull requests before they're merged. **Add rule**
- Continuous integration has not been set up:** GitHub Actions and several other apps can be used to automatically catch bugs and enforce style.
- This branch has no conflicts with the base branch:** Merging can be performed automatically.

At the bottom, there are buttons for 'Merge pull request' and 'or view command line instructions.'

Figure 5.6.: Time to review the pull request.

Here, the reviewer can check the commit, the files that were changed, and see if there are any conflicts between this code and the code base on the master (or trunk) branch. Github also tells us two interesting things: the owner can add a rule that

5.1. Collaborating as a team

states that any pull request must be approved, and also that continuous integration has not been set up (we are going to see what this means in the second part of this book).

Let's go ahead and add a rule forcing each pull request to be approved. By clicking on “Add rule”, the following screen appears:

The screenshot shows a configuration interface for protecting the 'master' branch. At the top, there is a field labeled 'Branch name pattern *' containing 'master'. Below this, a section titled 'Protect matching branches' contains several options, each preceded by a checkbox:

- Require a pull request before merging**: When enabled, all commits must be made to a non-protected branch and submitted via a pull request before they can be merged into a branch that matches this rule.
- Require status checks to pass before merging**: Choose which status checks must pass before branches can be merged into a branch that matches this rule. When enabled, commits must first be pushed to another branch, then merged or pushed directly to a branch that matches this rule after status checks have passed.
- Require conversation resolution before merging**: When enabled, all conversations on code must be resolved before a pull request can be merged into a branch that matches this rule. Learn more.
- Require signed commits**: Commits pushed to matching branches must have verified signatures.
- Require linear history**: Prevent merge commits from being pushed to matching branches.
- Require deployments to succeed before merging**: Choose which environments must be successfully deployed to before branches can be merged into a branch that matches this rule.

Figure 5.7.: Choose how to protect the master branch.

By clicking the first option, more sub-options appear:

5. Collaborating using Trunk-based development

The screenshot shows the 'Branch name pattern *' field set to 'master'. Below it is a section titled 'Protect matching branches' containing several configuration options:

- Require a pull request before merging**: A checked checkbox with a descriptive subtitle: "When enabled, all commits must be made to a non-protected branch and submitted via a pull request before they can be merged into a branch that matches this rule."
- Require approvals**: A checked checkbox with a subtitle: "When enabled, pull requests targeting a matching branch require a number of approvals and no changes requested before they can be merged." A dropdown menu shows the value is currently set to 1.
- Dismiss stale pull request approvals when new commits are pushed**: An unchecked checkbox with a subtitle: "New reviewable commits pushed to a matching branch will dismiss pull request review approvals."
- Require review from Code Owners**: An unchecked checkbox with a subtitle: "Require an approved review in pull requests including files with a designated code owner."
- Require approval of the most recent reviewable push**: An unchecked checkbox with a subtitle: "Whether the most recent reviewable push must be approved by someone other than the person who pushed it."

Figure 5.8.: Reviews are now required.

By choosing these options, the owner can basically enforce trunk-based development (well, collaborators still have to submit pull requests frequently enough though, because if they don't, we can be in a situation where merging can be very difficult).

Let's choose one last option: by scrolling down, it's possible to select the option "Do not allow bypassing the above settings". This makes sure that even administrations (the owners of the project) must abide by the same rules.

Let's go back to the pull request. We can see now that a review is required:

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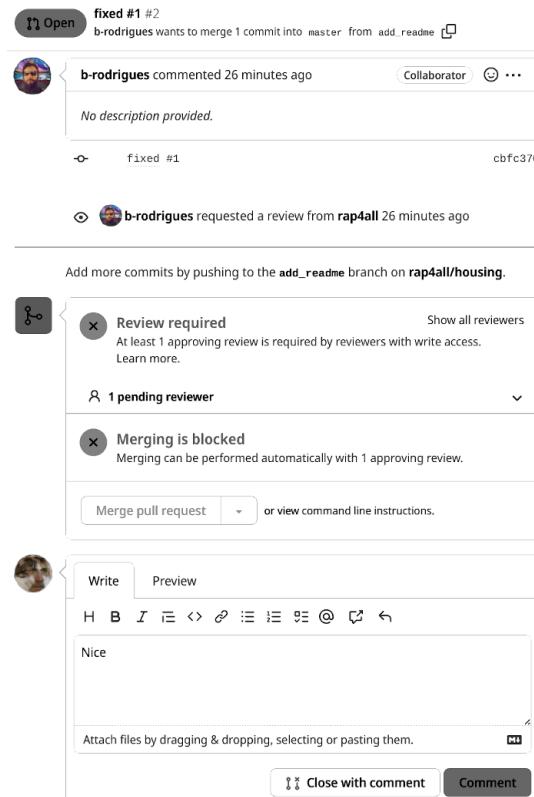


Figure 5.9.: Time to review.

So now the owner actually has to go and see the files that were changed:

5. Collaborating using Trunk-based development

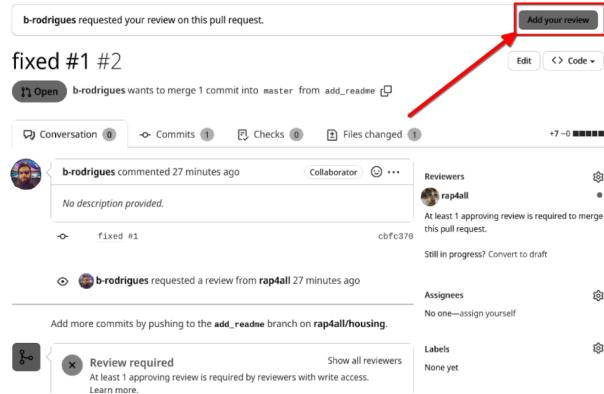


Figure 5.10.: Check the code and add comments if needed.

It's possible to add comments to single lines if needed:

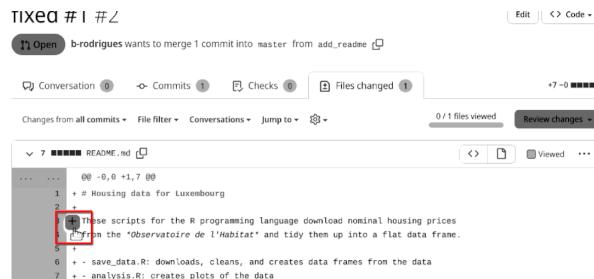


Figure 5.11.: It's possible to add comments to lines.

By clicking on the plus sign, a box appears and it's possible to leave a comment. In this case, everything is fine, so the owner is going to click on the “Viewed” button:

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Figure 5.12.: Good job!

Then, by clicking on “Review changes”, it’s possible to either add a general comment, approve the pull request, or request changes that must be addressed before merging. Let’s go ahead and approve:

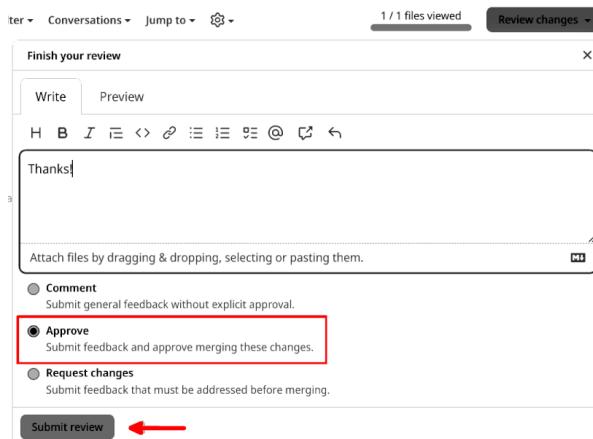


Figure 5.13.: Nothing to complain about.

By submitting the review, the reviewer is taken back to the issue:

5. Collaborating using Trunk-based development

fixed #1 #2

The screenshot shows a GitHub pull request interface. At the top, a message from b-rodrigues says "wants to merge 1 commit into master from add_readme". Below this are tabs for Conversation (1), Commits (1), Checks (0), and Files changed (1). A comment from b-rodrigues states "No description provided." and lists the commit "fixed #1" with hash cbfc370. A review from rap4all is shown with a checkmark and the message "approved these changes now". A comment from rap4all says "Thanks!". Below the pull request details, a message encourages adding more commits to the add_readme branch. The main section displays review status: "Changes approved" (1 approval), "Continuous integration has not been set up" (GitHub Actions and several other apps can be used to automatically catch bugs and enforce style), and "This branch has no conflicts with the base branch" (Merging can be performed automatically). A red arrow points to the "Merge pull request" button at the bottom.

Figure 5.14.: We're done, we can merge the pull request.

The reviewer can now merge the pull request by clicking on the “Merge pull request” button. Github even suggests we delete the branch, which has served its purpose:

5.1. Collaborating as a team

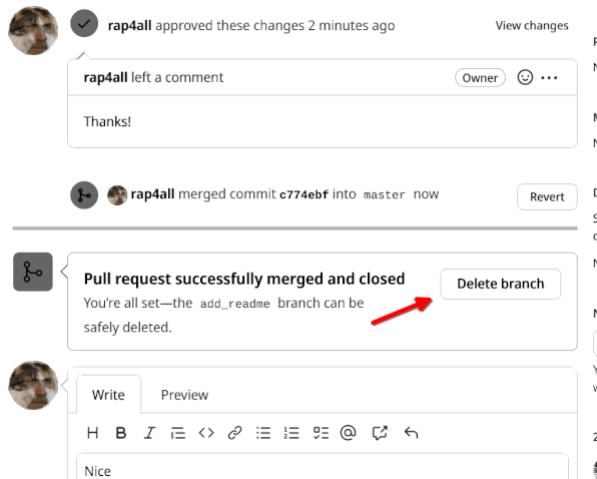


Figure 5.15.: Let's get rid of this branch.

Let's delete it (it's always possible to restore it).

5.1.2. Handling conflicts

As mentioned in the previous chapter, Git makes it easy to handle conflicts. Well, let's be clear; even with Git, it can sometimes be very tricky to resolve conflicts. But you should know that when solving a conflict with Git is difficult, this usually means that it would be impossible to do any other way, and would inevitably result in someone having to reconcile the files by hand. What makes handling conflicts easier with Git though, is that Git is able to tell you where you can find clashes on a per-line basis. So for instance, if you change the first ten lines of a script, and I change the next ten lines, there would be no conflict, and Git will automatically merge both our contributions into a single file. Other tools, like Dropbox, would fail in a situation like this, because these tools can only handle conflicts

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on a per-file basis. The same file was changed by two different persons? Regardless of where these changes happened, you now have a conflict to deal with on your hands... and worse, you don't even know where the conflicts are in the file! You will need to scan the two resulting copies of the file by hand. Git, in the case where the same lines were changed, highlights them very clearly so that you can quickly find them and deal with the problems.

We will see all of this in the coming sections.

So how do conflicts happen? Let's imagine the following scenario. Both Bruno and the project owner create branches, and edit the same file. Perhaps they talked over the phone and decided to add a feature or correct a bug. Perhaps they decided that it wasn't worth opening an issue on Github and assign someone to do it. After all, they discussed this on the phone and decided that Bruno should do it. Or was it the owner who needed to solve the issue? No one remembers now. Either way, they both did, and changed the same file, so a conflict will ensue.

First, Bruno needs to switch back to the master branch on his computer:

```
bruno@computer $ git checkout master  
  
Switched to branch 'master'  
Your branch is behind 'origin/master' by 2  
→ commits, and can be fast-forwarded.  
(use "git pull" to update your local branch)
```

Git tells us to update the code on our computer by running `git pull`. We use `git push` to upload code to Github, and use `git pull` to download code from Github. Let's run it and see what happens:

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```
bruno@computer $ git pull
```

```
Updating b7f82ee..c774ebf
Fast-forward
 README.md | 7 ++++++
 1 file changed, 7 insertions(+)
 create mode 100644 README.md
```

Files on Bruno's computer have been updated. The owner of the project (called `owner`, remember?) can do the same and will see the same. Now, Bruno creates a new branch to work on the new feature:

```
bruno@computer $ git checkout -b
 ↵ add_cool_feature
```

And the project owner also creates a new branch:

```
owner@localhost $ git checkout -b
 ↵ add_nice_feature
```

They now edit the same file, `analysis.R`. Bruno added this function:

```
make_plot <- function(country_level_data,
                      commune_level_data,
                      commune){
  filtered_data <- commune_level_data %>%
    filter(locality == commune)
```

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```
data_to_plot <- bind_rows(  
  country_level_data,  
  filtered_data  
)  
  
ggplot(data_to_plot) +  
  geom_line(aes(y = pl_m2,  
                x = year,  
                group = locality,  
                colour = locality))  
}
```

This way, Bruno could delete the repeating code and create plots like this:

```
lux_plot <- make_plot(country_level_data,  
                      commune_level_data,  
                      communes[1])  
  
# Esch sur Alzette  
  
esch_plot <- make_plot(country_level_data,  
                      commune_level_data,  
                      communes[2])  
  
# and so on...
```

The end effect is the same, but by using this function, the code is now shorter, and clearer. Also, if someone wants to change, say, the theme of the plot, now this only needs to be changed in one place and not for each commune. Now, what did the owner change? The owner started by removing the line that loaded

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the `{purrr}` package, as no function from the package was used in the script, and then also changed every `%>%` to `|>`. It seems that much more than just who would make the changes got lost in translation... Anyways, both now push their changes to their respective branches. This is Bruno:

```
bruno@computer $ git add .
bruno@computer $ git commit -m "make_plot() for
  ↵ plotting"
bruno@computer $ git push origin
  ↵ add_cool_feature
```

```
Enumerating objects: 5, done.
Counting objects: 100% (5/5), done.
Delta compression using up to 12 threads
Compressing objects: 100% (3/3), done.
Writing objects: 100% (3/3), 647 bytes | 647.00
  ↵ KiB/s, done.
Total 3 (delta 1), reused 0 (delta 0),
  ↵ pack-reused 0
remote: Resolving deltas: 100% (1/1), completed
  ↵ with 1 local object.
remote:
remote: Create a pull request for
  ↵ 'add_cool_feature' on GitHub by visiting:
remote:
  ↵ https://github.com/rap4all/housing/pull/
  ↵ new/add_cool_feature
remote:
To github.com:rap4all/housing.git
 * [new branch]      add_cool_feature ->
  ↵ add_cool_feature
```

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and this is the owner:

```
owner@localhost $ git add .
owner@localhost $ git commit -m "cleanup"
owner@localhost $ git push origin
    ↵ add_sweet_feature

Enumerating objects: 5, done.
Counting objects: 100% (5/5), done.
Delta compression using up to 4 threads
Compressing objects: 100% (3/3), done.
Writing objects: 100% (3/3), 449 bytes | 449.00
    ↵ KiB/s, done.
Total 3 (delta 1), reused 0 (delta 0)
remote: Resolving deltas: 100% (1/1), completed
    ↵ with 1 local object.
remote:
remote: Create a pull request for
    ↵ 'add_sweet_feature' on GitHub by visiting:
remote:
    ↵ https://github.com/rap4all/housing/pull/
    ↵ new/add_sweet_feature
remote:
To github.com:rap4all/housing.git
 * [new branch]      add_sweet_feature ->
    ↵ add_sweet_feature
```

So, let's think about what just happened: two developers changed the same file, `analysis.R`, in two separate branches. These two branches need to be merged back to the trunk.

So Bruno does a pull request:

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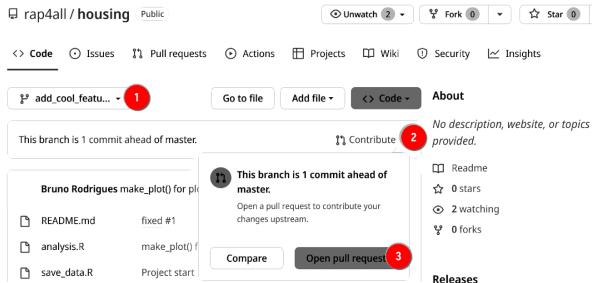


Figure 5.16.: Bruno opens a pull request after finishing his changes.

First, Bruno selects the feature branch (1), then clicks on “Contribute” (2) and then “Open pull request” (3). Bruno gets taken to this screen:

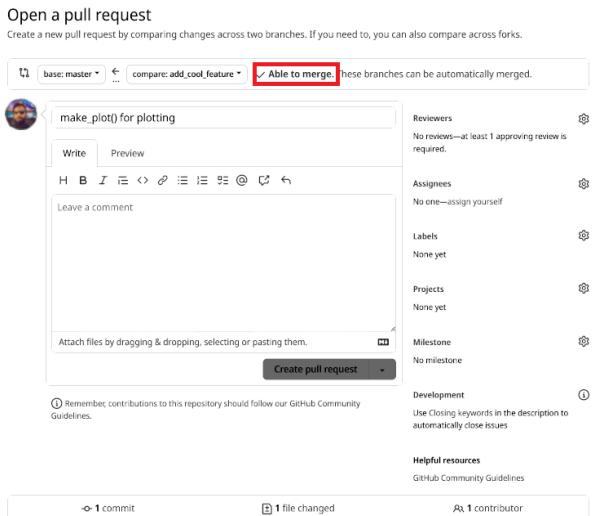


Figure 5.17.: No conflicts, for now...

Now Bruno can click on “Create pull request”, but remember, because reviews are required, automatic merging is disabled.

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If now we go see what happens from the project owner's side of things, first of all, there's now a notification for a pending review:

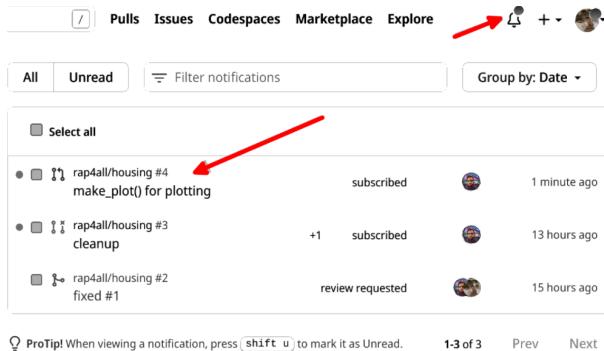


Figure 5.18.: New review pending.

By clicking on it, the project owner can review the pull request and decide what to do with it. So at this point, the owner did not open a pull request for the feature he or she worked on yet. And maybe that's a good thing, because now the project owner can see that the changes that Bruno made on the file will conflict with the project owner's changes.

So how to move forward? Simple: the project owner can decide to approve the pull request, which will merge Bruno's changes into the master branch (or the trunk). Then, instead of opening a pull request for merging his or her changes into trunk, which will cause a conflict, the project owner can instead merge the changes from the trunk into his or her feature branch. This will also create a conflict, but now the project owner can easily deal with it on his or her machine, and then push a new commit with both changes integrated gracefully. The image below illustrates this workflow:

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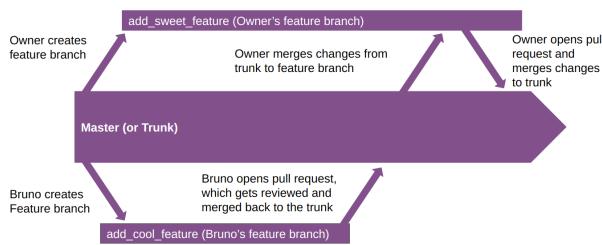


Figure 5.19.: Conflict solving with trunk-based development.

First step, the owner reviews and approves Bruno's pull request:

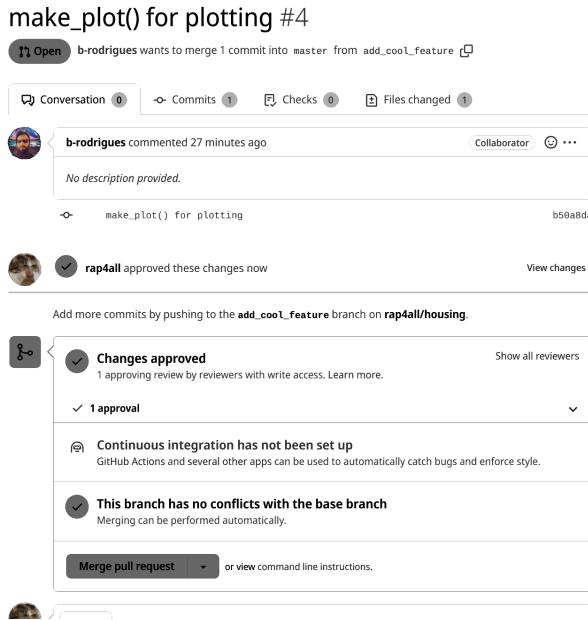


Figure 5.20.: First, let's approve the changes.

The pull request can get merged and Bruno's feature branch deleted. Now, it wouldn't make sense for the project owner to

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create a pull request to merge his or her changes. They would conflict with what Bruno did. So the project owner goes back to his or her computer and essentially updates the code in his or her feature branch by merging master into it.

So, the project owner checks that he or she is working on the feature branch:

```
owner@localhost $ git status
```

```
On branch add_sweet_feature
nothing to commit, working tree clean
```

Ok, so now let's get the updated code from master, by pulling from master:

```
owner@localhost $ git pull origin master
```

The owner now sees this:

```
remote: Enumerating objects: 6, done.
remote: Counting objects: 100% (6/6), done.
remote: Compressing objects: 100% (3/3), done.
remote: Total 4 (delta 1), reused 3 (delta 1),
  ↳ pack-reused 0
Unpacking objects: 100% (4/4), 1.23 KiB | 418.00
  ↳ KiB/s, done.
From github.com:rap4all/housing
 * branch                  master      -> FETCH_HEAD
   c774ebf..a43c68f  master      -> origin/master
Auto-merging analysis.R
CONFLICT (content): Merge conflict in analysis.R
```

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```
Automatic merge failed; fix conflicts and then
↪ commit the result.
```

Git detects that there are some conflicts and tells the owner to fix them, and then commit the results. So let's open `analysis.R` and see how it looks (you can view the file online on this link¹. First of all, you will see Git deals with conflicts on a per-line basis. So each line that the owner changed that does not conflict with Bruno's change gets immediately updated to reflect the owner's changes. For example, remember that the owner removed the line that loaded the `{purrr}` package? This line was also removed by pulling the changes from master into the feature branch. Also, you should notice that every `%>%` was changed into `|>` as well. These two changes happened without any issues.

Then, you should understand what happens when a conflict gets detected on some lines. For example, this is the first conflict you should see:

```
<<<<< HEAD
filtered_data <- commune_level_data |>
  filter(locality == communes[1])
=====
filtered_data <- commune_level_data %>%
  filter(locality == commune)
>>>>> a43c68f5596563ffca33b3729451bffc762782c3
```

We see how the lines look on the owner's computer and how they look in the master branch (or trunk). The lines between `<<<<< HEAD` and `=====` are the lines in the owner's feature branch. The lines between `=====` and `>>>>> a43c68f5596563ffca33b3729451bffc762782c3` are how they

¹<https://is.gd/ktWtjr>

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look in the master branch (or trunk). This very long chain of characters that starts with `a43c68f` is the hash of the commit from which these lines come from.

So this makes things quite easy; one simply needs to remove the outdated code, and then commit and push the fixed file! The project owner only needs to remove `<<<<< HEAD` and `=====` and what's between these lines, as well as the lines that show the hash commit. The project owner can now commit and push the changes, open a pull request, ask Bruno to review the changes one last time and merge everything back to master.

Add sweet feature #5

Open rap4all wants to merge 4 commits into master from add_sweet_feature

Conversation 0 Commits 4 Checks 0 Files changed 1

rap4all commented 1 minute ago Owner Tip ...
No description provided.

Rap4all - rpi added 4 commits 14 hours ago

- cleanup 2a7c963
- Revert "cleanup" 38ed775
- cleanup 55804cc
- removed call to purrr and replace magrittr pipe with base pipe 1 77a181c

rap4all requested a review from b-rodrigues now 2

b-rodrigues approved these changes now 3 View changes

Add more commits by pushing to the `add_sweet_feature` branch on `rap4all/housing`.

Changes approved 1 approving review by reviewers with write access. Learn more. Show all reviewers

1 approval

This branch has no conflicts with the base branch Merging can be performed automatically.

Merge pull request or view command line instructions. 4

The screenshot shows a GitHub pull request titled 'Add sweet feature #5'. The pull request summary indicates it merges 4 commits from 'add_sweet_feature' into the 'master' branch. The main commit message is 'Rap4all - rpi added 4 commits 14 hours ago' with four detailed commits: 'cleanup', 'Revert "cleanup"', 'cleanup', and 'removed call to purrr and replace magrittr pipe with base pipe'. A comment from 'rap4all' asks for a review from 'b-rodrigues'. The review section shows 'b-rodrigues' has approved the changes. Below the pull request, there is a note to 'Add more commits by pushing to the add_sweet_feature branch on rap4all/housing'. At the bottom, there is a summary of the merge status: 'Changes approved' (1 approval), 'This branch has no conflicts with the base branch', and a button to 'Merge pull request'.

Figure 5.21.: The conflict has been gracefully solved.

In (1) we see the commit that deals with the conflict, in (2) the

owner asks Bruno for a review and then in (3) we see that Bruno reviewed and approved. Finally, the pull request can be merged (4) and the feature branch deleted.

5.1.3. Make sure you blame the right person

If many people contribute to a single project, it might sometimes be difficult to know who changed what and when exactly. This is where the `git blame` command is useful. If you want to know who changed the file called `analysis.R` for example, simply run:

```
owner@localhost $ git blame analysis.R
```

and you will see a detailed history, line by line, with the user name of the contributors and a date stamp:

```
b7f82ee1 (Bruno 2023-02-05 18:03:37 +0100 24)
    ↵ #Let's also compute it...
b7f82ee1 (Bruno 2023-02-05 18:03:37 +0100 25)
55804ccb (Owner 2023-02-11 22:33:20 +0000 26)
    ↵ country_level_data <- ...
55804ccb (Owner 2023-02-11 22:33:20 +0000 27)
    ↵ mutate(p0 = ifelse(y...
```

We can see that Bruno edited lines 24 and 25 on the 5th of February as part of the commit with the hash `b7f82ee1`, while the owner of the repository changed lines 26 and 27 on the 11th of February as part of the commit with the hash `55804ccb`.

Take advantage of `git blame` to have a clear overview of each file's changes.

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5.1.4. Simplified trunk-based development

The workflow that we showed here may seem a bit too rigid for smaller teams (below 4 or 5 contributors). It is possible to adopt a simplified version of trunk-based development, where contributors don't have to open pull requests to merge their feature branches into the trunk, and no reviewer is needed. In cases like this, Git forces you to pull changes if someone already merged his or her feature branch into the trunk before you could. This way, when pulling, conflicts (if any) arise at that point. It is then your responsibility to solve the conflicts (and this works just like in the previous section) and then commit and push the commits with the conflicts resolved. Another contributor who then wishes to merge his or her feature branch into the trunk will have to pull again, ensuring that conflicts get resolved before they can merge. If no conflicts arise (for example, you both worked on different files, or on different lines of the same files), then no resolution is needed and the feature branch can be merged into master.

5.1.5. Conclusion

The main ideas of trunk-based development are:

- Each contributor opens a new branch to develop a feature or fix a bug, and works alone on his or her own little branch;
- At the end of the day at the latest (or a previously agreed upon duration), branches need all to get merged;
- Conflicts need to be taken care of at that point;
- If adding a feature would take more time than just one day, then the task needs to be split in a manner that

5.2. Contributing to public repositories

small contributions can be merged daily. In the beginning, these contributions can be simple placeholders that will be gradually enriched with functioning code until the feature is successfully implemented. This strategy is called branching by abstraction;

- The master branch (or trunk) always contains working, production-grade, code;
- To enforce discipline, it might be worth it to make opening pull requests mandatory for merging back to the trunk, and require a review.

5.2. Contributing to public repositories

In this last section, we are going to briefly discuss how to contribute to a project when we are not a team member of that project. For example, maybe we use an R package and notice a bug, and want to propose a fix. Or maybe we simply spotted a typo in the README of said package, and want to propose a correction. Whatever it may be, if the repository is public, anyone can propose a fix. For example, consider this repository:

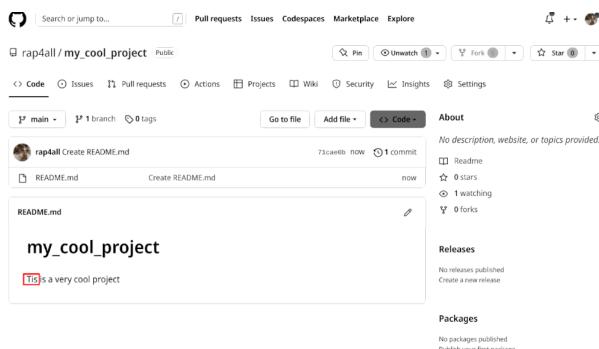


Figure 5.22.: A public repository.

5. Collaborating using Trunk-based development

This repository contains code written by a fellow called “rap4all”, and Bruno uses this code daily. However, Bruno notices a typo in the readme, and wants to propose a fix.

First, Bruno visits the repository on Github (since it’s a public repository, anyone can view it online) and creates a fork:

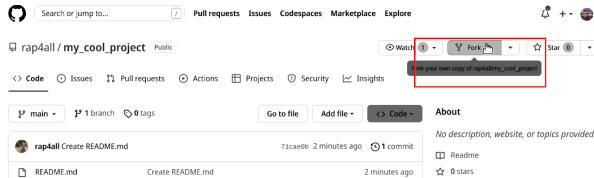


Figure 5.23.: Bruno needs to create a fork of the repository.

Forking creates a copy of the repository in Bruno’s account:

Create a new fork

A *fork* is a copy of a repository. Forking a repository allows you to freely experiment with changes without affecting the original project.

Owner * **Repository name ***

 b-rodrigues - / my_cool_project ✓

By default, forks are named the same as their upstream repository. You can customize the name to distinguish it further.

Description (optional)

Copy the main branch only
Contribute back to rap4all/my_cool_project by adding your own branch. Learn more.

ⓘ You are creating a fork in your personal account.

Create fork

Figure 5.24.: Bruno goes ahead with forking.

5.2. Contributing to public repositories

Bruno now sees the fork on his account as well:

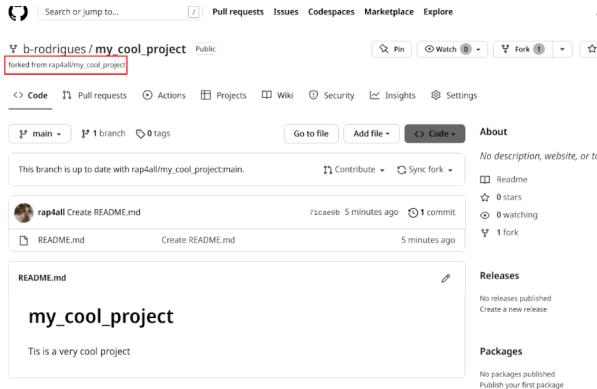


Figure 5.25.: Bruno's fork.

So now, Bruno can clone this repository and work on it, because he is working on a copy of the repository that he owns. Anything Bruno does on this copy will not affect the original repository:

```
bruno@computer $ git clone
  ↳  git@github.com:b-rodrigues/my_cool_project.git
  ↳
```

Bruno now fixes the typo in the `README.md` file, commits and pushes to his fork:

5. Collaborating using Trunk-based development

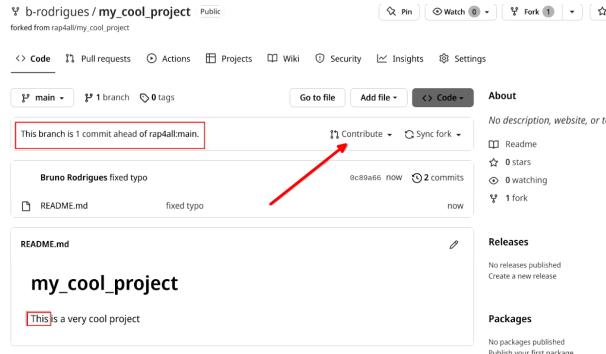


Figure 5.26.: Bruno fixed the typo in his fork.

As you can see, Bruno's fork is now ahead of the original repo by one commit. By clicking on “Contribute”, Bruno can open a pull request to propose his fix to the original repository.

This pull request will be opened over at the original repository:

5.2. Contributing to public repositories

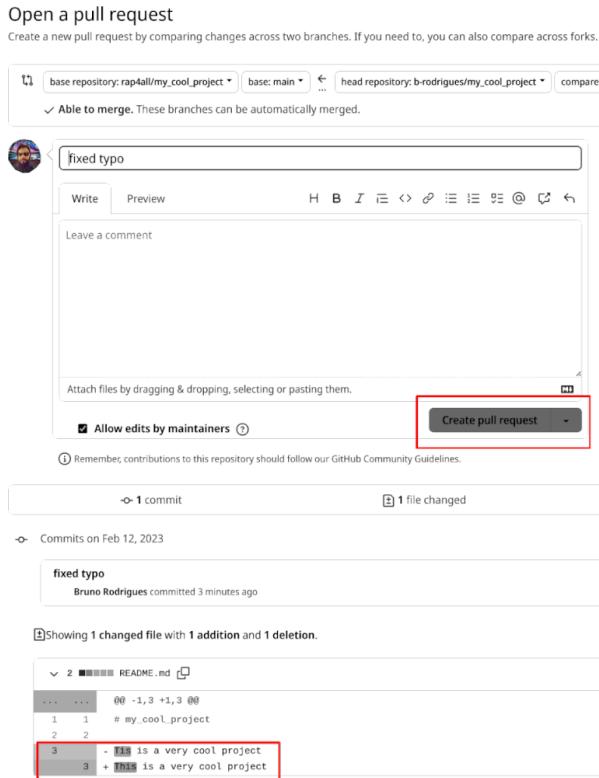


Figure 5.27.: Bruno opens a pull request to contribute his fix upstream.

What does the owner of the original repository, “rap4all”, see? The pull request Bruno opened is now in the original repository’s “Pull request” menu, and the owner can check what the contribution is, if it breaks code or not, etc. This is essentially the same workflow as the one presented before in trunk-based development with pull requests and reviews before merging (minus the forking of the repository).

5. Collaborating using Trunk-based development

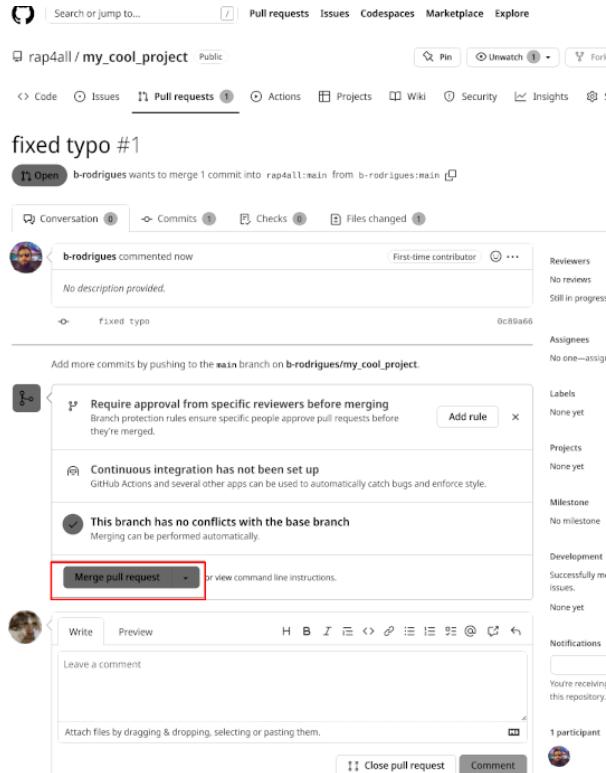


Figure 5.28.: The owner of the original repository can now accept Bruno's fix.

By merging the fix, the owner can now benefit from a grammatically correct Readme file as well:

5.3. Further reading

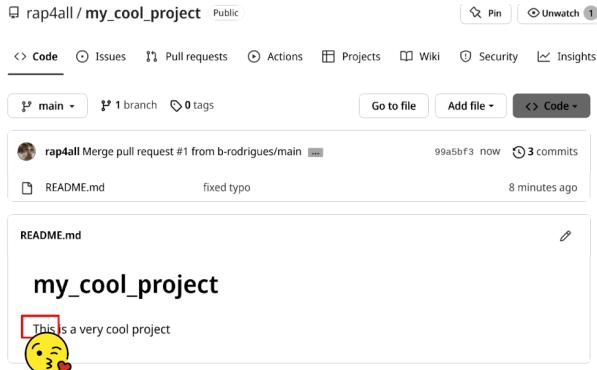


Figure 5.29.: The beauty of open source.

5.3. Further reading

To know everything about trunk-based development, check out Hammant (2020). A free, online, version of the book is available at <https://trunkbaseddevelopment.com/>.

6. Functional programming

Now that we are familiar with Git and Github, we can start with writing code. We will learn how to write code using the functional programming paradigm. Programming paradigms are ways to structure programs (or scripts).

This chapter will teach you the fundamentals of functional programming. *Functional programming* might sound scary, but we will focus on only a handful of concepts that are quite accessible but still provide many benefits. Using these functional programming concepts will make your code more reliable, easier to test, document, share, and ultimately rerun.

6.1. Introduction

Remember that the philosophy of part one of this book is “don’t repeat yourself”. In this chapter we will see how we can reduce the amount of code as much as possible. In the previous chapter we’ve seen how Bruno was able to get rid of many lines of code (that were all the same) by writing a single function:

```
make_plot <- function(country_level_data,  
                      commune_level_data,  
                      commune){
```

6. Functional programming

```
filtered_data <- commune_level_data %>%
  filter(locality == commune)

data_to_plot <- bind_rows(
  country_level_data,
  filtered_data
)

ggplot(data_to_plot) +
  geom_line(aes(y = pl_m2,
    x = year,
    group = locality,
    colour = locality))
}
```

Now we are going to go one step further and not only learn how to write good functions, but also how we can push the concept of “not repeating oneself” to the extreme by using higher-order functions and function factories.

You are very likely already familiar with at least two elements of functional programming: functions and lists. But functional programming is a complete programming paradigm, so using functional programming is more than simply using functions and lists (which you can use with other programming paradigms as well).

Functional programming is a paradigm that relies exclusively on the evaluation of functions to achieve the desired result. If you have already written your own functions in the past, what follows will not be very new. But in order to write a good functional program, the functions that you write and evaluate have to have certain properties. Before discussing these properties,

let's start with *state*.

6.1.1. The state of your program

Let's suppose that you start a fresh R session, and immediately run this line:

```
ls()
```

If you did not modify any of R's configuration files that get automatically loaded on startup, you should see the following:

```
character(0)
```

Let's suppose that now you load some data:

```
data(mtcars)
```

and define a variable a:

```
a <- 1
```

Running `ls()` now shows the following:

```
[1] "a"      "mtcars"
```

You have just altered the state of your program. You can think of the *state* as a box that holds everything that gets defined by the user and is accessible at any time. Let's now define a simple function that prints a sentence:

6. Functional programming

```
f <- function(name){  
  print(paste0(name, " likes lasagna"))  
}  
  
f("Bruno")
```

and here's the output:

```
[1] "Bruno likes lasagna"
```

Let's run `ls()` again:

```
[1] "a"        "f"        "mtcars"
```

Function `f()` is now listed there as well. This function has two nice properties:

- For a given input, it always returns exactly the same output. So `f("Bruno")` will always return “Bruno likes lasagna”.
- When running this function, the state of the program does not get altered in any way.

6.1.2. Predictable functions

Let's now define another function called `g()`, which does not have the same properties as `f()`. First, let's define a function which does not always return the same output given a particular input:

```
g <- function(name){
  food <- sample(c("lasagna", "cassoulet",
  ~ "feijoada"), 1)
  print(paste0(name, " likes ", food))
}
```

For the same input, “Bruno”, this function now produces (potentially) a different output:

```
g("Bruno")
[1] "Bruno likes lasagna"
```

```
g("Bruno")
[1] "Bruno likes feijoada"
```

And now let’s consider function `h()` that modifies the state of the program:

```
h <- function(name){
  food <- sample(c("lasagna", "cassoulet",
  ~ "feijoada"), 1)

  if(exists("food_list")){
    food_list <- append(food_list, food)
  } else {
    food_list <- append(list(), food)
  }

  print(paste0(name, " likes ", food))
}
```

This function uses the `<<-` operator. This operator saves def-

6. Functional programming

initions that are made inside the body of functions (the body of a function are all the instructions that go between the curly braces) in the global environment. Before calling this function, run `ls()` again. You should see the same objects as before, plus the new functions we've defined:

```
[1] "a"          "f"          "g"          "h"  
↳ "mtcars"
```

Let's now run `h()` once:

```
h("Bruno")  
[1] "Bruno likes feijoada"
```

And now `ls()` again:

```
[1] "a"          "f"          "food_list" "g"  
↳ "h"          "mtcars"
```

Running `h()` did two things: it printed the message, but also created a variable called “`food_list`” in the global environment with the following contents:

```
food_list  
[[1]]  
[1] "feijoada"
```

Let's run `h()` again:

```
h("Bruno")
[1] "Bruno likes cassoulet"
```

and let's check the contents of "food_list":

```
food_list

[[1]]
[1] "feijoada"

[[2]]
[1] "cassoulet"
```

If you keep running `h()`, this list will continue growing. Let me say that I hesitated to show you this; this is because if you didn't know `<-`, you might find the example above useful. But while useful, it is quite dangerous as well. Generally, we want to avoid using functions that change the state as much as possible because these functions are unpredictable, especially if randomness is involved. It is much safer to define `h()` like this instead:

```
h <- function(name, food_list = list()){

  food <- sample(c("lasagna", "cassoulet",
  "feijoada"), 1)

  food_list <- append(food_list, food)

  print(paste0(name, " likes ", food))

  food_list
```

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```
}
```

The difference now is that we made `food_list` the second argument of the function. Also, we defined it as being optional by writing:

```
food_list = list()
```

This means that if we omit this argument, the empty list will get used by default. This avoids the users from having to manually specify it.

We can call it like this:

```
food_list <- h("Bruno", food_list)
# since food_list is
# already defined, we don't
# need to start with an empty list
```

```
[1] "Bruno likes feijoada"
```

We save the output back to `food_list`. Let's now check its contents:

```
food_list
```

```
[[1]]
[1] "feijoada"
```

```
[[2]]
[1] "cassoulet"
```

```
[[3]]  
[1] "feijoada"
```

The only thing that we now still need to deal with is the fact that the food item gets chosen randomly. I'm going to show you the simple way of dealing with this, but later in this chapter we are going to use the `{withr}` package for situations like this. Let's redefine `h()` one last time:

```
h <- function(name, food_list = list(), seed =  
  ↵ 123){  
  
  # We set the seed, making sure that we get  
  # the same selection of food for a given seed  
  
  set.seed(seed)  
  food <- sample(c("lasagna", "cassoulet",  
  ↵ "feijoada"), 1)  
  
  # We now need to unset the seed, because  
  # if we don't, guess what, the seed will  
  # stay set for the whole session!  
  
  set.seed(NULL)  
  
  food_list <- append(food_list, food)  
  
  print(paste0(name, " likes ", food))  
  
  food_list  
}
```

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Let's now call `h()` several times with its default arguments:

```
h("Bruno")
```

```
[1] "Bruno likes feijoada"  
[[1]]  
[1] "feijoada"
```

```
h("Bruno")
```

```
[1] "Bruno likes feijoada"  
[[1]]  
[1] "feijoada"
```

```
h("Bruno")
```

```
[1] "Bruno likes feijoada"  
[[1]]  
[1] "feijoada"
```

As you can see, every time this function runs, it now outputs the same result. Users can change the seed to have this function output, consistently, another result.

6.1.3. Referentially transparent and pure functions

A referentially transparent function is a function that does not use any variable that is not also one of its inputs. For example,

the following function:

```
bad <- function(x){
  x + y
}
```

is not referentially transparent, because `y` is not one of the function's inputs. What happens if you run `bad()` is that `bad()` needs to look for `y`. Because `y` is not one of its inputs, `bad()` then looks for it in the global environment. If `y` is defined there, it then gets used. Defining and using such functions must be avoided at all costs because these functions are unpredictable. For example:

```
y <- 10

bad <- function(x){
  x + y
}

bad(5)
```

This will return 15. But if `y <- 45` then `bad(5)` would this time around return 50. It is much safer, and clearer to make `y` an explicit input of the function instead of having to keep track of `y`'s value (and it's so easy to do, why just not do it):

```
good <- function(x, y){
  x + y
}
```

`good()` is a referentially transparent function; it is much safer than `bad()`. `good()` is also a pure function, because it's a func-

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tion that does not interact in any way with the global environment. It does not write anything to the global environment, nor requires anything from the global environment. Function `h()` from the previous section was not pure, because it created an object and wrote it to the global environment (the `food_list` object). Turns out that pure functions are thus necessarily referentially transparent.

So the first lesson in your functional programming journey that you have to remember is to only use pure functions.

6.2. Writing good functions

6.2.1. Functions are first-class objects

In a functional programming language, functions are first-class objects. Contrary to what the name implies, this means that functions, especially the ones you define yourself, are nothing special. A function is an object like any other, and can thus be manipulated as such. Think of anything that you can do with any object in R, and you can do the same thing with a function. For example, let's consider the `+()` function. It takes two numeric objects and returns their sum:

```
1 + 5.3
```

```
[1] 6.3
```

```
# or alternatively: `+`(1, 5.3)
```

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You can replace the numbers with functions that return numbers:

```
sqrt(1) + log(5.3)
```

```
[1] 2.667707
```

It's also possible to define a function that explicitly takes another function as an input:

```
h <- function(number, f){  
  f(number)  
}
```

You can then use `h()` as a wrapper for `f()`:

```
h(4, sqrt)
```

```
[1] 2
```

```
h(10, log10)
```

```
[1] 1
```

Because `h()` takes another function as an argument, `h()` is called a higher-order function.

If you don't know how many arguments `f()`, the function you're wrapping, has, you can use the `...`:

```
h <- function(number, f, ...){  
  f(number, ...)  
}
```

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... are simply a place-holder for any potential additional argument that `f()` might have:

```
h(c(1, 2, NA, 3), mean, na.rm = TRUE)
```

```
[1] 2
```

```
h(c(1, 2, NA, 3), mean, na.rm = FALSE)
```

```
[1] NA
```

`na.rm` is an argument of `mean()`. As the developer of `h()`, I don't necessarily know what `f()` might be, but even if I knew what `f()` would be and knew all its arguments, I might not want to list them all. So I can use ... instead. The following is also possible:

```
w <- function(...){  
  paste0("First argument: ", ..1,  
        ", second argument: ", ..2,  
        ", last argument: ", ..3)  
}  
  
w(1, 2, 3)
```

```
[1] "First argument: 1, second argument: 2, last  
argument: 3"
```

If you want to learn more about ..., type `?dots` in an R console.

Because functions are nothing special, you can also write functions that return functions. As an illustration, we'll be writing

a function that converts warnings to errors. This can be quite useful if you want your functions to fail early, which often makes debugging easier. For example, try running this:

```
sqrt(-5)
```

```
Warning in sqrt(-5): NaNs produced
```

```
[1] NaN
```

This only raises a warning and returns NaN (Not a Number). This can be quite dangerous, especially when working non-interactively, which is what we will be doing a lot later on. It is much better if a pipeline fails early due to an error, than dragging a NaN value. This also happens with `sqrt()`:

```
sqrt(-10)
```

```
Warning in sqrt(-10): NaNs produced
```

```
[1] NaN
```

So it could be useful to redefine these functions to raise an error instead, for example like this:

```
strict_sqrt <- function(x){  
  if(x < 0) stop("x is negative")  
  sqrt(x)  
}
```

This function now throws an error for negative x:

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```
strict_sqrt(-10)
```

```
Error in strict_sqrt(-10) : x is negative
```

However, it can be quite tedious to redefine every function that we need in our pipeline, and remember, we don't want to repeat ourselves. So, because functions are nothing special, we can define a function that takes a function as an argument, converts any warning thrown by that function into an error, and returns a new function. For example:

```
strictly <- function(f){  
  function(...){  
    tryCatch({  
      f(...)  
    },  
    warning = function(warning)stop("Can't do  
      ↵ that chief"))  
  }  
}
```

This function makes use of `tryCatch()` which catches warnings raised by an expression (in this example the expression is `f(...)`) and then raises an error instead with the `stop()` function. It is now possible to define new functions like this:

```
s_sqrt <- strictly(sqrt)
```

```
s_sqrt(-4)
```

```
Error in value[[3L]](cond) : Can't do that chief
```

```
s_log <- strictly(log)
```

```
s_log(-4)
```

```
Error in value[[3L]](cond) : Can't do that chief
```

Functions that return functions are called *function factories* and they're incredibly useful. I use this so much that I've written a package, available on CRAN, called `{chronicler}`, that does this:

```
s_sqrt <- chronicler::record(sqrt)
```

```
result <- s_sqrt(-4)
```

```
result
```

```
NOK! Value computed unsuccessfully:
-----
```

```
Nothing
```

```
-----  
This is an object of type `chronicle`.
```

```
Retrieve the value of this object with pick(.c,  
"value").
```

```
To read the log of this object, call read_log(.c).
```

Because the expression above resulted in an error, `Nothing` is returned. `Nothing` is a special value defined in the `{maybe}` package (check it out, a very interesting package!). We can then even read a log to see what went wrong:

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```
chronicler::read_log(result)

[1] "Complete log:"
[2] "NOK! sqrt() ran unsuccessfully with following
exception: NaNs produced at 2023-07-10 10:31:47"
[3] "Total running time: 0.00120449066162109 secs"
```

The `{purrr}` package also comes with function factories that you might find useful (`{possibly}`, `{safely}` and `{quietly}`).

In part 2 we will also learn about assertive programming, another way of making our functions safer, as an alternative to using function factories.

6.2.2. Optional arguments

It is possible to make functions' arguments optional, by using `NULL`. For example:

```
g <- function(x, y = NULL){
  if(is.null(y)){
    print("optional argument y is NULL")
    x
  } else {
    if(y == 5) print("y is present"); x+y
  }
}
```

Calling `g(10)` prints the message “Optional argument y is `NULL`”, and returns 10. Calling `g(10, 5)` however, prints “y is present” and returns 15. It is also possible to use `missing()`:

```
g <- function(x, y){  
  if(missing(y)){  
    print("optional argument y is missing")  
    x  
  } else {  
    if(y == 5) print("y is present"); x+y  
  }  
}
```

I however prefer the first approach, because it is clearer which arguments are optional, which is not the case with the second approach, where you need to read the body of the function.

6.2.3. Safe functions

It is important that your functions are safe and predictable. You should avoid writing functions that behave like the `nchar()` base function. Let's see why this function is not safe:

```
nchar("10000000")
```

```
[1] 8
```

It returns the expected result of 8. But what if I remove the quotes?

```
nchar(10000000)
```

```
[1] 5
```

What is going on here? I'll give you a hint: simply type 10000000 in the console:

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```
10000000
[1] 1e+07
```

10000000 gets represented as `1e+07` by R. This number in scientific notation gets then converted into the character “`1e+07`” by `nchar()`, and this conversion happens silently. `nchar()` then counts the number of characters, and *correctly* returns 5. The problem is that it doesn’t make sense to provide a number to a function that expects a character. This function should have returned an error message, or at the very least raised a warning that the number got converted into a character. Here is how you could rewrite `nchar()` to make it safer:

```
nchar2 <- function(x, result = 0){

  if(!isTRUE(is.character(x))){
    stop(paste0("x should be of type
      ↴ 'character', but is of type '", 
      typeof(x), "' instead."))
  } else if(x == ""){
    result
  } else {
    result <- result + 1
    split_x <- strsplit(x, split = "")[[1]]
    nchar2(paste0(split_x[-1],
                  collapse = ""), result)
  }
}
```

This function now returns an error message if the input is not a character:

```
nchar2(10000000)
```

```
Error in nchar2(10000000) : x should be of type
'character', but is of type 'integer' instead.
```

This section is in a sense an introduction to assertive programming. As mentioned in the section on function factories, we will be learning about assertive programming in greater detail in part 2 of the book.

6.2.4. Recursive functions

You may have noticed in the last lines of `nchar2()` (defined above) that `nchar2()` calls itself. A function that calls itself in its own body is called a recursive function. It is sometimes easier to define a function in its recursive form than in an iterative form. The most common example is the factorial function. However, there is an issue with recursive functions (in the R programming language, other programming languages may not have the same problem, like Haskell): while it is sometimes easier to write a function using a recursive algorithm than an iterative algorithm, like for the factorial function, recursive functions in R are quite slow. Let's take a look at two definitions of the factorial function, one recursive, the other iterative:

```
fact_iter <- function(n){
  result = 1
  for(i in 1:n){
    result = result * i
    i = i + 1
  }
}
```

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```
    result
}

fact_recur <- function(n){
  if(n == 0 || n == 1){
    result = 1
  } else {
    n * fact_recur(n-1)
  }
}
```

Using the `{microbenchmark}` package we can benchmark the code:

```
microbenchmark::microbenchmark(
  fact_recur(50),
  fact_iter(50)
)
```

Unit: microseconds

	expr	min	lq	mean	median
	uq	max	neval		
fact_recur(50)	21.501	21.701	23.82701	21.901	
	22.0515	68.902	100		
fact_iter(50)	2.000	2.101	2.74599	2.201	
	2.3510	21.000	100		

We see that the recursive factorial function is 10 times slower than the iterative version. In this particular example it doesn't make much of a difference, because the functions only take microseconds to run. But if you're working with more complex functions, this is a problem. If you want to keep using the recursive function and not switch to an iterative algorithm, there

are ways to make them faster. The first is called *trampolining*. I won't go into details, but if you're interested, there is an R package that allows you to use trampolining with R, aptly called `{trampoline}`¹. Another solution is using the `{memoise}`² package. Again, I won't go into details. So if you want to use and optimize recursive functions, take a look at these packages.

6.2.5. Anonymous functions

It is possible to define a function and not give it a name. For example:

```
function(x) (x+1) (10)
```

Since R version 4.1, there is even a shorthand notation for anonymous functions:

```
(\ (x) (x+1)) (10)
```

Because we don't name them, we cannot reuse them. So why is this useful? Anonymous functions are useful when you need to apply a function somewhere inside a pipe once, and don't want to define a function just for this. This will become clearer once we learn about lists, but before that, let's philosophize a bit.

6.2.6. The Unix philosophy applied to R

This is the Unix philosophy: Write programs that do one thing and do it well. Write programs to work

¹<https://rdinnager.github.io/trampoline/>

²<https://memoise.r-lib.org/>

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together. Write programs to handle text streams, because that is a universal interface.

Doug McIlroy, in A Quarter Century of Unix³

We can take inspiration from the Unix philosophy and rewrite it for our purposes:

Write functions that do one thing and do it well. Write functions that work together. Write functions that handle lists, because that is a universal interface.

Strive for writing simple functions that only perform one task. Don't hesitate to split a big function into smaller ones. Small functions that only perform one task are easier to maintain, test, document and debug. These smaller functions can then be chained using the `|>` operator. In other words, it is preferable to have something like:

```
a |> f() |> g() |> h()
```

where `a` is for example a path to a data set, and where `f()`, `g()` and `h()` successively read, clean, and plot the data, than having something like:

```
big_function(a)
```

that does all the steps above in one go.

This idea of splitting the problem into smaller chunks, each chunk in turn split into even smaller units that can be handled by functions and then the results of these function combined into a final output is called composition.

The advantage of splitting `big_function()` into `f()`, `g()` and `h()` is that you can *eat the elephant one bite at a time*, and

³<https://stackoverflow.com/a/68690065/1298051>

also reuse these smaller functions in other projects more easily. So what's important is that you can make small functions work together by sharing a common interface. The list is usually a good candidate for this.

6.3. Lists: a powerful data-structure

Lists are the second important ingredient of functional programming. In the R philosophy inspired by the UNIX philosophy, I stated that *lists are a universal interface* in R, so our functions should handle lists. This of course depends on what it is you're doing. If you need functions to handle numbers, then there's little value in placing these numbers inside lists. But in practice, you will very likely manipulate objects that are more complex than numbers, and this is where lists come into play.

6.3.1. Lists all the way down

Lists are extremely flexible, and most of the very complex objects classes that you manipulate are actually lists, but just fancier. For example, a data frame is a list:

```
data(mtcars)  
typeof(mtcars)  
  
[1] "list"
```

A fitted model is a list:

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```
my_model <- lm(hp ~ mpg, data = mtcars)
```

```
typeof(my_model)
```

```
[1] "list"
```

A `ggplot` is a list:

```
library(ggplot2)
```

```
my_plot <- ggplot(data = mtcars) +  
  geom_line(aes(y = hp, x = mpg))
```

```
typeof(my_plot)
```

```
[1] "list"
```

It's lists all the way down, and it's not a coincidence; it's because lists are very powerful. So it's important to know what you can do with lists.

6.3.2. Lists can hold many things

If you write a function that needs to return many objects, the only solution is to place them inside a list. For example, consider this function:

```
sqrt_newton <- function(a,  
                        init = 1,  
                        eps = 0.01,  
                        steps = 1){
```

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```
stopifnot(a >= 0)
while(abs(init**2 - a) > eps){
    init <- 1/2 *(init + a/init)
    steps <- steps + 1
}
list(
    "result" = init,
    "steps" = steps
)
}
```

This function returns the square root of a number using Newton's algorithm, as well as the number of steps, or iterations, it took to reach the solution:

```
result_list <- sqrt_newton(1600)

result_list

$result
[1] 40

$steps
[1] 10
```

It is quite common to print the number of steps to the console instead of returning them. But the issue with a function that prints something to the console instead of returning it, is that such a function is not pure, as it changes something outside of its scope (it prints to the console!). And if you need the information that got printed (for example, if you want to count all the steps it took to run the script from start to finish), it is lost. It gets printed, and that's it. It is preferable to instead

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make the function pure by returning everything inside a neat list. It is then possible to separately save these objects if needed:

```
result <- result_list$result  
  
result_steps <- result_list$steps
```

Or you could define functions that know how to deal with the list:

```
f <- function(result_list){  
  list(  
    "result" = result_list$result * 10,  
    "steps" = result_list$steps + 1  
  )  
}  
  
f(result_list)  
  
$result  
[1] 400  
  
$steps  
[1] 11
```

It all depends on what you want to do. But it is usually better to keep everything neatly inside a list.

Lists can also hold objects of different types:

```
list(  
  "a" = head(mtcars),  
  "b" = lm(y ~ x)
```

6.3. Lists: a powerful data-structure

```
)  
  
$a  
  mpg cyl disp hp drat    wt  qsec  
  vs am  
Mazda RX4      21.0   6 160 110 3.90 2.620 16.46  
0 1  
Mazda RX4 Wag  21.0   6 160 110 3.90 2.875 17.02  
0 1  
Datsun 710     22.8   4 108  93 3.85 2.320 18.61  
1 1  
Hornet 4 Drive 21.4   6 258 110 3.08 3.215 19.44  
1 0  
Hornet Sportabout 18.7   8 360 175 3.15 3.440 17.02  
0 0  
Valiant        18.1   6 225 105 2.76 3.460 20.22  
1 0  
              gear carb  
Mazda RX4      4     4  
Mazda RX4 Wag  4     4  
Datsun 710     4     1  
Hornet 4 Drive 3     1  
Hornet Sportabout 3     2  
Valiant        3     1  
  
$b  
~lm(y ~ x)
```

The list above has two elements, the first is the head of the `mtcars` data frame, the second is a formula object. Lists can even hold other lists:

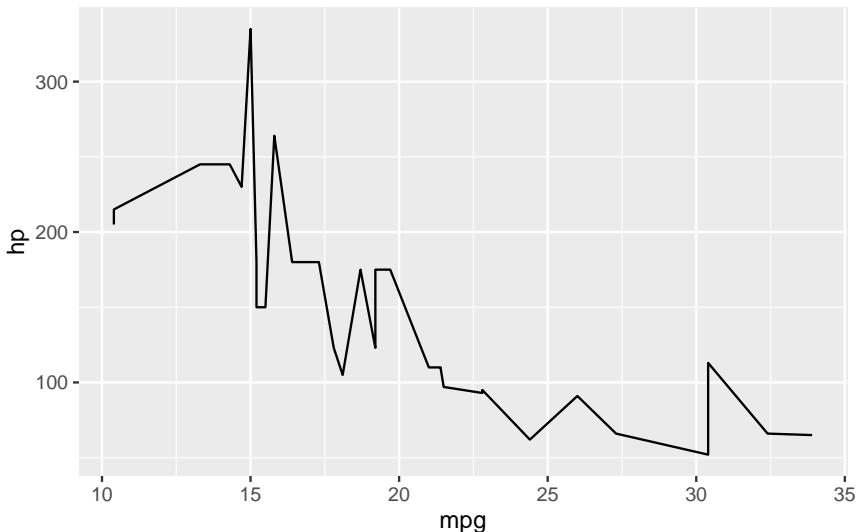
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```
list(  
  "a" = head(mtcars),  
  "b" = list(  
    "c" = sqrt,  
    "d" = my_plot # Remember this ggplot object  
    ↵ from before?  
  )  
)  
  
$a  
mpg cyl disp hp drat wt qsec  
vs am  
Mazda RX4 21.0 6 160 110 3.90 2.620 16.46  
0 1  
Mazda RX4 Wag 21.0 6 160 110 3.90 2.875 17.02  
0 1  
Datsun 710 22.8 4 108 93 3.85 2.320 18.61  
1 1  
Hornet 4 Drive 21.4 6 258 110 3.08 3.215 19.44  
1 0  
Hornet Sportabout 18.7 8 360 175 3.15 3.440 17.02  
0 0  
Valiant 18.1 6 225 105 2.76 3.460 20.22  
1 0  
gear carb  
Mazda RX4 4 4  
Mazda RX4 Wag 4 4  
Datsun 710 4 1  
Hornet 4 Drive 3 1  
Hornet Sportabout 3 2  
Valiant 3 1  
  
$b
```

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```
$b$c
function (x) .Primitive("sqrt")
```

```
$b$d
```



Use this to your advantage.

6.3.3. Lists as the cure to loops

Loops are incredibly useful, and you are likely familiar with them. The problem with loops is that they are a concept from iterative programming, not functional programming, and this is a problem because loops rely on changing the state of your program to run. For example, let's suppose that you wish to use a for-loop to compute the sum of the first 100 integers:

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```
result <- 0

for (i in 1:100){
  result <- result + i
}

print(result)
```

```
[1] 5050
```

If you run `ls()` now, you should see that there's a variable `i` in your global environment. This could cause issues further down in your pipeline if you need to re-use `i`. Also, writing loops is, in my opinion, quite error prone. But how can we avoid using loops? Looping in a functional programming language involves using higher-order functions and lists. A reminder: a higher-order function is a function that takes another function as an argument. Looping is a task like any other, so I can write a function that does the looping. This function, which I'll call `looping()`, will take a function as an argument, as well as a list. The list will serve as the container to hold our numbers:

```
looping <- function(a_list, a_func, init = NULL,
                     ...){

  # If the user does not provide an `init`
  # value,
  # set the head of the list as the initial
  # value
  if(is.null(init)){
    init <- a_list[[1]]
    a_list <- tail(a_list, -1)
  }
}
```

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```
}

# Separate the head from the tail of the list
# and apply the function to the initial value
#   and the head of the list
head_list = a_list[[1]]
tail_list = tail(a_list, -1)
init = a_func(init, head_list, ...)

# Check if we're done: if there is still some
#   tail,
# rerun the whole thing until there's no tail
#   left
if(length(tail_list) != 0){
  looping(tail_list, a_func, init, ...)
}
else {
  init
}
}
```

Now, this might seem much more complicated than a for loop. However, now that we have abstracted the loop away inside a function, we can keep reusing this function:

```
looping(as.list(seq(1, 100)), `+`)
```

```
[1] 5050
```

Of course, because this is so useful, `looping()` actually ships with R, and is called `Reduce()`:

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```
Reduce(`+`, seq(1, 100)) # the order of the
← arguments is `function` then `list` for
← `Reduce()`
```

```
[1] 5050
```

But this is not the only way that we can loop. We can also write a loop that applies a function to each element of a list, instead of operating on the whole list:

```
result <- as.list(seq(1, 5))
for (i in seq_along(result)){
  result[[i]] <- sqrt(result[[i]])
}

print(result)
```

```
[[1]]
```

```
[1] 1
```

```
[[2]]
```

```
[1] 1.414214
```

```
[[3]]
```

```
[1] 1.732051
```

```
[[4]]
```

```
[1] 2
```

```
[[5]]
```

```
[1] 2.236068
```

Here again, we have to pollute the global environment by first

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creating a vessel for our results, and then apply the function at each index. We can abstract this process away in a function:

```
applying <- function(a_list, a_func, ...){  
  
  head_list = a_list[[1]]  
  tail_list = tail(a_list, -1)  
  result = a_func(head_list, ...)  
  
  # Check if we're done: if there is still some  
  # tail, rerun the whole thing until there's  
  # no tail left  
  if(length(tail_list) != 0){  
    append(result, applying(tail_list, a_func,  
                           ...))  
  }  
  else {  
    result  
  }  
}
```

Once again this might seem complicated, and I would agree. Abstraction is complex. But once we have it, we can focus on the task at hand, instead of having to always tell the computer what we want:

```
applying(as.list(seq(1, 5)), sqrt)
```

```
[1] 1.000000 1.414214 1.732051 2.000000 2.236068
```

Of course, R ships with its own, much more efficient, implementation of this function:

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```
lapply(list(seq(1, 5)), sqrt)  
[[1]]  
[1] 1.000000 1.414214 1.732051 2.000000 2.236068
```

In other programming languages, `lapply()` is often called `map()`. The `{purrr}` package ships with other such useful higher-order functions that abstract loops away. For example, there's the function called `map2()`, that maps a function of two arguments to each element of two atomic vectors or lists, two at a time:

```
library(purrr)  
  
map2(  
  .x = seq(1, 5),  
  .y = seq(1, 5),  
  .f = `+`  
)  
  
[[1]]  
[1] 2  
  
[[2]]  
[1] 4  
  
[[3]]  
[1] 6  
  
[[4]]  
[1] 8  
  
[[5]]  
[1] 10
```

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If you have more than two lists, you can use `pmap()` instead.

Another important, idiomatic, way to deal with loops in R is to use matrix algebra instead. For example, to compute the sum of the first 100 integers, the following approach is possible:

```
rep(1, 100) %*% seq(1, 100)
```

```
[,1]  
[1,] 5050
```

Also, don't forget that many functions are vectorized by default, so no loop is required:

```
sqrt(seq(1, 5))
```

```
[1] 1.000000 1.414214 1.732051 2.000000 2.236068
```

or:

```
seq(1, 5) + seq(1, 5)
```

```
[1] 2 4 6 8 10
```

Before diving directly into loops, check if the functions you're using are vectorized, or if there is a simple way to express the computation you want to run in terms of matrix multiplication.

6.3.4. Data frames

As mentioned in the introduction of this section, data frames are a special type of list of atomic vectors. This means that just as I can use `lapply()` to compute the square root of the elements

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of an atomic vector, as shown previously, I can also operate on all the columns of a data frame. For example, it is possible to determine the class of every column of a data frame like this:

```
lapply(iris, class)

$Sepal.Length
[1] "numeric"

$Sepal.Width
[1] "numeric"

$Petal.Length
[1] "numeric"

$Petal.Width
[1] "numeric"

$Species
[1] "factor"
```

Unlike a list however, the elements of a data frame must be of the same length. Data frames remain very flexible though, and using what we have learned until now it is possible to use the data frame as a structure for all our computations. For example, suppose that we have a data frame that contains data on unemployment for the different subnational divisions of the Grand-Duchy of Luxembourg, the country the author of this book hails from. Let's suppose that I want to generate several plots, per subnational division and per year. Typically, we would use a loop for this, but we can use what we've learned here, as well as some functions from the `{dplyr}`, `{purrr}`, `{ggplot2}` and `{tidyverse}` packages. I will be downloading data that I made

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available inside a package, but instead of installing the package, I will download the `.rda` file directly (which is the file format of packaged data) and then load that data into our R session (instead of downloading from the long Github url, I download the data from a shortened `is.gd` link):

```
# Create a temporary file
unemp_path <- tempfile(fileext = ".rda")

# Download the data and save it to the path of
#   ↵ the temporary file
# avoids having to install the package from
#   ↵ Github
download.file(
  "https://is.gd/l57cNX",
  destfile = unemp_path)

# Load the data. The data is now available as
#   ↵ 'unemp'
load(unemp_path)
```

Let's load the required packages and take a look at the data:

```
library(dplyr)
```

Attaching package: 'dplyr'

The following objects are masked from
'package:stats':

`filter`, `lag`

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The following objects are masked from
'package:base':

```
intersect, setdiff, setequal, union
```

```
library(purrr)  
library(ggplot2)  
library(tidyr)
```

```
glimpse(unemp)
```

Rows: 472

Columns: 9

```
$ year                      <dbl> 2013, 2013,  
2013, 201~  
$ place_name                <chr> "Luxembourg",  
"Capell~  
$ level                     <chr> "Country",  
"Canton", ~  
$ total_employed_population <dbl> 223407, 17802,  
1703, ~  
$ of_which_wage_earners     <dbl> 203535, 15993,  
1535, ~  
$ of_which_non_wage_earners <dbl> 19872, 1809,  
168, 94, ~  
$ unemployed                <dbl> 19287, 1071,  
114, 25, ~  
$ active_population          <dbl> 242694, 18873,  
1817, ~  
$ unemployment_rate_in_percent <dbl> 7.947044,  
5.674773, 6~
```

Column names are self-descriptive, but the `level` column needs some explanations. `level` contains the administrative divisions

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of the country, so the country of Luxembourg, then the Cantons and then the Communes.

Remember that Luxembourg can refer to the country, the canton or the commune of Luxembourg. Now let's suppose that I want a separate plot for the three communes of Luxembourg, Esch-sur-Alzette and Wiltz. Instead of creating three separate data frames and feeding them to the same ggplot code, I can instead take advantage of the fact that data frames are lists, and are thus quite flexible. Let's start with filtering:

```
filtered_unemp <- unemp %>%
  filter(
    level == "Commune",
    place_name %in% c("Luxembourg",
  ~ "Esch-sur-Alzette", "Wiltz")
  )

glimpse(filtered_unemp)
```

```
Rows: 12
Columns: 9
$ year                               <dbl> 2013, 2013,
2013, 201~
$ place_name                          <chr>
"Esch-sur-Alzette", "~
$ level                               <chr> "Commune",
"Commune", ~
$ total_employed_population          <dbl> 12725, 39513,
2344, 1~
$ of_which_wage_earners              <dbl> 12031, 35531,
2149, 1~
$ of_which_non_wage_earners         <dbl> 694, 3982, 195,
703, ~
```

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```
$ unemployed           <dbl> 2054, 3855,  
318, 1997~  
$ active_population    <dbl> 14779, 43368,  
2662, 1~  
$ unemployment_rate_in_percent <dbl> 13.898099,  
8.889043, ~
```

We are now going to use the fact that data frames are lists, and that lists can hold any type of object. For example, remember this list from before where one of the elements is a data frame, and the second one a formula:

```
list(  
  "a" = head(mtcars),  
  "b" = ~lm(y ~ x)  
)
```



```
$a  
              mpg cyl disp  hp drat      wt  qsec  
vs am  
Mazda RX4        21.0   6 160 110 3.90 2.620 16.46  
0  1  
Mazda RX4 Wag    21.0   6 160 110 3.90 2.875 17.02  
0  1  
Datsun 710       22.8   4 108  93 3.85 2.320 18.61  
1  1  
Hornet 4 Drive    21.4   6 258 110 3.08 3.215 19.44  
1  0  
Hornet Sportabout 18.7   8 360 175 3.15 3.440 17.02  
0  0  
Valiant          18.1   6 225 105 2.76 3.460 20.22  
1  0  
                  gear carb  
Mazda RX4         4      4
```

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```
Mazda RX4 Wag      4      4
Datsun 710        4      1
Hornet 4 Drive    3      1
Hornet Sportabout 3      2
Valiant           3      1
```

```
$b
~lm(y ~ x)
```

{dplyr} comes with a function called `group_nest()` which groups the data frame by a variable (such that the next computations will be performed group-wise) and then nests the other columns into a smaller data frame. Let's try it and see what happens:

```
nested_unemp <- filtered_unemp %>%
  group_nest(place_name)
```

Let's see what this looks like:

```
nested_unemp

# A tibble: 3 x 2
  place_name          data
  <chr>                <list<tibble[,8]>>
1 Esch-sur-Alzette    [4 x 8]
2 Luxembourg          [4 x 8]
3 Wiltz               [4 x 8]
```

`nested_unemp` is a new data frame of 3 rows, one per commune (“Esch-sur-Alzette”, “Luxembourg”, “Wiltz”), and of two columns, one for the names of the communes, and the other contains every other variable inside a smaller data frame. So this is a data frame that has one column where each element of

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that column is itself a data frame. Such a column is called a list-column. This is essentially a list of lists.

Let's now think about this for a moment. If the column titled `data` is a list of data frames, it should be possible to use a function like `map()` or `lapply()` to apply a function on each of these data frames. Remember that `map()` or `lapply()` require a list of elements of whatever type and a function that accepts objects of this type as input. So this means that we could apply a function that plots the data to each element of the column titled `data`. Since each element of this column is a data frame, this function needs a data frame as an input. As a first and simple example to illustrate this, let's suppose that we want to determine the number of rows of each data frame. This is how we would do it:

```
nested_unemp %>%
  mutate(nrows = map(data, nrow))

# A tibble: 3 x 3
#>   place_name          data nrows
#>   <chr>              <list<tibble[,8]>> <list>
#> 1 Esch-sur-Alzette    [4 x 8] <int [1]>
#> 2 Luxembourg          [4 x 8] <int [1]>
#> 3 Wiltz               [4 x 8] <int [1]>

# 'data' is the name of
# the list-column that contains
# the smaller data frames
```

The new column, titled `nrows` is a list of integers. We can simplify it by converting it directly to an atomic vector of integers by using `map_int()` instead of `map()`:

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```
nested_unemp %>%
  mutate(nrows = map_int(data, nrow))

# A tibble: 3 x 3
  place_name          data nrows
  <chr>              <list<tibble[,8]>> <int>
1 Esch-sur-Alzette   [4 x 8]     4
2 Luxembourg          [4 x 8]     4
3 Wiltz               [4 x 8]     4
```

Let's try a more complex example now. What if we want to filter rows (of course, the simplest way would be to filter the rows we need before nesting the data frame)? We need to apply the function `filter()` where its first argument is a data frame and the second argument is a predicate:

```
nested_unemp %>%
  mutate(nrows = map(data, \(x)filter(x, year ==
  ↪ 2015)))
```



```
# A tibble: 3 x 3
  place_name          data nrows
  <chr>              <list<tibble[,8]>> <list>
1 Esch-sur-Alzette   [4 x 8] <tibble [1 x
8]>
2 Luxembourg          [4 x 8] <tibble [1 x
8]>
3 Wiltz               [4 x 8] <tibble [1 x
8]>
```

In this case, we need to use an anonymous function. This is because `filter()` has two arguments and we need to make clear what it is we are mapping over and what argument stays fixed;

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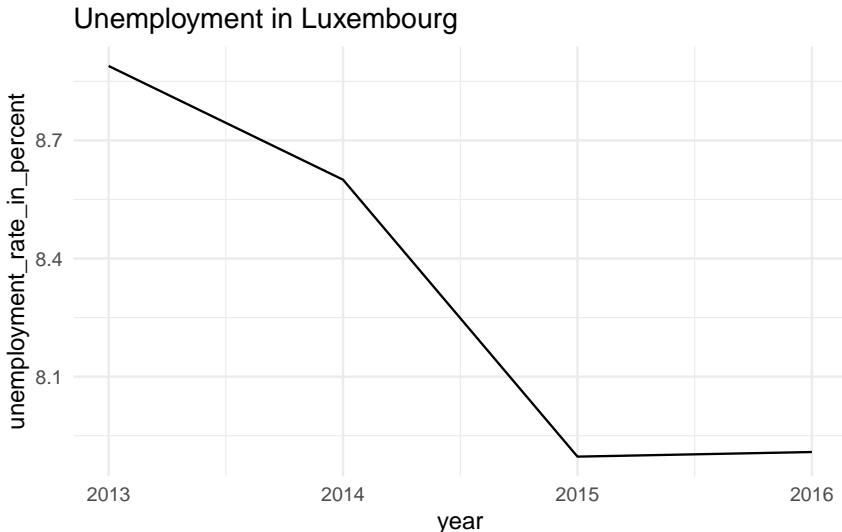
we are mapping over (iterating) the data frames but the predicate `year == 2015` stays fixed.

We are now ready to plot our data. The best way to continue is to first get the function right by creating one plot for one single commune. Let's select the dataset for the commune of Luxembourg:

```
lux_data <- nested_unemp %>%
  filter(place_name == "Luxembourg") %>%
  unnest(data)
```

To plot this data, we can now write the required `ggplot2()` code:

```
ggplot(data = lux_data) +
  theme_minimal() +
  geom_line(
    aes(year, unemployment_rate_in_percent,
        group = 1)
  ) +
  labs(title = "Unemployment in Luxembourg")
```



To turn the lines of code above into a function, you need to think about how many arguments that function would have. There is an obvious one, the data itself (in the snippet above, the data is the `lux_data` object). Another one that is less obvious is in the title:

```
labs(title = "Unemployment in Luxembourg")
```

Ideally, we would want that title to change depending on the data set. So we could write the function like so:

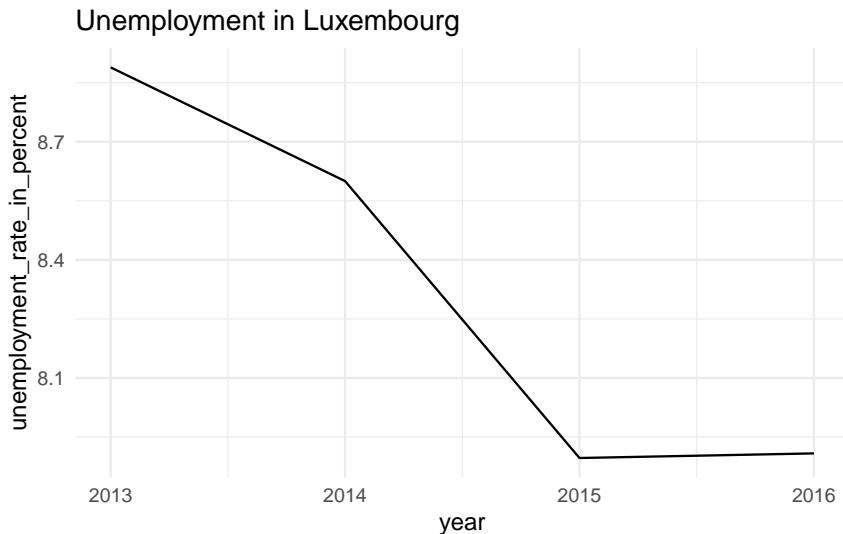
```
make_plot <- function(x, y){
  ggplot(data = x) +
    theme_minimal() +
    geom_line(
      aes(year, unemployment_rate_in_percent,
          group = 1)
    ) +
```

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```
    labs(title = paste("Unemployment in", y))  
  }
```

Let's try it on our data:

```
make_plot(lux_data, "Luxembourg")
```



Ok, so now, we simply need to apply this function to our nested data frame:

```
nested_unemp <- nested_unemp %>%  
  mutate(plots = map2(  
    .x = data, # column of data frames  
    .y = place_name, # column of commune names  
    .f = make_plot  
  ))
```

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```
nested_unemp
```

```
# A tibble: 3 x 3
  place_name      data_plots
  <chr>           <list<tibble[,8]>> <list>
1 Esch-sur-Alzette [4 x 8] <gg>
2 Luxembourg      [4 x 8] <gg>
3 Wiltz           [4 x 8] <gg>
```

If you look at the `plots` column, you see that it is a list of `gg` objects: these are our plots. Let's take a look at them:

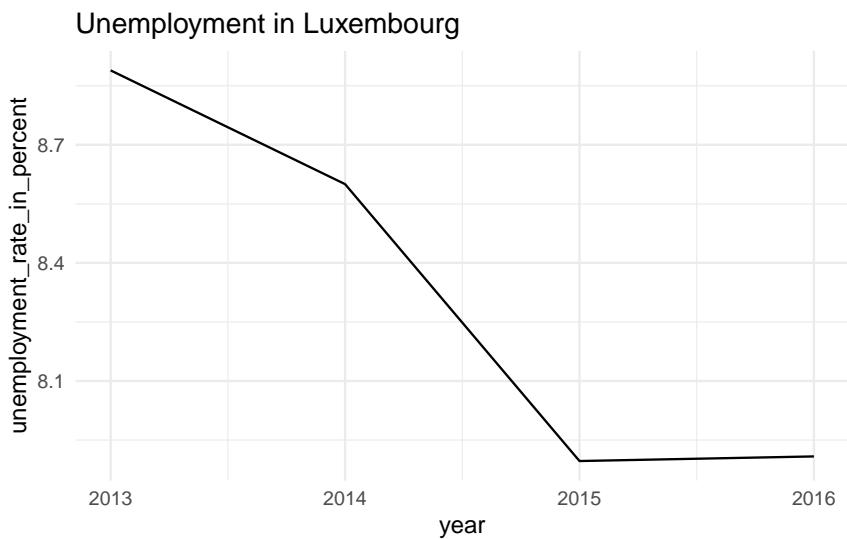
```
nested_unemp$plots
```

```
[[1]]
```



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[[2]]



[[3]]

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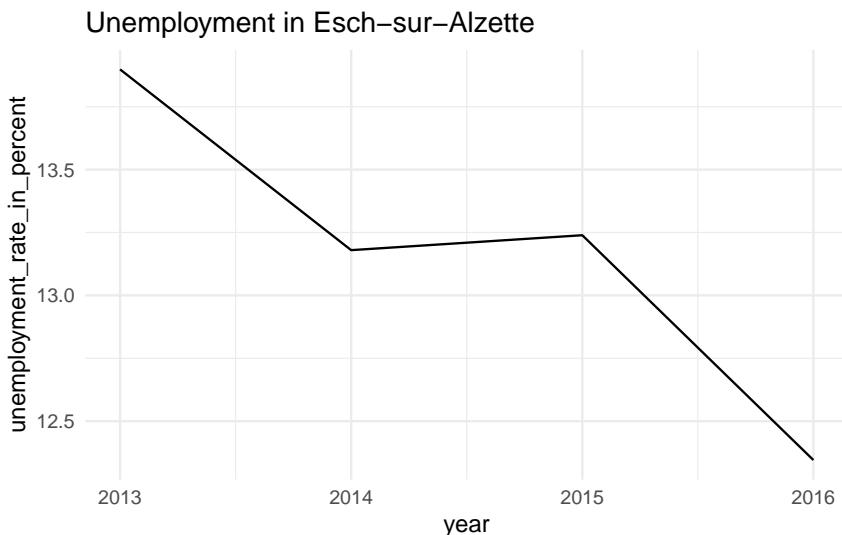
We could also have used an anonymous function (but it is more difficult to get right):

```
nested_unemp %>%
  mutate(plots2 = map2(
    .x = data,
    .y = place_name,
    .f = \(.x,.y)(
      ggplot(data = .x) +
        theme_minimal() +
        geom_line(
          aes(year,
              ↵  unemployment_rate_in_percent,
              ↵  group = 1)
    ) +
```

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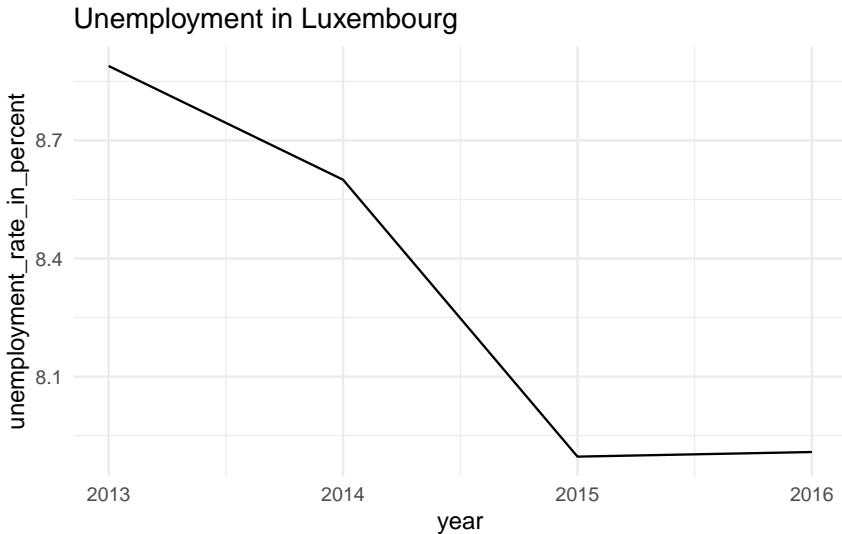
```
    labs(title =
      ↵  paste("Unemployment in",
      ↵  .y))
  )
) %>%
pull(plots2)
```

[[1]]



[[2]]

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[[3]]



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This list-column based workflow is extremely powerful and I highly advise you to take the required time to master it. Remember, we never want to have to repeat ourselves. This approach might seem more complicated than calling `make_plot()` three times, but imagine that you need to do this for several countries, several variables, etc... What are you going to do, copy and paste code everywhere? This gets very tedious and more importantly, very error-prone, because now you've just introduced many points of failure by having so much copy-pasted code. You could of course use a loop instead of this list-column based workflow. But as mentioned, the issue with loops is that you have to interact with the global environment, which can lead to other issues. But whatever you end up using, you need to avoid copy and pasting at all costs.

6.4. Functional programming in R

Up until now I focused on general concepts rather than on specifics of the R programming language when it comes to functional programming. In this section, we will be focusing entirely on R-specific capabilities and packages for functional programming.

6.4.1. Base capabilities

R is a functional programming language (but not only), and as such it comes with many functions out of the box to write functional code. We have already discussed `lapply()` and `Reduce()`. You should know that depending on what you want to achieve, there are other functions that are similar to `lapply()`: `apply()`, `sapply()`, `vapply()`, `mapply()` and `tapply()`. There's also

`Map()` which is a wrapper around `mapply()`. Each function performs the same basic task of applying a function over all the elements of a list or list-like structure, but it can be hard to keep them apart and when you should use one over another. This is why `{purrr}`, which we will discuss in the next section, is quite an interesting alternative to base R's offering.

Another one of the quintessential functional programming functions (alongside `Reduce()` and `Map()`) that ships with R is `Filter()`. If you know `dplyr::filter()` you should be familiar with the concept of filtering rows of a data frame where the elements of one particular column satisfy a predicate. `Filter()` works the same way, but focusing on lists instead of data frame:

```
Filter(is.character,
       list(
         seq(1, 5),
         "Hey")
     )
```

```
[[1]]
[1] "Hey"
```

The call above only returns the elements where `is.character()` evaluates to TRUE.

Another useful function is `Negate()` which is a function factory that takes a boolean function as an input and returns the opposite boolean function. As an illustration, suppose that in the example above we wanted to get everything *but* the character:

```
Filter(Negate(is.character),
       list(
```

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```
    seq(1, 5),  
    "Hey")  
)
```

```
[[1]]  
[1] 1 2 3 4 5
```

There are some other functions like this that you might want to check out: type `?Negate` in console to read more about them.

Sometimes you may need to run code with side-effects, but want to avoid any interaction between these side-effects and the global environment. For example, you might want to run some code that creates a plot and saves it to disk, or code that creates some data and writes them to disk. `local()` can be used for this. `local()` runs code in a temporary environment that gets discarded at the end:

```
local({  
  a <- 2  
)
```

Variable `a` was created inside this local environment. Checking if it exists now yields `FALSE`:

```
exists("a")
```

```
[1] FALSE
```

We will be using this technique later in the book to keep our scripts pure.

Before continuing with R packages that extend R's functional programming capabilities it's also important to stress that just

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as R is a functional programming language, it is also an object oriented language. In fact, R is what John Chambers called a *functional OOP* language (Chambers (2014)). I won't delve too much into what this means (read Wickham (2019) for this), but as a short discussion, consider the `print()` function. Depending on what type of object the user gives it, it seems as if somehow `print()` knows what to do with it:

```
print(5)
```

```
[1] 5
```

```
print(head(mtcars))
```

	mpg	cyl	disp	hp	drat	wt	qsec
	vs	am					
Mazda RX4	21.0	6	160	110	3.90	2.620	16.46
0 1							
Mazda RX4 Wag	21.0	6	160	110	3.90	2.875	17.02
0 1							
Datsun 710	22.8	4	108	93	3.85	2.320	18.61
1 1							
Hornet 4 Drive	21.4	6	258	110	3.08	3.215	19.44
1 0							
Hornet Sportabout	18.7	8	360	175	3.15	3.440	17.02
0 0							
Valiant	18.1	6	225	105	2.76	3.460	20.22
1 0							
	gear	carb					
Mazda RX4	4	4					
Mazda RX4 Wag	4	4					
Datsun 710	4	1					
Hornet 4 Drive	3	1					

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```
Hornet Sportabout      3      2
Valiant                3      1
```

```
print(str(mtcars))

'data.frame':   32 obs. of  11 variables:
 $ mpg : num  21 21 22.8 21.4 18.7 18.1 14.3 24.4
22.8 19.2 ...
 $ cyl  : num  6 6 4 6 8 6 8 4 4 6 ...
 $ disp : num  160 160 108 258 360 ...
 $ hp   : num  110 110 93 110 175 105 245 62 95 123
...
 $ drat: num  3.9 3.9 3.85 3.08 3.15 2.76 3.21 3.69
3.92 3.92 ...
 $ wt   : num  2.62 2.88 2.32 3.21 3.44 ...
 $ qsec: num  16.5 17 18.6 19.4 17 ...
 $ vs   : num  0 0 1 1 0 1 0 1 1 1 ...
 $ am   : num  1 1 1 0 0 0 0 0 0 0 ...
 $ gear: num  4 4 4 3 3 3 3 4 4 4 ...
 $ carb: num  4 4 1 1 2 1 4 2 2 4 ...
NULL
```

This works by essentially mixing both functional and object-oriented programming, hence functional OOP. Let's take a closer look at the source code of `print()` by simply typing `print` without brackets, into a console:

```
print

function (x, ...)
UseMethod("print")
<bytecode: 0x5608721ec598>
<environment: namespace:base>
```

Quite unexpectedly, the source code of `print()` is one line long and is just `UseMethod("print")`. So all `print()` does is use a generic method called “print”. If your text editor has auto-completion enabled, you might see that there are actually many `print()` functions. For example, type `print.data.frame` into a console:

```
print.data.frame

function (x, ..., digits = NULL, quote = FALSE,
right = TRUE,
row.names = TRUE, max = NULL)
{
  n <- length(row.names(x))
  if (length(x) == 0L) {
    cat(sprintf(ngettext(n, "data frame with 0
columns and %d row",
"data frame with 0 columns and %d
rows"), n), "\n",
sep = ""))
  }
  else if (n == 0L) {
    print.default(names(x), quote = FALSE)
    cat(gettext("<0 rows> (or 0-length
row.names)\n"))
  }
  else {
    if (is.null(max))
      max <-getOption("max.print", 99999L)
    if (!is.finite(max))
      stop("invalid 'max' /
getOption(\"max.print\"): ",
max)
  }
}
```

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```
omit <- (n0 <- max%/%length(x)) < n
m <- as.matrix(format.data.frame(if (omit)
  x[seq_len(n0), , drop = FALSE]
else x, digits = digits, na.encode = FALSE))
if (!isTRUE(row.names))
  dimnames(m)[[1L]] <- if
  (isFALSE(row.names))
    rep.int("", if (omit)
      n0
    else n)
  else row.names
print(m, ..., quote = quote, right = right,
max = max)
if (omit)
  cat(" [ reached 'max' /
getOption(\"max.print\") -- omitted",
  n - n0, "rows ]\n")
}
invisible(x)
}
<bytecode: 0x5608732ad808>
<environment: namespace:base>
```

This is the `print` function for `data.frame` objects. So what `print()` does, is look at the class of its argument `x`, and then look for the right `print` function to call. In more traditional OOP languages, users would type something like:

```
mtcars.print()
```

In these languages, objects encapsulate methods (the equivalent of our functions), so if `mtcars` is a data frame, it encapsulates a `print()` method that then does the printing. R is different, because classes and methods are kept separate. If a

package developer creates a new object class, then the developer also must implement the required methods. For example in the `{chronicler}` package, the `chronicler` class is defined alongside the `print.chronicler()` function to print these objects.

All of this to say that if you want to extend R by writing packages, learning some OOP essentials is also important. But for data analysis, functional programming does the job perfectly well. To learn more about R's different OOP systems (yes, R can do OOP in different ways and the one I sketched here is the simplest, but probably the most used as well), take a look at Wickham (2019).

6.4.2. purrr

The `{purrr}` package, developed by Posit (formerly RStudio), contains many functions to make functional programming with R more smooth. In the previous section, we discussed the `apply()` family of function; they all do a very similar thing, which is looping over a list and applying a function to the elements of the list, but it is not quite easy to remember which one does what. Also, for some of these functions like `apply()`, the list argument comes first, and then the function, but in the case of `mapply()`, the function comes first. This type of inconsistencies can be frustrating. Another issue with these functions is that it is not always easy to know what type the output is going to be. List? Atomic vector? Something else?

`{purrr}` solves this issue by offering the `map()` family of functions, which behave in a very consistent way. The basic function is called `map()` and we've already used it:

```
map(seq(1, 5), sqrt)
```

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```
[[1]]
```

```
[1] 1
```

```
[[2]]
```

```
[1] 1.414214
```

```
[[3]]
```

```
[1] 1.732051
```

```
[[4]]
```

```
[1] 2
```

```
[[5]]
```

```
[1] 2.236068
```

But there are many interesting variants:

```
map_dbl(seq(1, 5), sqrt)
```

```
[1] 1.000000 1.414214 1.732051 2.000000 2.236068
```

`map_dbl()` coerces the output to an atomic vector of doubles instead of a list of doubles. Then there's:

```
map_chr(letters, toupper)
```

```
[1] "A" "B" "C" "D" "E" "F" "G" "H" "I" "J" "K" "L"
```

```
"M" "N"
```

```
[15] "O" "P" "Q" "R" "S" "T" "U" "V" "W" "X" "Y" "Z"
```

for when the output needs to be an atomic vector of characters.

There are many others, so take a look at the documentation with `?map`. There's also `walk()` which is used if you're only interested in the side-effect of the function (for example if the function takes paths as input and saves something to disk).

`{purrr}` also has functions to replace `Reduce()`, simply called `reduce()` and `accumulate()`, and there are many, many other useful functions. Read through the documentation of the package⁴ and take the time to learn about all it has to offer.

6.4.3. `withr`

`{withr}` is a powerful package that makes it easy to “purify” functions that behave in a way that can cause problems. Remember the function from the introduction that randomly gave out a dish Bruno liked? Here it is again:

```
h <- function(name, food_list = list()){

  food <- sample(c("lasagna", "cassoulet",
  ↴ "feijoada"), 1)

  food_list <- append(food_list, food)

  print(paste0(name, " likes ", food))

  food_list
}
```

For the same input, this function may return different outputs so this function is not referentially transparent. So we improved

⁴<https://purrr.tidyverse.org/reference/index.html>

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the function by adding calls to `set.seed()` like this:

```
h2 <- function(name, food_list = list(), seed =
  ↵  123){

  # We set the seed, making sure that we get the
  ↵  same selection of food for a given seed
  set.seed(seed)
  food <- sample(c("lasagna", "cassoulet",
  ↵  "feijoada"), 1)

  # We now need to unset the seed, because if we
  ↵  don't, guess what, the seed will stay set
  ↵  for the whole session!
  set.seed(NULL)

  food_list <- append(food_list, food)

  print(paste0(name, " likes ", food))

  food_list
}
```

The problem with this approach is that we need to modify our function. We can instead use `withr::with_seed()` to achieve the same effect:

```
withr::with_seed(seed = 123,
                 h("Bruno"))
```

```
[1] "Bruno likes feijoada"
```

```
[[1]]
```

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```
[1] "feijoada"
```

It is also easier to create a wrapper if needed:

```
h3 <- function(..., seed){  
  withr::with_seed(seed = seed,  
                  h(...))  
}  
  
h3("Bruno", seed = 123)
```

```
[1] "Bruno likes feijoada"
```

```
[[1]]  
[1] "feijoada"
```

In a previous example we downloaded a dataset and loaded it into memory; we did so by first creating a temporary file, then downloading it and then loading it. Suppose that instead of loading this data into our session, we simply wanted to test whether the link was still working. We wouldn't want to keep the loaded data in our session, so to avoid having to delete it again manually, we could use `with_tempfile()`:

```
withr::with_tempfile("unemp", {  
  download.file(  
    "https://is.gd/l57cNX",  
    destfile = unemp)  
  load(unemp)  
  nrow(unemp)  
})
```

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[1] 472

The data got downloaded, and then loaded, and then we computed the number of rows of the data, without touching the global environment, or state, of our current session.

Just like for `{purrr}`, `{withr}` has many useful functions which I encourage you to familiarize yourself with⁵.

6.5. Conclusion

If there is only one thing that you should remember from this chapter, it would be pure functions. Writing pure functions is in my opinion not very difficult to do and comes with many benefits. But avoiding loops and replacing them with higher-order functions (`lapply()`, `Reduce()`, `purrr::map()` – and its variants –) also pays off. While this chapter stresses the advantages of functional programming, you should not forget that R is not a pure, and solely, functional programming language and that other paradigms, like object-oriented programming, are also available to you. So if your goal is to master the language (instead of “just” using it to solve data analysis problems), then you also need to know about R’s OOP capabilities.

⁵<https://withr.r-lib.org/reference/index.html>

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You now know about version control, how to collaborate using Github.com and functional programming. By only learning about this, you have already made some massive steps towards making your projects reproducible. Especially by using Git and Github. Even if you're using private repos and work in the private sector, by using version control, you ensure that reusing this code for future projects is much easier. Auditing is greatly simplified as well.

But this book is still far from over. Let's think about our project up until now. We have downloaded some data, and wrote code to analyse it. Fair enough. But usually, we don't really stop there. We now need to write a report, or maybe a Powerpoint presentation. If you're a researcher, you still need to write a paper, just getting the results is not enough, and if you work in the private sector, you also need to present the results of your analysis to management.

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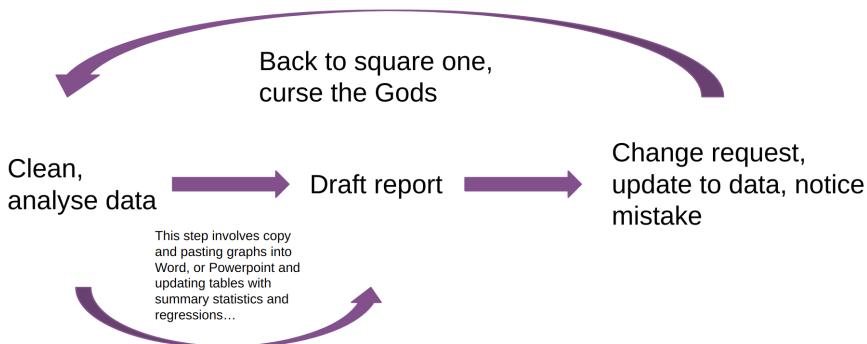


Figure 7.1.: The cursed report drafting loop.

The problem is that writing code, getting some results, and putting these results into a document (it doesn't matter what kind) is often very tedious. The picture above illustrates this cursed report drafting loop. Get some results, copy and paste images into Word or Powerpoint, get a change request, or notice a mistake, and start from scratch again. If you're using LaTeX it'll be easier for pictures, but you'll still need to update tables by hand each time you need to touch your analysis code.

Worse, what if you start with a Word or LaTeX document, but then get asked to make a Powerpoint presentation as well? Then you need to copy and paste everything again, but this time into Powerpoint... and if you get a change request after you're done and need to start over, you might seriously consider raising goats instead of dealing with this again.

But if we can make the loop look like this instead:

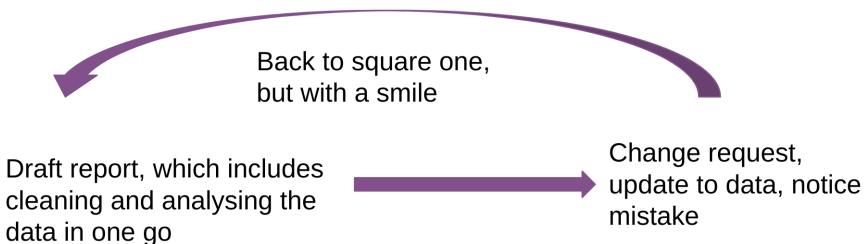


Figure 7.2.: The holy report drafting loop.

Basically, everything from cleaning, analysing and drafting is done in one single step? Well, this is what literate programming enables you to do. And even if you get asked to make a Powerpoint presentation, you can start from the same source code as the original report, and remove everything that you don't need and compile to a Powerpoint (or Beamer) presentation.

7.1. A quick history of literate programming

In literate programming, authors mix code and prose, which makes the output of their programs not just a series of tables, or graphs or predictions, but a complete report that contains the results of the analysis directly embedded into it. Scripts written using literate programming are also very easy to compile, or render, into a variety of document formats like `html`, `docx`, `pdf` or even `pptx`. R supports several frameworks for literate programming: `Sweave`, `knitr` and `Quarto`.

`Sweave` was the first tool available to R (and S) users, and allowed the mixing of R and LaTeX code to create a document. Friedrich Leisch developed `Sweave` in 2002 and described it in

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his 2002 paper (Leisch 2002). As Leisch argues, *the traditional way of writing a report as part of a statistical data analysis project uses two separate steps*: running the analysis using some software, and then copy and pasting the results into a word processing tool (as illustrated above). To really drive that point home: the problem with this approach is that much time is wasted copy and pasting things, so experimenting with different layouts or data analysis techniques is very time-consuming. Copy and paste mistakes will also happen (it's not a question of if, but when) and updating reports (for example, when new data comes in) means that someone will have, again, to copy and paste the updated results into a new document.

Sweave makes it possible to embed the analysis in the final document itself, by providing a way to mix LaTeX and R code which gets executed whenever the final, output document gets compiled. This gives practitioners considerable time savings because it eliminates the copy and pasting of results from R outputs into a document.

The snippet below shows the example from Leisch's paper:

```
\documentclass[a4paper]{article}  
  
\begin{document}
```

In this example we embed parts of the examples from the
\texttt{kruskal.test} help page into a LaTeX document:

```
<<>>=  
data (airquality)  
kruskal.test(Ozone ~ Month, data = airquality)  
@
```

which shows that the location parameter of the Ozone distribution varies significantly from month to month.

Finally we include a boxplot of the data:

```
\begin{center}
<<fig=TRUE,echo=FALSE>>=
boxplot(Ozone ~ Month, data = airquality)
@
\end{center}

\end{document}
```

Even if you've never seen a LaTeX source file, you should be able to figure out what's going on. The first line states what type of document we're writing. Then comes `\begin{document}` which tells the compiler where the document starts. Then comes the content. You can see that it's a mixture of plain English with R code defined inside chunks starting with `<<>>=` and ending with `@`. Finally, the document ends with `\end{document}`. Getting a human-readable PDF from this source is a two-step process: first, this source gets converted into a `.tex` file and then this `.tex` file into a PDF. Sweave is included with every R installation since version 1.5.0, and still works to this day. For example, we can test that our Sweave installation works just fine by compiling the example above. This is what the final output looks like:

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In this example we embed parts of the examples from the `kruskal.test` help page into a L^AT_EX document:

```
> data (airquality)
> kruskal.test(Ozone ~ Month, data = airquality)

Kruskal-Wallis rank sum test

data: Ozone by Month
Kruskal-Wallis chi-squared = 29.267, df = 4, p-value = 6.901e-06
```

which shows that the location parameter of the Ozone distribution varies significantly from month to month. Finally we include a boxplot of the data:

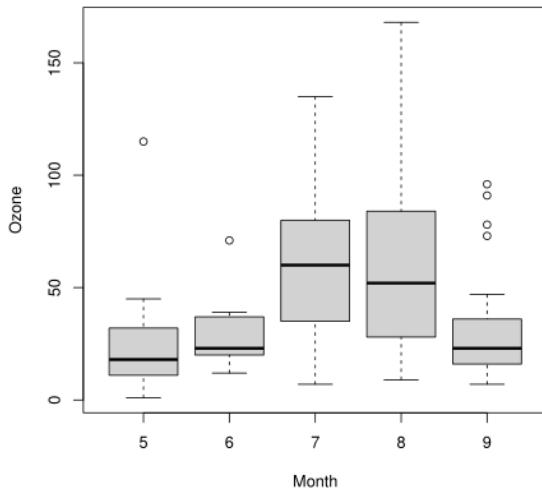


Figure 7.3.: More than 20 years later, the output is still the same.

Let me just state that the fact that it is still possible to compile this example more than 20 years later is an incredible testament to how mature and stable this software is (both R, Sweave, and

7.1. A quick history of literate programming

LaTeX). But as impressive as this is, LaTeX has a steep learning curve, and Leisch even advocated the use of the Emacs text editor to edit Sweave files, which also has a very steep learning curve (but this is entirely optional; for example, I've edited and compiled the example on the RStudio IDE).

The next generation of literate programming tools was provided by a package called `{knitr}` in 2012. From the perspective of the user, the biggest change from Sweave is that `{knitr}` is able to use many different formats as source files. The one that became very likely the most widely used format is a flavour of the Markdown markup language, R Markdown (Rmd). But this is not the only difference with Sweave: `{knitr}` can also run code chunks for other languages, such as Python, Perl, Awk, Haskell, bash and more (Xie 2014). Since version 1.18, `{knitr}` uses the `{reticulate}` package to provide a Python engine for the Rmd format.

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To illustrate the Rmd format, let's rewrite the example from Leisch's Sweave paper into it:

```
---
```

```
output: pdf_document
```

```
--
```

In this example we embed parts of the examples
↳ from the
\texttt{kruskal.test} help page into a LaTeX
↳ document:

```
```{r}  
data (airquality)
kruskal.test(Ozone ~ Month, data = airquality)
```
```

which shows that the location parameter of the
↳ Ozone
distribution varies significantly from month to
↳ month.

Finally we include a boxplot of the data:

```
```{r, echo = FALSE}  
boxplot(Ozone ~ Month, data = airquality)
```
```

This is what the output looks like:

7.1. A quick history of literate programming

In this example we embed parts of the examples from the `kruskal.test` help page into a L^AT_EX document:

```
data (airquality)
kruskal.test(Ozone ~ Month, data = airquality)

##
## Kruskal-Wallis rank sum test
##
## data: Ozone by Month
## Kruskal-Wallis chi-squared = 29.267, df = 4, p-value = 6.901e-06
```

which shows that the location parameter of the Ozone distribution varies significantly from month to month.
Finally we include a boxplot of the data:

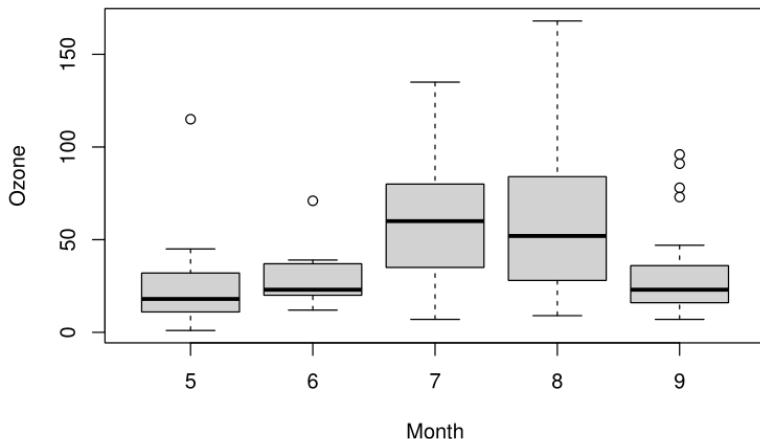


Figure 7.4.: It's very close to the Sweave output.

Just like in a Sweave document, an Rmd source file also has a header in which authors can define a number of general options. Here I've only specified that I wanted a pdf document as an output file. I then copy and pasted the contents from the Sweave source, but changed the chunk delimiters from <>>= and @ to `r` to start an R chunk and `r` to end it. Remember; we need to specify the engine in the chunk because {knitr} supports many engines. For example, it is possible to run a

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bash command by adding this chunk to the source:

```
---
```

```
output: pdf_document
```

```
--
```

In this example we embed parts of the examples
↳ from the
`\texttt{kruskal.test}` help page into a LaTeX
↳ document:

```
```{r}
data (airquality)
kruskal.test(Ozone ~ Month, data = airquality)
```
```

which shows that the location parameter of the
↳ Ozone
distribution varies significantly from month to
↳ month.

Finally we include a boxplot of the data:

```
```{r, echo = FALSE}
boxplot(Ozone ~ Month, data = airquality)
```
```

```
```{bash}
pwd
```
```

(bash's `pwd` command shows the current working directory). You may have noticed that I've also keep two LaTeX commands in the source Rmd, `\texttt{()}` and `\LaTeX`. This is because Rmd

7.1. A quick history of literate programming

files get first converted into `LaTeX` files and then into a PDF. If you’re using RStudio, this document can be compiled by clicking a button or using a keyboard shortcut, but you can also use the `rmarkdown::render()` function. This function does two things transparently: it first converts the Rmd file into a source `LaTeX` file, and then converts it into a PDF. It is of course possible to convert the document to a Word document as well, but in this case, `LaTeX` commands will be ignored. `Html` is another widely used output format.

If you’re a researcher and prefer working with `LaTeX` directly instead of having to switch to Markdown, you can either use `Sweave`, or use `{knitr}` but instead of writing your documents using the R Markdown format, you can use the `Rnw` format which is basically the same as `Sweave`, but uses `{knitr}` for compilation. Take a look at this example¹ from the `{knitr}` Github repository for example.

You should know that `{knitr}` makes it possible to author many, many different types of documents. It is possible to write books, blogs, package documentation (and even entire packages, as we shall see later in this book), Powerpoint slides... It is extremely powerful because we can use the same general R Markdown knowledge to build many different outputs.

¹<https://is.gd/Z7VS09>

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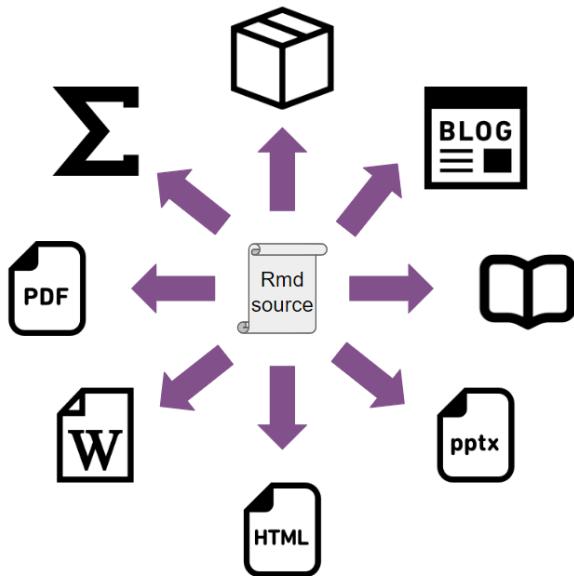


Figure 7.5.: One format to rule them all.

Finally, the latest in literate programming for R is a new tool developed by Posit, called Quarto. If you're an R user and already know `{knitr}` and the Rmd format, you should be able to immediately use Quarto. So what's the difference? In practice and for R users not much but there are some things that Quarto is able to do out of the box for which you'd need extensions with `{knitr}`. Quarto has some nice defaults; in fact, this book is written in Quarto's Markdown flavour and compiled with Quarto instead of `{knitr}` because the default Quarto output looks nicer than the default `{knitr}` output. However, there may even be things that Quarto can't do at all (at least for now) when compared to `{knitr}`. So why bother switching? Well, Quarto provides sane defaults and some nice features out of the box, and the cost of switching from the Rmd format to Quarto's Qmd format is basically 0. Also, and this is probably

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the biggest reason to use Quarto, Quarto is not tied to R. Quarto is actually a standalone tool that needs to be installed alongside your R installation, and works completely independently. In fact, you can use Quarto without having R installed at all, as Quarto, just like `{knitr}` supports many engines. This means that if you're primarily using Python, you can use Quarto to author documents that mix Python chunks and prose. Quarto also supports the Julia programming language and Observable JS, making it possible to include interactive visualisations into an Html document. Let's take a look at how the example from Leisch's paper looks as a Qmd (Quarto's flavour of Markdown) file:

```
---
```

```
output: pdf
```

```
--
```

```
In this example we embed parts of the examples
↳   from the
\texttt{\{kruskal.test\}} help page into a LaTeX
↳   document:
```

```
```{r}
data (airquality)
kruskal.test(Ozone ~ Month, data = airquality)
```
```

```
which shows that the location parameter of the
↳   Ozone
```

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```
distribution varies significantly from month to
↪ month.
```

Finally we include a boxplot of the data:

```
```{r, echo = FALSE}
boxplot(Ozone ~ Month, data = airquality)
```
```

(I've omitted the bash chunk from before, not because Quarto does not support it, but to keep close to the original example from the paper.)

As you can see, it's exactly the same as the Rmd file from before. The only difference is in the header. In the Rmd file I specified the output format as:

```
---
output: pdf_document
---
```

whereas in the Qmd file we changed it to:

```
---
output: pdf
---
```

7.1. A quick history of literate programming

While Quarto is the latest option in literate programming, it is quite recent, and as such, I feel it might be better to stick with `{knitr}` and the Rmd format for now, so that's what we're going to use going forward. Also, the `{knitr}` and the Rmd format are here to stay, so there's little risk in keeping using it, and anyways, as already stated, if switching to Quarto becomes a necessity, the cost of switching would be very, very low. In what follows, I won't be focused on anything really `{knitr}` or Rmd specific, so should you want to use Quarto instead, you should be able to follow along without any problems at all, since the Rmd and Qmd formats have so much overlap. Also, Quarto needs to be installed separately, but to use `{knitr}` and RMarkdown, no specific tools are necessary.

In the next two sections, I will show you how to set up and use `{knitr}` as well as give you a quick overview of the R Markdown syntax. However, we will very quickly focus on the templating capabilities of `{knitr}`: expanding text, using child documents, and parameterised reports. These are advanced topics and not easy to tackle if you're not comfortable with R already. Just as functions and higher-order functions like `lapply()` avoid having to repeat yourself, so does templating, but for literate programming. The goal is to write functions that return literal R Markdown code, so that you can loop over these functions to build entire sections of your documents. However, the learning curve for these features is quite steep, but by now, you should have noticed that this book expects a lot from you. Keep going, and you shall be handsomely rewarded.

7.2. {knitr} basics

This section will be a very small intro to {knitr}. I'm going to teach you just enough to get started writing Rmd files. Most, if not all, of what I'll be explaining here is also applicable to the Qmd format. There are many resources out there that you can use if you want to dig deeper, for instance the R Markdown website² from Posit, or the R Markdown: The Definitive Guide³ and R Markdown Cookbook⁴ eBooks. I will also not assume that you are using the RStudio IDE and give you instead the lower level commands to render documents. If you use RStudio and want to know how to use it effectively to author Rmd documents, you should take a look at this⁵ page. In fact, this section will basically focus on the same topics, but without RStudio.

7.2.1. Set up

The first step is to install the {knitr} and the {rmarkdown} packages. That's easy, just type:

```
install.packages("rmarkdown")
```

in an R console. Since {knitr} is required to install {rmarkdown}, it gets installed automatically. If you want to compile PDF documents, you should also have a working LaTeX distribution. You can skip this next part if you're only interested in generating Html and Word files. For what follows in the book, we will only be rendering Html documents,

²<https://rmarkdown.rstudio.com/lesson-1.html>

³<https://bookdown.org/yihui/rmarkdown/>

⁴<https://bookdown.org/yihui/rmarkdown-cookbook/>

⁵https://rmarkdown.rstudio.com/authoring_quick_tour.html

so no need to install LaTeX (by the way, you don't even need a working Word installation to compile documents to the `docx` format). However, if you already have a working LaTeX installation, you shouldn't have to do anything else to generate PDF documents. If you don't have a working LaTeX distribution, then Yihui Xie, the creator of `{knitr}` created an R package called `{tinytex}` which you can use to install a working LaTeX distribution very easily. In fact, this is the way I recommend installing LaTeX even if you're not an R user (it is possible to use the `tinytex` distribution without R; it's just that the `{tinytex}` R package provides many functions that makes installing and maintaining it very easy). Simply run these commands in an R console to get started:

```
install.packages("tinytex")
tinytex::install_tinytex()
```

and that's it! If you need to install specific LaTeX packages, then refer to the **Maintenance** section on `tinytex`'s⁶ website. For example, to compile the example from Leisch's article on Sweave discussed previously, the `grfext` LaTeX package needs to be installed (as explained by the error output in the console when I tried compiling). To install this package, you can use the `tlmgr_install()` function from `{tinytex}`:

```
tlmgr_install("grfext")
```

After you've installed `{knitr}`, `{rmarkdown}` and, optionally, `{tinytex}`, simply try to compile the following document:

⁶<https://yihui.org/tinytex/#maintenance>

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```
---
```

```
output: html_document
```

```
--
```

```
# Document title
```

```
## Section title
```

```
### Subsection title
```

```
This is **bold** text. This is *text in
```

```
↳ italics*.
```

```
My favourite programming language for statistics
```

```
↳ is ~~SAS~~ R.
```

save this document into a file called `rmd_intro.rmd` using your favourite text editor. Then render it into an Html file by running the following command in the R console:

```
rmarkdown::render("path/to/rmd_test.rmd")
```

This should create a file called `rmd_test.html`; open it with your web browser and you should see the following:

Document title

Section title

Subsection title

This is **bold** text. This is *text in italics*.

My favourite programming language for statistics is ~~SAS~~ R.

Figure 7.6.: This is how formatting looks like, once the document is compiled.

Congratulations, you just *knitted* your first Rmd document!

7.2.2. Markdown ultrabasics

R Markdown is a flavour of Markdown, which means that you should know some Markdown to really take full advantage of R Markdown. The example document from before should have already shown you some basics: titles, sections and subsections all start with a # and the depth level is determined by the number of #s. For bold text, simply put the words in between ** and for italics use only one *. If you want **bold and italics**, use ***. The original designer of Markdown did not think that underlining text was important, so there is no *easy* way of doing it, unfortunately. For this, you need to use a somewhat hidden feature; without going into too many technical details, the

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program that converts Rmd files to the final output format is called Pandoc, and it's possible to use some of Pandoc's features to format text. For example, for underlining:

```
[This is some underlined text in a R Markdown
↳ document]{.underline}
```

This will underline the text between square brackets.⁷

The next step is to mix code and prose. As you've seen from Leisch's canonical example, this is quite easily achieved by using R code chunks. The R Markdown example below shows various code chunks alongside some options. For example, a code chunk that uses the `echo = FALSE` option will not appear (but the output of the computation will):

```
---
title: "Document title"
output: html_document
date: "2023-01-28"
---

# R code chunks

This below is an R code chunk:

```{r}
data(mtcars)

plot(mtcars)
```

```

⁷<https://stackoverflow.com/a/68690065/1298051>

The code chunk above will appear in the final
↳ output.

The code chunk below will be hidden:

```
```{r, echo = FALSE}
data(iris)

plot(iris)
```
```

This next code chunk will not be evaluated:

```
```{r, eval = FALSE}
data(titanic)

str(titanic)
```
```

The last one below runs, but code and output
↳ from the code is
not shown in the final document. This is useful
↳ for loading

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libraries and hiding startup messages:

```
```{r, include = FALSE}
library(dplyr)
```
```

If you use RStudio and create a new R Markdown file from the menu, a template R Markdown file is generated for you to fill out. The first R chunk is this one:

```
```{r setup, include=FALSE}
knitr::opts_chunk$set(echo = TRUE)
```
```

This is an R chunk named `setup` with the option `include = FALSE` (so neither the chunk itself, nor the output it produces will be shown in the compiled document). Naming chunks is optional, but we are going to make use of this later on. The code that runs in this chunk defines a global option to show the source code from all the chunks by default (which is the default behaviour). You can change `TRUE` to `FALSE` if you want to hide every code chunk instead (if you're using Quarto, global options are set differently⁸).

Something else you might have noticed in the previous example, is that we've added some more content in the header:

```
---
title: "Document title"
output: html_document
date: "2023-01-28"
```

⁸<https://quarto.org/docs/computations/execution-options.html>

```
---
```

There are several other options available that you can define in the header. Later on, I will show you some more options, for example how to define a table of contents.

To finish this part on code chunks, you should know about inline code chunks. Take a look at the following example:

```
---
```

```
title: "Document title"  
output: html_document  
date: "2023-01-28"
```

```
---
```

```
# R code chunks
```

```
```{r, echo = FALSE}  
data(iris)
```
```

The iris dataset has `r nrow(iris)` rows.

The last sentence from this example has an inline code chunk. This is quite useful, as it allows to parameterise sentences and paragraphs, and thus avoids needing to copy and paste (and we will go quite far into how to avoid copy and pasting, thanks to more advanced features we will shortly discuss).

To finish this crash course, you should know that to use footnotes you need to write the following:

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This sentence has a footnote.^[^1]

[^1]: This is the footnote.

or the following (which I prefer):

This sentence has a footnote.<sup>[This is the
→ footnote]</sup>

and that you can write LaTeX formulas as well. For example, add the lines below into the example from before and render either a PDF or an HTML document (don't put the LaTeX formula below inside a chunk, simply paste it as if it were normal text. This doesn't work for Word output because Word does not support LaTeX equations):

```
\begin{align*}
S(\omega)
&= \frac{\alpha g^2}{\omega^5} e^{[-0.74\bigl(\frac{\omega U_\omega}{19.5}\bigr)g]}
&= \frac{\alpha g^2}{\omega^5} \exp\Bigl[-0.74\Bigl(\frac{\omega U_\omega}{19.5}\Bigr)g\Bigr]
\end{align*}
```

The LaTeX code above results in this equation:

$$\begin{aligned} S(\omega) &= \frac{\alpha g^2}{\omega^5} e^{[-0.74\left\{\frac{\omega U_{\omega} 19.5}{g}\right\}^{-4}]} \\ &= \frac{\alpha g^2}{\omega^5} \exp\left[-0.74\left\{\frac{\omega U_{\omega} 19.5}{g}\right\}^{-4}\right] \end{aligned}$$

Figure 7.7.: A rendered LaTeX equation.

7.3. Keeping it DRY

Remember; we never, ever, want to have to repeat ourselves. Copy and pasting is forbidden. Striving for 0 copy and pasting will make our code much more robust and likely to be correct.

To keep DRY, we started by using functions, as discussed in the previous chapter, but we can go much further than that. For example, suppose that we need to write a document that has the following structure:

- A title
- A section
- A table inside this section
- Another section
- Another table inside this section
- Yet another section
- Yet another table inside this section

Is there a way to automate the creation of such a document by taking advantage of the repeating structure? Of course there is. The question is not, *is it possible to do X?*, but *how to do X?*.

7. Literate programming

7.3.1. Generating R Markdown code from code

The example below is a fully working minimal example of this. Copy it inside a document titled something like `rmd_templating.Rmd` and render it. You will see that the output contains more sections than defined in the source. This is because we use templating at the end. Take some time to read the document, as the text inside explains what is going on:

```
---
```

```
title: "Templating"
output: html_document
date: "2023-01-27"
---
```

```
```{r setup, include=FALSE}
knitr::opts_chunk$set(echo = TRUE)
```
```

```
## A function that creates tables
```

```
```{r}
create_table <- function(dataset, var){
 table(dataset[var]) |>
 knitr::kable()
}
```
```

The function above uses the `table()` function
↳ to create frequency tables, and then this gets passed to
↳ the `knitr::kable()` function that produces a good
↳ looking table for our rendered document:

```
```{r}  
create_table(mtcars, "am")
```
```

Let's suppose that we want to generate a
↳ document that would look like this:

- first a section title, with the name of the
↳ variable of interest
- then the table

So it would look like this:

```
## Frequency table for variable: "am"  
```{r}  
create_table(mtcars, "am")
```

## 7. Literate programming

```
```
```

We don't want to create these sections for every variable by hand.

Instead, we can define a function that returns the R markdown code required to create this. This is this function:

```
```{r}
return_section <- function(dataset, var){
 a <- knitr::knit_expand(text = c(
 ## Frequency table for variable:
 {{variable}}",
 create_table(dataset, var)),
 variable = var)
 cat(a, sep = "\n")
}
```

```

This new function, `return_section()` uses `knitr::knit_expand()` to generate RMarkdown code. Words between `{{}}` get replaced by the provided `var` argument to the function. So when we call `return_section("am")`, `{{variable}}` is replaced by `"am"`. `"am"`

then gets passed down to `create_table()` and the frequency table gets generated.

We can now generate all the section by simply applying our function to a list of column names:

```
```{r, results = "asis"}
invisible(lapply(colnames(mtcars),
 ~ return_section, dataset = mtcars))
```

```

The last function, named `return_section()` uses `knit_expand()`, which is the function that does the heavy lifting. This function returns literal R Markdown code. It returns `## Frequency table for variable: {{variable}}` which creates a level 2 section title with the text *Frequency table for variable: xxx* where the `xxx` will get replaced by the variable passed to `return_section()`. So calling `return_section(mtcars, "am")` will print the following in your console:

```
## Frequency table for variable: am
am	Freq
0	19
1	13
```

We now simply need to find a clever way to apply this function to each variable in the `mtcars` dataset. For this, we are going to use `lapply()` which implements a for loop (you could use `purrr::map()` just as well for this):

```
invisible(lapply(colnames(mtcars),
  return_section,
  dataset = mtcars))
```

7. Literate programming

This will create, for each variable in `mtcars`, the same R Markdown code as above. Notice that the R Markdown chunk where the call to `lapply()` is has the option `results = "asis"`. This is because the function returns literal Markdown code, and we don't want the parser to have to parse it again. We tell the parser “don't worry about this bit of code, it's already good”. As you see, the call to `lapply()` is wrapped inside `invisible()`. This is because `return_section()` does not return anything, it just prints something to the console. No object is returned. `return_section()` is a function with only a side-effect: it changes something outside its scope. So if you don't wrap the call to `lapply()` inside `invisible()`, then a bunch of NULLs will also get printed (NULLs get returned by functions that don't return anything). To avoid this, use `invisible()` (and use `purrr::walk()` rather than `purrr::map()` if you want to use tidyverse packages and functions).

See the output here⁹.

This is not an easy topic, so take the time to play around with the example above. Try to print another table, try to generate more complex Markdown code, remove the call to `invisible()` and knit the document and see what happens with the output, replace the call to `lapply()` with `purrr::walk()` or `purrr::map()`. Really take the time to understand what is going on.

While extremely powerful, this approach using `knit_expand()` only works if your template only contains text. If you need to print something more complicated in the document, you need to use child documents instead. For example, suppose that instead of a table we wanted to show a plot made using `{ggplot2}`. This would not work, because a ggplot object is not made of

⁹<https://is.gd/EzdUtt>

text, but is a list with many elements. The `print()` method for `ggplot` objects then does some magic and prints a plot. But if you want to show plots using `knitr::knit_expand()`, then the contents of the list will be shown, not the plot itself. This is where child documents come in. Child documents are exactly what you think they are: they're smaller documents that get knitted and then embedded into the parent document. You can define anything within these child documents, and as such you can even use them to print more complex objects, like a `ggplot` object. Let's go back to the example from before and make use of a child document (for ease of presentation, we will not use a separate Rmd file, but will inline the child document into the main document). Read the Rmd example below carefully, as all the steps are explained:

```
---
```

```
title: "Templating with child documents"
output: html_document
date: "2023-01-27"
---
```

```
```{r setup, include=FALSE}
knitr::opts_chunk$set(echo = TRUE)
library(ggplot2)
```
```

```
## A function that creates ggplots
```

```
```{r}
create_plot <- function(dataset, aesthetic){
```

```
 ggplot(dataset) +
```

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```
geom_point(aesthetic)
}
```
```

The function above takes a dataset and an
↳ aesthetic
made using `ggplot2::aes()` to create a plot:

```
```{r}  
create_plot(mtcars, aes(y = mpg, x = hp))
```
```

Let's suppose that we want to generate a
↳ document
that would look like this:

- first a section title, with the dataset used;
- then a plot

So it would look like this:

```
## Dataset used: "mtcars"  
```{r}  
create_plot(mtcars, aes(y = mpg, x = hp))
```
```

We don't want to create these sections for every
↳
aesthetic by hand.

Instead, we can make use of a child document
↳ that
gets knitted separately and then embedded in the
↳
parent document. The chunk below makes use of
↳ this trick:

```
```{r, results = "asis"}  

x <- list(aes(y = mpg, x = hp),
 aes(y = mpg, x = hp, size = am))

res <- lapply(x,
 function(dataset, x){

knitr:::knit_child(text = c(

'\n',
'## Dataset used: `r
↳ deparse(substitute(dataset))`',
'\n',
'```{r, echo = F}',
'print(create_plot(dataset, x))',
'```'

)
envir = environment(),
quiet = TRUE)

}, dataset = mtcars)
```

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```
cat(unlist(res), sep = "\n")
```
```

The child document is the `text` argument to the
`knit_child()` function. `text` is literal R
Markdown code: we define a level 2 header, and then an R
chunk.

This child document gets knitted, so we need to
specify the environment in which it should get knitted.
This means that the child document will get knitted in the
same environment as the parent document (our current
global environment). This way, every package that gets
loaded and every function or variable that got defined
in the parent document will also be available to the
child document.

To get the dataset name as a string, we use the
`deparse(substitute(dataset))` trick; this
substitutes "dataset" by its bound value, so `mtcars`. But
`mtcars` is an expression and we don't want it to get
evaluated, or the

```
contents of the entire dataset would be used in
↳ the title
of the section. So we use `deparse()` which
↳ turns unevaluated
expressions into strings.
```

We then use `lapply()` to loop over two
 ↳ aesthetics with an
 anonymous function that encapsulates the child
 ↳ document. So we
 get two child documents that get knitted, one
 ↳ per aesthetic.
 This gets saved into variable `res`. This is
 ↳ thus a list of
 knitted Markdown.

Finally, we need unlist `res` to actually merge
 ↳ the Markdown
 code from the child documents into the parent
 ↳ document.

See the output here¹⁰.

Here again, take some time to play with the above example. Change the child document, try to print other types of output, really take your time to understand this. To know more about child documents, take a look at this section¹¹ of the R Markdown Cookbook (Xie, Dervieux, and Riederer 2020).

By the way, if you wish to add a table of contents to your document, change the header to this:

¹⁰<https://is.gd/aR2hyz>

¹¹<https://is.gd/gAqzf9>

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```
---
```

```
title: "Templating with child documents and TOC"
output:
  html_document:
    toc: true
    toc_float: true
date: "2023-01-27"
---
```

```
---
```

7.3.2. Tables in R Markdown documents

Getting tables right in Rmd documents is not always an easy task. There are several packages specifically made just for this task, and the package that I recommend tick the following two important boxes:

- Work the same way regardless of output format (Word, PDF or Html);
- Work for any type of table: summary tables, regression tables, two-way tables, etc.

Let's start with the simplest type of table, which would is a table that simply shows some rows of data. `{knitr}` comes with the `kable()` function, but this function generates a very plain looking output. For something publication-worthy, we recommend the `{flextable}` package, developed by Gohel and Skintzos (2023):

```
library(flextable)

my_table <- head(mtcars)
```

```
flextable(my_table) |>
  set_caption(caption = "Head of the mtcars
    ↵ dataset") |>
  theme_booktabs()
```

| mpg | cyl | disp | hp | drat | wt | qsec | vs | am | gear | carb |
|------|-----|------|-----|------|-------|-------|----|----|------|------|
| 21.0 | 6 | 160 | 110 | 3.90 | 2.620 | 16.46 | 0 | 1 | 4 | 4 |
| 21.0 | 6 | 160 | 110 | 3.90 | 2.875 | 17.02 | 0 | 1 | 4 | 4 |
| 22.8 | 4 | 108 | 93 | 3.85 | 2.320 | 18.61 | 1 | 1 | 4 | 1 |
| 21.4 | 6 | 258 | 110 | 3.08 | 3.215 | 19.44 | 1 | 0 | 3 | 1 |
| 18.7 | 8 | 360 | 175 | 3.15 | 3.440 | 17.02 | 0 | 0 | 3 | 2 |
| 18.1 | 6 | 225 | 105 | 2.76 | 3.460 | 20.22 | 1 | 0 | 3 | 1 |

Figure 7.8.: The output of the code above.

Note that the example above will work pretty much the same way for any table that you can coerce into a data frame! I won't explain how `{flextable}` works, but it is very powerful, and the fact that it works for PDF, Html, Word and Powerpoint outputs is really a massive plus. If you want to learn more about `{flextable}`, there's a whole, free, ebook on it¹². `{flextable}` can create very complicated tables, so really take the time to dig in!

The next package is `{modelsummary}`, by Arel-Bundock (2022), and this one focuses on regression and summary tables. It is extremely powerful as well, and just like `{flextable}`, works for any type of output. It is very simple to get started:

¹²<https://ardata-fr.github.io/flextable-book/index.html>

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```
library(modelsummary)

model_1 <- lm(mpg ~ hp + am, data = mtcars)
model_2 <- lm(mpg ~ hp, data = mtcars)

models <- list("Model 1" = model_1,
               "Model 2" = model_2)

modelsummary(models)
```

| | Model 1 | Model 2 |
|-------------|-------------------|-------------------|
| (Intercept) | 26.585
(1.425) | 30.099
(1.634) |
| hp | -0.059
(0.008) | -0.068
(0.010) |
| am | 5.277
(1.080) | |
| Num.Obs. | 32 | 32 |
| R2 | 0.782 | 0.602 |
| R2 Adj. | 0.767 | 0.589 |
| AIC | 164.0 | 181.2 |
| BIC | 169.9 | 185.6 |
| Log.Lik. | -78.003 | -87.619 |
| RMSE | 2.77 | 3.74 |

Figure 7.9.: Estimated models are shown side by side.

Here again, I won't get into much detail, but recommend instead that you read the package's website¹³ which has very detailed documentation.

These packages can help you keeping it DRY, so take some time

¹³<https://is.gd/pjIKmV>

to learn them.

And one last thing: if you're a researcher, take a look at the `{rticles}`¹⁴ package, which provides Rmd templates to write articles for many scientific journals.

7.3.3. Parametrized reports

Templating and child documents are very powerful, but sometimes you don't want to have one section dedicated to each unit of analysis within the same report, but rather, you want a complete separate report by unit of analysis. This is possible thanks to parameterised reports.

Let's change the example from before, which consisted of creating one section per column of the `mtcars` dataset and a frequency table, and make it now one separate report for each column. The R Markdown file will look like this:

```
---
title: "Report for column `r params$var` of
  ↵ dataset `r params$dataset`"
output: html_document
date: "2023-01-27"
params:
  dataset: mtcars
  var: "am"
---

```{r setup, include=FALSE}
knitr::opts_chunk$set(echo = TRUE)
```

---

<sup>14</sup><https://pkgs.rstudio.com/rticles/articles/examples.html>

## 7. Literate programming

```

```
## Frequency table for `r params$var`  
  
```{r, echo = F}  
create_table <- function(dataset, var){

 dataset <- get(dataset)

 table(dataset[var]) |>
 knitr::kable()
}
```
```

The table below is for variable `r params\$var`
 ↳ of
dataset `r params\$dataset`.

```
```{r}  
create_table(params$dataset, params$var)
```
```

```
```{r, eval = FALSE, echo = FALSE}  
Run these lines to compile the document
Set eval and echo to FALSE, so that this does
 ↳ not appear
```

```

in the output, and does not get evaluated when
knitting
rmarkdown::render(
 input = "param_report_example.Rmd",
 params = list(
 dataset = "mtcars",
 var = "cyl"
)
)
```

```

Save the code above into an Rmd file titled something like `param_report_example.Rmd` (preferably inside its own folder). Note that at the end of the document, I wrote the lines to render this document inside a chunk that does not get shown to the reader, nor gets evaluated:

```

```{r, eval = F, echo = FALSE}
rmarkdown::render(
 input = "param_report_example.Rmd",
 params = list(
 dataset = "mtcars",
 var = "cyl"
)
)
```

```

You need to run these lines yourself to knit the document.

This will pass the list `params` with elements “`mtcars`” and “`cyl`” down to the report. Every `params$dataset` and `params$var` in the report gets replaced by “`mtcars`” and “`cyl`” respectively.

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Also, notice that in the header of the document, I defined default values for the params. Something else you need to be aware of, is that the function `create_table()` inside the report is slightly different than before. It now starts with the following line:

```
dataset <- get(dataset)
```

Let's break this down. `params$dataset` contains the string "mtcars". I made the decision to pass the dataset as a string, so that I could use it in the title of the document. But then, inside the `create_table()` function, I have the following code:

```
dataset[var]
```

`dataset` can't be a string here, but needs to be a variable name, so `mtcars` and not "mtcars". This means that I need to *convert* that string into a name. `get()` searches an object by name, and then makes it possible to save it to a new variable called `dataset`. The rest of the function is then the same as before. This little difficulty can be avoided by hard-coding the dataset inside the R Markdown file, or by passing the dataset as the `params$dataset` and not the string, in the render function. However, if you pass down the name of the dataset as a variable instead of the dataset name as a string, then you need to convert it to a string if you want to use it in the text (so `mtcars` to "mtcars", using `deparse(substitute(dataset))` as in child documents example).

If you instead want to create one report per variable, you could compile all the documents at once with:

```
```{r, eval = F, echo = F}
columns <- colnames(mtcars)
```

```
lapply(columns,
 (\(x)rmarkdown::render(
 input =
 "param_report_example.Rmd",
 output_file = paste0(
 "param_report_example_",
 x, ".html"
),
 params = list(
 dataset = "mtcars",
 var = x
)
)
)
```
}
```

By now, this should not intimidate you anymore; I use `lapply()` to loop over a list of column names (that I get using `colnames()`). Because I don't want to overwrite the report I need to change the name of the output file. I do so by using `paste0()` which creates a new string that contains the variable name, so each report gets its own name. `x` inside the `paste0()` function is each element, one after the other, of the `columns` variable I defined first. Think of it as the `i` in a for loop. I then must also pass this to the `params` list, hence the `var = x`. The complete call to `rmarkdown::render()` is wrapped inside an anonymous function, because I need to use the argument `x` (which is each column defined in the `columns` list) in different places.

7.4. Conclusion

Before continuing, I highly recommend that you try running this yourself, and also that you try to build your own little parameterised reports. Maybe start by replacing “mtcars” by “iris” in the code to compile the reports and see what happens, and then when you’re comfortable with parameterised reports, try templating inside a parameterised report!

It is important not to succumb to the temptation of copy and pasting sections of your report, or parts of your script, instead of using these more advanced features provided by the language. It is tempting, especially under time pressure, to just copy and paste bits of code and get things done instead of writing what seems to be unnecessary code to finally achieve the same thing. The problem, however, is that in practice copy and pasting code to simply get things done will come bite you sooner rather than later. Especially when you’re still in the exploration/drafting phase of the project. It may take more time to set up, but once you’re done, it is much easier to experiment with different parameters, test the code or even re-use the code for other projects. Not only that but forcing you to actually think about how to set up your code in a way that avoids repeating yourself also helps with truly understanding the problem at hand. What part of the problem is constant and does not change? What does change? How often, and why? Can you also fix these parts or not? What if instead of five sections that I need to copy and paste, I had 50 sections? How would I handle this?

Asking yourself these questions, and solving them, will ultimately make you a better programmer.

Remember: don’t repeat yourself!

8. Conclusion of part 1

We're at the end of part 1, and I need to congratulate you for making it this far. If you took the time to digest what we've learned up until now, you should be ready for what's coming, which should be a bit easier, at least some of the parts.

But before continuing, let's quickly summarise what we've learned so far.

We started our journey with two scripts that download and analyse data about housing in Luxembourg. We then learned about tools and programming paradigms that we will now use in part 2 to make our scripts more robust:

- Version control;
- Functional programming;
- Literate programming.

In some ways, you might think that we've made our life unnecessarily complicated for very little gain. For example, functional programming seems to be only about putting restrictions on how you code. Same with using trunk-based development; why make it so restrictive?

What you need to understand is that these restrictions actually play a role. They force us to work in a much more structured way, which then ensures that our projects will be well-managed and ultimately reproducible. So while these techniques come with a cost, the benefits are far greater.

8. Conclusion of part 1

We will start part 2 by rewriting our scripts using what we've learned, and then, we will think about approaching the core problem differently, and structuring our project not as a series of scripts (or R Markdown files in the case of literate programming) but instead as a pipeline. Because until now, there's still no pipeline and let me remind you that this book has the word "pipeline" in its title.

We will also learn about tools that capture the computational environment that was used to set up this pipeline and how to use them effectively to make sure that our project is reproducible.

Part II.

Part 2: Write IT down

In this part of the book, we are now going to focus on the second main idea of this book: Write IT down. We now need to acknowledge that our brains are fallible (and ageing) and thus we need to write down many safeguards to ensure that our analyses can be of high quality.

We cannot leave code quality, documentation and finally its reproducibility to chance. We need to write down everything we need to ensure the long-term reproducibility of our pipelines.

The reproducibility iceberg

I think it is time to reflect on why I bothered with the first part of the book at all, because for now, I didn't really teach you anything directly related to reproducibility, so why didn't I just jump straight to the reproducibility part?

Remember the introduction, where I talked about the reproducibility continuum or spectrum? It is now time to discuss this in greater detail. I propose a new analogy, *the reproducibility iceberg*:

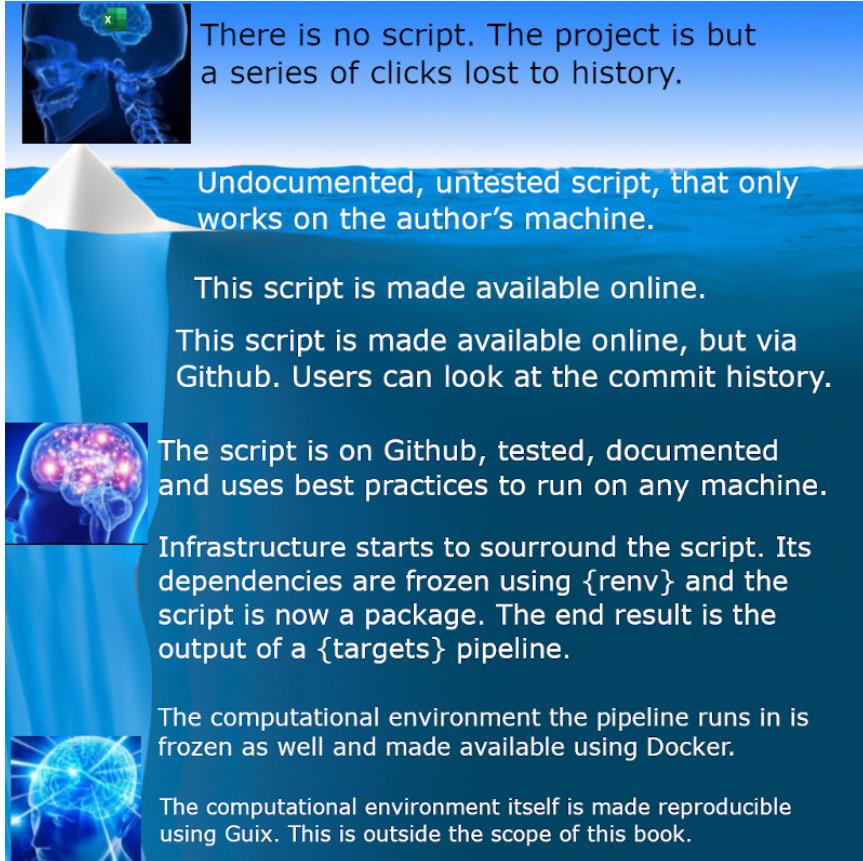


Figure 8.1.: The reproducibility iceberg.

Why an iceberg? Because the parts of the iceberg that you see, those that are obvious, are like running your analyses in a click-based environment like Excel. This is what's obvious, what's easy. No special knowledge or even training is required. All that's required is time, so people using these tools are not efficient and thus compensate by working insane hours (*I can't go home and enjoy time with my family I have to stay at the office and update the spreadsheet furiously*).

Let's go one level deeper: let's write a script. This is where we started. Our script was not too bad, it did the job. Unlike a click-based workflow, we could at least re-read it, someone else could read it, and it would be possible to run in the future but likely with some effort unless we're lucky. By that, I mean that for such a script to run successfully in the future, that script cannot rely on packages that got updated in such a way that the script cannot run anymore (for example, if functions get renamed, or if their arguments get renamed). Furthermore, if that script relies on a data source, the original authors also have to make sure that the same data source stays available. Another issue is collaborating when writing this script. Without any version control tools nor code hosting platform, collaborating on this script can very quickly turn into a nightmare.

This is where Git and Github.com came into play, one level deeper. The advantage now is that collaboration was streamlined. The commit history is available to all the teammates and it is possible to revert changes, experiment with new features using branches and overall manage the project. In this layer we also employ new programming paradigms to make the code of the project less verbose, using functional programming, with the added benefits of making it easier to test, document and share (which we will discuss to its fullest in this part of the book). Using literate programming, it is also much easier to go to our final output (which is usually a report). We implemented DRY ideas to the fullest to ensure that our code was of high quality.

At this depth, we are at a pivotal moment: in many cases, analysts may want to stop here because there is no more time or budget left. After all, the results were obtained and shared with higher-ups. It can be difficult, in some contexts, to justify spending more time to go deeper and write tests, documentation and otherwise ensure total reproducibility. So at this stage, we

will see what we can do that is *very cheap* (in both time and effort) to ensure the minimal amount of reproducibility, which is recording packages versions. Recording packages means that the exact same versions of the packages that were used originally will get used regardless of *when* in the future we rerun the analysis.

But if budget and time allow we can still go deeper, and definitely should. One day, you will want to update your script to use the newest functionality of your preferred package, but with package version recording, you will be stuck in the past with a very old version and its dependencies. How will you know that upgrading this package will not break anything anywhere in your workflow? Also, we want to make running the script as easy as possible, and ideally, *as non-interactively as possible*. Indeed, any human interaction with the analysis is a source of errors. That's why we need to thoroughly and systematically test our code. These tests also need to run non-interactively. Using the tools described in part two of this book, we can actually set up the project, right from the very beginning, in a way that it will be reproducible quite naturally. By using the right tools and setting things up right, we don't really need to invest more time to make things reproducible. The project will simply be reproducible because it was engineered that way. And I insist, at practically no additional cost!

Another problem with only recording packages's version is that in practice, it is very often not enough. This is because installing older versions of packages can be a challenge. This can be the case for two reasons:

- These older packages need also an older version of R, and installing old versions of R can be tricky, depending on your operating system;

- These older packages might need to get compiled and thus depend themselves on older versions of development libraries needed for compilation.

So to solve this issue, we will also need a way to freeze the computational environment itself, and this is where we will use Docker.

Finally, and this is the last level of the iceberg and not part of this book, is the need to make the building of the computational environment reproducible as well. *Guix* is the tool that enables one to do just that. However, this is a very deep topic unto itself, and there are workarounds to achieve this using Docker, so that's why we will not be discussing *Guix*.

We will travel down the iceberg in the coming chapters. First, we will use what we've learned up until now to rewrite our project using functional and literate programming. Our project will not be two scripts anymore, but two Rmarkdown files that we can knit and that we can then read and also send to non-technical stakeholders.

Then, we are going to turn these two Rmds files into a package. This will be done by using Sébastien Rochette's package `{fusen}`¹. `{fusen}` makes it very easy to go from our Rmd files to a package, by using what Sébastien named the *Rmarkdown first* method. If at this stage it's not clear why you would want to turn your analysis into a package, don't worry, it'll be once we're done with this chapter.

Once we have a package, we can use `{testthat}` for unit testing, and base R functions for assertive programming. At this stage, our code should be well-documented, easy to share, and thoroughly tested.

¹<https://thinkr-open.github.io/fusen/>

I think I should emphasize the following: I started from very simple scripts, which is how most analyses are done. Then, using functional and literate programming, these scripts got turned into RMarkdown files, and in this part of the book these RMarkdown files will get turned into a package. It is important to understand the following point: I did this to illustrate how we can go from these simple scripts to something more robust, step by step. Of course, later, you can immediately start from either the RMarkdown files or from the package. My advice is to start from the package, because as you shall see, starting from the package is basically the same amount of effort as starting from a simple RMarkdown file, thanks to `{fusen}`, but now you have the added benefits of using package development facilities to improve your analysis.

Once you have the package, you can build a true pipeline using `{targets}`, an incredibly useful library for build automation (but if you prefer to keep it at simple RMarkdown files, you can also use `{targets}`, you *don't have to* build a package).

Once we reached this stage, this is when we can finally start introducing reproducibility concretely. The reason it will take so long to actually make our pipeline reproducible is that we need solid foundations. There is no point in making a shaky analysis reproducible.

9. Rewriting our project

In this chapter, we will use what we've learned until now to rewrite our project. As a reminder, here are the scripts we wrote together:

- `save_data.R`: <https://is.gd/7PhUjd>
- `analysis.R`: <https://is.gd/X7XXJg>

The `analysis.R` file already includes one change: the one from the chapter on collaborating with Github, where Bruno wrote a function to make the plots for each commune.

If you skipped part one of the book, or for any other reason do not have a Github repository with these two files yet, then now is the time to do so. Create a repository and name it *housing_lux* or anything you'd like, and put these two files there. I will assume that you have these files safely versioned, and will not be telling you systematically when to commit and push. Simply do so as often as you'd like! You should have a repository with a *master* or *main* branch containing these two scripts. On your computer, calling `git status` in Git Bash (on Windows) or in a terminal (for Linux and macOS) should result in this:

```
owner@localhost $ git status
```

9. Rewriting our project

```
On branch master  
nothing to commit, working tree clean
```

If that's the case, congrats, we can start working. Start by creating a new branch, and call it `rmd`:

```
owner@localhost $ git checkout -b rmd
```

```
Switched to a new branch 'rmd'
```

We will now be working on this branch, simply work as usual, but when pushing, make sure to push to the `rmd` branch:

```
owner@localhost $ git add .  
owner@localhost $ git commit -m "some changes"  
owner@localhost $ git push origin rmd
```

This will push whatever changes you've made to files to the `rmd` branch. By using two branches like this, you keep the original `.R` scripts in the main branch, and then will end up with the `.Rmd` files in the `rmd` branch.

Before moving forward now is the right moment to actually discuss why you would want to convert the script into Rmds. There are several reasons. First, as argued in the chapter on literate programming, a document that mixes prose and code is easier to read and share than a script. Next, since this Rmd file can get knitted into any type of document (PDF, Word, etc...), it also makes it easier to arrive at what interests us, the output. A script is simply a means, it's not an end. The end is (in most cases) a document so we might as well use literate programming to avoid the cursed loop of changing the script, editing the doc-

ument, going back to the script, etc.

But there is yet another benefit; even if the Rmd file is not supposed to get shared with anyone else, we will, later on, use it as our starting point for the *Rmd first* method of package development as promoted by Sébastien Rochette, the author of `{fusen}`. This Rmd first method involves making use of a *development* Rmd file that contains all the usual steps that we would take to create a package. This is in contrast with the usual package development process, in which we would type the required commands to build the package in the terminal. The functions, tests, and documentation that we want to add to the package get defined using Rmd files as well. This makes them much easier to read and also share with a non-technical audience. All these Rmd files can then be converted (or *inflated* in `{fusen}` jargon) to create a fully working package. If this sounds complicated or confusing, don't worry. Trust the process, push on, and all the pieces of the puzzle will elegantly fit together in a couple of chapters.

In the following sections I will rewrite the scripts by using functional and literate programming: if you don't want to rewrite everything, don't worry, I link the final Rmd files at the end of each section. But I would advise that you follow along by writing everything as it will make absorbing the contents much simpler.

9.1. An Rmd for cleaning the data

So, let's start with the `save_data.R` script. Since we are going to use functional programming and literate programming, we are going to start from an empty `.Rmd` file. So open an empty `.Rmd` file and start with the following lines:

9. Rewriting our project

```
---
```

```
title: "Nominal house prices data in Luxembourg"
  ↵ - Data cleaning"
author: "Put your name in here"
date: "`r Sys.Date()`"
```

```
---
```

```
```{r, warning=FALSE, message=FALSE}
library(dplyr)
library(ggplot2)
library(janitor)
library(purrr)
library(readxl)
library(rvest)
library(stringr)
```
```

```
## Downloading the data
```

We start by writing a header to define the title of the document, the name of the author and the current date using inline R code (you can also hardcode the date as a string if you prefer). We then load packages in a chunk with options `warning=FALSE` and `message=FALSE` which will avoid showing packages' startup messages in the knitted document.

Then we start with a new section called `## Downloading the data`. We then add a paragraph explaining from where and how we are going to download the data:

9.1. An Rmd for cleaning the data

This data is downloaded from the Luxembourgish
↳ [Open Data
Portal] ([https://data.public.lu/fr/datasets/
↳ prix-annonces-des-logements-par-commune/](https://data.public.lu/fr/datasets/prix-annonces-des-logements-par-commune/))
(the data set called *Série rétrospective des
↳ prix
annoncés des maisons par commune, de 2010 à
↳ 2021*),
and the original data is from the "Observatoire
↳ de
l'habitat". This data contains prices for houses
↳ sold
since 2010 for each luxembourgish commune.

The function below uses the permanent URL from
↳ the Open Data
Portal to access the data, but I have also
↳ rehosted the data,
and use my link to download the data (for
↳ archival purposes):

This is much more detailed than using comments in a script, one of the benefits of literate programming. Then comes a function to download and get the data. This function simply wraps the lines from our original script that did the downloading and the cleaning. As a reminder, here are the lines from the original script, which I will then rewrite as a function:

```
url <- "https://is.gd/1vvBAC"  
  
raw_data <- tempfile(fileext = ".xlsx")
```

9. Rewriting our project

```
download.file(url, raw_data, method = "auto",
← mode = "wb")

sheets <- excel_sheets(raw_data)

read_clean <- function(..., sheet){
  read_excel(..., sheet = sheet) |>
    mutate(year = sheet)

  raw_data <- map(
    sheets,
    ~read_clean(raw_data,
                skip = 10,
                sheet = .)
  ) |>
    bind_rows() |>
    clean_names()

  raw_data <- raw_data |>
    rename(
      locality = commune,
      n_offers = nombre_doffres,
      average_price_nominal_euros =
        ↵ prix_moyen_annonce_en_courant,
      average_price_m2_nominal_euros =
        ↵ prix_moyen_annonce_au_m2_en_courant,
      average_price_m2_nominal_euros =
        ↵ prix_moyen_annonce_au_m2_en_courant
    ) |>
    mutate(locality = str_trim(locality)) |>
    select(year, locality, n_offers,
          ↵ starts_with("average"))
```

9.1. An Rmd for cleaning the data

and here is the same code, but as a function:

```
```{r, eval = FALSE}
get_raw_data <- function(url =
 "https://is.gd/1vvBAc"){

 raw_data <- tempfile(fileext = ".xlsx")

 download.file(url,
 raw_data,
 mode = "wb")

 sheets <- excel_sheets(raw_data)

 read_clean <- function(..., sheet){
 read_excel(..., sheet = sheet) %>%
 mutate(year = sheet)
 }

 raw_data <- map_dfr(
 sheets,
 ~read_clean(raw_data,
 skip = 10,
 sheet = .)) %>%
 clean_names()

 raw_data %>%
 rename(
 locality = commune,
 n_offers = nombre_doffres,
 average_price_nominal_euros =
 prix_moyen_annonce_en_courant,
```

## 9. Rewriting our project

```
 average_price_m2_nominal_euros =
 ↵ prix_moyen_annonce_au_m2_en_courant,
 average_price_m2_nominal_euros =
 ↵ prix_moyen_annonce_au_m2_en_courant
) %>%
 mutate(locality = str_trim(locality)) %>%
 select(year, locality, n_offers,
 ↵ starts_with("average"))

}
```
```

As you see, it's almost exactly the same code. So why use a function? Our function has the advantage that it uses the url of the data as an argument. This means that we can use it on other datasets (let's remember that we are here focusing on prices of houses, but there's another dataset of prices of apartments) or use it on an updated version of this dataset (which gets updated yearly). We can now more easily re-use this function later on (especially once we've turned this Rmd into a package in the next chapter). You can decide to show the source code of the function or hide it with the chunk option `include=FALSE` or `echo=FALSE` (the difference between `include` and `echo` is that `include` hides both the source code chunk and the output of that chunk). Showing the source code in the output of your Rmd file can be useful if you want to share it with other developers. The next part of the Rmd file is simply using the function we just wrote:

```
```{r}  
raw_data <- get_raw_data(url =
 ↵ "https://is.gd/1vvBAc")
```

## 9.1. An Rmd for cleaning the data

```

We can now continue by explaining what's wrong with the data and what cleaning steps need to be taken:

We need clean the data: "Luxembourg" is
↳ "Luxembourg-ville" in 2010 and 2011,
then "Luxembourg". "Pétange" is also spelt
↳ non-consistently, and we also need
to convert columns to the right type. We also
↳ directly remove rows where the
locality contains information on the "Source":

```
```{r}
clean_raw_data <- function(raw_data){
 raw_data %>%
 mutate(locality =
 ifelse(grepl("Luxembourg-Ville", locality),
 "Luxembourg",
 locality),
 locality = ifelse(grepl("P.tange",
 locality),
 "Pétange",
 locality)
) %>%
 filter(!grepl("Source", locality)) %>%
 mutate(across(starts_with("average"),
 as.numeric))
}
```
```{r}
```

## 9. Rewriting our project

```
flat_data <- clean_raw_data(raw_data)
````
```

The chunk above explains what we're doing and why we're doing it, and so we write a function (based on what we already wrote). Here again, the advantage of having this as a function will make it easier to run on updated data.

We now continue with establishing a list of communes:

```
We now need to make sure that we got all the
↳ communes/localities
in there. There were mergers in 2011, 2015 and
↳ 2018. So we need
to account for these localities.
```

```
We're now scraping data from Wikipedia of former
↳ Luxembourgish communes:
```

```
```{r}
get_former_communes <- function(
 url = "https://w.wiki/_wFe7",
 min_year = 2009,
 table_position = 3
){

 read_html(url) %>%
 html_table() %>%
 pluck(table_position) %>%
 clean_names() %>%
 filter(year_dissolved > min_year)
}
```

## 9.1. An Rmd for cleaning the data

```
```{r}
former_communes <- get_former_communes()
````
```

We can scrape current communes:

```
```{r}
get_current_communes <- function(
    url = "https://w.wiki/6nPu",
    table_position = 1
){

  read_html(url) %>%
    html_table() %>%
    pluck(table_position) %>%
    clean_names()
}

````

```{r}
current_communes <- get_current_communes()
````
```

This is quite a long chunk, but there is nothing new in here, so I won't explain it line by line. What's important is that the code doing the actual work is all being wrapped inside functions. I reiterate: this will make reusing, testing and documenting much easier later on. Using the objects `former_communes` and `current_communes` we can now build the complete list:

## 9. Rewriting our project

Let's now create a list of all communes:

```
```{r}
get_test_communes <- function(former_communes,
  ↵  current_communes){

  communes <- unique(c(former_communes$name,
  ↵  current_communes$commune))
  # we need to rename some communes

  # Different spelling of these communes between
  ↵  wikipedia and the data

  communes[which(communes == "Clemency")] <-
  ↵  "Clémency"
  communes[which(communes == "Redange")] <-
  ↵  "Redange-sur-Attert"
  communes[which(communes ==
  ↵  "Erpeldange-sur-Sûre")] <- "Erpeldange"
  communes[which(communes == "Luxembourg-City")]
  ↵  <- "Luxembourg"
  communes[which(communes == "Käerjeng")] <-
  ↵  "Kaerjeng"
  communes[which(communes == "Petange")] <-
  ↵  "Pétange"

  communes
}

```
```{r}
```

9.1. An Rmd for cleaning the data

```
former_communes <- get_former_communes()  
current_communes <- get_current_communes()  
  
communes <- get_test_communes(former_communes,  
                                ↵ current_communes)  
```
```

Once again, we write a function for this. We need to merge these two lists, and need to make sure that the spelling of the communes' names is unified between this list and between the communes' names in the data.

We now run the actual test:

```
Let's test to see if all the communes from our
↪ dataset are represented.
```

```
```{r}  
setdiff(flat_data$locality, communes)  
```
```

```
If the above code doesn't show any communes,
↪ then this means that we are
accounting for every commune.
```

This test is quite simple, and we will see how to create something a bit more robust and useful later on.

Now, let's extract the national average from the data and create a separate dataset with the national level data:

## 9. Rewriting our project

Let's keep the national average in another  
↪ dataset:

```
```{r}
make_country_level_data <- function(flat_data){
  country_level <- flat_data %>%
    filter(grepl("nationale", locality)) %>%
    select(-n_offers)

  offers_country <- flat_data %>%
    filter(grepl("Total d.offres", locality))
  ↵ %>%
    select(year, n_offers)

  full_join(country_level, offers_country) %>%
    select(year, locality, n_offers,
  ↵ everything()) %>%
    mutate(locality = "Grand-Duchy of
  ↵ Luxembourg")

}

```
```{r}
country_level_data <-
  ↵ make_country_level_data(flat_data)
```
```

```

and finally, let's do the same but for the commune level data:

9.1. An Rmd for cleaning the data

We can finish cleaning the commune data:

```
```{r}
make_communе_level_data <- function(flat_data){
 flat_data %>%
 filter(!grepl("nationale|offres", locality),
 !is.na(locality))
}

```

```{r}
commune_level_data <-
 `> make_communе_level_data(flat_data)
```

```

We can finish with a chunk to save the data to disk:

```
We now save the dataset in a folder for further
`> analysis (keep chunk option to
`eval = FALSE` to avoid running it when
`> knitting):

```{r, eval = FALSE}
write.csv(commune_level_data,
 "datasets/house_prices_communе_level_data.csv",
 row.names = FALSE)
write.csv(country_level_data,
 "datasets/house_prices_country_level_data.csv",
 row.names = FALSE)
```

## 9. Rewriting our project

...

This last chunk is something I like to add to my Rmd files.

Instead of showing it in the final document but not evaluating its contents using the chunk option `eval = FALSE`, like I did, you could use `include = FALSE`, so it doesn't appear in the compiled document at all. The first time you compile this document, you could change the option to `eval = TRUE`, so that the data gets written to disk, and then change it to `eval = FALSE` to avoid overwriting the data on subsequent knittings. This is up to you, and it also depends on who the audience of the knitted output is (do they want to see this chunk at all?).

Ok, and that's it. You can take a look at the finalised file here<sup>1</sup>. You can now remove the `save_data.R` script, as you have successfully ported the code over to an RMarkdown file. If you have not done it yet, you can commit these changes and push.

Let's now do the same thing for the analysis script.

## 9.2. An Rmd for analysing the data

We will follow the same steps as before to convert the analysis script into an analysis RMarkdown file. Instead of showing the whole file here, I will show you two important points.

The first point is removing redundancy. In the original script, we had the following lines:

---

<sup>1</sup><https://is.gd/eBbcsR>

## 9.2. An Rmd for analysing the data

```
#Let's compute the Laspeyeres index for each
↪ commune:

commune_level_data <- commune_level_data %>%
 group_by(locality) %>%
 mutate(p0 = ifelse(year == "2010",
 ↪ average_price_nominal_euros,
 NA)) %>%
 fill(p0, .direction = "down") %>%
 mutate(p0_m2 = ifelse(year == "2010",
 ↪ average_price_m2_nominal_euros,
 NA)) %>%
 fill(p0_m2, .direction = "down") %>%
 ungroup() %>%
 mutate(
 pl = average_price_nominal_euros/p0*100,
 pl_m2 = average_price_m2_nominal_euros/p0_m2
 ↪ * 100)
```

```
#Let's also compute it for the whole country:
```

```
country_level_data <- country_level_data %>%
 mutate(p0 = ifelse(year == "2010",
 ↪ average_price_nominal_euros,
 NA)) %>%
 fill(p0, .direction = "down") %>%
 mutate(p0_m2 = ifelse(year == "2010",
```

## 9. Rewriting our project

```
 ↵ average_price_m2_nominal_euros,
 ↵ NA)) %>%
fill(p0_m2, .direction = "down") %>%
mutate(
 pl = average_price_nominal_euros/p0*100,
 pl_m2 = average_price_m2_nominal_euros/p0_m2
 ↵ * 100)
```

As you can see, this is almost exactly the same code twice. The only difference between the two code snippets, is that we need to group by commune when computing the Laspeyeres index for the communes (remember, this index will make it easy to make comparisons). Instead of repeating 99% of the lines, we should create a function that will group the data if the data is the commune level data, and not group the data if it's the national data. Here is this function:

```
get_laspeyeres <- function(dataset, start_year =
 ↵ "2010"){

 which_dataset <- deparse(substitute(dataset))

 group_var <- if(grepl("commune",
 ↵ which_dataset)){
 quo(locality)
 } else {
 NULL
 }

 dataset %>%
 group_by (!!group_var) %>%
 mutate(p0 = ifelse(year == start_year,
```

```

 ↵ average_price_nominal_euros,
 NA)) %>%
 fill(p0, .direction = "down") %>%
 mutate(p0_m2 = ifelse(year == start_year,
 ↵ average_price_m2_nominal_euros,
 NA)) %>%
 fill(p0_m2, .direction = "down") %>%
 ungroup() %>%
 mutate(
 pl = average_price_nominal_euros/p0*100,
 pl_m2 =
 ↵ average_price_m2_nominal_euros/p0_m2*100)

}

```

So, the first step is naming the function. We'll call it `get_laspeyeres()`, and it'll be a function of two arguments. The first is the data (commune or national level data) and the second is the starting date of the data. This second argument has a default value of “2010”. This is the year the data starts, and so this is the year the Laspeyeres index will have a value of 100.

The following lines are probably the most complicated:

```

which_dataset <- deparse(substitute(dataset))

group_var <- if(grepl("commune",
 ↵ which_dataset)){
 quo(locality)
}

```

## 9. Rewriting our project

```
 } else {
 NULL
 }
```

The first line replaces the variable `dataset` by its bound value (that's what `substitute()` does) for example, `commune_level_data`, and then converts this variable name into a string (using `deparse()`). So when the user provides `commune_level_data`, `which_dataset` will be defined as equal to "`commune_level_data`". We then use this string to detect whether the data needs to be grouped or not. So if we detect the word "commune" in the `which_dataset` variable, we set the grouping variable to `locality`, if not to `NULL`. But you might have the following questions: why is `locality` given as an input to `quo()`, and what is `quo()`?

A simple explanation: `locality` is a variable in the `commune_level_dataset`. If we don't *quote* it using `quo()`, our function will look for a variable called `locality` in the body of the function, but since there is no variable defined that is called `locality` in there, the function will look for this variable in the global environment. But this is not a variable defined in the global environment either, it is a column in our dataset. So we need a way to tell this to our function: *don't worry about evaluating this just yet, I'll tell you when it's time.*

So by using `quo()`, we can delay evaluation. So how can we tell the function that it's time to evaluate `locality`? This is where we need `!!` (pronounced *bang-bang*). You'll see that `!!` gets used on `group_var` inside `locality`:

```
group_by(!!group_var)
```

So if we are calling the function on `commune_level_dataset`, then `group_var` is equal to `locality`, if not it's `NULL`. `!!group_var` means that now it's time to evaluate `group_var` (or rather, `locality`). Because `!!group_var` gets replaced by `quo(locality)`, and because `group_by()` is a `{dplyr}` function that knows how to deal with quoted variables, `locality` gets looked up among the columns of the data frame. If it's `NULL` nothing happens, so the data doesn't get grouped.

This is a big topic unto itself, so if you want to know more you can start by reading the famous `{dplyr}` vignette called *Programming with dplyr* here<sup>2</sup>. In case you use `{dplyr}` a lot, I recommend you study this vignette because mastering *tidy evaluation* (the name of this framework) is key to becoming comfortable with programming using `{dplyr}` (and other *tidyverse* packages). You can also read the chapter I wrote on this in my other free ebook<sup>3</sup>.

The next lines of the script that we need to port over to the Rmd are quite standard, we write code to create some plots (which were already refactored into a function in the chapter on collaborating on Github). But remember, we want to have an Rmd file that can be compiled into a document that can be read by humans. This means that to make the document clear, I suggest that we create one subsection by commune that we plot. Thankfully, we have learned all about child documents in the literate programming chapter, and this is what we will be using to avoid having to repeat ourselves. The first part is simply the function that we've already written:

---

<sup>2</sup><https://dplyr.tidyverse.org/articles/programming.html>

<sup>3</sup><https://is.gd/f11De1>

## 9. Rewriting our project

```
```{r}
make_plot <- function(commune){

  commune_data <- commune_level_data %>%
    filter(locality == commune)

  data_to_plot <- bind_rows(
    country_level_data,
    commune_data
  )

  ggplot(data_to_plot) +
    geom_line(aes(y = pl_m2,
                  x = year,
                  group = locality,
                  colour = locality))
}

```

```

Now comes the interesting part:

```
```{r, results = "asis"}
res <- lapply(communes, function(x){

  knitr::knit_child(text = c(
    '\n',
    '## Plot for commune: `r x`',
    '\n',
    '```{r, echo = FALSE}' ,
    'print(make_plot(x))' ,
    '\n'
  ))
})
```

```

  ````

) ,
 envir = environment(),
 quiet = TRUE)

}

cat(unlist(res), sep = "\n")

```

```

I won't explain this now in great detail, since that was already done in the chapter on literate programming. Before continuing, really make sure that you understand what is going on here. Take a look at the finalised file here⁴. You'll notice that at the start of the RMarkdown file, I also load some package and the data saved by the `save_data.Rmd` RMarkdown file.

You can see how the outputs look like by browsing to the links below:

- `save_data.html`, compiled from the `save_data.Rmd` source⁵
- `analyse_data.html`, compiled from the `analyse_data.Rmd` source⁶

Of course, you could compile the files into Word documents or PDF, depending on your needs, and you could of course write many more details than me. I wanted to keep it short; the point

⁴<https://is.gd/L2GICG>

⁵<https://is.gd/Z15Ycy>

⁶<https://is.gd/D1o4XJ>

9. Rewriting our project

of this chapter was to show you how to use literate programming and not to write a very detailed analysis.

9.3. Conclusion

This chapter was short, but quite dense, especially when we converted the analysis script to an Rmd, because we've had to use two advanced concepts, *tidy evaluation* and Rmarkdown child documents. *Tidy* evaluation is not a topic that I wanted to discuss in this book, because it doesn't have anything to do with the main topic at hand. However, part of building a robust, reproducible pipeline is to avoid repetition. In this sense, programming with `{dplyr}` and tidy evaluation are quite important. As suggested before, take a look at the linked vignette above, and then the chapter from my other free ebook. This should help get you started.

The end of this chapter marks an important step: many analyses stop here, and this can be due to a variety of reasons. Maybe there's no time left to go further, and after all, you've got the results you wanted. Maybe this analysis is useful, but you don't necessarily need it to be reproducible in 5, 10 years, so all you want is to make sure that you can at least rerun it in some months or only a couple of years later (but be careful with this assessment, sometimes an analysis that wasn't supposed to be reproducible for too long turns out to need to be reproducible for way longer than expected...).

Because I want this book to be a pragmatic guide, I will now talk about putting the least amount of effort to make your current analysis reproducible, and this is by freezing package versions, which I will show you in the next chapter.

10. Basic reproducibility: freezing packages

We are at a stage where the analysis is done. Converting our scripts into Rmds was quite easy to justify because writing the Rmds is also writing the report that we need to send to our boss (or our research paper, etc). But it might be harder to justify writing further documentation or package the functions we've had to write for reuse later and otherwise ensure that the analysis is and stays reproducible. So we are going to start with the simplest and most cost-effective solution to the reproducibility issue, which is recording the versions of the packages that were used. This is quite easy and quick to do and provides at least some hope that the analysis will stay reproducible. But this will not do anything to make the analysis more easily re-usable, will not improve the documentation, nor ensure that what we wrote is indeed correct. For this, we would need to write tests, which are missing from our current analysis. We only wrote one test, which made sure that all the communes were accounted for. This is why going with a package is so useful (and I need to stress here that the aim of writing a package is NOT to upload it to CRAN): packages offer us a great framework for documenting, testing and sharing our code (even if only sharing internally in your company/team, or even just future you). So in order to take advantage of what packaging our code has to offer, we will learn about the `{fusen}` package in the next chapter. `{fusen}`

10. Basic reproducibility: freezing packages

will enable us to convert our Rmd files into a package quite quickly; your analysis is much closer to being a package than you think. As you shall see in the next chapter, going from our Rmds to a fully functioning package is much easier than you expect, even if you've never written a package in your life.

So I hope that I made my point clear: it is not recommended to stop at this stage, but I also recognize that we live in the real world with real physical constraints. So because we live in this imperfect world, sometimes we need to deliver imperfect work. So let's see what we can do that is very cheap in terms of effort and time, but that still allows us to have some hope of having our analysis reproducible, all thanks to the `{renv}` package. It is quite easy to get started with `{renv}`: simply install it, and get a record of the used packages and their versions with one single command. This record gets saved inside a file that can then be used to restore this project's library in the future, and without interfering with the other packages that you already have installed on your machine. You see, `{renv}` creates a per-project library (a library is the set of R packages installed on your machine) which means that you can have as many versions of `{dplyr}` as needed (one per project). The right version of `{dplyr}` will be installed and used for the right project only, and without interfering with other installed versions.

Let's see how this works by creating such a project-specific library for our little project.

10.1. Recording packages' version with `{renv}`

So now that you've used functional and literate programming, we need to start thinking about the infrastructure surrounding our code. By infrastructure I mean:

- the R version;
- the packages used for the analysis;
- and otherwise the whole computational environment, even the computer hardware itself.

`{renv}` enables you to create **R**eproducible **E**nvironments and is a package that takes care of point number 2: it allows you to easily record the packages that were used for a specific project. This record is a file called `renv.lock` which will appear at the root of your project once you've set up `{renv}` and run it. You can use `{renv}` once you're done with an analysis like in our case, or better yet, immediately at the start of the project. You can keep updating the `renv.lock` file as you add or remove packages from your analysis. The `renv.lock` file can then be used to restore the exact same package library that was used for your analysis on another computer, or on the same computer but in the future.

This works because `{renv}` does more than simply create a list of the used packages and recording their versions inside the `renv.lock` file: it actually creates a per-project library that is completely isolated for the main, default, R library on your machine, but also from the other `{renv}` libraries that you might have set up for your other projects (remember, the *library* is the set of R packages installed on your computer). To save time when setting up an `{renv}` library, packages simply get copied over from your main library instead of being re-downloaded and

10. Basic reproducibility: freezing packages

re-installed (if the required packages are already installed in your default library).

To get started, install the `{renv}` package (make sure to start a fresh R session):

```
install.packages("renv")
```

and then go to the folder containing the Rmds we wrote together in the previous chapter. Make sure that you have the two following files in that folder:

- `save_data.Rmd`, the script that downloads and prepares the data;
- `analyse_data.Rmd`, the script that analyses the data.

Also, make sure that the changes are correctly backed up on Github.com, so if you haven't already, commit and push any change to the `rmd` branch. Because we will be experimenting with a new feature, create a new branch called `renv`. You should know the drill by now, but if not simply follow along:

```
owner@localhost $ git checkout -b renv
```

```
Switched to a new branch 'renv'
```

We will now be working on this branch. Simply work as usual, but when pushing, make sure to push to the `renv` branch:

```
owner@localhost $ git add .
owner@localhost $ git commit -m "some changes"
owner@localhost $ git push origin renv
```

10.1. Recording packages' version with `{renv}`

Once this is done, start an R session, and simply type the following in a console:

```
renv::init()
```

You should see the following:

```
* Initializing project ...
* Discovering package dependencies ... Done!
* Copying packages into the cache ... [76/76]
  ↵ Done!

The following package(s) will be updated in the
  ↵ lockfile:

# CRAN =====
***and then a long list of packages***

The version of R recorded in the lockfile will
  ↵ be updated:
- R           [*] -> [4.2.2]

* Lockfile written to
  ↵ 'path/to/housing/renv.lock'.
* Project 'path/to/housing' loaded. [renv
  ↵ 0.16.0]
* renv activated -- please restart the R
  ↵ session.
```

Let's take a look at the files that were created (if you prefer using your file browser, feel free to do so, but I prefer the command line):

10. Basic reproducibility: freezing packages

```
owner@localhost $ ls -la

total 1070
drwxr-xr-x 1 owner Domain Users      0 Feb 27
    ↵ 12:44 .
drwxr-xr-x 1 owner Domain Users      0 Feb 27
    ↵ 12:35 ..
-rw-r--r-- 1 owner Domain Users     27 Feb 27
    ↵ 12:44 .Rprofile
drwxr-xr-x 1 owner Domain Users      0 Feb 27
    ↵ 12:40 .git
-rw-r--r-- 1 owner Domain Users   306 Feb 27
    ↵ 12:35 README.md
-rw-r--r-- 1 owner Domain Users  2398 Feb 27
    ↵ 12:38 analyse_data.Rmd
drwxr-xr-x 1 owner Domain Users      0 Feb 27
    ↵ 12:44 renv
-rw-r--r-- 1 owner Domain Users 20502 Feb 27
    ↵ 12:44 renv.lock
-rw-r--r-- 1 owner Domain Users  6378 Feb 27
    ↵ 12:38 save_data.Rmd
```

As you can see, there are two new files and one folder. The new files are the `renv.lock` file that I mentioned before and a file called `.Rprofile`. The new folder is simply called `renv`. The `renv.lock` is the file that lists all the packages used for the analysis. `.Rprofile` files are files that get read by R automatically at startup (as discussed at the very beginning of part one of this book). You should have a system-wide one that gets read on startups of R, but if R discovers an `.Rprofile` file in the directory it starts on, then that file gets read instead. Let's see the contents of this file (you can open this file in any text editor,

10.1. Recording packages' version with `{renv}`

like Notepad on Windows, but then again I prefer the command line):

```
owner@localhost $ cat .Rprofile
```

The files contains the single line:

```
source("renv/activate.R")
```

`activate.R` is an R script that was also created by `renv::init()`, which you can find in the `renv` folder. Let's take a look at the contents of this folder:

```
owner@localhost $ ls renv
```

```
total 107
drwxr-xr-x 1 owner Domain Users      0 Feb 27
  ↘ 12:44 .
drwxr-xr-x 1 owner Domain Users      0 Feb 27
  ↘ 12:35 ..
-rw-r--r-- 1 owner Domain Users     27 Feb 27
  ↘ 12:44 activate.R
drwxr-xr-x 1 owner Domain Users      0 Feb 27
  ↘ 12:40 .gitignore
drwxr-xr-x 1 owner Domain Users      0 Feb 27
  ↘ 12:40 library
-rw-r--r-- 1 owner Domain Users   6378 Feb 27
  ↘ 12:38 settings.dcf
```

So inside the `renv` folder, there is another folder called `library`: this is the folder that contains our isolated library for just this project. That's something that we would not want to back up on

10. Basic reproducibility: freezing packages

Github as it grows quite large. To avoid tracking this folder and backing it up on Github.com a file called `.gitignore` (notice the `.` at the start of the name) gets used. This is a file that contains the paths to other files and folders that should be ignored. If you open it, you will see that the `library/` folder is listed there so it will be ignored. You can have as many `.gitignore` files as necessary, but if you put one in the root folder of your project, then that `.gitignore` will work project-wide.

For example, if you are working with sensitive data, you could also add a `.gitignore` file in the root of the project's directory, and simply list the folder containing the sensitive data. Create this file using your favourite text editor and simply add, for example if you're working with sensitive data, the following:

```
datasets/
```

This will prevent the `datasets/` folder from being tracked and backed up.

Let's restart a fresh R session in our project's directory; you should see the following startup message:

```
* Project 'path/to/housing' loaded. [renv
  ↵ 0.16.0]
```

This means that this R session will use the packages installed in the isolated library we've just created. Let's now take a look at the `renv.lock` file:

```
owner@localhost $ cat renv.lock
```

10.1. Recording packages' version with `{renv}`

```
{
  "R": {
    "Version": "4.2.2",
    "Repositories": [
      {
        "Name": "CRAN",
        "URL": "https://packagemanager.rstudio.com/
          ↴ all/latest"
      }
    ]
  },
  "Packages": {
    "MASS": {
      "Package": "MASS",
      "Version": "7.3-58.1",
      "Source": "Repository",
      "Repository": "CRAN",
      "Hash": "762e1804143a332333c054759f89a706",
      "Requirements": []
    },
    "Matrix": {
      "Package": "Matrix",
      "Version": "1.5-1",
      "Source": "Repository",
      "Repository": "CRAN",
      "Hash": "539dc0c0c05636812f1080f473d2c177",
      "Requirements": [
        "lattice"
      ]
    }
  }
}

***and many more packages***
```

The `renv.lock` file is a json file listing all the packages, as well as

10. Basic reproducibility: freezing packages

their dependencies, that are used for the project. At the top of the file, the R version that was used to generate the `renv.lock` file is also named. It is important to remember that when you'll use `{renv}` to restore a project's library on a new machine, the R version will not be restored: so in the future, you might be restoring this project and running old versions of packages on a newer version of R, which may sometimes be a problem (but we're going to discuss this later).

So... that's it. You've generated the `renv.lock` file, which means that future you, or someone else, can restore the library that you used to write this analysis. All that's required is for that person (or future you) to install `{renv}` and then use the `renv.lock` file that you generated to restore the library. Let's see how this works by cloning the following Github repository on this link¹ (forked from this one here²):

```
owner@localhost $ git clone  
→ git@github.com:b-rodrigues/targets-minimal.git
```

You should see a `targets-minimal` folder on your computer now. Start an R session in that folder and type the following command:

```
renv::restore()
```

You should be prompted to activate the project before restoring:

¹<https://is.gd/jMVfCu>

²<https://is.gd/AAnByB>

10.1. Recording packages' version with `{renv}`

```
This project has not yet been activated.  
Activating this project will ensure the project  
  ↳ library  
is used during restore.  
Please see `?renv::activate` for more details.
```

```
Would you like to activate this project before  
  ↳ restore? [Y/n] :
```

Type Y and you should see a list of packages that need to be installed. You'll get asked once more if you want to proceed, type y and watch as the packages get installed. If you pay attention to the links, you should see that many of them get pulled from the CRAN archive, for example:

```
Retrieving  
  ↳ 'https://cloud.r-project.org/src/contrib/Archive  
  ↳ /vroom/vroom_1.5.5.tar.gz'
```

Notice the word “Archive” in the url? That’s because this project uses `{vroom}` 1.5.5, but as of writing (early 2023), `{vroom}` is at version 1.6.1.

Now, maybe you’ve run `renv::restore()`, but the installation of the packages may have failed. If that’s the case, let me explain what likely happened.

I tried restoring the project’s library on two different machines: a Windows laptop and a Linux workstation. `renv::restore()` failed on the Windows laptop, but succeeded on the Linux workstation.

Why does that happen? Well in the case of the Windows laptop, compilation of the `{dplyr}` package failed. This is likely

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because my Windows laptop does not have the right version of Rtools installed. If you look inside the `renv.lock` file that came with the `targets-minimal` project, you should notice that the recorded R version is 4.1.0, but I'm running R 4.2.2 on my computers. So libraries get compiled using Rtools 4.2 and not Rtools 4.0 (which includes the libraries for R 4.1 as well).

So in order to run this project successfully, I should install the right version of R and Rtools which on Windows should not be too complicated. But that might be a problem on other operating systems. Does that mean that `{renv}` is useless? No, not at all.

At a minimum, `{renv}` ensures that a project's library doesn't interfere with another project's library while you're working on different projects. You can be working on several projects and be sure that if you update your library (for example, to use a nice new function from one specific package), that update will only affect the project where the library was updated, and not the other libraries from the other projects. When working with a system-wide library, updating packages for a project could introduce breaks in other projects. Without `{renv}`, such breaks could happen because another function coming from some other package that also got updated and that you use in another long-term project got removed, or renamed, or simply works differently now. This types of issues can be avoided by using a per-project library, which is exactly what `{renv}` does.

But also, apart from that already quite useful feature, `renv.lock` files provide a very useful blueprint for Docker, which we are going to explore in a future chapter. Only to give you a little taste of what's coming: since the `renv.lock` file lists the R version that was used to record the packages, we can start from a Docker image that contains the right version of R. From there, restoring the project using `renv::restore()`

should succeed without issues. If you have no idea what this all means, do not worry, you will know by the end of the book, so hang in there.

So should you use `{renv}`? I see two scenarios where it makes sense:

- You're done with the project and simply want to keep a record of the packages used. Simply call `renv::init()` at the end of the project and commit and push the `renv.lock` file on Github.
- You want to use `{renv}` from the start to isolate the project's library from your whole R installation's library to avoid any interference (I would advise you to do it like this).

In the next section, we'll quickly review how to use `{renv}` on a “daily basis”.

10.1.1. Daily `{renv}` usage

So let's say that you start a new project and want to use `{renv}` right from the start. You start with an empty directory, and add a template `.Rmd` file, and let's say it looks like this:

```
---
```

```
title: "My new project"
output: html_document
---
```

```
```{r setup, include=FALSE}
library(dplyr)
```
```

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```
## Overview
```

```
## Analysis
```

Before continuing, make sure that it correctly compiles into a HTML file by running `rmarkdown::render("test.Rmd")` in the correct directory.

In the `setup` chunk you load the packages that you need. Now, save this file, and start a fresh session in the same directory and run `renv::init()`. You should see the familiar prompts described above, as well as the `renv.lock` file (which will only contain `{dplyr}` and its dependencies).

Now, after the `library(dplyr)` line, add the following `library(ggplot2)` (or any other package that you use on a daily basis). Make sure to save the `.Rmd` file and try to render it again by using `rmarkdown::render("test.Rmd")` (or if you're using RStudio, by clicking the right button), but, spoiler alert, it won't work. Instead you should see this:

```
Quitting from lines 7-9 (my_new_project.Rmd)
Error in library(ggplot2) : there is no package
  ↵ called 'ggplot2'
```

Don't be confused: remember that `{renv}` is now activated, and that each project where `{renv}` is enabled has its own project-specific library. You may have `{ggplot2}` installed on your system-wide library, but this `{renv}`-enabled project does not have it yet on its own specific library. This means

10.1. Recording packages' version with `{renv}`

that you need to install `{ggplot2}` for your project. To do so, simply start an R session within your project and run `install.packages("ggplot2")`. If the version installed on your system-wide library is the latest version available on CRAN, the package will simply be copied over from the system-wide to the project-specific library, if not, the latest version will be downloaded onto your project's library. You can now update the `renv.lock` file. This is done using `renv::snapshot()`; this will show you a list of new packages to record inside the `renv.lock` file and ask you to continue:

```
**list of many packages over here**
```

```
Do you want to proceed? [y/N] :
```

```
* Lockfile written to
  ↳ 'path/to/my_new_project/renv.lock'.
```

If you now open the `renv.lock` file, and look for the string "ggplot2" you should see it listed there alongside its dependencies. Let me reiterate: this version of `{ggplot2}` is now unique to this project. You can work on other projects with other versions of `{ggplot2}` without interfering with this one. If for some reason you didn't want to have the latest version of `{ggplot2}` installed in the project-specific library, you could have installed an older version, still thanks to `{renv}`. For example, to install an older version of `{AER}`:

```
renv::install("AER@1.0-0") # this is a version
  ↳ from August 2008
```

But just like in the previous section, where we wanted to restore an old project that used `{renv}`, installation of older packages may fail. If you need to use old packages there are other easier

10. Basic reproducibility: freezing packages

approaches which we are also going to explore in this chapter.

When you install more of the required packages for your project, you need to call `renv::snapshot()` to add the packages to the `renv.lock` file. Once you're done with your project, call `renv::snapshot()` one last time to make sure that every dependency is correctly accounted for. Don't forget to version the `renv.lock` file using Git!

10.1.2. Collaborating with {renv}

{renv} is also quite useful when collaborating. You can start the project and generate the lock file, and when your teammates clone the repository from Github, they can get the exact same package versions as you. All of you only need to make sure that everyone is running the same R version to avoid any issues.

There is a vignette on just this that I invite you to read for more details, see here³.

10.1.3. {renv}'s shortcomings

As useful as {renv} is, it also comes with some shortcomings (which I've already alluded to before). It is quite important to understand what {renv} does and what it doesn't do, and why {renv} alone is not enough to ensure the long-term reproducibility of your projects.

The first problem, and I'm repeating myself here, is that {renv} only records the R version used for the project, but does not restore it when calling `renv::restore()`. You need to install the

³<https://is.gd/sXpWVp>

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right R version yourself. On Windows this should be fairly easy to do, but then you need to start juggling R versions and know which scripts need which R version, which can get confusing.

There is the `{rig}` package that makes it easy to install and switch between R versions that you could check out⁴ if you're interested. However, I don't think that `{rig}` should be used for our purposes. I believe that it is safer to use Docker instead, and we shall see how to do so in the coming chapters.

The other issue of using `{renv}` is that future you, or your teammates or people that want to reproduce your results need to install packages that may be quite difficult to install, either because they're very old by now, or because their dependencies are difficult to satisfy. Have you ever tried to install a package that depended on `{rJava}`? Or the `{rgdal}` package? Installing these packages can be quite challenging because they need specific system requirements that may be impossible for you to install (either because you don't have admin rights on your workstation, or because the required version of these system dependencies is not available anymore). Having to install these packages (and potentially quite old versions at that) can really hinder the reproducibility of your project. Here again, Docker provides a solution. Future you, your teammates or other people simply need to be able to run a Docker container, which is a much lower bar than installing these old libraries.

Note also that during your journey, you will want to improve your scripts, you maybe will also want to upgrade some dependencies to take advantage of recent developments in some packages. This will require upgrading the `{renv}` environment. To do so, run `update.packages()` to update the packages, and then `renv::snapshot()` to generate a new `renv.lock` file. But

⁴<https://is.gd/dvH2Sj>

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how will you be sure that these upgrades will not impair some other parts of your code? Turning the analysis into a package will help with this, as I'll explain in the next chapter, because once the analysis is turned into a package, testing gets much easier. If the tests indicate that something went wrong, you can simply restore the previous lock file using Git and restore the old library.

I want to stress that this does not mean that `{renv}` is useless: we will keep using it, but together with Docker to ensure the reproducibility of our project. As I've written above already, *at a minimum `{renv}` ensures that a project's library doesn't interfere with another project's library* and this is in itself already quite useful. The `renv.lock` file also provides a blueprint that can be used (by you or someone else) to build a Docker image for long-term reproducibility.

Let's now quickly discuss two other packages before finishing this chapter, which provide an answer to the question: *how to rerun an old analysis if no `renv.lock` file was made available at the time the analysis was made?*.

10.2. Becoming an R-cheologist

So let's say that you need to run an old script, and there's no `renv.lock` file around for you to restore the right package library. There might still be a solution (apart from running the script on the current version on R and packages, and hope that everything goes well), but for this you need to at least know roughly *when* that script was written. Let's say that you know that this script was written back in 2017, somewhere around October. If you know that, you can use the `{rang}` or `{groundhog}`

packages to download the packages as of October 2018 in a separate library and then run your script.

`{rang}` is fairly recent as of writing (February 2023) so I won't go into too much detail now, as it is likely that the package will keep evolving rapidly in the coming weeks. So if you want to use it and follow its development, take a look at its Github repository here⁵ and read the preprint⁶ (Chan and Schoch 2023).

`{groundhog}` (website⁷) is another option that has been around for more time and is fairly easy to use. Suppose that you have a script from October 2018 that looks like this:

```
library(purrr)
library(ggplot2)

data(mtcars)

myplot <- ggplot(mtcars) +
  geom_line(aes(y = hp, x = mpg))

ggsave("/home/project/output/myplot.pdf",
       myplot)
```

If you want to run this script with the versions of `{purrr}` and `{ggplot2}` that were current in October 2017, you can achieve this by simply changing the `library()` calls:

```
groundhog::groundhog.library(
  library(purrr)
```

⁵<https://is.gd/sQu7NV>

⁶<https://arxiv.org/abs/2303.04758>

⁷<https://groundhog.com>

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```
library(ggplot2)",  
"2017-10-04"  
)  
  
data(mtcars)  
  
myplot <- ggplot(mtcars) +  
  geom_line(aes(y = hp, x = mpg))  
  
ggsave("/home/project/output/myplot.pdf",  
       myplot)
```

but you will get the following message:

| **IMPORTANT.**

| Groundhog says: you are using R-4.2.2, but
| ↵ the version of R current
| for the entered date, '2017-10-04', is
| ↵ R-3.4.x. It is recommended
| that you either keep this date and switch
| ↵ to that version of R, or
| you keep the version of R you are using but
| ↵ switch the date to
| between '2022-04-22' and '2023-01-08'.
|
| You may bypass this R-version check by
| ↵ adding:
| `tolerate.R.version='4.2.2'` as an option in
| ↵ your groundhog.library()
| call. Please type 'OK' to confirm you have
| ↵ read this message.

```
| >ok
```

Groundhog is speaking to us, advising us to switch to the version of R that was current at that time the script was written. If we want to ignore the message's advice, and add `tolerate.R.version = '4.2.2'`, we may get the script to run anyways:

```
groundhog.library("purrr")
library(ggplot2)",
"2017-10-04",
tolerate.R.version = "4.2.2")

data(mtcars)

myplot <- ggplot(mtcars) +
  geom_line(aes(y = hp, x = mpg))

ggsave("/home/project/output/myplot.pdf",
  myplot)
```

But just like for `{renv}` (or `{rang}`), installation of the packages can fail, and for the same reasons (unmet system requirements most of the time).

So here again, the solution is to take care of the missing piece of the reproducibility puzzle, which is the whole computational environment itself.

10.3. Conclusion

In this chapter you had a first (maybe a bit sour) taste of reproducibility. This is because while the tools presented here are very useful, they will not be sufficient if we want our project to be truly reproducible, especially in the long term. There are too many things that can go wrong when re-installing old package versions, so we must instead provide a way for users to not have to do it at all. This is where Docker is going to be helpful. But before that, we need to hit the development bench again. We are actually not quite done with our project; before going to full reproducibility, we should turn our analysis into a package. And as you will see, this is going to be much, much, easier than you might expect. You already did 95% of the job! There are many advantages to turning our analysis into a package, and not only from a reproducibility perspective.

11. Packaging your code

In this chapter, you’re going to learn how to create your own package. And let me be clear right from the start: the goal here is not to convert your analysis as a package to then get it published on CRAN. No, that’s not it. The goal is to convert your analysis into a package because when your analysis goes into *package development mode*, you can, as the developer, leverage many tools that will help you improve the quality of your analysis. These tools will make it easier for you to:

- document the functions you had to write for your analysis;
- test these functions;
- properly define dependencies;
- use all the code you wrote into a true reproducible pipeline.

Turning the analysis into a package will also make the separation between the software development work you had to write for your analysis (writing functions to clean data for instance) from the analysis itself much clearer. The package itself can be published on Github (if there’s nothing particularly sensitive about it) and can also be very easily installed from R itself from Github, or you can store it inside your organisation and then simply install it locally.

By turning your analysis into a package you will essentially end up with two *things*:

- a well-documented, and tested package;

11. Packaging your code

- an analysis that uses this package like any other package.

Making this separation will then make it easier to record dependencies of your analysis using `{renv}`, as your package will be a package like any other that needs to be recorded. And what's more, we can start with the `.Rmd` files that we have already written! The `{fusen}` package (Rochette 2022) will bridge the gap between the `.Rmd` files and the package: as Sébastien Rochette, the author of `{fusen}`, says:

If you have written an Rmd file, you have (almost)
already written a package.

But you could just as well start directly with an empty `{fusen}` package template, and then start your analysis from there. Package development with `{fusen}` is simply writing RMarkdown code.

11.1. Benefits of

Let's first go over the benefits of turning your analysis into a package once again, as this is crucial.

The main point is not to turn the analysis into a package to publish on CRAN (but you can if you want to). The point is that when you analyse data, you have to write a lot of custom code, and very often, you don't expect to write that much custom code when starting. Let's think about our little project: all we wanted was to create some plots from Luxembourgish houses' price data. And yet, we had to scrape Wikipedia on two occasions, clean an Excel file, and write a test... the project is quite modest but the amount of code (and thus opportunities to make mistakes) is quite large. But, that's not something that

we could have anticipated, hence why we didn't start the analysis by writing a package but a script (or an `.Rmd`) instead. But then as this script grows larger and larger, we realise that we might need something else than a simple `.Rmd` file and this is when we would start writing a package. Without `{fusen}`, we would almost need to start from scratch.

The other benefit of turning all this code into a package is that we get a clear separation between the code that we wrote purely to get our analysis going (what I called the *software development part* before) from the analysis itself (which would then typically consist in computing descriptive statistics, running regression or machine learning models, and visualisation). This then in turn means that we can more easily maintain and update each part separately. So the pure software development part goes into the package, which then gives us the possibility to use many great tools to ensure that our code is properly documented and tested, and then the analysis can go inside a purely reproducible pipeline. Putting the code into a package also makes it easier to reuse across projects.

11.2. {fusen} quickstart

If you haven't already, install the `{fusen}` package:

```
install.packages("fusen")
```

`{fusen}` makes the *documentation first* method proposed by Sébastien Rochette, `{fusen}`'s author, simple to use. The idea is to start from documentation in the form of an `.Rmd` file and go from there to a package. Let's dive right into it by starting from a template included in the `{fusen}` package. Start an R

11. Packaging your code

session from your home (or Documents) directory and run the following:

```
fusen::create_fusen(path = "fusen.quickstart",
                     template = "minimal")
```

This will create a directory called `fusen.quickstart` inside your home (or Documents) directory. Inside that folder, you will find another folder called `dev/`. Let's see what's inside it (I use the command line to list the files, but you're free to use your file explorer program):

```
owner@localhost $ ls dev/
0-dev_history.Rmd  flat_minimal.Rmd
```

`dev/` contains two `.Rmd` files, `0-dev_history.Rmd` and `flat_minimal.Rmd`. They're both important, so let me explain what they do:

- `flat_minimal.Rmd` is only an example, a stand-in for our own `.Rmd` files. When doing actual work, we will be using the `Rmd` file(s) that we have written before (`analyse_data.Rmd` and `save_data.Rmd`) instead, or if this is a fresh project, we could rename `flat_minimal.Rmd` and use it as a template for our analysis.
- `0-dev_history.Rmd` contains lines of code that you typically run when you're developing a package. For example, a line to initialise Git for the project, a line to add some dependencies, etc. The idea is to **write down everything** that you type in the console in this file. This leaves a trace of what you have been doing and also acts as a checklist so that you can make sure that you didn't forget anything. You can also re-use for any other package

development project.

Before describing these files in detail, I want to show you this image taken from `{fusen}`'s website¹:

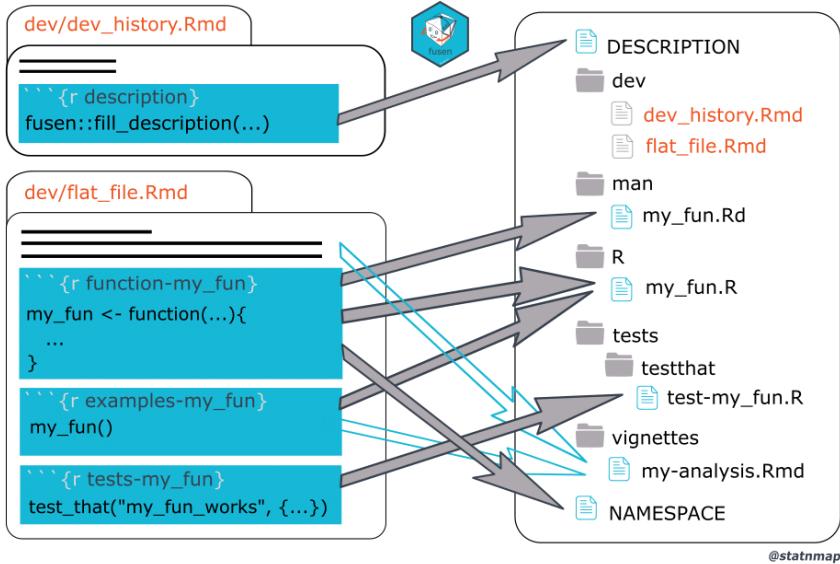


Figure 11.1.: `fusen` takes care of the boring stuff for you!

On the left-hand side of the image, we see the two template .Rmd files from `{fusen}`. `0-dev_history.Rmd` contains a chunk called `description`. This is the main chunk in that file that we need to execute to get started with `{fusen}`. Running this chunk will create the package's DESCRIPTION file (don't worry if you don't know about this file yet, I will explain). Then, the second file `flat_minimal.Rmd` (or our very own .Rmd files) contains functions, tests, examples, and everything we need for our analysis. When we *inflate* the Rmd file, `{fusen}` places

¹<https://is.gd/5pJi2h>

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every piece from this `.Rmd` file in the right place: the functions get copied into the package's `R/` folder, tests go into the `tests/` folder, and so on. `{fusen}` simply takes care of everything for us!

But for `{fusen}` to be able to work its magic, we do need to prepare our `.Rmd` files a bit. But don't worry, it is mostly simply giving adequate names to our code chunks. Let's take a look at the `flat_minimal.Rmd` file that was just generated. If you open it in a text editor, you should see that it is a fairly normal `.Rmd` file. There is a comment telling you to first run the `description` chunk in the `0-dev_history.Rmd` file before changing this one. But let's keep reading `flat_minimal.Rmd`. What's important comes next:

```
# my_fun

```{r function-my_fun}
#' my_fun Title
#
#' @return 1
#' @export
#
#' @examples
my_fun <- function() {
 1
}
```

```{r examples-my_fun}
my_fun()
```

```

```
```{r tests-my_fun}
test_that("my_fun works", {
})
```

```

This is a section titled `my_fun`. Then comes the definition of `my_fun()`, inside a chunk titled `function-my_fun`, then comes an example, inside a chunk titled `examples-my_fun` and finally a test in a chunk titled `tests-my_fun`.

This is how we need to rewrite our own `.Rmd` files to be able to use `{fusen}`, and what's really nice is that this is essentially what we did before, but with some added structure on it. Using `{fusen}` just *forces* us to clean up our code and define examples and tests (if we want them) more cleanly and explicitly. Also, you might have noticed that in the chunk with the function definition, there are a bunch of comments that start with `#'`. These are `{roxygen2}` type comments. As the package's documentation gets built, these comments get automatically turned into the documentation you see when you type `help("my_fun")` in an R console. So even the comments that you typically write to explain how your code works can be re-used to build documentation that will be much easier to browse than comments in source code!

So, basically, a `{fusen}`-ready `.Rmd` file is nothing more than an `.Rmd` file with some structure imposed on it. Instead of documenting your functions as simple comments, document them using `{roxygen2}` comments, which then get turned into the package's documentation automatically. Instead of trying your function out on some mock data in your console, write down that example inside the `.Rmd` file itself. Instead of writing ad-hoc tests, or worse, instead of testing your functions on your

11. Packaging your code

console manually, one by one (and we've all done this), write down the test inside the `.Rmd` file itself, right next to the function you're testing.

Write it down, write it down, write it down... you're already documenting and testing things (most of the time in the console only), so why not just write it down once and for all, so you don't have to rely on your ageing, mushy brain so much? Don't make yourself remember things, just write them down! `{fusen}` gives you a perfect framework to do this. The added benefit is that it will improve your package's quality through the tests and examples that are not directly part of the analysis itself but are still required to make sure that the analysis is of high quality, reproducible and maintainable. So that if you start messing with your functions, you have the tests right there to tell you if you introduced breaking changes.

Let's go back to the template and inflate it into a package. Open `0-dev_history.Rmd` and take a look at the `description` code chunk:

```
```{r description, eval=FALSE}
Describe your package
fusen::fill_description(
 pkg = here::here(),
 fields = list(
 Title = "Build A Package From Rmarkdown",
 File",
 Description = "Use Rmarkdown First method to
 build your package.
 Start your package with
 documentation.
```

```

Everything can be set from a
↳ Rmarkdown file
 in your project." ,
`Authors@R` = c(
 person("Sebastien", "Rochette", email =
↳ "sebastien@thinkr.fr",
 role = c("aut", "cre"),
 comment = c(ORCID =
↳ "0000-0002-1565-9313")),
 person(given = "ThinkR", role = "cph")
)
)
#
Define License with use_*_license()
usethis::use_mit_license("Sébastien Rochette")
```

```

The `fill_description()` function will create the package's `DESCRIPTION` file. Here² is an example of such a file. This file provides some information on who wrote the package, the purpose of the package, as well as some metadata such as the package's version. While developing your package, you will continuously fill in some important extra parts of this file, such that parts that list dependencies required to be able to use your package: `Depends:`, `Imports:` and `Suggests::`. `Depends:` is where you list packages (or R versions) that must be installed for your package to work (if they're not installed, they will be installed alongside your package). This is the same with `Imports::`, and the difference with `Depends:` is most of the time irrelevant: packages listed under `Depends:` will not only be loaded when you load your package, but also attached.

²<https://is.gd/PfvkSZ>

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This means that the functions from these packages will also be available to the end user when loading your package. Most of the time, you do not have to list packages under `Depends::`. Packages listed under `Imports:` will only be loaded, meaning that their functions will only be available to your packages' functions, not the end-users themselves. If that's confusing, don't worry too much about it, this will not be consequential for our purposes. Finally, `Suggests:` are dependencies that are not critical for your package to run, usually these are only necessary if you want to run the code from the package's vignettes or examples. As you can imagine, listing the right packages under the right category can be a daunting task. But don't worry, `{fusen}` takes care of this automatically for us! Simply focus on writing your `.Rmd` files.

The last line of this chunk runs `usethis::use_mit_license()`. `{usethis}` is a package that contains many helper functions to help you develop packages. You can choose among many licenses. Note that any open-source work should present a license so that users know how they are allowed to use it. Otherwise, theoretically, without a license, no one is allowed to re-use or share your work. You don't need to think too much about it at the start since you can always change the license later. And if you don't want to publish your package anywhere (nor CRAN, nor Github) and keep it completely internal to your organisation, you can just define a proprietary license with `usethis::use_proprietary_license("your name")`. My very personal take on licenses is that you should use copyleft licenses as much as possible (so licenses like the GPL) which ensure that if others take your code and change it, their changes also have to be republished to the public under the GPL – but only if they wish to publish their changes at all. They could always keep their modifications totally private, which means that companies can, and do, use GPL'ed code in their internal

products.

It's when that product gets released to the public that the source code must be released as well. This ensures that open code stays open.

However, licenses like the MIT allow private companies to take open source and freely available code and incorporate it inside their own proprietary tools, without having to give back their modifications to the community. Some people argue that this is the *true* free license because anyone is then also free to use any code and they also have the liberty of not having to give anything back to the community. I think that this is a very idiotic argument, and when proponents of permissive licenses like the MIT (or BSD) get their code taken and not even thanked for it (as per the license, which doesn't even force anyone to cite the software), and their software gets used for nefarious purposes, the levels of cope are through the roof³ (archived link for posterity). Anyway, I got side-tracked here, let's go back to our package.

Run the code of the two functions inside the `description` chunk in an R console (don't change anything for now, and make sure that the R session was started on the root of the project, so in the `fusen.quickstart/` folder), and see the `DESCRIPTION` file appear magically in the root of the folder (as well as the `LICENSE` file, containing the license).

For now, we can ignore the rest of the `0-dev_history.Rmd` file: actually, everything that follows the `description` code chunk is totally optional but still useful. If you look at them, you see that the lines that follow simply help you remember to do useful things, like initialising Git, creating a `Readme` file, add

³<https://is.gd/PS45xu>

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some usual dependencies, and so on. But let's ignore this for now, and go to the `flat_minimal.Rmd` file.

Go at the end of the file, and take a look at the chunk titled `development-inflate`. This is the chunk that will convert the `.Rmd` file into a fully functioning package. This process is called *inflating* the `.Rmd` file (because a *fusen* is a type of origami figure that you fold in a certain way, which can then get *literally* inflated into a box). Run the code in that chunk, and see your analysis become a package automagically.

If you look now at the projects' folder, you will see several new sub-folder:

- `R/`: the folder that contains the functions;
- `man/`: contains the functions' documentation;
- `tests/`: contains the tests;
- `vignettes/`: contains the vignettes.

Every function defined in the `flat_minimal.Rmd` file is now inside the `R/` folder; all the documentation written as `{roxygen2}` comments is now neatly inside `man/`, the tests are in `tests/`, and `flat_minimal.Rmd` has been converted to an actual vignette (without all the `development` chunks). This is now a package that can be installed immediately using `devtools::install()`, or that can be shared on Github and installed from there. Right now, without doing anything else. You can even generate a website for your package: got back to the `0-dev_history.Rmd` and check the last code chunk, under the title *Share the package*. Start a new, fresh session at the root of your project and run the two following lines from that last chunk:

```
# set and try pkgdown documentation website
usethis::use_pkdown()
```

```
pkgdown::build_site()
```

This will build a website for your package using the `{pkgdown}` website and open your web browser and show you what it looks like. The files for this website are in the newly created `docs/` folder in the root of your package folder. This can then be hosted, for free, with a service from Github called Github Pages so people can explore the package's functions and documentation without having to install the package! Later in this chapter, I will show you how to do this.

11.3. Turning our Rmds into a package

Ok, so I hope to have convinced you that `{fusen}` is definitely something that you should add to your toolbox. Let's now turn our analysis into a package, but before diving right into it, let's think about it for a moment.

We have two `.Rmd` files, one for getting and cleaning the data, which we called `save_data.Rmd` and another for analysing this data, called `analyse_data.Rmd`.

In both `.Rmd` files, we defined a bunch of functions, but most of the functions were defined in the `save_data.Rmd` script. In fact, in the `analyse_data.Rmd` file we defined only two functions, `get_laspeyeres()`, the function to get the Laspeyeres price index, and `make_plot()`, the function to create the plots for our analysis.

We are faced with the following choice here:

- make both these `.Rmd` files *fusen-ready*, and inflate them both. This would put the functions from both

11. Packaging your code

- save_data.Rmd and analyse_data.Rmd into the inflated package R/ folder;
- put all the functions into save_data.Rmd and only inflate that file. The other, analyse_data.Rmd can then be used exclusively for the analysis *stricto sensu*.

This is really up to you, there is no right or wrong answer. You could even go for another option if you wanted. It all depends on how much time you want to invest in this. If you want to get done quickly, the first option, where you simply inflate both files is the fastest. If you have more time, the last option, where you neatly split everything might be better. I propose that we go for the second option. This way, we only have to inflate one file, and in our case here, it won't take much time anyways. It's literally only moving two code chunks from analyse_data.Rmd to save_data.Rmd. So before continuing, let's go back to our repository and switch back to the rmd branch that contains the .Rmd files (let's ignore freezing packages with {renv} and thus the renv branch for now):

```
owner@localhost $ git checkout rmd
```

Using the rmd branch as a starting point, let's create a new branch called fusen:

```
owner@localhost $ git checkout -b fusen
```

```
Switched to a new branch 'fusen'
```

We will now be working on this branch. Simply work as usual, but when pushing, make sure to push to the fusen branch:

```
owner@localhost $ git add .
owner@localhost $ git commit -m "some changes"
owner@localhost $ git push origin fusen
```

By now, that repository should have four branches:

- *master*, or *main* with the simple .R scripts;
- *rmd*, with the .Rmd files
- *renv*, containing the .Rmd files as well, and the `renv.lock` file
- *fusen*, the branch we will be using now.

If you've skipped the first part of the book, or didn't diligently create the branches and push, you can fork this repository⁴ and then clone it to start from a sane base. Switch to the `rmd` branch, and create a branch called `fusen`.

First order of business: create a `{fusen}` flat template in a `dev/` folder. Start a fresh R session inside the `housing/` folder, and run the following:

```
fusen::create_fusen(path = ".",
                      template = "minimal",
                      overwrite = TRUE)
```

Because we already have a folder for our project, called `housing/` we use `"."` which essentially means “right here”. We need the `overwrite = TRUE` option because the folder exists already. Running the above command will add the `dev/` folder. Move `save_data.Rmd` inside `dev/`; remember, we only want to inflate that one: `analyse_data.Rmd` will be a simple .Rmd that will use our package to load the needed functions and data.

⁴<https://is.gd/jGZrMF>

11. Packaging your code

Next step, move the functions `get_laspeyeres()` and `make_plot()` from `analyse_data.Rmd` to `save_data.Rmd`. Simply cut and paste these functions from one `.Rmd` to the other. Make sure `save_data.Rmd` looks something like this⁵, take a look at the end of the script to find the functions we've moved over. The `analyse_data.Rmd` script is exactly the same, minus the functions that we've just moved over.

Ok, so now, we need to make `save_data.Rmd` ready to be inflated. Take inspiration from the `flat_minimal.Rmd` that `fusen::create_fusen()` put in the `dev/` folder. This is what the end-result should look like⁶ (no worries, I'm going to explain how I got there). For consistency with your future use of `{fusen}`, you could also rename the `save_data.Rmd` to `flat_save_data.Rmd`, although this won't avoid `{fusen}` to work properly.

Let's start with the first function, `get_raw_data()`. If you compare the before⁷ and after⁸, the differences are that we have named the chunk containing the function, `function-get_raw_data` and added documentation in the form of `{roxygen2}` comments. Naming the chunks is essential: this is how `{fusen}` knows that this chunk contains a function that should go into the `R/` folder. `{roxygen2}` comments are strictly speaking not required, but it is highly advised that you add them: this way, your function will get documented and users (including future you) will be able to read the documentation by typing `help(get_raw_data)`. And you're likely already adding comments explaining what the function does anyway. Another difference is that I have made all the functions

⁵<https://is.gd/SpzL88>

⁶<https://is.gd/anRjt4>

⁷<https://is.gd/n3m6In>

⁸<https://is.gd/anRjt4>

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referentially transparent. Take a closer look at `make_plot()` in the before and after .Rmd's. You will see that I've added two arguments to `make_plot()`, `country_level_data` and `commune_level_data`. This is really important, so don't forget to do it!

Remember when I mentioned that the good thing about turning our analysis into a package is that it gives us a framework to develop high-quality code by using nice development tools? `{roxygen2}` type comments for documentation is the first such tool in this list. By commenting your functions, you explain what the inputs are, what the outputs are going to be, and also how to use the functions with some examples. Using `{fusen}` (and `{roxygen2}`), you simply continue doing the same, but with some added structure. This added structure is not costly to impose on yourself, and comes with many added benefits (in this case, free documentation!). I'm repeating myself but I really want to drive this point home: the goal is not to have to *add* code on top of what you already did. The point is to do what you always do, but within a framework.

Let's now look at the functions' `{roxygen2}`-type comments. The first line:

```
#' get_raw_data Gets raw nominal house price
←   data from LU Open Data Portal
```

will create the title of the function's help page. Then come the `@param` lines (in this case we only have one):

```
#' @param url Optional: Persistent url to the
←   data
```

This lists the parameters of the function. Here you can explain

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exactly what the inputs should be. What happens if the function you're documenting has several parameters and you forget to document one? If that happens, when you will inflate the file, you will get a warning in the console that will look like this:

```
inflate warnings and errors: Undocumented
  ↵ arguments in documentation
object 'get_raw_data'
  'url'
```

Then come the `@importFrom` statements. This is where you list dependencies:

```
#' @importFrom readxl excel_sheets read_excel
#' @importFrom utils download.file
#' @importFrom dplyr mutate rename select
#' @importFrom stringr str_trim
#' @importFrom janitor clean_names
#' @importFrom purrr map_dfr
```

This is important, because the statements will write the dependencies into the package's `NAMESPACE` file. This file is important, because any function defined there will be available to your package's functions when you load the package. So if your function use `dplyr::mutate()` for example, your package needs to know where to look for `mutate()`. This is where the `NAMESPACE` file comes into play. Take the opportunity to list the dependencies of your function to review them: maybe you're using a package for a single dependency that you could easily remove. For example, I'm using `stringr::str_trim()` to remove whitespace around characters. But I could be using the base R function `trimws()` instead, which would remove this dependency. I'm going to keep it here, because I'm lazy though. It might seem

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like extra work to add these statements. But you have to see it this way: you are writing the functions here, once, that need to be available to your functions for them to work. The alternative is to have to write:

```
library("readxl")
library("utils")
library("dplyr")
library("stringr")
library("janitor")
library("purrr")
```

on top of each script that uses your functions. This gets old pretty fast and is error-prone. By declaring the dependencies here, you ensure that they get recorded by `{renv}` and will make using your project much easier.

You will also notice the following `importFrom` statement:

```
#' @importFrom utils download.file
```

`download.file()` is included in the `{utils}` package, itself included with a base installation of R. So you don't really need to specify it; but when inflating the file, you get the following message:

Consider adding
 `importFrom("utils", "download.file")`
to your NAMESPACE file.

hence why I've added it, to silence this message. Again, not mandatory, but why not do it?

Now comes the `@return` keyword: this simply tells your users

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what the function returns. If the function doesn't return anything, because it only has a side effect (for example, writing something to disk, or printing something on screen), then you could return `NULL`.

```
#' @return A data frame
```

Last but not least, the `@export` keyword:

```
#' @export
```

This makes the function available to users that load the package using `library(housing)`. If you don't add this keyword, the function will be only available to the other functions of the package. Another way to see this: functions decorated with the `@export` keyword are public and functions without it are private. But the concept of private functions doesn't really exist in R. You can always access a “private” function by using `:::` (three times the `:`), as in `package:::private_function()`.

The other functions are documented in the same manner, so I won't comment them here. Something else you might have noticed: I replaced every `%>%` by the base pipe `|>`. You don't have to do it, but the advantage of using the base pipe is that it removes the dependency on the `{magrittr}` package, needed for `%>%`. If you want to use `%>%`, you can keep it, but then should run the line:

```
usethis::use_pipe()
```

in the `0-dev_history.Rmd` file, which will take care of adding this dependency correctly for you (by editing the `NAMESPACE` file).

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Next comes the test we wrote. As a reminder, here is how it looked like in our original .Rmd file:

```
Let's test to see if all the communes from our
↪ dataset are represented.
```

```
```{r}
setdiff(flat_data$locality, communes)
```
```

The objects `communes` and `flat_data` have to obviously exist for this test to pass. This was a very simple test that must be monitored interactively. If commune names are returned here, then this means that there are communes left that we need to include in our data. But remember: we are aiming at building a RAP, and don't want to have to look at it as it is running to see if everything is alright. What we need is a test that returns an error if it fails and which should completely halt the pipeline. So for this we use the `{testthat}` package, and write a so-called *unit test*. We're going to deep-dive into unit testing (and assertive testing) in the next chapter, so for now, let me simply comment the test:

```
```{r tests-clean_flat_data}
We now need to check if we have them all in
↪ the data.
The test needs to be self-contained, hence
why we need to redefine the required
↪ variables:

former_communes <- get_former_communes()
```

## 11. Packaging your code

```
current_communes <- get_current_communes()

communes <- get_test_communes(
 former_communes,
 current_communes
)

raw_data <- get_raw_data(url =
 "https://is.gd/1vvBAc")

flat_data <- clean_raw_data(raw_data)

testthat::expect_true(
 all(communes %in% unique(flat_data$locality))
)
```

```

The first thing that you need to know is that tests need to be self-contained. This is why we define `former_communes` and `current_communes` again. The reason is that `{fusen}` will take this whole chunk and save it inside a script in the package's `tests/` folder. When executed, the test will run in a fresh session where the `communes` object is not defined. So that's why you need to redefine every variable the test needs to run. For the test itself, we use `testthat::expect_true()`. This function expects a piece of code that should evaluate to TRUE: if not, we get an error, and the whole pipeline stops here, forcing us to see what's going on. This is exactly what we want: when our code fails, it needs to fail as early and as spectacularly as possible. If you rely on future you to have to manually check console output or logs and look for errors, you deserve everything that's going to happen to you.

11.3. Turning our Rmds into a package

Under the section titled “Functions used for analysis”, I copy-and-pasted the functions from the `analyse_data.Rmd` and documented them as well. What’s new is that I’ve added examples:

```
```{r examples-get_laspeyeres, eval = FALSE}
#' \dontrun{
#' commune_level_data_laspeyeres <-
get_laspeyeres(commune_level_data)
#' }
````
```

But I don’t want these examples to run, I just want them to simply appear in the documentation. This is because, just like for tests, examples have to be self-contained. So for this example to run successfully, I would need to redefine `commune_level_data` from scratch. I don’t want to do this now, so hence why I wrapped the example around `\dontrun` and used roxygen-style comments with `#'`. I did the same with the function to plot the data.

We’re almost done; take a look again at the template `flat_minimal.Rmd`. I advised you to take inspiration from it to get `save_data.Rmd` fusen-ready. At the end of that file, we can see this chunk:

```
```{r development-inflate, eval=FALSE}
Run but keep eval=FALSE to avoid infinite loop
Execute in the console directly
fusen::inflate(flat_file =
 "dev/flat_minimal.Rmd",
 vignette_name = "Minimal")
````
```

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This chunk contains the code that we need to run, manually, to inflate the package. However, I've removed it from my `save_data.Rmd` file, and the reason is that I prefer to have it inside the `0-dev_history.Rmd` file. I think that it makes more sense to have it there. Take a look at my `0-dev_history.Rmd` here⁹. By reading that file, you see all the different developer actions that were taken. Your team-mates, or future you could read this, and immediately understand what happened, and what was done. Under the section title “Inflate `save_data.Rmd`”, you see that the chunk to inflate the `.Rmd` file and generate the package is there. I can run this chunk from `0-dev_history.Rmd` and have my package successfully generated. Something important to notice as well: my fusen-ready `.Rmd` file is simply called `save_data.Rmd`, while the generated, inflated file, that will be part of the package under the `vignettes/` folder is called `dev-save_data.Rmd`.

When you inflate you a flat file into a package, the R console will be verbose. This lists all files that are created or modified, but there is also a long list of checks that run automatically. This is the output of `devtools::check()` that is included inside `fusen::inflate()`. This function verifies that your package, once inflated, follows the rules of package development. This will likely result in some fails, warnings and notes. Your goal is to make it to 0 `errors`, 0 `warnings`, 0 `notes`. This will be a tricky part while developing packages, as you may not understand all outputs the first time. However, if you read the long list carefully, you will see that you are helped in many ways: position of the problems, type of problem,... Fix the problems in the flat file, and inflate again, until the number of errors is 0. I will not get deeper into this topic here, so you may want to search for `check()` in <https://r-pkgs.org>¹⁰ to go further.

⁹<https://is.gd/JsjJJVN>

¹⁰<https://r-pkgs.org>

I suggest that you stop here, and really try to get this working. You can start by simply cloning this repository¹¹ I linked in the beginning of this chapter, and follow along. After inflating, take a look at the vignette generated from the inflated `dev-save_data.Rmd`, which you can find under the `vignettes/` folder. One thing you need to understand is that the `save_data.Rmd` file that you inflate, under `dev/`, is a working file for *developers*. The generated vignette on the other hand, can be read by stakeholders other than developers as well. In my case, I've added the prefix `dev-` because this vignette deals with preparing data for including in the package, and there is not much point for a stakeholder other than a developer to read this vignette. You will notice that the generated vignette does not contain the function chunks. This is normal, because after inflating the `.Rmd` file, the functions get saved under the `R/` folder. Really take some time to understand this. Because what follows will assume that you have groked `{fusen}`.

11.4. Including datasets

Another difference between our initial `.Rmd` and the fusen-ready `.Rmd`, is that the fusen-ready `save_data.Rmd` file does not save the datasets as `.csv` files anymore. This is because it is much better to include them directly in the package, and make them available to users by running the line:

```
data("commune_level_data")
```

¹¹<https://is.gd/jGZrMF>

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To include data in a package, we need the package to already be built; only once the package exists can we include data sets. This is why we need to inflate `save_data.Rmd` first. So, how do we include data sets in a package? If you are developing packages in the usual manner (meaning, without `{fusen}`) then you have to do the following steps:

- write a script that generates the data set (and save this script inside the `data-raw/` folder for future reference)
- save the datasets inside the `data/` folder.

But we are using `{fusen}`, so instead, we can use the documentation first approach! And actually, the first step is done already: we have our vignette `save_data.Rmd`! Let's not forget that the whole point of `save_data.Rmd` file was, initially, to build these datasets and save them. So why not simply re-use this vignette? If you take a look at the inflated `dev-save_data.Rmd`, you will see that everything is right there! That's obvious because that was the Rmd file that we used to build the datasets in the first place. So remember, we don't want to have to repeat ourselves. The vignette is right there with the code we need, so we are going to use it.

If you look at `0-dev_history.Rmd`, everything is explained under the header “Including datasets”. The idea is to run the code inside the vignette, which creates our datasets, and then save these datasets in the right place using `useThis::use_data()`, mimicking the steps from “traditional” package development. In my `0-dev_history.Rmd` here¹², I wrapped all the code around the `local()` function to run all these steps inside a temporary, local environment. This way, any variable that gets made by knitting the vignette gets discarded once we're done saving the

¹²<https://is.gd/JsjJVN>

datasets. You may need to install your package before, using `remotes::install_local()`.

Finally, we need to document the datasets. For this, we use another `.Rmd` file that we inflate as well. You can find it under `dev/data_doc.Rmd`, or by clicking here¹³. Datasets get defined inside chunks, just like functions, using `{roxygen2}`-type comments.

This basically covers what you need to know to package code. Of course, there are many other topics that we could discuss, but for our purposes, this is enough. We now know how to take advantage of the tools that make package development easy, and have diverted them for our use. If you want to develop a proper package and push it to CRAN, then I highly recommend you read the second edition of *R packages*¹⁴ by Wickham and Bryan (2023). This book goes into all the nitty-gritty details of full package development. But let me be clear: this does not mean that you cannot develop a full, CRAN-ready, package using `{fusen}`. You absolutely can! It's just that this is outside the scope of the present book.

11.5. Installing and sharing the package

To install the package on the same machine that you developed it, you can simply run the line `remotes::install_local()` on line 46 of the `0-dev_history.Rmd` file (ideally in a fresh R session). But how can you share it with colleagues or future you?

Now that the package is ready, you need to be able to share it. This really depends on whether you can publish the code

¹³<https://is.gd/wjkNAO>

¹⁴<https://r-pkgs.org/>

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on Github or not, or whether your company/institution has a self-hosted version control system. In this section, we're going to explore the following two scenarios: the package is hosted on Github (or in a private self-hosted version control system), or the package cannot be hosted for whatever reason but you still need to share the package.

11.5.1. Code is hosted

So if the code is hosted on Github (or on a self-hosted, private, version control system), users of the package can install it directly from Github. This can be done using the `{remotes}` package, like this:

```
remotes::install_github(  
  "github_username/repository_name"  
)
```

It is also possible to install the package from a specific branch:

```
remotes::install_github(  
  "github_username/repository_name@repo_name"  
)
```

it is even possible to install the package exactly how it was at a specific commit:

```
remotes::install_github(  
  "github_username/repository_name@repo_name",  
  ref = "commit_hash"  
)
```

For example, if you want to install the package we have developed together from my Github account, you could run the following (the commit hash is actually wrong so you don't install this one by mistake):

```
remotes::install_github(
  "rap4all/housing@fusen",
  ref = "ae42601"
)
```

So the package in the `fusen` branch and at commit “ae42601” gets installed. Keep in mind that you can specify the commit hash to install the exact version you need, because this is going to do wonders for reproducibility.

11.5.2. Code cannot be hosted

If the code cannot be hosted, then you have to share it *manually*. That's less than ideal, but sometimes there simply is no alternative. In that case, you need to prepare a compressed archive that you can share. This is easily done using `devtools::build()`. Start a new session in the root directory of your package, and run `devtools::build()`. This will create a `.tar.gz` file that you can send to your teammates, or archive for future you. Ideally, before creating this file, you should go to `0-dev_history.Rmd` and update the version number in the `fusen::fill_description()` function, like so:

```
```{r description, eval=FALSE}
fusen::fill_description(
 pkg = here::here(),
```

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```
fields = list(
 Title = "Housing Data For Luxembourg",
 Version = "0.1", # notice that I've added a
 ↵ version number here
 Description = "This package contains
 ↵ functions to get,
 ↵ clean and analyse housing
 ↵ price data for Luxembourg.",
 `Authors@R` = c(
 person("Bruno", "Rodrigues", email =
 ↵ "bruno@brodrigues.co",
 role = c("aut", "cre"),
 comment = c(ORCID =
 ↵ "0000-0002-3211-3689"))
)
)
,
overwrite = TRUE) # you need to add overwrite
 ↵ = TRUE to overwrite the file
```

```

You have to be very disciplined here, because you have to make sure that you keep updating this and documenting which version of the package should get used for which project. Also, make sure that you can store generated `.tar.gz` alongside the project and that you provide clear installation instructions. To install a package from a `.tar.gz` file, open a new R session and run the following:

```
remotes::install_local(
  "path/to/package/housing_0.0.0.9000.tar.gz"
)
```

11.5.3. Marketing your work

Once your package is done, whether it is destined for CRAN or not, whether it can only be shared within your organisation or not, it is important to market it and make it discoverable. This is where building a website for the package is important, and thankfully, it takes two lines of code to build a fully functioning site. In the introduction we built the website for the template included with `{fusen}`, let's now build a website for our housing package.

This website can then be hosted online if you wish, or it can be shared internally to your organisation, offline, as a means of providing documentation.

Take a look at the very last section of the `0-dev_history.Rmd` file, titled “Share the package”. If you execute the lines in that chunk (ideally from a fresh R session), a website will be built automatically. You can find the website’s files in the `docs/` folder: open the `index.html` file using a web browser and you can start navigating the documentation!

If your package is on Github, you can also host the website for free on Github pages. For this, you can build the website locally and send it to GitHub, or use GitHub Actions to build and publish it automatically.

For the manual build, first make sure that the `.gitignore` file in the root of your package does not contain the `docs/` folder. If it does, remove it. Then, commit and push. This will upload the `docs/` package on Github. Then, go to the repository’s settings, and “Pages” and then choose the branch that contains the `docs/` folder:

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The screenshot shows the GitHub repository settings page for a repository named 'fusen'. The 'Pages' tab is selected, highlighted with a red box. On the left, a sidebar lists various settings categories: General, Access, Collaborators, Moderation options, Code and automation, Branches, Tags, Actions, Webhooks, Environments, Codespaces, and Pages. The 'Pages' category is highlighted with a red box. In the main content area, under the 'GitHub Pages' heading, it says 'GitHub Pages is designed to host your personal, organization, or project pages from a GitHub repository.' Below this, the 'Build and deployment' section has 'Source' set to 'Deploy from a branch'. A dropdown menu shows 'Branch' with options 'fusen' and 'docs', with 'docs' selected. A 'Save' button is also present. At the bottom, there's a 'Visibility' section with a 'GITHUB ENTERPRISE' button, a note about privately publishing sites, and a 'Try GitHub Enterprise risk-free for 30 days' button.

Figure 11.2.: Choose these options to host your package's website for free!

For the automatic build, first make sure that the `.gitignore` file in the root of your package does contain the `docs/` folder, so that you do not send your local verifications. Then go to your `0-dev_history.Rmd` to run:

```
usethis::use_github_action("pkgdown")
```

Commit the `.github/` directory with its `yml` files and push. GitHub Action is a service that automatically runs following instructions in the `yml` file, at each commit. When you commit to the `main` or `master` branch, the website will be built. As above, in the GitHub settings, you will need to define the root of the `gh-pages` branch to be published as GitHub Pages. This is called Continuous Integration and Continuous Deployment. Note that you may want to set the other GitHub Actions listed in the `0-dev_history.Rmd` to make it check your package on a

different computer than yours. There is a chapter about CI/CD later in this book.

As an example of the website, you can visit the website of the package we've built together here¹⁵.

The package's `README` will be shown, if available, on the starting page of the website. So if you want to add a `README` to your package, go to the `0-dev_history.Rmd` file and execute the line `usethis::use_readme_rmd()`, which adds a template `README` file in the root of your package. Regardless of whether you want to build a website, adding a `README` to it is always a good idea! You could explain what the main features of the package are, and how to install it, especially if you want your users or future you to install the package at a certain commit, it is quite useful to write it down clearly in the instructions. Something like:

```
To install this package, run the following lines
↳ of code:

```
remotes::install_github("rap4all/housing@fusen",
 ref = "ae42601")
```

```

You can also include the link to your website documentation.

11.6. Conclusion

Turning our analysis into a package is useful, because we can divert a lot of tools that are originally intended for package

¹⁵<https://rap4all.github.io/housing/>

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development towards improving our analysis. We can now more easily document the code, define its dependencies, and also share it with teammates, our future selves or the world. What's more, we clearly separate two tasks from each other: the pure software engineering part, which consisted in building the package, from the pure data analysis part, which will eventually become our pipeline.

But turning the analysis into a package *is* optional; this is not something that you absolutely have to do to turn your analysis reproducible. However, the entry cost of package development is really lowered thanks to `{fusen}` and the benefits are really great, so I think that is important to do.

There is one chapter left before we actually build a full-fledged pipeline. In the next chapter, we will learn how to use unit and assertive testing to further improve the code of our package, which will thus also improve the quality of our analysis.

12. Testing your code

Testing code is crucial, and we all do it in some form or another. The problem is that it is not something that we do consistently: usually code gets tested at the beginning of a project, but then, as we start focusing on the analysis more and more and need to respect deadlines, testing gets forgotten.

In this chapter, you are going to learn how to make testing your code consistent and, very importantly, fully automatic. Just like in the previous chapter, the key is to *write everything down*. Don't just do a little test in the console to see if the function you've just written works as expected. Write it down! And don't rely on future you to run tests, because future you is just as unreliable as you are. Tests need to be run each time *any* of the code from a project gets changed. This might seem overkill (why test a function that you didn't even touch for weeks?), but because there are dependencies between your functions, a change in one function can affect another function. Especially if the output of function A is the input of function B: you changed function A and now the output of function A changed in a way that it breaks function B, or also modifies its output in an unexpected way.

There are several types of tests that we can use:

- unit testing: these are written while developing, and executed while developing;

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- assertive testing: these are executed at runtime. These make sure, for example, that the inputs a function receives are sane.

Let's start with unit testing.

12.1. Unit testing

Unit testing is the testing of units. What's a unit? Functions are units! We actually already encountered one unit test before, in the `save_data.Rmd` script:

```
```{r tests-clean_flat_data}
We now need to check if we have them all in
the data.
The test needs to be self-contained, hence
why we need to redefine the required
variables:

former_communes <- get_former_communes()

current_communes <- get_current_communes()

communes <- get_test_communes(
 former_communes,
 current_communes
)

raw_data <- get_raw_data(url =
 "https://is.gd/1vvBAc")
```

```
flat_data <- clean_raw_data(raw_data)

testthat::expect_true(
 all(communes %in%
 unique(flat_data$locality)))
)
````
```

When using `{fusen}`, a unit test should be a self-contained chunk that can be executed completely independently. This is why in this chunk we re-created the different variables that were needed, `communes` and `flat_data`. If you were developing the package without `{fusen}`, you would need to do the same, so don't think that this is somehow a limitation of `{fusen}`.

The test above ensures that we find all the former and current communes of Luxembourg in our dataset. Let me explain again why we want to write such a test down in a script and not simply try it out in our console “manually” to check if the code works.

For this test to pass, a lot of moving pieces have to fall together. If anything changes, be it because you changed something in either `get_raw_data()` or `clean_raw_data()` or because something changed with the Wikipedia tables you scraped, this test will not pass. And you should be made aware of failures as soon as possible! Also, this test ensures that when the data gets updated, you are certain that if you use the code in `save_data.Rmd` you will get a new dataset that is likely correct, even if new communes merge. And mergers will happen around 2024 by the way, the communes of Groussbous and Wal will merge, and the communes of Bous and Waldbredimus as well. So you need to make sure that when this happens, your code knows how to handle this, or at least returns an error as early as possible.

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Ideally, you need to test every function that you wrote, but sometimes that's not really possible, either due to lack of time, or because the function is quite trivial, so maybe no test is warranted. But be careful what you consider trivial though, I have personally been bitten in the past by “trivially” simple functions! For example, a function like this one:

```
```{r function-make_commune_level_data}
#' make_commune_level_data Makes the final data
#< at commune level
#'
#' @param flat_data Flat data df as returned by
#< clean_flat_data()
#' @importFrom dplyr filter
#' @return A data frame
#' @export
make_commune_level_data <- function(flat_data){
 flat_data |>
 filter(!grepl("nationale|offres", locality),
 !is.na(locality))
}

````
```

might not need to be unit-tested. An assertion, which we will learn about in the next section, is likely better suited to the above function. However, as functions become more complex, unit tests are highly recommended. This is because it can become very difficult to make sure that changing some part of the function somewhere does not affect some other part. This is where writing several unit tests can be useful. As long as all unit tests keep succeeding (or passing) you are somewhat sure that what you're doing is not breaking stuff. And unit tests are

especially useful when collaborating using trunk-based development! As the project leader, you could for example refuse to merge changes that break unit tests.

Before continuing, let's rewrite the test we have already. While it is fully working, I didn't really write it in the canonical form. Inside `dev/save_data.Rmd`, change the code of the test to the following:

```
```{r tests-clean_flat_data}
We now need to check if we have them all in
the data.
The test needs to be self-contained, hence
why we need to redefine the required
variables:

former_communes <- get_former_communes()

current_communes <- get_current_communes()

communes <- get_test_communes(
 former_communes,
 current_communes
)

raw_data <- get_raw_data(url =
 "https://is.gd/1vvBAc")

flat_data <- clean_raw_data(raw_data)

test_that("Check if all communes are accounted
for", {
```

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```
expect_true(
 all(communes %in%
 unique(flat_data$locality))
)
}
```
```

The only difference is that instead of calling `expect_true()` directly, I wrapped this call inside `test_that()`. This way, I can add a description to the test. This is useful if the test fails.

Save `dev/save_data.Rmd` and go back to `0-dev_history.Rmd` to inflate `save_data.Rmd` again. Everything should work without problems.

If the test fails, you get an informative message. To illustrate, I've added a typo in the test and inflated `save_data.Rmd`. Because tests always run when a fusen-package gets inflated, this test failed and here is the output:

```
Failed tests  
Error ('test-get_raw_data.R:18'): Check if all  
communes are accounted for  
Error in `communs %in% unique(flat_data$locality)`:  
object 'communs' not found  
Backtrace:  
1.  testthat::expect_true(all(communs %in%  
unique(flat_data$locality)))  
   at test-get_raw_data.R:18:2  
2.  testthat::quasi_label(enquo(object), label,  
arg = "object")
```

```

3.      rlang::eval_bare(expr, quo_get_env(quo))
4.  communs %in% unique(flat_data$locality)

[ FAIL 1 | WARN 2 | SKIP 0 | PASS 0 ]
Error: Test failures
Execution halted

```

The file `test-get_raw_data.R` contains our test, generated by inflating `save_data.Rmd`. You can find it under the `tests/testthat/` folder of your inflated package. You can also see the description that we've added, which helps us find the test that failed. In cases like this, you should go back to the function that makes the test fail and correct it, until the test passes. You should also make sure that everything is alright with the test itself. If there really is a typo in the test, you should of course correct the test (in `dev/save_data.Rmd`, not in `tests/testthat/`)!

Now, let's add a unit test to another function, `get_laspeyeres()`. This function seems to me like a good candidate for testing, as it is not that trivial.

Let's try with something simple. `get_laspeyeres()` expects either `commune_level_data` or `country_level_data`. What happens if we provide another dataset? The function very likely returns an error. So let's test for this. Go back to the `save_data.Rmd` file and add the following, under the function definition of `get_laspeyeres()`:

```

```{r tests-get_laspeyeres}
test_that("Wrong data", {

 expect_error(
 get_laspeyeres(mtcars)
}

```

## 12. Testing your code

```
)
})

```

Since we expect an error, we used `expect_error()`, which succeeds if the code fails! If you're confused, no worries, we've all been there. But let's think about it: what would you want to happen if you provided a wrong data set? Surely, you'd like for the function to scream an error at you, and not somehow do something and return *something*. So testing that functions fail when they should is actually quite important as well. Let's add another, similar, test:

```
```{r tests-get_laspeyeres}  
  
test_that("Wrong data", {  
  
  expect_error(  
    get_laspeyeres(mtcars)  
  )  
  
})  
  
test_that("Empty data", {  
  
  expect_error(  
    # this subsetting results in an empty dataset  
    get_laspeyeres(subset(mtcars, am == 2))  
  )  
  
})
```

...

This second test checks what happens if we provide an empty dataset. This should not happen, but hey, it's always a good idea to see what could happen. Here we also expect an error, so we use `expect_error()` as well. Inflating `save_data.Rmd` runs the tests again, and all of them succeed.

Now, I know what you're thinking. Probably something along the lines of “*Bruno, you told me that making my projects reproducible and reliable and robust would not take much more time than what I was already doing before. This certainly doesn't feel like it!*”, to which I answer that your feelings on the issue are wrong. It may not feel like it, but doing this does two things:

- It ultimately saves you time. You typed the test once, and can now rerun it automatically every time you inflate the `.Rmd` files. You don't need to remember to test the code, and don't need to remember how to test the code.
- This saves you a lot of headaches. You don't have to live in fear that you might forget to test the code, or forget how to test the code. You wrote the tests down, and now you're free to concentrate on adding features or using the existing code knowing that you can trust its outputs.

Trust the process.

Let's go back to the two tests from before: `get_laspeyeres()` fails, as expected, when we provide a random dataset to it. But it would be interesting to know why it fails. Simply run `get_laspeyeres(mtcars)` in the console. This is what we get back:

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```
Error in `mutate()`:
! Problem while computing `p0 = ifelse(year ==
"2010",
  average_price_nominal_euros, NA)`.

Caused by error in `ifelse()`:
! object 'year' not found
Run `rlang::last_error()` to see where the error
occurred.
```

So the function fails but for the wrong reason. It fails because the column `year` cannot be found in the data. But what if there was a column `year` in the data? The code would continue, but then likely fail for some other reason. It would be much safer to make it fail as soon as possible, by detecting right from the start if the provided data sets are not one of `commune_level_data` or `country_level_data`. But for this, we need assertive programming, which we will discuss in the next section. Why an assertive test and not a unit test? Because unit tests should run during development time, and assertive tests run at run-time (when the function is executed). So in this case, we want the input to get checked at run-time. In the next section, we will be changing the function to fail when the right datasets are not provided, but our unit test will not need to change; the function still fails, but this time it'll be for the right reasons.

This is another advantage of writing tests: it forces you to think about what you're doing. The simple act of thinking and writing tests very often improves your code quite a lot, and not just from a pure algorithmic perspective, but also from a user experience perspective. Writing these tests made us think about the failure of our function when users provide a wrong dataset and made us realise that it would be much better for users if the returned error message is something along the lines of “Wrong dataset, please provide either `commune_level_data` or

`country_level_data”.`

Let’s continue with testing `get_laspeyeres()`. It would be nice to see if the function actually does what it’s supposed to do correctly. For this, we need to start from an input, and then create the expected output. It doesn’t matter how you create this output, what matters is that you make absolutely sure that it is correct, and then, never touch it ever again. Let’s call this output the “truth”. Then, you provide `get_laspeyeres()` with this input and save the output that `get_laspeyeres()` generates. You then compare the “truth” to this output. If everything matches, congratulations, your function produces the right output.

So let’s start. Remember that unit tests should be self-contained, so I’m going to create the input dataset and the expected data set (what I called the “truth”) in the test itself. This is the code I’m going to use to create the mock, input dataset:

```
input_df <- expand.grid(
  list("year" = c(2010, 2011),
       "locality" = c("Bascharage",
                     "Luxembourg")))
)

input_df$n_offers <- c(123, 101, 1230, 1010)
input_df$average_price_nominal_euros <- c(234,
                                            345, 560, 670)
input_df$average_price_m2_nominal_euros <- c(23,
                                              34, 56, 67)
```

This creates a data frame with two years, two communes and some mock prices. Now, I need to create the output. I start from the input, and add the columns that get computed by running

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`get_laspeyeres()` myself, “by hand”. Remember, you need to make sure that these results are correct!

```
expected_df <- input_df

# p0 should be always equal to the value in the
# first year
expected_df$p0 <- c(234, 234, 560, 560)
expected_df$p0_m2 <- c(23, 23, 56, 56)

# pl should be equal to the price divided by p0
expected_df$pl <-
  expected_df$average_price_nominal_euros/
  expected_df$p0 * 100

expected_df$pl_m2 <-
  expected_df$average_price_m2_nominal_euros/
  expected_df$p0_m2 * 100
```

If you look at each line, you see that this is exactly what `get_laspeyeres()` does. We can inspect the results and maybe even verify the value of each cell using a pocket calculator. It doesn’t matter, what’s important is that `expected_df` is correct and saved. This is what the full test looks like:

```
```{r, eval = F}
test_that("get_laspeyeres() produces correct
results", {

 input_df <- expand.grid(
 list("year" = c(2010, 2011),
```

```
 "locality" = c("Bascharage",
 ↵ "Luxembourg"))
)

input_df$n_offers <- c(123, 101, 1230, 1010)
input_df$average_price_nominal_euros <- c(234,
 ↵ 345, 560, 670)
input_df$average_price_m2_nominal_euros <-
 ↵ c(23, 34, 56, 67)

expected_df <- input_df

p0 should be always equal to the value in
 ↵ the first year
expected_df$p0 <- c(234, 234, 560, 560)
expected_df$p0_m2 <- c(23, 23, 56, 56)

p1 should be equal to the price divided by
 ↵ p0
expected_df$p1 <-
 ↵ expected_df$average_price_nominal_euros /
 ↵ expected_df$p0 * 100
expected_df$p1_m2 <-
 ↵ expected_df$average_price_m2_nominal_euros /
 ↵ expected_df$p0_m2 * 100

expect_equivalent(
 ↵ expected_df, get_laspeyeres(input_df)
)

})
...
```

## 12. Testing your code

Notice that I've used `expect_equivalent()` and not `expect_equal()` to check if `expected_df` is equal to the output of `get_laspeyeres(input_df)`. This is because `expected_df` is of class `data.frame`, while `get_laspeyeres()` outputs a `tibble`. So if you use `expect_equal()` the test would not pass, because the classes of both objects are not strictly equal. Sometimes, this level of strictness is required, but not always, as is the case here.

Once again, inflate `save_data.Rmd`. This will run the tests, and if everything went well, you should end up, again, with a functioning package. I highly advise that you consult `{testthat}`'s documentation to learn about all the other functions that you can use for writing unit tests.

If you've managed to write the unit tests and inflate the package successfully, then let's move on to assertive programming.

## 12.2. Assertive programming

Remember in Chapter 6, where I discussed safe functions? As a refresher, here's the `nchar()` function, providing a correct output when the input is a character:

```
nchar("100000000")
```

```
[1] 9
```

and here is `nchar()` providing a *surprising* result when the input is a number:

```
nchar(100000000)
```

```
[1] 5
```

This is because 100000000 gets converted to `1e+08` and then this gets converted into the string "`1e+08`" which is 5 characters long. So in that section, I suggested defining your own `nchar2()` that makes sure that the provided input is a character:

```
nchar2 <- function(x, result = 0){

 if(!isTRUE(is.character(x))){
 stop(paste0("x should be of type
 'character', but is of type '",
 typeof(x), "' instead."))
 } else if(x == ""){
 result
 } else {
 result <- result + 1
 split_x <- strsplit(x, split = "")[[1]]
 nchar2(paste0(split_x[-1],
 collapse = ""), result)
 }
}
```

This now returns an error if the input is a number, instead of doing all these silent conversions. The technique we have used here is what we call assertive programming. `stop()` and `stopifnot()` are functions included with R that can be used for assertive programming. Here is an example using `stopifnot()`:

```
nchar3 <- function(x, result = 0){

 stopifnot("Input x must be a character" =

```

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```
isTRUE(is.character(x)))\n\nif(x == ""){\n result\n} else {\n result <- result + 1\n split_x <- strsplit(x, split = "")[[1]]\n nchar3(paste0(split_x[-1],\n collapse = "")), result)\n}\n}
```

If we go back to `get_laspeyeres()`, we should be using assertive programming to make sure that the provided datasets are one of `commune_level_data` or `country_level_data`. This is how we could rewrite the function:

```
get_laspeyeres <- function(dataset){\n\n which_dataset <- deparse(substitute(dataset))\n\n stopifnot("dataset must be one of\n `commune_level_data`\n or `country_level_data`" =\n (which_dataset %in% c(\n \"commune_level_data\",\n \"country_level_data\")))\n\n group_var <- if(grepl(\"commune\", \n which_dataset)){\n quo(locality)\n } else {
```

```

 NULL
 }

dataset |>
 group_by (!!group_var) |>
 mutate(
 p0 = ifelse(
 year == "2010",
 average_price_nominal_euros,
 NA)
) |>
 fill(p0, .direction = "down") |>
 mutate(
 p0_m2 = ifelse(
 year == "2010",
 average_price_m2_nominal_euros,
 NA)
) |>
 fill(p0_m2, .direction = "down") |>
 ungroup() |>
 mutate(
 pl = average_price_nominal_euros/p0*100,
 pl_m2 =
 ↵ average_price_m2_nominal_euros/p0_m2*100)

}

```

We can now also edit the unit test from before, the one where we provide the wrong data. With this new specification of the function, this unit test would still pass (the function returns an error), as expected, but for the wrong reason. We now want to make sure that it fails for the right reason, in other words, that it fails not because no `year` column is found, but because the provided data set is neither `commune_level_data`

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nor `country_level_data`, so for this we change the unit tests like this:

```
test_that("Wrong data", {

 expect_error(
 get_laspeyeres(mtcars),
 regexp = "dataset must be one of"
)

})
```

I use the `regexp` argument of `expect_error` to enter a regular expression that matches the error message. So the string “dataset must be one of” will match the message returned by the error, and if they match (remember, the provided string is a regular expression), then I know I get the *correct* error. Here is what happens if I use the wrong message as the `regex` argument:

```
Failed tests
Failure ('test-get_laspeyeres.R:6'): Wrong data

'get_laspeyeres(mtcars)' threw an error with
unexpected message.
Expected match: "message is wrong"
Actual message: "dataset must be one of
'commune_level_data'
 or `country_level_data`"
```

So now, not only does our function fail for the right reasons, our test is able to tell us that as well!

Before inflating to run these tests, you should also change the test titled “`get_laspeyeres()` provides correct answers”. This

is because the name of the input dataset used for the test is `input_df`. So if you leave it like this, the assertion that we've included in the function will make this test fail. So change this test by simply saving `input_df` `commune_level_data`:

```
rename data to make assertion pass
commune_level_data <- input_df

expect_equivalent(
 expected_df,
 `get_laspeyeres(commune_level_data)
)
```

if you forget to do this, don't worry, the unit test would not fail to remind you!

Go back to `0-dev_history.Rmd` and inflate the file again to update it. Everything should work without any issues. If not, take the time to make the unit tests pass and inflate the package successfully!

Something else that is well-suited for assertive programming is checking whether the provided inputs are of the right class:

```
any_function <- function(dataset){

 stopifnot(``dataset` must be a data frame" =
 inherits(dataset, "data.frame"))

 print("No problem")
}
```

This will succeed:

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```
any_function(mtcars)
```

```
[1] "No problem"
```

But this will fail:

```
any_function("this is not a data frame")
```

```
Error in any_function("this is not a data frame") :
`dataset` must be a data frame
```

`inherits()` checks if an object inherits from a certain class. So for example, a `tibble` or a `data.table` that are classes that are defined by inheriting attributes from the `data.frame` class, will also successfully pass the test above. You can be as strict as you need: for example, do you need any type of number? You could do the following:

```
inherits(2, "numeric")
```

```
[1] TRUE
```

But do you actually need integers, and want to force this? Then you could be stricter in your assertion:

```
inherits(2, "integer")
```

```
[1] FALSE
```

If you want the above to evaluate to `TRUE`, an integer must be provided:

```
inherits(2L, "integer")
```

```
[1] TRUE
```

Do you want, for some reason, that your functions only accept `tibbles` and not `data.frames`? Be as strict as you need. This will succeed:

```
inherits(tibble::as_tibble(mtcars), "tbl_df")
```

```
[1] TRUE
```

This will fail:

```
inherits(mtcars, "tbl_df")
```

```
[1] FALSE
```

You could also use more complex assertions. For example, suppose that you need to clean data using many functions, with several filters. Something could go wrong in any of these functions for a variety of reasons. So each of these functions could test if all the individuals are still in the data, and that you didn't remove any of them by mistake. A test like this could make sure that each level of the variable `am` are still in the data:

```
summary_stats <- function(dataframe, var){
 stopifnot("Some individuals are missing!" =
 all((unique(dataframe[[var]]))
 %in% c(0,1)))

 # and then some computations here
}
```

## 12. Testing your code

Now, when running `summary_stats(mtcars, "am")`, if somehow the level “1” or “0” is missing from `mtcars`, the function would throw an error.

There are several packages for assertive programming that you might want to check out:

- `{assertthat}`<sup>1</sup>
- `{chk}`<sup>2</sup>
- `{checkmate}`<sup>3</sup>

I won’t discuss any of them; what’s important is for you to know that assertive programming is something that is useful and that you should add to your toolbox.

### 12.3. Test-driven development

Test-driven development, or TDD, is the programming paradigm in which instead of writing a function and then several tests to ensure that the code is working as expected, you start by writing tests, and then the function. Of course, since there is no function to test, these tests will all obviously fail at first. But the goal is to then write a function such that the tests pass.

TDD is interesting in at least two scenarios:

- You want to write a function, but don’t know exactly where to start. Maybe it’s a very complex function. So writing tests can help you think about it, and already fix certain properties that this function should have.

---

<sup>1</sup><https://github.com/hadley/assertthat>

<sup>2</sup><https://poissonconsulting.github.io/chk/>

<sup>3</sup><https://mllg.github.io/checkmate/>

- You use the tests as a way to write requirements for a code-base. This can be useful when working in a team, and you don't want to "waste" time writing requirements, so instead you write tests that describe how the function should work, what type of inputs get accepted, how its output looks like... Careful though, because a "smart" programmer could write code that passes the tests but doesn't actually do anything otherwise useful.

I tend to use TDD when I need to write a function but don't quite know where to start. I start by writing the most basic tests and make them ever more complicated. At some point, I start having an idea for the function's implementation and have a go at it.

Some programmers only do TDD; so they start by writing many, many tests, and then only start writing their functions. Personally, I think that this is also not ideal, because you could waste a lot of time writing meaningless tests.

## 12.4. Code coverage

It is useful to have an idea of which functions are tested and which are not, but also *how much* of a function is being tested. For example, suppose that you have an `if...else...` clause somewhere in a function. Did you write a test for each of the outcomes of this clause? Maybe you only wrote a test when this clause evaluates to `TRUE`, but forgot to write a test for the case it is `FALSE`.

The packages `{covr}` allows you to track the test coverage of your package. Install `{covr}` and run `report()` in the console to get the results:

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```
covr::report()
```

This should open a tab in your web browser with some statistics. You can click on the individual scripts to see the source code of your functions: each line that is highlighted in green represents a line that is being tested, and lines in red are lines that are not being tested:

housing coverage - 73.33%

```
1 # WARNING - Generated by {fusen} from /dev/save_data.Rmd: do not edit by hand
2
3 #' Draw some plots
4 #
5 #' @param dataset The dataset for which the index needs to be computed
6 #' @importFrom dplyr group_by ungroup mutate
7 #' @importFrom rlang quo
8 #' @importFrom tidyverse fill
9 #' @return The input dataset with added columns: p0, p0_m2, pl and pl_m2. p0 are prices
10 #' @export
11 #' @examples
12 #' \dontrun{
13 #' commune_level_data_laspeyeres <- get_laspeyeres(commune_level_data)
14 #' }
15 get_laspeyeres <- function(dataset){
16
17 3x which_dataset <- deparse(substitute(dataset))
18
19 3x stopifnot("dataset must be one of `commune_level_data` or `country_level_data`" =
20 3x (which_dataset %in% c("commune_level_data", "country_level_data")))
21
22 1x group_var <- if(grepl("commune", which_dataset)){
23 1x quo(locality)
24 } else {
25 ! NULL
26 }
27 1x dataset |>
28 1x group_by(!|group_var) |>
29 1x mutate(n0 = ifelse/year == "2010", average price nominal euros. NA) |>
```

Figure 12.1.: The output of report() inside a web browser.

You could strive to get 100% coverage by painting all the lines green (by writing unit tests that test these lines). But in practice, it is not always so easy to get 100% coverage, so don't fret if you don't achieve perfection.

If you're working on a server (and thus do not have access to a graphical user interface) you can instead use the

`covr::package_coverage()` function which provides you with the following results (printed in the console):

```
housing Coverage: 73.33%
R/get_laspeyeres.R: 57.14%
R/get_raw_data.R: 80.65%
```

The percentage represents the share of lines of code that are tested by our unit tests. We see that the share of lines being tested in `get_laspeyeres.R` is 57%: this is because the script `get_laspeyeres.R` contains two functions, `get_laspeyeres()` and `make_plot()`. We do not test `make_plot()` at all, hence why the percentage is so low. We could move `make_plot()` to another script by simply putting the function under a level two header in the original `.Rmd` file and then inflating again. But in any case, this would not improve the overall coverage of the package; we would ideally need to write a test for `make_plot()`. This is left as an exercise to the reader.

## 12.5. Conclusion

Testing is crucial and useful. Not just because it gives you peace of mind but also because writing tests forces you to think about your code, by putting yourself in the shoes of your users (which include future you as well). In most cases, it is even something that you've been doing but perhaps not as systematically as you should.

There really is no other way to say this: you need to consider writing tests as an integral part of the project, and need to take the required time it takes to write them into account when planning projects. But keep in mind that writing them makes you gain a lot of time in the long run, so actually, you might even be

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faster by writing tests! Tests also allow you to immediately see where something went wrong, when something goes wrong. So tests save you time here as well. Without tests, when something goes wrong, you have a hard time finding where the bug comes from, and end up wasting precious time. And worse, sometimes things go wrong and break, but silently. You still get an output that may look ok at first glance, and only realise something is wrong way too late. Testing helps to avoid such situations.

So remember: it might *feel* like packaging your code and writing tests for it takes time, but you're actually already doing it, but non-systematically and manually and it ends up saving you time in the long run instead. Testing also helps with developing complex functions.

The tools I've shown you in this and the previous chapter are probably the fastest, easiest options to go from your analysis to a documented and tested package in a matter of hours. The benefits these provide however are measured in days of work.

# 13. Build automation with targets

We are finally ready to actually build a pipeline. For this, we are going to be using a package called `{targets}` (Landau 2021) which is a so-called “build automation tool”.

If you go back to the reproducibility iceberg, you will see that we are quite low now.

Without a build automation tool, a pipeline is nothing but a series of scripts that get called one after the other, or perhaps the pipeline is only one very long script that does the required operations successfully.

There are several problems with this approach, so let’s see how build automation can help us.

## 13.1. Introduction

Script-based workflows are problematic for several reasons. The first is that scripts can, and will, be executed out of order. You can mitigate some of the problems this can create by using pure functions, but you still need to make sure not to run the scripts out of order. But what does that actually mean? Well, suppose that you changed a function, and only want to re-execute the

### *13. Build automation with targets*

parts of the pipeline that are impacted by that change. But this supposes that you can know, in your head, which part of the script was impacted and which was not. And this can be quite difficult to figure out, especially when the pipeline is huge. So you will run certain parts of the script, and not others, in the hope that you don't need to re-run everything.

Another issue is that pipelines written as scripts are usually quite difficult to read and understand. To mitigate this, what you'd typically do is write a lot of comments. But here again you face the problem of needing to maintain these comments, and once the comments and the code are out of synch... the problems start (or rather, they continue).

Running the different parts of the pipeline in parallel is also very complicated if your pipeline is defined as script. You would need to break the script into independent parts (and make really sure that these parts are independent) and execute them in parallel, perhaps using a separate R session for each script. The good news is that if you followed the advice from this book you have been using functional programming and so your pipeline is a series of pure function calls, which simplifies running the pipeline in parallel.

But by now you should know that software engineers also faced similar problems when they needed to build their software, and you should also suspect that they likely came up with something to alleviate these issues. Enter build automation tools.

When using a build automation tool, what you end up doing is writing down a recipe that defines how the source code should be “cooked” into the software (or in our case, a report, a cleaned dataset or any data product).

The build automation tool then tracks:

- any change in any of the code. Only the outputs that are affected by the changes you did will be re-computed (and their dependencies as well);
- any change in any of the tracked files. For example, if a file gets updated daily, you can track this file and the build automation tool will only execute the parts of the pipeline affected by this update;
- which parts of the pipeline can safely run in parallel (with the option to thus run the pipeline on multiple CPU cores).

Just like many of the other tools that we have encountered in this book, what build automation tools do is allow you to not have to rely on your brain. You *write down* the recipe once, and then you can focus again on just the code of your actual project. You shouldn't have to think about the pipeline itself, nor think about how to best run it. Let your computer figure that out for you, it's much better at such tasks than you.

## 13.2. `{targets}` quick-start

First thing's first: to know everything about the `{targets}` package, you should read the excellent `{targets}` manual<sup>1</sup>. Everything's in there. So what I'm going to do is really just give you a very quick intro to what I think are really the main points you should know about to get started.

Let's start with a "hello-world" type pipeline. Create a new folder called something like `targets_intro/`, and start a fresh R session in it. For now, let's ignore `{renv}`. We will see how `{renv}` works together with `{targets}` to provide an (almost

---

<sup>1</sup><https://is.gd/VS6vSs>

## 13. Build automation with targets

reproducible) pipeline later. In that fresh session inside the `targets_intro/` run the following line:

```
targets::tar_script()
```

this will create a template `_targets.R` file in that directory. This is the file in which we will define our pipeline. Open it in your favourite editor. A `_targets.R` pipeline is roughly divided into three parts:

- first is where packages are loaded and helper functions are defined;
- second is where pipeline-specific options are defined;
- third is the pipeline itself, defined as a series of *targets*.

Let's go through all these parts one by one.

### 13.2.1. `_targets.R`'s anatomy

The first part of the pipeline is where packages and helper functions get loaded. In the template, the very first line is a `library(targets)` call followed by a function definition. There are two important things here that you need to understand.

If your pipeline needs, say, the `{dplyr}` package to run, you could write `library(dplyr)` right after the `library(targets)` call. However, it is best to actually do as in the template, and load the packages using `tar_option_set(packages = "dplyr")`. This is because if you execute the pipeline in parallel, you need to make sure that all the packages are available to all the workers (typically, one worker per CPU core). If you load the packages at the top of the `_targets.R` script, the packages will be available for the original session that called

`library(...)`, but not to any worker sessions spawned for parallel execution.

So, the idea is that at the very top of your script, you only load the `{targets}` library and other packages that are required for running the pipeline itself (as we shall see in coming sections). But packages that are required by functions that are running inside the pipeline should ideally be loaded as in the template. Another way of saying this: at the top of the script, think “pipeline infrastructure” packages (`{targets}` and some others), but inside `tar_option_set()` think “functions that run inside the pipeline” packages.

Part two is where you set some global options for the pipeline. As discussed previously, this is where you should load packages that are required by the functions that are called inside the pipeline. I won’t list all the options here, because I would simply be repeating what’s in the documentation<sup>2</sup>. This second part is also where you can define some functions that you might need for running the pipeline. For example, you might need to define a function to load and clean some data: this is where you would do so. We have developed a package, so we do not need such a function, we will simply load the data from the package directly. But sometimes your analysis doesn’t require you to write any custom functions, or maybe just a few, and perhaps you don’t see the benefit of building a package just for one or two functions. So instead, you have two other options: you either define them directly inside the `_targets.R` script, like in the template, or you create a `functions/` folder next to the `_targets.R` script, and put your functions there. It’s up to you, but I prefer this second option. In the example script, the following function is defined:

---

<sup>2</sup><https://is.gd/lm4QoO>

### 13. Build automation with targets

```
summarize_data <- function(dataset) {
 colMeans(dataset)
}
```

Finally, comes the pipeline itself. Let's take a closer look at it:

```
list(
 tar_target(data,
 data.frame(x = sample.int(100),
 y = sample.int(100))),

 tar_target(data_summary,
 summarize_data(data)) # Call your
 ↵ custom functions.
)
```

The pipeline is nothing but a list (told you lists where a very important object) of *targets*. A target is defined using the `tar_target()` function and has at least two inputs: the first is the name of the target (without quotes) and the second is the function that generates the target. So a target defined as `tar_target(y, f(x))` can be understood as `y <- f(x)`. The next target can use the output of the previous target as an input, so you could have something like `tar_target(z, f(y))` (just like in the template).

## 13.3. A pipeline is a composition of pure functions

You can run this pipeline by typing `tar_make()` in a console:

### 13.3. A pipeline is a composition of pure functions

```
targets::tar_make()
```

- start target data
- built target data [0.82 seconds]
- start target data\_summary
- built target data\_summary [0.02 seconds]
- end pipeline [1.71 seconds]

The pipeline is done running! So, now what? This pipeline simply built some summary statistics, but where are they? Typing `data_summary` in the console to try to inspect this output results in the following:

```
data_summary
```

```
Error: object 'data_summary' not found
```

What is going on?

First, you need to remember our chapter on functional programming. We want our pipeline to be a sequence of pure functions. This means that our pipeline running successfully should not depend on anything in the global environment (apart from loading the packages in the first part of the script, and the options set with `tar_option_set()` for the others) and it should not change anything outside of its scope. This means that the pipeline should not change anything in the global environment either. This is exactly how a `{targets}` pipeline operates. A pipeline defined using `{targets}` will be pure and so the output of the pipeline will not be saved in the global environment. Now, strictly speaking, the pipeline is not exactly pure. Check the folder that contains the `_targets.R` script. There should

### 13. Build automation with targets

now be a `_targets/` folder in there as well. If you go inside that folder, and then open the `objects/` folder, you should see two objects, `data` and `data_summary`. These are the outputs of our pipeline.

So each target that is defined inside the pipeline gets saved there in the `.rds` format. This is an R-specific format that you can use to save *any* type of object. It doesn't matter what it is: a simple data frame, a fitted model, a ggplot, whatever, you can write any R object to disk in this format using the `saveRDS()` function, and then read it back into another R session using `readRDS()`. `{targets}` makes use of these two functions to save every target computed by your pipeline, and simply retrieves them from the `_targets/` folder instead of recomputing them. Keep this in mind if you use Git to version the code of your pipeline (which you are doing of course), and add the `_targets/` folder to the `.gitignore` (unless you really want to also version it, but it shouldn't be necessary).

So because the pipeline is pure, and none of its outputs get saved into the global environment, calling `data_summary` results in the error above. So to retrieve the outputs you should use `tar_read()` or `tar_load()`. The difference is that `tar_read()` simply reads the output and shows it in the console but `tar_load()` reads and saves the object into the global environment. So to retrieve our `data_summary` object let's use `tar_load(data_summary)`:

```
tar_load(data_summary)
```

Now, typing `data_summary` shows the computed output:

```
data_summary
```

### 13.3. A pipeline is a composition of pure functions

```
x y
50.5 50.5
```

It is possible to load all the outputs using `tar_load_everything()` so that you don't need to load each output one by one.

Before continuing with more `{targets}` features, I want to really stress the fact that the pipeline is the composition of pure functions. So functions that only have a side-effect will be difficult to handle. Examples of such functions are functions that read data, or that print something to the screen. For example, plotting in base R consists of a series of calls to functions with side-effects. If you open an R console and type `plot(mtcars)`, you will see a plot. But the function `plot()` does not create any output. It just prints a picture on your screen, which is a side-effect. To convince yourself that `plot()` does not create any output and only has a side-effect, try to save the output of `plot()` in a variable:

```
a <- plot(mtcars)
```

doing this will show the plot, but if you then call `a`, the plot will not appear, and instead you will get `NULL`:

```
a
```

```
NULL
```

This is also why saving plots in R is awkward, it's because there's no object to actually save!

So because `plot()` is not a pure function, if you try to use it in a `{targets}` pipeline, you will get `NULL` as well when loading

### 13. Build automation with targets

the target that should be holding the plot. To see this, change the list of targets like this:

```
list(
 tar_target(data,
 data.frame(x = sample.int(100),
 y = sample.int(100))),

 tar_target(data_summary,
 summarize_data(data)), # Call your
 ↵ custom functions.

 tar_target(
 data_plot,
 plot(data)
)
)
```

I've simply added a new target using `tar_target()` at the end, to generate a plot. Run the pipeline again using `tar_make()` and then type `tar_load(data_plot)` to load the `data_plot` target. But typing `data_plot` only shows `NULL` and not the plot!

There are several workarounds for this. The first is to use `ggplot()` instead. This is because the output of `ggplot()` is an object of type `ggplot`. You can do something like `a <- ggplot() + etc...` and then type `a` to see the plot. Doing `str(a)` also shows the underlying list holding the structure of the plot, as a list.

The second workaround is to save the plot to disk. For this, you need to write a new function, for example:

### 13.3. A pipeline is a composition of pure functions

```
save_plot <- function(filename, ...){

 png(filename = filename)
 plot(...)
 dev.off()

}
```

If you put this in the `_targets.R` script, before defining the list of `tar_target` objects, you could use this instead of `plot()` in the last target:

```
summarize_data <- function(dataset) {
 colMeans(dataset)
}

save_plot <- function(filename, ...){
 png(filename = filename)
 plot(...)
 dev.off()

 filename
}

Set target-specific options such as packages.
tar_option_set(packages = "dplyr")

End this file with a list of target objects.
list(
 tar_target(data,
 data.frame(x = sample.int(100),
 y = sample.int(100))),
```

### 13. Build automation with targets

```
tar_target(data_summary,
 summarize_data(data)), # Call your
 ↵ custom functions.

tar_target(
 data_plot,
 save_plot(
 filename = "my_plot.png",
 data),
 format = "file")
)
```

After running this pipeline you should see a file called `my_plot.png` in the folder of your pipeline. If you type `tar_load(data_plot)`, and then `data_plot` you will see that this target returns the `filename` argument of `save_plot()`. This is because a target needs to return something, and in the case of functions that save a file to disk returning the path where the file gets saved is recommended. This is because if I then need to use this file in another target, I could do `tar_target(x, f(data_plot))`. Because the `data_plot` target returns a path, I can write `f()` in such a way that it knows how to handle this path. If instead I write `tar_target(x, f("path/to/my_plot.png"))`, then `{targets}` would have no way of knowing that the target `x` depends on the target `data_plot`. The dependency between these two targets would break. Hence why the first option is preferable.

Finally, you will have noticed that the last target also has the option `format = "file"`. This will be topic of the next section.

It is worth noting that the `{ggplot2}` package includes a func-

tion to save ggplot objects to disk called `ggplot2::ggsave()`. So you could define two targets, one to compute the `ggplot` object itself, and another to generate a `.png` image of that `ggplot` object.

## 13.4. Handling files

In this section, we will learn how `{targets}` handles files. First, run the following lines in the folder that contains the `_targets.R` script that we've been using up until now:

```
data(mtcars)

write.csv(mtcars,
 "mtcars.csv",
 row.names = F)
```

This will create the file "`mtcars.csv`" in that folder. We are going to use this in our pipeline.

Write the pipeline like this:

```
list(
 tar_target(
 data_mtcars,
 read.csv("mtcars.csv")
),

 tar_target(
 summary_mtcars,
 summary(data_mtcars)
```

### 13. Build automation with targets

```
) ,

tar_target(
 plot_mtcars,
 save_plot(
 filename = "mtcars_plot.png",
 data_mtcars),
 format = "file")
)
```

You can now run the pipeline and will get a plot at the end. The problem however, is that the input file "`mtcars.csv`" is not being tracked for changes. Try to change the file, for example by running this line in the console:

```
write.csv(head(mtcars), "mtcars.csv", row.names
 = F)
```

If you try to run the pipeline again, our changes to the data are ignored:

```
skip target data_mtcars
skip target plot_mtcars
skip target summary_mtcars
skip pipeline [0.1 seconds]
```

As you can see, because `{targets}` is not tracking the changes in the `mtcars.csv` file, from its point of view nothing changed. And thus the pipeline gets skipped because according to `{targets}`, it is up-to-date.

Let's change the csv back:

```
write.csv(mtcars, "mtcars.csv", row.names = F)
```

and change the first target such that the file gets tracked. Remember that targets need to be pure functions and return something. So we are going to change the first target to simply return the path to the file, and use the `format = "file"` option in `tar_target()`:

```
path_data <- function(path){
 path
}

list(
 tar_target(
 path_data_mtcars,
 path_data("mtcars.csv"),
 format = "file"
),
 tar_target(
 data_mtcars,
 read.csv(path_data_mtcars)
),
 tar_target(
 summary_mtcars,
 summary(data_mtcars)
),
 tar_target(
 plot_mtcars,
 save_plot(filename = "mtcars_plot.png",
 data_mtcars),
 format = "file")
)
```

### 13. Build automation with targets

To drive the point home, I use a function called `path_data()` which takes a path as an input and simply returns it. This is totally superfluous, and you could define the target like this instead:

```
tar_target(
 path_data_mtcars,
 "mtcars.csv",
 format = "file"
)
```

This would have exactly the same effect as using the `path_data()` function.

So now we got a target called `path_data_mtcars` that returns nothing but the path to the data. But because we've used the `format = "file"` option, `{targets}` now knows that this is a file that must be tracked. So any change on this file will be correctly recognised and any target that depends on this input file will be marked as being out-of-date. The other targets are exactly the same.

Run the pipeline now using `tar_make()`. Now, change the input file again:

```
write.csv(head(mtcars),
 "mtcars.csv",
 row.names = F)
```

Now, run the pipeline again using `tar_make()`: this time you should see that `{targets}` correctly identified the change and runs the pipeline again accordingly!

## 13.5. The dependency graph

As you've seen in the previous section (and as I told you in the introduction) `{targets}` keeps track of changes in files, but also in the functions that you use. Any change to the code of any of these functions will result in `{targets}` identifying which targets are now out-of-date and which should be re-computed (alongside any other target that depends on them). It is possible to visualise this using `tar_visnetwork()`. This opens an interactive network graph in your web browser that looks like this:

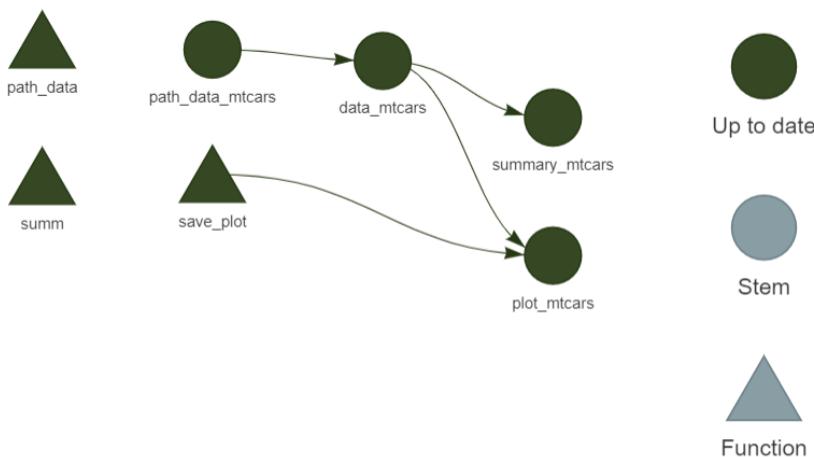


Figure 13.1.: This image opens in your web-browser.

In the image above, each target has been computed, so they are all up-to-date. If you now change the input data, here is what you will see instead:

### 13. Build automation with targets

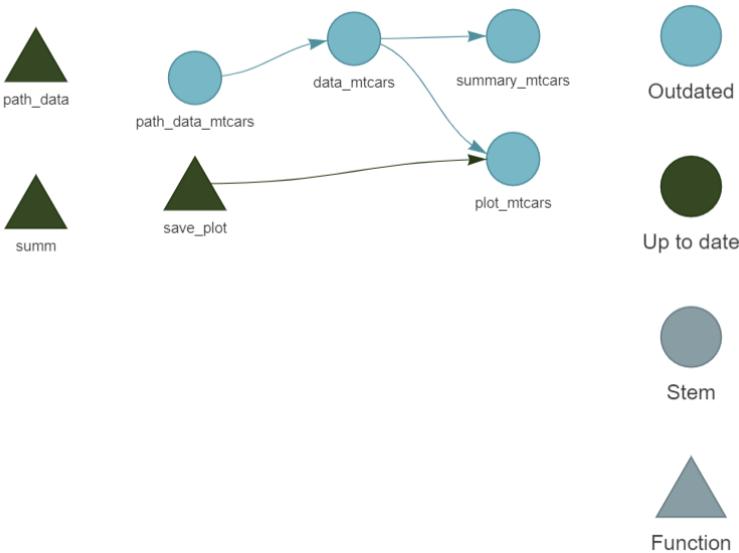


Figure 13.2.: Because the input data was changed, we need to run the pipeline again.

Because all the targets depend on the input data, we need to re-run everything. Let's run the pipeline again to update all the targets using `tar_make()` before continuing.

Now let's add another target to our pipeline, one that does not depend on the input data. Then, we will modify the input data again, and call `tar_visnetwork()` again. Change the pipeline like so:

```
list(
 tar_target(
 path_data_mtcars,
 "mtcars.csv",
```

```
 format = "file"
),
tar_target(
 data_iris,
 data("iris")
),
tar_target(
 summary_iris,
 summary(data_iris)
),
tar_target(
 data_mtcars,
 read.csv(path_data_mtcars)
),
tar_target(
 summary_mtcars,
 summary(data_mtcars)
),
tar_target(
 plot_mtcars,
 save_plot(
 filename = "mtcars_plot.png",
 data_mtcars),
 format = "file")
)
```

Before running the pipeline, we can call `tar_visnetwork()` again to see the entire workflow:

### 13. Build automation with targets

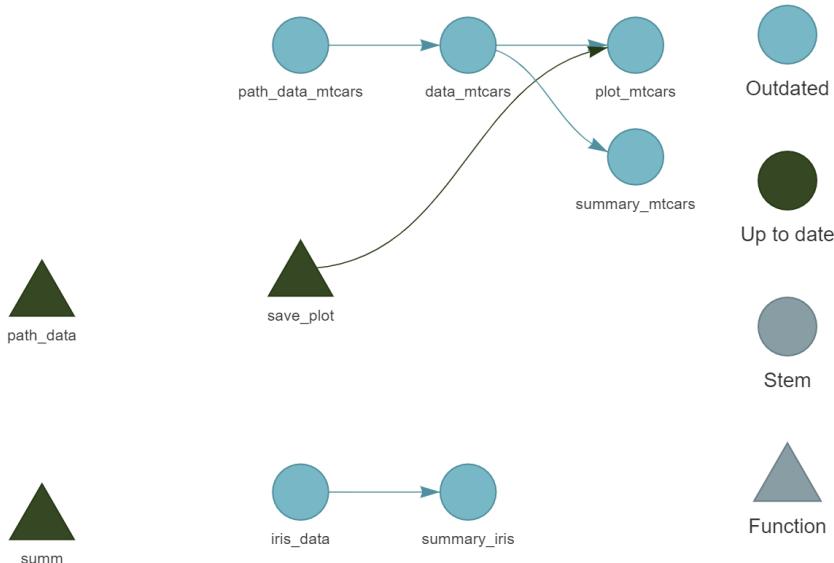


Figure 13.3.: We clearly see that the pipeline has two completely independent parts.

We can see that there are now two independent parts, as well as two unused functions, `path_data()` and `summ()` which we could remove.

Running the pipeline using `tar_make()` builds everything successfully. Let's add the following target, just before the very last one:

```
tar_target(
 list_summaries,
 list(
 "summary_iris" = summary_iris,
 "summary_mtcars" = summary_mtcars
)
```

),

This target creates a list with the two summaries that we compute. Call `tar_visnetwork()` again:

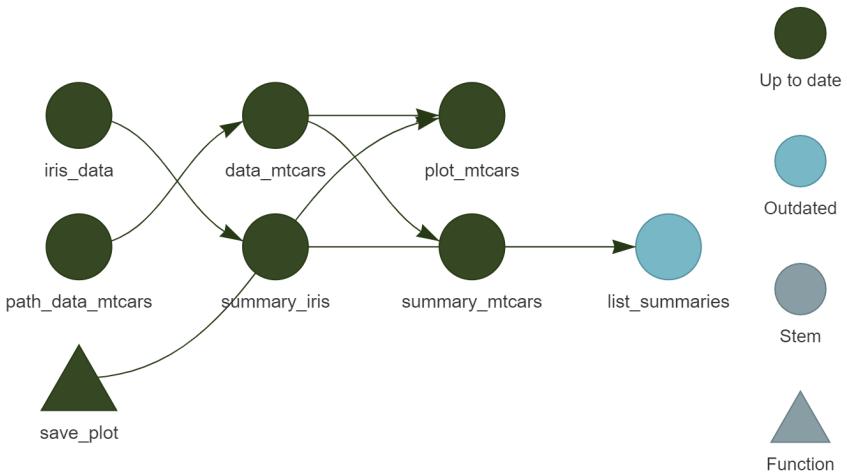


Figure 13.4.: The two separate workflows end up in one output.

Finally, run the pipeline one last time to compute the final output.

## 13.6. Running the pipeline in parallel

{targets} makes it easy to run independent parts of our pipeline in parallel. In the example from before, it was quite obvious to know which parts were independent, but when the pipeline grows in complexity, it can be very difficult to see which parts are independent.

### 13. Build automation with targets

Let's now run the example from before in parallel. But first, we need to create a function that takes some time to run. `summary()` is so quick that running both of its calls in parallel is not worth it (and would actually even run slower, I'll explain why at the end). Let's define a new function called `slow_summary()`:

```
slow_summary <- function(...){
 Sys.sleep(30)
 summary(...)
}
```

and replace every call to `summary()` with `slow_summary()` in the pipeline:

```
list(
 tar_target(
 path_data_mtcars,
 "mtcars.csv",
 format = "file"
),
 tar_target(
 data_iris,
 data("iris")
),
 tar_target(
 summary_iris,
 slow_summary(data_iris)
),
 tar_target(
 data_mtcars,
 read.csv(path_data_mtcars)
```

### 13.6. Running the pipeline in parallel

```
),
tar_target(
 summary_mtcars,
 slow_summary(data_mtcars)
),
tar_target(
 list_summaries,
 list(
 "summary_iris" = summary_iris,
 "summary_mtcars" = summary_mtcars
)
),
tar_target(
 plot_mtcars,
 save_plot(filename = "mtcars_plot.png",
 data_mtcars),
 format = "file")
)
```

here's what the pipeline looks like before running:

### 13. Build automation with targets

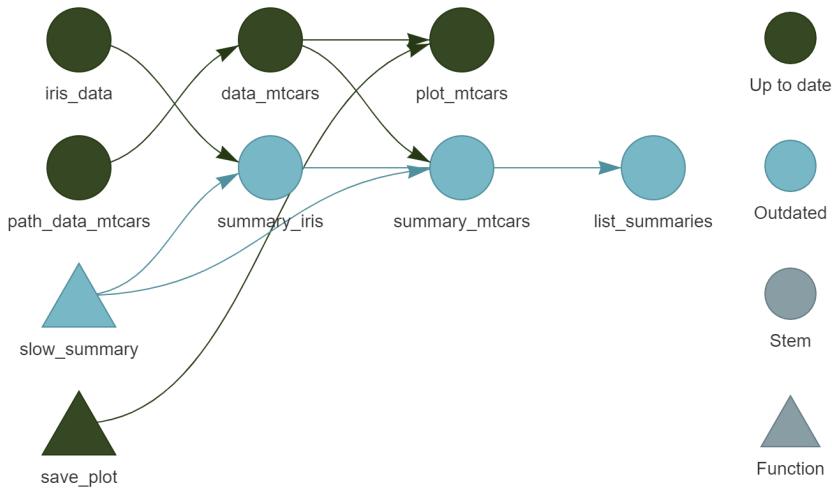


Figure 13.5.: `slow_summary()` is used instead of `summary()`.

(You will also notice that I've removed the unneeded functions, `path_data()` and `summ()`).

Running this pipeline sequentially will take about a minute, because each call to `slow_summary()` takes 30 seconds. To re-run the pipeline completely from scratch, call `tar_destroy()`. This will make all the targets outdated. Then, run the pipeline from scratch with `tar_make()`:

```
targets::tar_make()
```

- start target path\_data\_mtcars
- built target path\_data\_mtcars [0.18 seconds]
- start target data\_iris
- built target data\_iris [0 seconds]
- start target data\_mtcars

### 13.6. Running the pipeline in parallel

- built target data\_mtcars [0 seconds]
- start target summary\_iris
- built target summary\_iris [30.26 seconds]
- start target plot\_mtcars
- built target plot\_mtcars [0.16 seconds]
- start target summary\_mtcars
- built target summary\_mtcars [30.29 seconds]
- start target list\_summaries
- built target list\_summaries [0 seconds]
- end pipeline [1.019 minutes]

Since computing `summary_iris` is completely independent of `summary_mtcars`, these two computations could be running at the same time on two separate CPU cores. To do this, we need to first load two additional packages, `{future}` and `{future.callr}` at the top of the script. Then, we also need to call `plan(callr)` before defining our pipeline. Here is what the complete `_targets.R` looks like:

```
library(targets)
library(future)
library(future.callr)
plan(callr)

Sometimes you gotta take your time
slow_summary <- function(...) {
 Sys.sleep(30)
 summary(...)
}

Save plot to disk
save_plot <- function(filename, ...){
```

### 13. Build automation with targets

```
png(filename = filename)
plot(...)
dev.off()

 filename
}

Set target-specific options such as packages.
tar_option_set(packages = "dplyr")

list(
 tar_target(
 path_data_mtcars,
 "mtcars.csv",
 format = "file"
),
 tar_target(
 data_iris,
 data("iris")
),
 tar_target(
 summary_iris,
 slow_summary(data_iris)
),
 tar_target(
 data_mtcars,
 read.csv(path_data_mtcars)
),
 tar_target(
 summary_mtcars,
 slow_summary(data_mtcars)
),
)
```

### 13.6. Running the pipeline in parallel

```
tar_target(
 list_summaries,
 list(
 "summary_iris" = summary_iris,
 "summary_mtcars" = summary_mtcars
)
,
tar_target(
 plot_mtcars,
 save_plot(
 filename = "mtcars_plot.png",
 data_mtcars),
 format = "file")
)
```

You can now run this pipeline in parallel using `tar_make_future()` (and sequentially as well, just as usual with `tar_make()`). To run the pipeline from scratch to test this, call `tar_destroy()` and then `tar_make()` will build the entire pipeline from scratch:

### 13. Build automation with targets

```
Set workers = 2 to use 2 cpu cores
targets::tar_make_future(workers = 2)
```

- start target path\_data\_mtcars
- start target data\_iris
- built target path\_data\_mtcars [0.2 seconds]
- start target data\_mtcars
- built target data\_iris [0.22 seconds]
- start target summary\_iris
- built target data\_mtcars [0.2 seconds]
- start target plot\_mtcars
- built target plot\_mtcars [0.35 seconds]
- start target summary\_mtcars
- built target summary\_iris [30.5 seconds]
- built target summary\_mtcars [30.52 seconds]
- start target list\_summaries
- built target list\_summaries [0.21 seconds]
- end pipeline [38.72 seconds]

As you can see, this was faster but not quite twice as fast, but almost. The reason this isn't exactly twice as fast is because there is some overhead to run code in parallel. New R sessions have to be spawned by `{targets}`, data needs to be transferred and packages must be loaded in these new sessions. This is why it's only worth parallelizing code that takes some time to run. If you decrease the number of sleep seconds in `slow_summary(...)` (for example to 10), running the code in parallel might be slower than running the code sequentially, because of that overhead. But if you have several long-running computations, it's really worth the very small price that you pay for the initial setup. Let me re-iterate again that in order to run your pipeline in parallel, the extra worker sessions that get spawned by `{targets}` need

to know which packages they need to load, which is why you should load the packages your pipeline needs using:

```
tar_option_set(packages = "dplyr")
```

## 13.7. {targets} and RMarkdown (or Quarto)

It is also possible to compile documents using RMardown (or Quarto) with {targets}. The way this works is by setting up a pipeline that produces the outputs you need in the document, and then defining the document as a target to be computed as well. For example, if you're showing a table in the document, create a target in the pipeline that builds the underlying data. Do the same for a plot, or a statistical model. Then, in the .Rmd (or .Qmd) source file, use `targets::tar_read()` to load the different objects you need.

Consider the following `_targets.R` file:

```
library(targets)

tar_option_set(packages = c("dplyr", "ggplot2"))

list(
 tar_target(
 path_data_mtcars,
 "mtcars.csv",
 format = "file"
),
 ...)
```

### 13. Build automation with targets

```
tar_target(
 data_mtcars,
 read.csv(path_data_mtcars)
) ,
tar_target(
 summary_mtcars,
 summary(data_mtcars)
) ,
tar_target(
 clean_mtcars,
 mutate(data_mtcars,
 am = as.character(am))
) ,
tar_target(
 plot_mtcars,
 {ggplot(clean_mtcars) +
 geom_point(aes(y = mpg,
 x = hp,
 shape = am))}
)
)
```

This pipeline loads the `.csv` file from before and creates a summary of the data as well as plot. But we don't simply want these objects to be saved as `.rds` files by the pipeline, we want to be able to use them to write a document (either in the `.Rmd` or `.Qmd` format). For this, we need another package, called `{tarchetypes}`. This package comes many functions that allow you to define new types of targets (these functions are called *target factories* in `{targets}` jargon). The new target factory that we need is `tarchetypes::tar_render()`. As you can probably guess from the name, this function renders an `.Rmd` file. Write the following lines in an `.Rmd` file and save it next to the

### 13.7. `{targets}` and RMarkdown (or Quarto)

pipeline:

```

```

```
title: "mtcars is the best data set"
author: "mtcars enjoyer"
date: today
```

```

```

```
Load the summary
```

```
```{r}
tar_read(summary_mtcars)
```
```

Here is the `_targets.R` file again, where I now load `{tarchetypes}` at the top and add a new target at the bottom:

```
library(targets)
library(tarchetypes)

tar_option_set(packages = c("dplyr", "ggplot2"))

list(
 tar_target(
 path_data_mtcars,
 "mtcars.csv",
 format = "file"
),
 tar_target(
 data_mtcars,
 read.csv(path_data_mtcars)
```

### 13. Build automation with targets

```
) ,
tar_target(
 summary_mtcars,
 summary(data_mtcars)
) ,
tar_target(
 clean_mtcars,
 mutate(data_mtcars,
 am = as.character(am))
) ,
tar_target(
 plot_mtcars,
 {ggplot(clean_mtcars) +
 geom_point(aes(y = mpg,
 x = hp,
 shape = am))}
) ,
tar_render(
 my_doc,
 "my_document.Rmd"
)
)
```

Running this pipeline with `tar_make()` will now compile the source `.Rmd` file into an `.html` file that you can open in your web-browser. Even if you want to compile the document into another format, I advise you to develop using the `.html` format. This is because you can open the `.html` file in the web-browser, and keep working on the source. Each time you run the pipeline after you made some changes to the file, you simply need to refresh the web-browser to see your changes. If instead you compile a Word document, you will need to always close the file, and then re-open it to see your changes, which is quite

## 13.7. $\{targets\}$ and RMarkdown (or Quarto)

annoying. A good second reason to have output in the `.html` format is that HTML is a text-only format, and thus can be tracked with version control systems covered in Chapter 5. The MS Word format is binary, and tracking it in Git is always an undecipherable mess. Keep in mind though that `.html` files can get large, in which case you may want to not track them, but only track the source `.Rmd` instead.

If you open the output file, you should be seeing something quite plain looking:

### mtcars is the best data set

```
mtcars enjoyer
today
```

#### Load the summary

```
tar_read(summary_mtcars)
```

```
mpg cyl disp hp
Min. :10.40 Min. :4.000 Min. : 71.1 Min. :52.0
1st Qu.:15.43 1st Qu.:4.000 1st Qu.:120.8 1st Qu.: 96.5
Median :19.20 Median :6.000 Median :196.3 Median :123.0
Mean :20.09 Mean :6.188 Mean :230.7 Mean :146.7
3rd Qu.:22.80 3rd Qu.:8.000 3rd Qu.:326.0 3rd Qu.:180.0
Max. :33.90 Max. :8.000 Max. :472.0 Max. :335.0
drat wt qsec vs
Min. :2.760 Min. :1.513 Min. :14.50 Min. :0.0000
1st Qu.:3.000 1st Qu.:2.581 1st Qu.:16.89 1st Qu.:0.0000
Median :3.695 Median :3.325 Median :17.71 Median :0.0000
Mean :3.597 Mean :3.217 Mean :17.85 Mean :0.4375
3rd Qu.:3.920 3rd Qu.:3.610 3rd Qu.:18.90 3rd Qu.:1.0000
Max. :4.930 Max. :5.424 Max. :22.90 Max. :1.0000
```

Figure 13.6.: The output of our pipeline. Our first data product!

Don't worry, we will make it look nice, but right at the end. Don't waste time making things look good too early on. Ideally, try to get the pipeline to run on a simple example, and then keep adding features. Also, try to get *as much feedback* as possible on the *content* as *early* as possible from your colleagues. No point in wasting time to make something look good if what you're writing is not at all what was expected. Let's now get the `ggplot` of the data to show in the document as well.

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For this, simply add:

```
```{r}
tar_read(plot_mtcars)
```
```

at the bottom of the `.Rmd` file. Running the pipeline again will now add the plot to the document. Before continuing, let me just remind you, again, of the usefulness of `{targets}` by changing the underlying data. Run the following:

```
write.csv(head(mtcars),
 "mtcars.csv",
 row.names = F)
```

and run the pipeline again. Because the data changed and every target depends on the data, the document gets entirely rebuilt. I hope that you see why this is really great: in case you need to build weekly, daily, heck, even hourly reports, by using `{targets}` the updated report can now get built automatically, and the targets that are not impacted by these recurrent updates will not need to be recomputed. Restore the data by running:

```
write.csv(mtcars,
 "mtcars.csv",
 row.names = F)
```

and rebuild the document by running the pipeline.

Now that the pipeline runs well, we can work a little on the document itself, by transforming the output into a nice looking table using `{flextable}`. But there is an issue however: the output of `summary()` on a `data.frame` object is not a

### 13.7. `{targets}` and RMarkdown (or Quarto)

`data.frame`, but a `table` and `flextable::flextable()` expects a `data.frame`. So if you call `flextable::flextable()` on the output of `summary()`, you'll get an error message. Instead, we need a replacement for `summary()` that outputs a `data.frame`. This replacement is `skimr::skim()`; let's go back to our pipeline and change the call to `summary()` to `skim()` (after adding the `{skimr}` to the list of loaded packages, as well as `{flextable}`):

```
library(targets)
library(tarchetypes)

tar_option_set(packages = c(
 "dplyr",
 "flextable",
 "ggplot2",
 "skimr"
)
)

list(
 tar_target(
 path_data_mtcars,
 "mtcars.csv",
 format = "file"
),
 tar_target(
 data_mtcars,
 read.csv(path_data_mtcars)
),
 tar_target(
 summary_mtcars,
```

### 13. Build automation with targets

```
skim(data_mtcars)
),
tar_target(
 clean_mtcars,
 mutate(data_mtcars,
 am = as.character(am))
),
tar_target(
 plot_mtcars,
 {ggplot(clean_mtcars) +
 geom_point(aes(y = mpg,
 x = hp,
 shape = am))}

),
tar_render(
 my_doc,
 "my_document.Rmd"
)
)
```

In the .Rmd file, we can now pass the output of `tar_read(summary_mtcars)` to `flextable()`:

```
Load the summary

```{r}
tar_read(summary_mtcars) %>%
  flextable()
```

```

If you run the pipeline and look at the output now, you'll see a nice table with a lot of summary statistics. Since the output of `skim()` is a `data.frame`, you can only keep the stats you want

### 13.7. $\{targets\}$ and RMarkdown (or Quarto)

by `dplyr::select()`ing the columns you need:

```
Load the summary

```{r}
tar_read(summary_mtcars) %>%
  select(Variable = skim_variable,
         Mean = numeric.mean,
         SD = numeric.sd,
         Histogram = numeric.hist) %>%
  flextable()
```

```

If you want to hide all the R code in the output document, simply use `knitr::opts_chunk$set(echo = F)` in the source .Rmd file, or if you want to hide the code from individual chunks use `echo = FALSE` in the chunks header. Here is what the final source code of the .Rmd could look like:

```

title: "mtcars is the best data set"
author: "mtcars enjoyer"
date: today

```{r, include = FALSE}
# Hides all source code
knitr::opts_chunk$set(echo = F)
```

```

### 13. Build automation with targets

```
Load the summary statistics
```

I really like to see the distribution of the variables as a cell of a table:

```
```{r}
tar_read(summary_mtcars) %>%
  select(Variable = skim_variable,
         Mean = numeric.mean,
         SD = numeric.sd,
         Histogram = numeric.hist) %>%
  flextable() %>%
  set_caption("Summary statistics for mtcars")
```

```

```
Graphics
```

The plot below is really nice, just look at it:

```
```{r, fig.cap = "Scatterplot of `mpg` and `hp`  
  by type of transmission"}
tar_read(plot_mtcars) +
  theme_minimal() +
  theme(legend.position = "bottom")
```

```

As you can see, once I've used `tar_read()`, I get back the object just as if I had generated it from within the .Rmd source file, and can simply add stuff to it (like changing the theme

### 13.8. Rewriting our project as a pipeline and `{renv}` redux

of the ggplot). Once you’re happy with the contents, you can add `output: word_document` to the header of the document (just below `date: today` for example) to generate a Word document.

Let me reiterate the advantages of using `{targets}` to compile RMarkdown documents: because the computation of all the objects is handled by `{targets}`, compiling the document itself is very quick. All that needs to happen is loading pre-computed targets. This also means that you benefit from all the other advantages of using `{targets}`: only the outdated targets get recomputed, and the computation of the targets can happen in parallel. Without `{targets}`, compiling the RMarkdown document would always recompute all the objects, and all the objects’ recomputation would happen sequentially.

## 13.8. Rewriting our project as a pipeline and `{renv}` redux

It is now time to return our little project into a full-fledged reproducible pipeline. For this, we’re going back to our project’s folder and specifically to the `fusen` branch. This is the branch where we used `{fusen}` to turn our `.Rmd` into a package. This package contains the functions that we need to update the data. But remember, we wrote the analysis in another `.Rmd` file that we did not inflate, `analyse_data.Rmd`. We are now going to write a `{targets}` pipeline that will make use of the inflated package and compute all the targets required for the analysis. The first step is to create a new branch, but you could also create an entirely new repository if you want. It’s up to you. If you create a new branch, start from the `rmd` branch, since this will provide a nice starting point.

### 13. Build automation with targets

```
#switch to the rmd branch
owner@localhost $ git checkout rmd

#create and switch to the new branch called
→ pipeline
owner@localhost $ git checkout -b pipeline
```

If you start with a fresh repository, you can grab the `analyse_data.Rmd` from here<sup>3</sup>.

First order of business, let's delete `save_data.Rmd` (unless you started with an empty repo). We don't need that file anymore, since everything is now available in the package we developed:

```
owner@localhost $ rm save_data.Rmd
```

Let's now start an R session in that folder and install our `{housing}` package. Whether you followed along and developed the package, or skipped the previous parts and didn't develop the package by following along, install it from my Github repository. This ensures that you have exactly the same version as me. Run the following line:

```
remotes::install_github("rap4all/housing@fusen",
 ref = "1c86095")
```

This will install the package from my Github repository, and very specifically the version from the `fusen` branch at commit `1c86095` (you may need to install the `{remotes}` package first). Now that the package is installed, we can start building the pipeline. In the same R session, call `tar_script()` which will give us a nice template `_targets.R` file:

---

<sup>3</sup><https://is.gd/L2GICG>

### 13.8. Rewriting our project as a pipeline and `{renv}` redux

```
targets::tar_script()
```

You should at most have three files: `README.md`, `_targets.R` and `analyse_data.Rmd` (unless you started with an empty repo, in which case you don't have the `README.md` file). We will now change `analyse_data.Rmd`, to load pre-computed targets, instead of computing them inside the `analyse_data.Rmd` at compilation time.

First, we need to load the data. The two datasets we use are now part of the package, so we can simply load them using `data(commune_level_data)` and `data(country_level_data)`. But remember, `{targets}` only loves pure functions, and `data()` is not pure! Let's see what happens when you call `data(mtcars)`. If you're using RStudio, this is really visible: in a fresh session, calling `data(mtcars)` shows the following in the Environment pane:

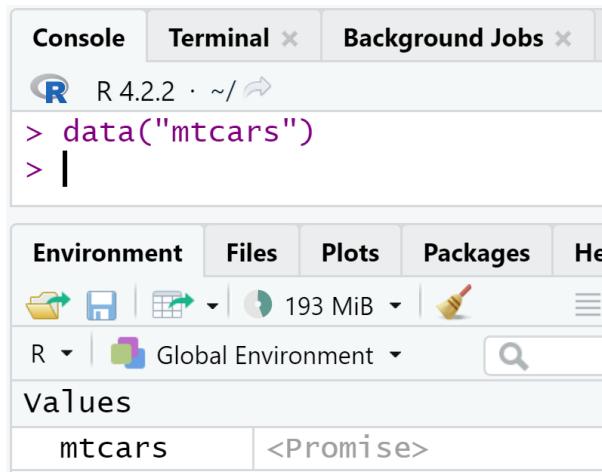


Figure 13.7.: What's described as 'mtcars' is not a 'data.frame', yet.

### 13. Build automation with targets

At this stage, `mtcars` is only a promise. It's only if you need to interact with `mtcars` that the promise becomes a `data.frame`. So `data()` returns a promise, does this mean that we can save that into a variable? If you try the following:

```
x <- data(mtcars)
```

And check out `x`, you will see that `x` contains the string "`mtcars`" and is of class character! So `data()` returns a promise by saving it directly to the global environment (this is a side-effect) but it returns a string. Because `{targets}` needs pure functions, if we write:

```
tar_target(
 target_mtcars,
 data(mtcars)
)
```

the `target_mtcars` target will be equal to the "`mtcars`" character string. This might be confusing, but just remember: a target must return something, and functions with side-effects don't always return something, or not the thing we want. Also remember the example on plotting with `plot()`, which does not return an object. It's actually the same issue here.

So to solve this, we need a pure function that returns the `data.frame`. This means that it first needs to load the data, which results in a promise (which gets loaded into the environment directly), and then evaluate that promise. The function to achieve this is as follows:

```
read_data <- function(data_name, package_name){
```

### 13.8. Rewriting our project as a pipeline and `{renv}` redux

```
temp <- new.env(parent = emptyenv())

data(list = data_name,
 package = package_name,
 envir = temp)

get(data_name, envir = temp)
}
```

This function takes `data_name` and `package_name` as arguments, both strings.

Then, I used `data()` but with two arguments: `list =` and `package =`. `list =` is needed because we pass `data_name` as a string. If we did something like `data(data_name)` instead, hoping that `data_name` would get replaced by its bound value ("commune\_level\_data") it would result in an error. This is because `data()` would be looking for a data set literally called `data_name` instead of replacing `data_name` by its bound value. The second argument, `package =` simply states that we're looking for that dataset in the `{housing}` package and uses the bound value of `package_name`. Now comes the `envir =` argument. This argument tells `data()` where to load the data set. By default, `data()` loads the data in the global environment. But remember, we want our function to be pure, meaning, it should only return the data object and not load anything into the global environment! So that's where the temporary environment created in the first line of the body of the function comes into play. What happens is that the functions loads the data object into this temporary environment, which is different from the global environment. Once we're done, we can simply discard this environment, and so our global environment stays clean.

The final step is using `get()`. Remember that once the line

### 13. Build automation with targets

`data(list = data_name...)` has run, all we have is a promise. So if we stop there, the target would simply hold the character "commune\_level\_data". In order to turn that promise into the data frame, we use `get()`. We've already encountered this function in Chapter 7. `get()` searches an object by name, and returns it. So in the line `get(data_name)`, `data_name` gets first replaced by its bound value, so `get("commune_level_data")` and hence we get the dataset back. Also, `get()` looks for that name in the temporary environment that was set up. This way, there is literally no interaction with the global environment, so that function is pure: it always returns the same output for the same input, and does not pollute, in any way, the global environment. After that function is done running, the temporary environment is discarded.

This seems overly complicated, but it's all a consequence of `{targets}` needing pure functions that actually return something to work well. Unfortunately some of R's default functions are not pure, so we need this kind of workaround. However, all of this work is not in vain! By forcing us to use pure functions, `{targets}` contributes to the general quality and safety of our pipeline. Once our pipeline is done running, the global environment will stay clean. Having stuff pollute the global environment can cause interactions with subsequent runs of the pipeline.

Let's continue the pipeline: here is what it will ultimately look like:

```
library(targets)
library(tarchetypes)

tar_option_set(packages = "housing")
```

### 13.8. Rewriting our project as a pipeline and `{renv}` redux

```
source("functions/read_data.R")

list(
 tar_target(
 commune_level_data,
 read_data("commune_level_data",
 "housing")
),
 tar_target(
 country_level_data,
 read_data("country_level_data",
 "housing")
),
 tar_target(
 commune_data,
 get_laspeyeres(commune_level_data)
),
 tar_target(
 country_data,
 get_laspeyeres(country_level_data)
),
 tar_target(
 communes,
 c("Luxembourg",
 "Esch-sur-Alzette",
 "Mamer",
 "Schengen",
 "Wiltz"
)
)
)
```

### 13. Build automation with targets

```
"Wincrange")
) ,

tar_render(
 analyse_data,
 "analyse_data.Rmd"
)
)
```

And here is what `analyse_data.Rmd` now looks like:

```

title: "Nominal house prices data in Luxembourg"
author: "Bruno Rodrigues"
date: "`r Sys.Date()`"

```

Let's load the datasets (the Laspeyeres price  
↳ index is already computed):

```
```{r}  
tar_load(commune_data)  
tar_load(country_data)  
```
```

We are going to create a plot for 5 communes and  
↳ compare the  
price evolution in the communes to the national  
↳ price evolution.  
Let's first load the communes:

### 13.8. Rewriting our project as a pipeline and `{renv}` redux

```
```{r}
tar_load(communes)
```

```{r, results = "asis"}
res <- lapply(communes, function(x){

  knitr::knit_child(text = c(
    '\n',
    '## Plot for commune: `r x`',
    '\n',
    ```{r, echo = F}',
 'print(make_plot(country_data, commune_data,
 x))',
    ```

  ),
  envir = environment(),
  quiet = TRUE)

})

cat(unlist(res), sep = "\n")
```

```

As you can see, the data gets loaded by using `tar_load()` which loads the two pre-computed data sets. The end portion of the document looks fairly similar to what we had before turning our analysis into a package and then a pipeline. We use a child document to generate as many sections as required automatically (remember, *Don't Repeat Yourself!*). Try to change

## 13. Build automation with targets

something in the pipeline, for example remove some communes from the `communes` object, and rerun the whole pipeline using `tar_make()`.

We are now done with this introduction to `{targets}`: we have turned our analysis into a pipeline, and now we need to ensure that the outputs it produces are reproducible. So the first step is to use `{renv}`; but as already discussed, this will not be enough, but it is essential that you do it! So let's initialize `{renv}`:

```
renv::init()
```

This will create an `renv.lock` file with all the dependencies of the pipeline listed. Very importantly, our Github package also gets listed:

```
"housing": {
 "Package": "housing",
 "Version": "0.1",
 "Source": "GitHub",
 "RemoteType": "github",
 "RemoteHost": "api.github.com",
 "RemoteRepo": "housing",
 "RemoteUsername": "rap4all",
 "RemoteRef": "fusen",
 "RemoteSha":
 ↵ "1c860959310b80e67c41f7bbdc3e84cef00df18e",
 "Hash": "859672476501daeea9b719b9218165f1",
 "Requirements": [
 "dplyr",
 "ggplot2",
 "janitor",
 "purrr",
```

### 13.8. Rewriting our project as a pipeline and `{renv}` redux

```
 "readxl",
 "rlang",
 "rvest",
 "stringr",
 "tidyverse"
]
},
```

If you look at the fields titled `RemoteSha` and `RemoteRef` you should recognize the commit hash and repository that were used to install the package:

```
"RemoteRef": "fusen",
"RemoteSha":
 "1c860959310b80e67c41f7bbdc3e84cef00df18e",
```

This means that if someone wants to re-run our project, by running `renv::restore()` the correct version of the package will get installed! To finish things, we should edit the `Readme.md` file and add instructions on how to re-run the project. This is what the `Readme.md` file could look like:

```
How to run

- Clone the repository: `git clone
 git@github.com:rap4all/housing.git`
- Switch to the `pipeline` branch: `git checkout
 pipeline`
- Start an R session in the folder and run
 `renv::restore()`
 to install the project's dependencies.
- Run the pipeline with `targets::tar_make()`.
```

## 13. Build automation with targets

- Checkout `analyse\_data.html` for the output.

If you followed along, don't forget to change the `url` of the repository to your own in the first bullet point of th Readme.

## 13.9. Some little tips before concluding

In this section I'll be showing you some other useful functions included in the `{targets}` package that I think you should know!

### 13.9.1. Load every target at once

It is possible to load every target included in the cache at once using `tar_load_everything()`. But be careful, if your pipeline builds many targets, this can take some time!

### 13.9.2. Get metadata information on your pipeline

`tar_meta()` will return a data frame with some information about the pipeline. I find it quite useful after running the pipeline, and it turns out that some warnings or errors were raised. This is how this data frame looks like:

```
targets::tar_meta()
```

### 13.9. Some little tips before concluding

```
A tibble: 11 × 18
 name type data command depend [...]
 <chr> <chr> <chr> <chr> <chr> [...]
 1 analyse_d... stem c251... 995812... 3233e... [...]
 2 commune_d... stem 024d... 85c2ab... ec7f2... [...]
 3 commune_l... stem fb07... f48470... ce0d8... [...]
 4 commune_l... stem fb07... 2549df... 15e48... [...]
 5 communes stem b097... be3c56... a3dad... [...]
 6 country_d... stem ae21... 9dc7a6... 1d321... [...]
```

There are more columns than those I'm showing, of great interest are the columns `warnings` and `error`. In the example below, I have changed the code to `read_data()`, and now it raises a warning:

```
targets::tar_make()
• built target commune_level_data [0.61 seconds]
• start target country_level_data
• built target country_level_data [0.02 seconds]
 skip target communes
 skip target commune_data
 skip target country_data
 skip target analyse_data
• end pipeline [0.75 seconds]

Warning messages:
1: this is a warning
2: this is a warning
3: 2 targets produced warnings. Run
 ↵ tar_meta(fields = warnings,
```

## 13. Build automation with targets

```
complete_only = TRUE) for the messages.
```

```
>
```

Because warnings were raised, the pipeline raises another warning telling you to run `tar_meta(fields = warnings, complete_only = TRUE)` so let's do it:

```
tar_meta(fields = warnings, complete_only =
 ↵ TRUE)
```

This code returns a data frame with the name of the targets that produced the warning, alongside the warning.

```
A tibble: 2 × 2
 name warnings
 <chr> <chr>
1 commune_level_data this is a warning
2 country_level_data this is a warning
```

So now you can better see what is going on.

### 13.9.3. Make a target (or the whole pipeline) outdated

With `tar_invalidate()` you can make a target outdated, so that when you rerun the pipeline, it gets re-computed (alongside every target that depends on it). This can sometimes be useful to make sure that everything is running correctly. Try running `tar_invalidate("communes")` and see what happens. It is also possible to completely nuke the whole pipeline and rerun it from scratch using `tar_destroy()`. You'll get asked to confirm if

that's what you want to do, and if yes, rerunning the pipeline after that will start from scratch.

#### 13.9.4. Customize the network's visualisation

By calling `visNetwork::visNetworkEditor(tar_visnetwork())`, a Shiny app gets started that lets you customize the look of your pipeline's network. You can play around with the options and see the effect they have on the look of the network. It is also possible to generate R code that you can then paste into a script to consistently generate the same look.

#### 13.9.5. Use targets from one pipeline in another project

If you need to load some targets inside another project (for example, because you need to reference an older study), you can do so easily with `{withr}`:

```
withr::with_dir(
 "path/to/root/of/project",
 targets::tar_load(target_name))
```

#### 13.9.6. Understanding this cryptic error message

Sometimes, when you try to run the pipeline, you get the following error message:

## 13. Build automation with targets

```
Error:
! Error running targets::tar_make()
 Target errors: targets::tar_meta(fields =
 ↴ error, complete_only = TRUE)
 Tips: https://books.ropensci.org/targets/
 ↴ debugging.html
Last error: argument 9 is empty
```

The last line is what interests us here: “Last error: argument 9 is empty”. It is not clear which target is raising this error: that’s because it’s not a target that is raising this error, but the pipeline itself! Remember that the pipeline is nothing but a list of targets. If your last target ends with a , character, `list()` is expecting another element. But because there’s none, this error gets raised. Type `list(1,2,)` in the console and you will get the same error message. Simply check your last target, there is a , in there that you should remove!

## 13.10. Conclusion

I hope to have convinced you that you need to add build automation tools to your toolbox. `{targets}` is a fantastic package, because it takes care of something incredibly tedious for you. By using `{targets}` you don’t have to remember which objects you need to recompute when you need to change code. You don’t need to rewrite your code to make it run in parallel. And by using `{renv}`, other users can run your pipeline in a couple of lines and reproduce the results.

In the next chapter, we will be going deeper in the iceberg of reproducibility still.

# 14. Reproducible analytical pipelines with Docker

If the book ended at the end of the previous chapter, it would have been titled “Building analytical pipelines with R”, because we have not ensured that the pipeline we built is reproducible. We did our best though:

- we used functional and literate programming;
- we documented, tested and versioned the code;
- we used `{renv}` to record the dependencies of the project;
- the project was rewritten as a `{targets}` pipeline and re-running it is as easy as it can possibly get.

But there are still many variables that we need to consider. If we go back to the reproducibility iceberg, you will notice that we can still go deeper. As the code stands now, we did our best using programming paradigms and libraries, but now we need to consider other aspects.

As already mentioned in the introduction and Chapter 10, `{renv}` *only* restores package versions. The R version used for the analysis only gets recorded. So to make sure that the pipeline reproduces the same results, you’d need to install the same R version that was used to build the pipeline originally. But installing the right R version can be difficult sometimes; it depends on the operating system you want to install it on,

## *14. Reproducible analytical pipelines with Docker*

and how old a version we're talking about. Installing R 4.0 on Windows should be quite easy, but I wouldn't be very keen on trying to install R 2.15.0 (released on March 2012) on a current Linux distribution (and it might be problematic even on Windows as well).

Next comes the operating system on which the pipeline was developed. In practice, this rarely matters, but there have been cases where the same code produced different results on different operating systems, sometimes even on different versions of the same operating system! For example, Bhandari Neupane et al. (2019) discuss their attempt at reproducing a paper from 2014. The original scripts and data were available, and yet they were not able to reproduce the results, even though they made sure to use the same version of Python that the original authors from 2014 were using. The reason was the operating system: they were conducting their replication exercise on a different operating system, and this was causing the results to be different. What was going on? The original script relied on how the operating system ordered the files for analysis. If the files were ordered in a different way, the results would be different. And file ordering is operating system dependent! The table below, from Bhandari Neupane et al. (2019), shows how the results vary depending on which operating system the script runs:

**Table 2. Variability in Calculated Carbon Chemical Shifts of 1b**

| no. | LINUX<br>(Ubuntu16) | Windows<br>(ver. 10) | Mac<br>(Mavericks) | Mac<br>(Mojave) |
|-----|---------------------|----------------------|--------------------|-----------------|
| 1   | 172.4               | 173.2                | 173.2              | 172.7           |
| 2   | 36.0                | 37.7                 | 37.7               | 39.3            |
| 3   | 68.3                | 68.4                 | 68.4               | 69.0            |
| 4   | 70.6                | 70.5                 | 70.5               | 71.2            |
| 5   | 79.0                | 78.4                 | 78.4               | 79.0            |
| 6   | 15.5                | 13.3                 | 13.3               | 13.3            |
| 7   | 162.4               | 162.5                | 162.5              | 161.8           |
| 8   | 110.4               | 109.8                | 109.8              | 110.3           |
| 9   | 155.0               | 156.5                | 156.5              | 155.5           |
| 10  | 116.2               | 115.5                | 115.5              | 116.0           |
| 11  | 131.6               | 131.6                | 131.6              | 131.7           |
| 12  | 127.1               | 126.6                | 126.6              | 127.0           |
| 13  | 126.7               | 125.6                | 125.6              | 126.3           |

Figure 14.1.: Different operating system yield different results.

and this table shows how Windows and Ubuntu (Linux) sort files:

**Table 2. Variability in Calculated Carbon Chemical Shifts of 1b**

| no. | LINUX<br>(Ubuntu16) | Windows<br>(ver. 10) | Mac<br>(Mavericks) | Mac<br>(Mojave) |
|-----|---------------------|----------------------|--------------------|-----------------|
| 1   | 172.4               | 173.2                | 173.2              | 172.7           |
| 2   | 36.0                | 37.7                 | 37.7               | 39.3            |
| 3   | 68.3                | 68.4                 | 68.4               | 69.0            |
| 4   | 70.6                | 70.5                 | 70.5               | 71.2            |
| 5   | 79.0                | 78.4                 | 78.4               | 79.0            |
| 6   | 15.5                | 13.3                 | 13.3               | 13.3            |
| 7   | 162.4               | 162.5                | 162.5              | 161.8           |
| 8   | 110.4               | 109.8                | 109.8              | 110.3           |
| 9   | 155.0               | 156.5                | 156.5              | 155.5           |
| 10  | 116.2               | 115.5                | 115.5              | 116.0           |
| 11  | 131.6               | 131.6                | 131.6              | 131.7           |
| 12  | 127.1               | 126.6                | 126.6              | 127.0           |
| 13  | 126.7               | 125.6                | 125.6              | 126.3           |

Figure 14.2.: Different OS order files differently!

So the operating system can have an impact, and often an un-

## 14. Reproducible analytical pipelines with Docker

expected impact, on our pipeline!

And finally, I believe that we are in a transition period when it comes to hardware architecture. Apple will very likely completely switch over to an ARM architecture with their Apple silicon CPUs (as of writing, the Mac Pro is the only computer manufactured by Apple that doesn't use an Apple silicon CPU and only because it was released in 2019) and it wouldn't surprise me if other manufacturers follow suit and develop their own ARM cpus. This means that projects written today may not run anymore in the future, because of this architecture changes. Libraries compiled for current architectures would need to be recompiled for ARM, and that may be difficult.

So, as I explained in the previous chapter, we want our pipeline to be the composition of pure functions. Nothing in the global environment (apart from `{target}`-specific options) should influence the runs of the pipeline. But, what about the environment R is running in? The R engine is itself running in some kind of environment. This is what I've explained above: operating system (and all the math libraries that are included in the OS that R relies on to run code) and hardware are variables that need to be recorded and/or frozen as much as possible.

Think about it this way: when you running a pure function `f()` of one argument you think you do this:

`f(1)`

but actually what you're doing is:

```
f(1, "windows 10 - build 22H2 - patch
10.0.19045.2075",
 "intel x86_64 cpu i9-13900F",
 "R version 4.2.2")
```

and so on. `f()` is only pure as far as the R version currently running `f()` is concerned. But everything else should also be taken into account! Remember, in technical terms, this means that our function is not referentially transparent. This is exactly what happened in the paper from Bhandari Neupane et al. (2019) that I described before. The authors relied on a *hidden* state (the order of the files) to program their script; in other words, their pipeline was not referentially transparent.

To deal with this, I will now teach you how to use Docker. Docker will essentially allow you to turn your pipeline referentially transparent, by freezing R's and the operating system's versions (and the CPU architecture as well).

Before continuing, let me warn you: if you're using an Apple computer with an Apple Silicon CPU (M1 or M2), then you may have issues following along. I don't own such a machine so I cannot test if the code below works flawlessly. What I can say is that I've read some users of these computers have had trouble using Docker in the past. These issues might have been solved in the meantime. It seems that enabling the option “use Rosetta for x86/amd64 emulation on Apple Silicon” in Docker Desktop (I will discuss Docker Desktop briefly in the following sections) may solve the issue.

## 14.1. What is Docker?

Let me first explain in very simple terms what Docker is.

In very simple (and technically wrong) terms, Docker makes it easy to run a Linux virtual machine (VM) on your computer. A VM is a computer within a computer: the idea is that you turn on your computer, start Windows (the operating system you use

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every day), but then start Ubuntu (a very popular Linux distribution) as if it were any other app installed on your computer and use it (almost) as you would normally. This is what a classic VM solution like *Virtualbox* offers you. You can start and use Ubuntu interactively from within Windows. This can be quite useful for testing purposes for example.

The way Docker differs from Virtualbox (or VMware) is that it strips down the VM to its bare essentials. There's no graphical user interface for example, and you will not (typically) use a Docker VM interactively. What you will do instead is write down in a text file the specifications of the VM you want. Let's call this text file a *Dockerfile*. For example, you want the VM to be based on Ubuntu. So that would be the first line in the Dockerfile. You then want it to have R installed. So that would be the second line. Then you need to install R packages, so you add those lines as well. Maybe you need to add some system dependencies? Add them. Finally, you add the code of the pipeline that you want to make reproducible as well.

Once you're done, you have this text file, the Dockerfile, with a complete recipe to generate a Docker VM. That VM is called an *image* (as I said previously it's technically not a true VM, but let's not discuss this). So you have a text file, and this file helps you define and generate an image. Here, you should already see a first advantage of using Docker over a more traditional VM solution like Virtualbox: you can very easily write these Dockerfiles and version them. You can easily start off from another Dockerfile from another project and adapt it to your current pipeline. And most importantly, because everything is written down, it's reproducible (but more on that at the end of this chapter...).

Ok, so you have this image. This image will be based on some Linux distribution, very often Ubuntu. It comes with a specific

version of Ubuntu, and you can add to it a specific version of R. You can also download a specific version of all the packages required for your pipeline. You end up with an environment that is tailor-made for your pipeline. You can then run the pipeline with this Docker image, and *always get exactly the same results, ever*. This is because, regardless of how, where or when you will run this *dockerized* pipeline, the same version of R, with the same version of R packages, on the same Linux distribution will be used to reproduce the results of your pipeline. By the way, when you run a Docker image, as in, you're executing your pipeline using that image definition, this now is referred to as a Docker container.

So: a Dockerfile defines a Docker image, from which you can then run containers. I hope that the pictures below will help. The first picture shows what happens when you run the same pipeline on two different R versions and two different operating systems:

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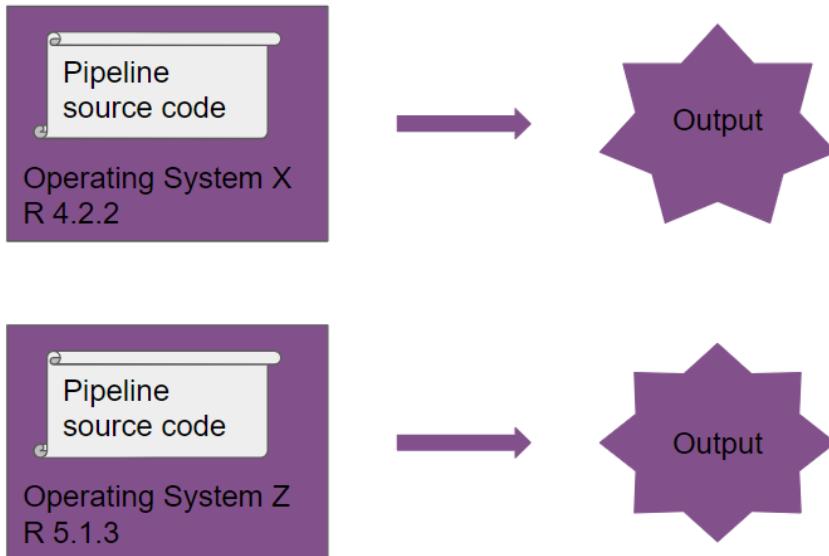


Figure 14.3.: Running a pipeline without Docker results (potentially) in different outputs.

Take a close look at the output, you will notice it's different!

Now, you run the same pipeline, which is now *dockerized*:

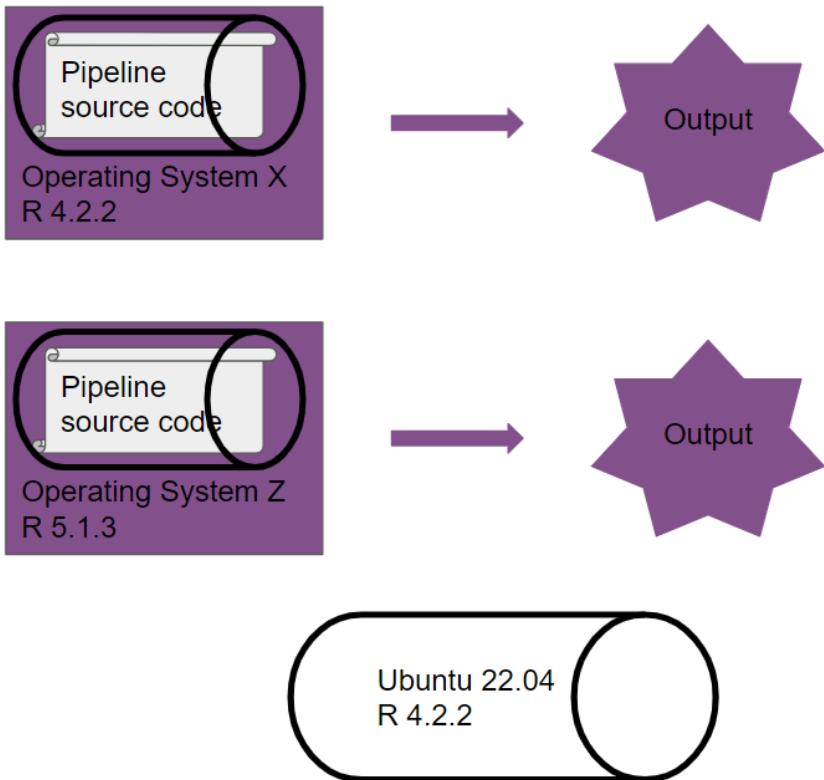


Figure 14.4.: Running a pipeline with Docker results in the same outputs.

Another way of looking at a Docker image: it's an immutable sandbox, where the rules of the game are always the same. It doesn't matter where or when you run this sandbox, the pipeline will always be executed in this same, well-defined space. Because the pipeline runs on the same versions of R (and packages) and on the same operating system defined within the Docker image, our pipeline is now truly reproducible.

But why Linux though; why isn't it possible to create Docker

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images based on Windows or macOS? Remember in the introduction, where I explained what reproducibility is? I wrote:

Open source is a hard requirement for reproducibility.

Open source is not just a requirement for the programming language used for building the pipeline but extends to the operating system that the pipeline runs on as well. So the reason Docker uses Linux is because you can use Linux distributions like Ubuntu for free and without restrictions. There aren't any licenses that you need to buy or activate, and Linux distributions can be customized for any use case imaginable. Thus Linux distributions are the only option available to Docker for this task.

## **14.2. A primer on Linux**

Up until this point, you could have followed along using any operating system. Most of the code shown in this book is R code, so it doesn't matter on what operating system you're running it. But there was some code that I ran in the Linux console (for example, I've used `ls` to list files). These commands should also work on macOS, but on Windows, I told you to run them in the Git Bash terminal instead. This is because `ls` (and other such commands) don't work in the default Windows command prompt (but should work in Powershell though). Instead of using the terminal (or Git Bash) to navigate your computer's file system, you could have followed along using the user interface of your operating system as well. For example, in Chapter 11, I list the contents of the `dev/` directory using the following command:

```
owner@localhost $ ls dev/
```

but you could have just opened the `dev/` folder in the file explorer of your operating system of choice. But to use Docker, you will need to get to know Linux and the Linux ecosystem and concepts a little bit. No worries, it's not as difficult as it sounds, and I think that you likely aren't afraid of difficult things, or else you would have stopped reading this book much earlier.

*Linux* is not the name of any one specific operating system, but of an operating system kernel. A kernel is an important component of an operating system. Linux is free and open-source, and among the most successful free and open source projects ever. Because its license allows (and encourages) re-use, anyone can take that kernel, and add all the other components needed to build a complete operating system and release the finished product. This is why there are many *Linux distributions*: a Linux distribution is a complete operating system that uses Linux as its kernel. The most popular Linux distribution is called Ubuntu, and if one time you googled something along the lines of “easy linux os for beginners” the answer that came out on top was likely Ubuntu, or one of the other variants of Ubuntu (yes, because Ubuntu itself is also open-source and free software, it is possible to build a variant using Ubuntu as a basis, like Linux Mint).

To define our Docker images, we will be using Ubuntu as a base. The Ubuntu operating system has two releases a year, one in April and one in October. On even years, the April release is a long-term support (LTS) release. LTS releases get security updates for 5 years, and Docker images generally use an LTS release as a base. As of writing (May 2023), the current LTS is Ubuntu 22.04 *Jammy Jellyfish* (Ubuntu releases are named with a number of the form YY.MM and then a code name based on

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some animal).

If you want, you can install Ubuntu on your computer. But there's no need for this, since you can use Docker to ship your projects!

A major difference between Ubuntu (and other Linux distributions) and macOS and Windows is how you install software. In short, software for Linux distributions is distributed as packages. If you want to install, say, the Emacs text editor, you can run the following command in the terminal:

```
sudo apt-get install emacs-gtk
```

Let's break this down: `sudo` makes the next commands run as root. `root` is Linux jargon for the administrator account. So if I type `sudo xyz`, the command `xyz` will run with administrator privileges. Then comes `apt-get install`. `apt-get` is Ubuntu's package manager, and `install` is the command that installs `emacs-gtk`. `emacs-gtk` is the name of the Emacs package. Because you're an R user, this should be somewhat familiar: after all, extensions for R are also installed using a package manager and a command: `install.packages("package_name")`. Just like in R, where the packages get downloaded from CRAN, Ubuntu downloads packages from a repository which you can browse here<sup>1</sup>. Of course, because using the command line is intimidating for beginners, it is also possible to install packages using a software store, just like on macOS or Windows. But remember, Docker only uses what it absolutely needs to function, so there's no interactive user interface. This is not because Docker's developers don't like user interfaces, but because the point of Docker is not to use Docker images interactively, so

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<sup>1</sup><https://packages.ubuntu.com/jammy/>

there's no need for the user interface. So you need to know how to install Ubuntu packages with the command line.

Just like for R, it is possible to install software from different sources. It is possible to add different repositories, and install software from there. We are not going to use this here, but just as an aside, if you are using Ubuntu on your computer as your daily driver operating system, you really should check out r2u<sup>2</sup>, an Ubuntu repository that comes with pre-compiled R packages that can get installed, very, very quickly. Even though we will not be using this here (and I'll explain why later in this chapter), you should definitely consider r2u to provide binary R packages if you use Ubuntu as your daily operating system.

Let's suppose that you are using Ubuntu on your machine, and are using R. If you want to install the {dplyr} R package, something interesting happens when you type:

```
install.packages("dplyr")
```

On Windows and macOS, a compiled binary gets downloaded from CRAN and installed on your computer. A “binary” is the compiled source code of the package. Many R packages come with C++ or Fortran code, and this code cannot be used as is by R. So these bits of C++ and Fortran code need to be compiled to be used. Think of it this way: if the source code is the ingredients of a recipe, the compiled binary is the cooked meal. Now imagine that each time you want to eat Bouillabaisse, you have to cook it yourself... or you could get it delivered to your home. You'd probably go for the delivery (especially if it would be free) instead of cooking it each time. But this supposes that there are people out there cooking Bouillabaisse for you.

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<sup>2</sup><https://github.com/eddelbuettel/r2u>

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CRAN essentially cooks the package source codes into binaries for Windows and macOS, as shown below:

**Downloads:**

Package source: [tidyverse\\_2.0.0.tar.gz](#)

Windows binaries: r-devel: [tidyverse\\_2.0.0.zip](#), r-release: [tidyverse\\_2.0.0.zip](#),

macOS binaries: r-release (arm64): [tidyverse\\_2.0.0.tgz](#), r-oldrel (arm64): [tid](#)

Old sources: [tidyverse archive](#)

Figure 14.5.: Download links to pre-compiled tidyverse binaries.

In the image above, you can see links to compiled binaries of the `{tidyverse}` package for Windows and macOS, but none for any Linux distribution. This is because, as stated in the introduction, there are many, many, many Linux distributions. So at best, CRAN could offer binaries for Ubuntu, but Ubuntu is not the only Linux distribution, and Ubuntu has two releases a year, which means that every CRAN package (that needs compilation) would need to get compiled twice a year. This is a huge undertaking unless CRAN decided to only offer binaries for LTS releases. But that would still be every two years.

So instead, what happens, is that the burden of compilation is pushed to the user. Every time you type `install.packages("package_name")`, and if that package requires compilation, that package gets compiled on your machine which not only takes some time, but can also fail. This is because very often, R packages that require compilation need some additional system-level dependencies that need to be installed. For example, here are the Ubuntu dependencies that need to be installed for the installation of the `{tidyverse}` package to succeed:

```
libicu-dev
zlib1g-dev
make
libcurl4-openssl-dev
libssl-dev
libfontconfig1-dev
libfreetype6-dev
libfribidi-dev
libharfbuzz-dev
libjpeg-dev
libpng-dev
libtiff-dev
pandoc
libxml2-dev
```

This why r2u is so useful: by adding this repository, what you're essentially doing is telling R to not fetch the packages from CRAN, but from the r2u repository. And this repository contains compiled R packages for Ubuntu. So the required system-level dependencies get installed automatically and the R package doesn't need compilation. So installation of the `{tidyverse}` package takes less than half a minute on a modern machine.

But if r2u is so nice, why did I say above that we would not be using it? Unfortunately, this is because r2u does not archive compiled binaries of older packages, and this is exactly what we need for reproducibility. So when you're building a Docker image to make a project reproducible, because that image will be based on Ubuntu, we will need to make sure that our Docker image contains the right system-level dependencies so that compilation of the R packages doesn't fail. Thankfully, you're reading the right book.

### 14.3. First steps with Docker

Let's start by creating a "Hello World" Docker image. As I explained in the beginning, to define a Docker image, we need to create a Dockerfile with some instructions. But first, you need of course to install Docker. To install Docker on any operating system (Windows, macOS or Ubuntu or other Linuxes), you can install Docker Desktop<sup>3</sup>. If you're running Ubuntu (or another Linux distribution) and don't want the GUI, you could install the Docker engine<sup>4</sup> and then follow the post-installation steps for Linux<sup>5</sup> instead.

In any case, whatever operating system you're using, we will be using the command line to interact with Docker. Once you're done with installing Docker, create a folder somewhere on your computer, and create inside of this folder an empty text file with the name "Dockerfile". This can be tricky on Windows, because you have to remove the .txt extension that gets added by default. You might need to turn on the option "File name extensions" in the **View** pane of the Windows file explorer to make this process easier. Then, open this file with your favourite text editor, and add the following lines:

```
FROM ubuntu:jamm
```

```
RUN uname -a
```

This very simple Dockerfile does two things: it starts by stating that it's based on the Ubuntu Jammy (so version 22.04) operat-

---

<sup>3</sup><https://docs.docker.com/desktop/>

<sup>4</sup><https://docs.docker.com/engine/install/ubuntu/#install-using-the-repository>

<sup>5</sup><https://docs.docker.com/engine/install/linux-postinstall/#manage-docker-as-a-non-root-user>

ing system, and then runs the `uname -a` command. This command, which gets run inside the Ubuntu command line, prints the Linux kernel version from that particular Ubuntu release. `FROM` and `RUN` are Docker commands; there are a couple of others that we will discover a bit later. Now, what do you do with this Dockerfile? Remember, a Dockerfile defines an image. So now, we need to build this image to run a container. Open a terminal/command prompt in the folder where the Dockerfile is and type the following:

```
owner@localhost $ docker build -t raps_hello .
```

The `docker build` command builds an image from the Dockerfile that is in the path `.` (a single `.` means “this current working directory”). The `-t` option tags that image with the name `raps_hello`. If everything goes well, you should see this output:

```
Sending build context to Docker daemon 2.048kB
Step 1/2 : FROM ubuntu:jammy
--> 08d22c0ceb15
Step 2/2 : RUN uname -a
--> Running in 697194b9a519
Linux 697194b9a519 6.2.6-1-default #1 SMP
 PREEMPT_DYNAMIC
 Mon Mar 13 18:57:27 UTC 2023 (fa1a4c6)
 x86_64 x86_64 x86_64 GNU/Linux
Removing intermediate container 697194b9a519
--> a0ea59f23d01
Successfully built a0ea59f23d01
Successfully tagged raps_hello:latest
```

Look at Step 2/2: you should see the output of the `uname -a`

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command:

```
Linux 697194b9a519 6.2.6-1-default #1 SMP
 ↳ PREEMPT_DYNAMIC
 Mon Mar 13 18:57:27 UTC 2023 (fa1a4c6)
 ↳ x86_64 x86_64 x86_64 GNU/Linux
```

Every RUN statement in the Dockerfile gets executed at build time: so this is what we will use to install R and needed packages. This way, once the image is built, we end up with an image that contains all the software we need.

Now, we would like to be able to use this image. Using a built image, we can start one or several containers that we can use for whatever we want. Let's now create a more realistic example. Let's build a Docker image that comes with R pre-installed. But for this, we need to go back to our Dockerfile and change it a bit:

```
FROM ubuntu:jessie

ENV TZ=Europe/Luxembourg

RUN ln -snf /usr/share/zoneinfo/$TZ /etc/localtime
&& echo $TZ > /etc/timezone

RUN apt-get update && apt-get install -y r-base

CMD ["R"]
```

First we define a variable using ENV, called TZ and we set that to the Europe/Luxembourg time zone (you can change this to your own time zone). We then run a rather complex looking command that sets the defined time zone system-wide. We had

to do all this, because when we will later install R, a system-level dependency called `tzdata` gets installed alongside it. This tool then asks the user to enter his or her time zone interactively. But we cannot interact with the image interactively as it's being built, so the build process gets stuck at this prompt. By using these two commands, we can set the correct time zone and once `tzdata` gets installed, that tool doesn't ask for the time zone anymore, so the build process can continue. This is a rather known issue when building Docker images based on Ubuntu, so the fix is easily found with a Google search (but I'm giving it to you, dear reader, for free).

Then come `RUN` statements. The first one uses Ubuntu's package manager to first refresh the repositories (this ensures that our local Ubuntu installation repositories are in synch with the latest software updates that were pushed to the central Ubuntu repos). Then we use Ubuntu's package manager to install `r-base`. `r-base` is the package that installs R. We then finish this Dockerfile by running `CMD ["R"]`. This is the command that will be executed when we run the container. Remember: `RUN` commands get executed at build-time, `CMD` commands at run-time. This distinction will be important later on.

Let's build the image (this will take some time, because a lot of software gets installed):

```
owner@localhost $ docker build -t raps_ubuntu_r
↳ .
```

This builds an image called `raps_ubuntu_r`. This image is based on Ubuntu 22.04 Jammy Jellyfish and comes with R pre-installed. But the version of R that gets installed is the one made available through the Ubuntu repositories, and as of writing that is version 4.1.2, while the latest version available is

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R version 4.2.3. So the version available through the Ubuntu repositories lags behind the actual release. But no matter, we will deal with that later.

We can now start a container with the following command:

```
owner@localhost $ docker run raps_ubuntu_r
```

And this is the output we get:

```
Fatal error: you must specify '--save',
↳ '--no-save' or '--vanilla'
```

What is going on here? When you run a container, the command specified by `CMD` gets executed, and then the container quits. So here, the container ran the command `R`, which started the R interpreter, but then quit immediately. When quitting R, users should specify if they want to save or not save the workspace. This is what the message above is telling us. So, how can we use this? Is there a way to use this R version interactively?

Yes, there is a way to use this R version boxed inside our Docker image interactively, even though that's not really what we want to achieve. What we want instead is that our pipeline gets executed when we run the container. We don't want to mess with the container interactively. But let me show you how we can interact with this dockerized R version. First, you need to let the container run in the background. You can achieve this by running the following command:

```
owner@localhost $ docker run -d -it --name
↳ ubuntu_r_1 raps_ubuntu_r
```

This runs the container that we name “ubuntu\_r\_1” from the image “raps\_ubuntu\_r” (remember that we can run many containers from one single image definition). Thanks to the option `-d`, the container runs in the background, and the option `-it` states that we want an interactive shell to be waiting for us. So the container runs in the background, with an interactive shell waiting for us, instead of launching (and then immediately stopping) the R command. You can now “connect” to the interactive shell and start R in it using:

```
owner@localhost $ docker exec -it ubuntu_r_1 R
```

You should now see the familiar R prompt:

```
R version 4.1.2 (2021-11-01) -- "Bird Hippie"
Copyright (C) 2021 The R Foundation for
 Statistical Computing
Platform: x86_64-pc-linux-gnu (64-bit)

R is free software and comes with ABSOLUTELY NO
 WARRANTY.
You are welcome to redistribute it under certain
 conditions.
Type 'license()' or 'licence()' for distribution
 details.

R is a collaborative project with many
 contributors.
Type 'contributors()' for more information and
'citation()' on how to cite R or R packages in
 publications.
```

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```
Type 'demo()' for some demos, 'help()' for
↳ on-line help, or
'help.start()' for an HTML browser interface to
↳ help.
Type 'q()' to quit R.
```

```
>
```

Welcome to a dockerized version of R. Now, all of this might have felt overly complicated to you. And of course if this is the first time that you have played around with Docker, it is tricky indeed. However, you shouldn't worry too much about it, for several reasons:

- we are not going to use Docker containers interactively, that's not really the point, but it can be useful to log in into the running container to check if things are working as expected;
- we will build our images on top of pre-built images from the Rocker project<sup>6</sup> and these images come with a lot of software pre-installed and configuration taken care of.

What you should take away from this section is that you need to write a Dockerfile which then allows you to build an image. This image can then be used to run one (or several) containers. These containers, at run-time, will execute our pipeline in an environment that is frozen, such that the output of this run will stay constant, forever.

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<sup>6</sup><https://rocker-project.org/>

## 14.4. The Rocker project

The Rocker project offers a very large collection of “R-ready” Docker images that you can use as starting points for building your own Docker images. Before using these images though, I still need to explain one very important Docker concept. Let’s go back to our “Hello World” Docker image:

```
FROM ubuntu:jammy
```

```
RUN uname -a
```

The very first line, `FROM ubuntu:jammy` downloads an Ubuntu Jammy image, but from where? All these images get downloaded from *Docker Hub*, which you can browse here<sup>7</sup>. If you create an account you can even push your own images on there. For example, we could push the image we built before, which we called `raps_ubuntu_r`, on Docker Hub. Then, if we wanted to create a new Docker image that builds upon `raps_ubuntu_r` we could simply type `FROM username:raps_ubuntu_r` (or something similar).

It’s also possible to not use Docker Hub at all, and share the image you built as a file. I’ll explain how later.

The Rocker project offers many different images, which are described here<sup>8</sup>. We are going to be using the *versioned* images. These are images that ship specific versions of R. This way, it doesn’t matter when the image gets build, the same version of R will be installed by getting built from source. Let me explain why building R from source is important. When we build the image from the Dockerfile we wrote before, R gets installed from the

---

<sup>7</sup><https://hub.docker.com/>

<sup>8</sup><https://rocker-project.org/images/>

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Ubuntu repositories. For this we use Ubuntu’s package manager and the following command: `apt-get install -y r-base`. As of writing, the version of R that gets installed is version 4.1.3. There’s two problems with installing R from Ubuntu’s repositories. First, we have to use whatever gets installed, which can be a problem with reproducibility. If we ran our analysis using R version 4.2.1, then we would like to dockerize that version of R. The second problem is that when we build the image today we get version 4.1.3. But it is not impossible that if we build the image in 6 months, we get R version 4.2.0, because it is likely that the version that ships in Ubuntu’s repositories will get updated at some point.

This means that depending on *when* we build the Docker image, we might get a different version of R. There are only two ways of avoiding this problem: either we build the image once and archive it and make sure to always keep a copy and ship that copy forever (or for as long as we want to make sure that pipeline is reproducible) just as you would ship data, code and any documentation required to make the pipeline reproducible. Or we write the Dockerfile in such a way that it always produces the same image, regardless of *when* it gets built. I very strongly advise you to go for the second option, but to *also* archive the image. But of course, this also depends on how critical your project is. Maybe you don’t need to start archiving images, or maybe you don’t even need to make sure that the Dockerfile always produces the same image. But I would still highly recommend that you write your Dockerfiles in such a way that they always output the same image. It is safer, and it doesn’t really mean extra work, thanks to the Rocker project.

So, let’s go back to the Rocker project, and specifically their *versioned* images which you can find here<sup>9</sup>. When you use one

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<sup>9</sup><https://rocker-project.org/images/versioned/r-ver.html>

of the versioned images as a base for your project, you get the following guarantees:

- a fixed version of R that gets built from source. It doesn't matter *when* you build the image, it will always ship with the same version of R;
- the operating system will be the LTS release that was current when that specific version of R was current;
- the R repositories are set to the Posit Public Package Manager (PPPM) at a specific date. This ensures that R packages don't need to be compiled as PPPM serves binary packages for the amd64 architecture (which is the architecture that virtually all non-Apple computers use these days).

This last point requires some more explanations. You should know that versioned Rocker images use the PPPM set at a specific date. This is a very neat feature of the PPPM. For example, the versioned Rocker image that comes with R 4.2.2 has the repos set at the 14th of March 2023, as you can see for yourself here<sup>10</sup>. This means that if you use `install.packages("dplyr")` inside a container running from that image, then the version of `{dplyr}` that will get installed is the one that was available on the 14th of March.

This can be convenient in certain situations, and you may want, depending on your needs, to use the PPPM set a specific date to define Docker images, as the Rocker project does. You could even set the PPPM at a specific date for your main development machine (just follow the instructions here<sup>11</sup>). But keep in mind that you will not be getting any updates to packages, so

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<sup>10</sup><https://is.gd/fdrq4p>

<sup>11</sup><https://is.gd/jbdTKC>

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if you want to install a fresh version of a package that may introduce some nice new features, you'll need to change the repos again. This is why I highly advise you to stay with your default repositories (or use r2u if you are on Ubuntu) and manage your projects' package libraries using `{renv}`. This way, you don't have to mess with anything, and have the flexibility to have a separate package library per project. The other added benefit is that you can then use the project's `renv.lock` file to install the exact same package library inside the Docker image.

As a quick introduction to using Rocker images, let's grab our pipeline's `renv.lock` file which you can download from here<sup>12</sup>. This is the latest `renv.lock` file that we generated for our pipeline, it contains all the needed packages to run our pipeline, including the right versions of the `{targets}` package and the `{housing}` package that we developed. An important remark: it doesn't matter if the `renv.lock` file contains packages that were released after the 14th of March. Even if the repositories inside the Rocker image that we will be using are set to that date, the lock file also specifies the URL of the right repository to download the packages from. So that URL will be used instead of the one defined for the Rocker image.

Another useful aspect of the `renv.lock` file is that it also records the R version that was used to originally develop the pipeline, in this case, R version 4.2.2. So that's the version we will be using in our Dockerfile. Next, we need to check the version of `{renv}` that we used to build the `renv.lock` file. You don't necessarily need to install the same version, but I recommend you do. For example, as I'm writing these lines, `{renv}` version 0.17.1 is available, but the `renv.lock` file was written by `{renv}` version 0.16.0. So to avoid any compatibility issues, we will also install the exact same version. Thankfully, that is quite easy to

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<sup>12</sup><https://is.gd/5UcuxW>

do (to check the version of `{renv}` that was used to write the lock file simply look for the word “renv” in the lock file).

While `{renv}` takes care of installing the right R packages, it doesn’t take care of installing the right system-level dependencies. So that’s why we need to install these system-level dependencies ourselves. I will give you a list of system-level dependencies that you can install to avoid any issues below, and I will also explain to you how I was able to come up with this list. It is quite easy thanks to Posit and their PPPM. For example, here<sup>13</sup> is the summary page for the `{tidyverse}` package. If you select “Ubuntu 22.04 (Jammy)” on the top right, and then scroll down, you will see a list of dependencies that you can simply copy and paste into your Dockerfile:

The screenshot shows a web-based software dependency manager interface. At the top, there's a header with the text "INSTALL SYSTEM PREREQUISITES ON UBUNTU 22.04 (JAMMY)" and two buttons: "i" and "Copy". Below the header is a code block containing several apt-get commands to install system dependencies. The code is as follows:

```
apt-get install -y libicu-dev
apt-get install -y zlib1g-dev
apt-get install -y make
apt-get install -y libcurl4-openssl-dev
apt-get install -y libssl-dev
apt-get install -y libfontconfig1-dev
```

Figure 14.6.: System-level dependencies for the `{tidyverse}` package on Ubuntu.

We will use this list to install the required dependencies for our pipeline.

Create a new folder and call it whatever you want and save the `renv.lock` file linked above inside of it. Then, create an empty text file and call it Dockerfile. Add the following lines:

---

<sup>13</sup><https://is.gd/ZaXHwa>

## 14. Reproducible analytical pipelines with Docker

```
FROM rocker/r-ver:4.2.2

RUN apt-get update && apt-get install -y \
 libglpk-dev \
 libxml2-dev \
 libcairo2-dev \
 libgit2-dev \
 default-libmysqlclient-dev \
 libpq-dev \
 libsasl2-dev \
 libsqlite3-dev \
 libssh2-1-dev \
 libxtst6 \
 libcurl4-openssl-dev \
 libharfbuzz-dev \
 libfribidi-dev \
 libfreetype6-dev \
 libpng-dev \
 libtiff5-dev \
 libjpeg-dev \
 libxt-dev \
 unixodbc-dev \
 wget \
 pandoc

RUN R -e "install.packages('remotes')"

RUN R -e
"remotes::install_github('rstudio/renv@0.16.0')"

RUN mkdir /home/housing

COPY renv.lock /home/housing/renv.lock
```

```
RUN R -e
"setwd('/home/housing');renv::init();renv::restore()"
```

The first line states that we will be basing our image on the image from the Rocker project that ships with R version 4.2.2, which is the right version that we need. Then, we install the required system-level dependencies using Ubuntu's package manager, as previously explained. Then comes the `{remotes}` package. This will allow us to download a specific version from `{renv}` from Github, which is what we do in the next line. I want to stress again that I do this simply because the original `renv.lock` file was generated using `{renv}` version 0.16.0 and so to avoid any potential compatibility issues, I also use this one to restore the required packages for the pipeline. But it is very likely that I could have installed the current version of `{renv}` to restore the packages, and that it would have worked without problems. But just to be on the safe side, I install the right version of `{renv}`. By the way, I knew how to do this because I read this vignette<sup>14</sup> that explains all these steps (but I've only kept the absolute essential lines of code to make it work). Next comes the line `RUN mkdir /home/housing`, which creates a folder (`mkdir` stands for *make directory*), inside the Docker image, in `/home/housing`. On Linux distributions, `/home/` is the directory that users use to store their files, so I create the `/home/` folder and inside of it, I create a new folder, `housing` which will contain the files for my project. It doesn't really matter if you keep that structure or not, you could skip the `/home/` folder if you wanted. What matters is that you put the files where you can find them.

Next comes `COPY renv.lock /home/housing/renv.lock`. This copies the `renv.lock` file from our computer (re-

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<sup>14</sup><https://rstudio.github.io/renv/articles/docker.html>

## 14. Reproducible analytical pipelines with Docker

member, I told you to save this file next to the Dockerfile) to `/home/housing/renv.lock`. By doing this, we include the `renv.lock` file inside of the Docker image which will be crucial for the next and final step: `RUN R -e "setwd('/home/housing');renv::init();renv::restore()"`.

This runs the R program from the Linux command line with the option `-e`. This option allows you to pass an R expression to the command line, which needs to be written between `" "`. Using `R -e` will quickly become an habit, because this is how you can run R non-interactively, from the command line. The expression we pass sets the working directory to `/home/housing`, and then we use `renv::init()` and `renv::restore()` to restore the packages from the `renv.lock` file that we copied before. Using this Dockerfile, we can now build an image that will come with R version 4.2.2 pre-installed as well as all the same packages that we used to develop the `housing` pipeline.

Build the image using `docker build -t housing_image .` (don't forget the `.` at the end).

The build process will take some time, so I would advise you to go get a hot beverage in the meantime. Now, we did half the work: we have an environment that contains the required software for our pipeline, but the pipeline files themselves are missing. But before adding the pipeline itself, let's see if the Docker image we built is working. For this, log in to a command line inside a running Docker container started from this image with this single command:

```
owner@localhost $ docker run --rm -it --name
← housing_container housing_image bash
```

This starts `bash` (Ubuntu's command line) inside the `housing_container` that gets started from the `housing_image`

image. We add the `--rm` flag do `docker run`, this way the Docker container gets stopped when we log out (if not, then the Docker container will continue running in the background). Once logged in, we can move to the folder's project using:

```
user@docker $ cd home/housing
```

and then start the R interpreter:

```
user@docker $ R
```

if everything goes well, you should see the familiar R prompt with a message from `{renv}` at the end:

```
R version 4.2.2 (2022-10-31) -- "Innocent and
 ↵ Trusting"
Copyright (C) 2022 The R Foundation for
 ↵ Statistical Computing
Platform: x86_64-pc-linux-gnu (64-bit)

R is free software and comes with ABSOLUTELY NO
 ↵ WARRANTY.
You are welcome to redistribute it under certain
 ↵ conditions.
Type 'license()' or 'licence()' for distribution
 ↵ details.

Natural language support but running in an
 ↵ English locale

R is a collaborative project with many
 ↵ contributors.
```

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```
Type 'contributors()' for more information and
'citation()' on how to cite R or R packages in
↳ publications.
```

```
Type 'demo()' for some demos, 'help()' for
↳ on-line help, or
'help.start()' for an HTML browser interface to
↳ help.
```

```
Type 'q()' to quit R.
```

```
* Project '/home/housing' loaded. [renv 0.16.0]
```

Try to load the `{housing}` package with `library("housing")`. This should work flawlessly!

## 14.5. Dockerizing projects

So we now have a Docker image that has the right environment for our project. We can now dockerize the project itself. There are two ways to do this: we either simply add the required lines to our Dockerfile, meaning copying the `_targets.R` script to the Docker image at build time and then use `targets::tar_make()` to run the pipeline, or we now create a new Dockerfile that will build upon this image and add the required lines there. In this section, we will use the first approach, and in the next section, we will use the second. The advantage of the first approach is that we have a single Dockerfile, and everything we need is right there. Also, each Docker image is completely tailor-made for each project. The issue is that building takes some time, so if for every project we restart from scratch it can be tedious to have

to wait for the build process to be done (especially if you use continuous integration, as we shall see in the next chapter).

The advantage of the second approach is that we have a base that we can keep using for as long as we want. You will only need to wait once for R and the required packages to get installed. Then, you can use this base for any project that requires the same version of R and packages. This is especially useful if you don't update your development environment very often, and develop a lot of projects with it.

In summary, the first approach is “dockerize pipelines”, and the second approach is “dockerize the dev environment and use it for many pipelines”. It all depends on how you work: in research, you might want to go for the first approach, as each project likely depends on bleeding-edge versions of R and packages. But in industry, where people tend to put the old adage “if ain’t broke don’t fix it” into practice, dev environments are usually frozen for some time and only get updated when really necessary (or according to a fixed schedule).

To dockerize the pipeline, we first need to understand something important with Docker, which I’ve already mentioned in passing: a Docker image is an immutable sandbox. This means that we cannot change it at run-time, only at build-time. So if we log in to a running Docker container (as we did before), and install an R package using `install.packages("package_name")`, that package will disappear if we stop that container. The same is true for any files that get created at run-time: they will also disappear once the container is stopped. So how are we supposed to get the outputs that our pipeline generates from the Docker container? For this, we need to create a volume. A volume is nothing more than a shared folder between the Docker container and the host machine that starts the container. We simply need

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to specify the path for this shared folder when running the container, and that's it.

Let's first write a Dockerfile that contains all the necessary files. We simply need to add the `_targets.R` script from our pipeline, the `analyse_data.Rmd` markdown file and all the functions from the `functions/` folder (you can find all the required files here<sup>15</sup>):

```
FROM rocker/r-ver:4.2.2
```

```
RUN apt-get update && apt-get install -y \
 libglpk-dev \
 libxml2-dev \
 libcairo2-dev \
 libgit2-dev \
 default-libmysqlclient-dev \
 libpq-dev \
 libsasl2-dev \
 libsqlite3-dev \
 libssh2-1-dev \
 libxtst6 \
 libcurl4-openssl-dev \
 libharfbuzz-dev \
 libfribidi-dev \
 libfreetype6-dev \
 libpng-dev \
 libtiff5-dev \
 libjpeg-dev \
 libxt-dev \
 unixodbc-dev \
 wget \
 pandoc
```

---

<sup>15</sup><https://github.com/rap4all/housing/tree/pipeline>

```
RUN R -e "install.packages('remotes')"

RUN R -e
"remotes::install_github('rstudio/renv@0.16.0')"

RUN mkdir /home/housing

RUN mkdir /home/housing/pipeline_output

RUN mkdir /home/housing/shared_folder

COPY renv.lock /home/housing/renv.lock

COPY functions /home/housing/functions

COPY analyse_data.Rmd /home/housing/analyse_data.Rmd

COPY _targets.R /home/housing/_targets.R

RUN R -e
"setwd('/home/housing');renv::init();renv::restore()"

RUN cd /home/housing && R -e "targets::tar_make()"

CMD mv /home/housing/pipeline_output/*
/home/housing/shared_folder/
```

I've added some `COPY` statements to copy the files from our computer to the Docker image, and also created some new directories: the `pipeline_output` and the `shared_folder` directories. `pipeline_output` is the folder that will contain all the outputs from the pipeline, and `shared_folder` (you guessed it) will be the folder that we will use to save the outputs of the pipeline to

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our computer.

I then use `targets::tar_make()` to run the pipeline, but I first need to use `cd /home/housing` to change directories to the project's folder. This is because in order to use the library that `{renv}` installed, we need to start the R session in the right directory. So we move to the right directory, then we run the pipeline using `R -e "targets::tar_make()"`. Notice that we do both operations within a `RUN` statement. This means that the pipeline will run at build-time (remember, `RUN` statements run at build-time, `CMD` statements at run-time). In other words, the image will contain the outputs. This way, if the build process and the pipeline take a long time to run, you can simply leave them running overnight for example. In the morning, while sipping on your coffee, you can then simply run the container to instantly get the outputs. This is because we move the outputs of the pipeline from the folder `pipeline_output` to the `shared_folder` folder using a `CMD` statement. Thus, when we run the container, the outputs get moved into the shared folder, and we can retrieve them.

One last thing I had to do: I needed to change the last target in the `_targets.R` script. Before dockerizing it, it was like this:

```
tar_render(
 analyse_data,
 "analyse_data.Rmd"
)
```

but I had to change it to this:

```
tar_render(
 analyse_data,
```

```

 "analyse_data.Rmd",
 output_dir = "/home/housing/pipeline_output"
)

```

The argument to `output_dir` gets passed to `knitr::knit()` and simply states that the output files should be saved in that folder. I can now build the image using `docker build -t housing_image ..`. Once the build process is done, we can log in to the container to see if our files are there. But let me repeat again, that you are not really supposed to do so. You could simply run the container now and get your files. But let's just take a quick look. You can log in to a bash session using:

```

owner@localhost $ docker run --rm -it --name
 ↵ housing_container housing_image bash

```

If you then move to `/home/housing/pipeline_output` and run `ls` in that folder, you should see `analyse_data.html`. That's our output! So how do we get it out?

You need to run the container with the `-v` flag which allows you to specify the path to the shared folder on your computer, and the shared folder inside the Docker container. The code below shows how to do it (I've used the \ to break this long command over two lines):

```

owner@localhost $ docker run --rm --name
 ↵ housing_container -v \
 /host/path/to/shared_folder:
 ↵ /home/housing/shared_folder:rw \
 housing_image

```

`/host/path/to/shared_folder` is the path to the shared folder

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on my computer. `/home/housing/shared_folder` is the path to the shared folder inside the Docker container. When these lines run, the very last `CMD` statement from the Dockerfile runs, moving the contents from inside the Docker container to our computer. If you check the contents of the `shared_folder` on your computer, you will see `analyse_data.html` in there.

That's it, we have now a complete reproducible analytical pipeline. We managed to tick every one of the following boxes when running our pipeline:

- Same version of R that was used for development;
- Same versions of all the packages that were used for development;
- The whole stack runs on a “frozen” environment;
- We can reproduce this environment (but more on that later...).

We now need to share all this with the world. One simple solution is to share the Dockerfile on Github. For example, this is the repository<sup>16</sup> with all the required code to build the Docker image and run the pipeline. But we could also share the built image so that users only need to run the pipeline to instantly get the results. In the next section, we will learn about dockerizing development environments, and then see how we can share images that have already been built.

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<sup>16</sup><https://github.com/rap4all/housing/tree/docker>

## 14.6. Dockerizing development environments

### 14.6.1. Creating a base image for development

In the previous section, I mentioned that you could either “dockerize pipelines” or “dockerize the dev environment and use it for many pipelines”. What we learned up until now was how to dockerize one single pipeline. In this section, we will learn how to build and dockerize an environment, and then build pipelines that use these environment as starting points.

Let me first explain, again, why (or when) you might want to use his approach instead of the “dockerizing pipelines” approach.

Depending on what or where you work, it is sometimes necessary to have a stable development environment that only gets rarely updated (following a strict schedule). In my own experience, when I was doing research I was almost always using the latest R version and packages. When I’ve joined the private sector, we worked on an environment that we developers could not update ourselves. That environment was updated according to a fixed schedule and now that I’m back in the public sector (but not doing research), I work in a similar manner, on a “frozen” environment. Working on frozen environments like this minimizes the unexpected issues that frequent updates can bring. So how can we use Docker to use such an approach?

The idea is to split up the Dockerfile we used in the previous section into two parts. The first part would consist in setting up everything that is “OS-related”. So installing R, packages, and system-level dependencies. The second Dockerfile would use the image defined thanks to the first Dockerfile as a base and then add the required lines to obtain the results from the pipeline.

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The first image, that focuses on the operating system, can be archived and re-used for as long as required to keep building pipelines. Once we update our environment, we can then regenerate a new Docker image that reflects this update.

Let's do this now. The first image would simply consist of these lines:

```
FROM rocker/r-ver:4.2.2

RUN apt-get update && apt-get install -y \
 libglpk-dev \
 libxml2-dev \
 libcairo2-dev \
 libgit2-dev \
 default-libmysqlclient-dev \
 libpq-dev \
 libsasl2-dev \
 libsqlite3-dev \
 libssh2-1-dev \
 libxtst6 \
 libcurl4-openssl-dev \
 libharfbuzz-dev \
 libfribidi-dev \
 libfreetype6-dev \
 libpng-dev \
 libtiff5-dev \
 libjpeg-dev \
 libxt-dev \
 unixodbc-dev \
 wget \
 pandoc

RUN R -e "install.packages('remotes')"
```

```
RUN R -e
"remotes::install_github('rstudio/renv@0.16.0')"
```

This image can then be built using `docker build -t dev_env_r`. (if you followed along, the cache will be used and this image should get built instantly). This simply installs all the packages and system-level dependencies that are common and needed for all pipelines. Then, each specific package libraries that are required for each pipeline will get installed using the pipeline-specific `renv.lock` file. This will be done with a second Dockerfile. But first, we need to make the `dev_env_r` image available to others, such that it becomes possible to build new images upon `dev_env_r`. There are two ways to make images available to anyone: either online through Docker Hub<sup>17</sup> (in case there's nothing preventing you from sharing the development environment through Docker Hub) or locally, by compressing the images and sharing them internally (in case you don't want to share your images with the world, because they contain proprietary software that you've developed within your company for example). I want to stress that making the image available through Docker Hub is different from sharing the Dockerfile through Github. You could just share the Dockerfiles through Github, and then tell users to first build the dev environment, and then build the pipeline image by building the second, pipeline-specific Dockerfile. But by sharing a built image from Docker Hub, users (including future you) will only need to build the pipeline-specific image and this is much faster. Just like we used `FROM ubuntu:jammy` in our Dockerfiles before, we will now use something like `FROM my_repo/my_image:version_number` from now on.

In the next section I will discuss sharing images on Docker Hub,

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<sup>17</sup><https://hub.docker.com/>

## 14. Reproducible analytical pipelines with Docker

but before that, let me first address the elephant in the room: the development environment that you are using may not be the one you are dockerizing. For example, if you are using Windows or macOS on your computer, then the environment that you are dockerizing will be different since it will be based on Ubuntu. There are only three solutions to this conundrum:

- You don't care, and maybe that's fine. As I stated multiple times, the same pipeline outputting different results due to different operating systems is in practice rare (but it can happen);
- You prefer being safe than sorry, and install Ubuntu on your pc as well. This is very often not an acceptable solution, however.
- You develop on your host environment, but after you're done you compare the results obtained from the Docker container to those obtained on your development environment.
- You use the Docker image not only to ship RAPs, but also for development.

The last option implies that you use Docker interactively, which is not ideal, but it is possible. For example, you could install RStudio server and run a Dockerized version of RStudio from a running Docker container. This is actually what happens if you follow the instructions on the Rocker project's homepage. You can get a dockerized RStudio instance by running:

```
owner@localhost $ docker run --rm -ti -e
 ↳ PASSWORD=yourpassword -p 8787:8787
 ↳ rocker/rstudio
```

and then going to `http://localhost:8787` on your web-browser. You can then log in with the username “rstudio”

and the password “yourpassword”. But you would also need to mount a volume (I called it “shared folder” previously) to keep the files you edit on your computer (remember, Docker container are immutable, so any files created within a Docker container will be lost when it’s stopped). Overall, I think that this is too cumbersome, especially because the risks of getting different results only because of your operating system are very, very, very low. I would simply advise the following:

- Use the same version of R on your computer and on Docker;
- Use the same package library on your computer and on Docker by using the same `renv.lock` file.

By following these two rules, you should keep any issues to a minimum. When or if you need to update R and/or the package library on your machine, simply create a new Docker image that reflects these changes.

However, if work in a field where operating system versions matter, then yes, you should find a way to either use the dockerized environment for development, or you should install Ubuntu on your computer (the same version as in Docker of course).

Let’s now discuss sharing images.

### **14.6.2. Sharing images through Docker Hub**

If you want to share Docker images through Docker Hub, you first need to create a free account. A free account gives you unlimited public repositories. If you want to make your images private, you need a paid account. For our purposes though, a free account is more than enough. Again, in the next section, we

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will discuss how you can build new images upon other images without using Docker Hub.

If you want to follow along, make sure that you have also written a Dockerfile and built an image that you can upload on Docker Hub. I will be uploading the image `dev_env_r` to Docker Hub, so if you want you could use for your own projects.

If you built an image to upload, now is the right moment to talk about the `docker images` command. This will list all the images available on your computer. You should see something like this:

| REPOSITORY       | TAG    | IMAGE ID     |   |
|------------------|--------|--------------|---|
| CREATED          | SIZE   |              |   |
| rver_intro       | latest | d3764d067534 | 2 |
| ↳ days ago       | 1.61GB |              |   |
| dev_env_r        | latest | 92fcf973ba42 | 2 |
| ↳ days ago       | 1.42GB |              |   |
| raps_ubuntu_r    | latest | 7dabadf3c7ee | 4 |
| ↳ days ago       | 1.04GB |              |   |
| rocker/tidyverse | 4.2.2  | 545e4538a28a | 3 |
| ↳ weeks ago      | 2.19GB |              |   |
| rocker/r-ver     | 4.2.2  | 08942f81ec9c | 3 |
| ↳ weeks ago      | 824MB  |              |   |

Take note of the image id of the `dev_env_r` image (second line), we will use it to push our image to Docker Hub. Also, don't be alarmed by the size of the images, because this is a bit misleading. Different images that use the same base (so here Ubuntu Jammy), will reuse "layers" such that they don't actually take up the size that is printed by `docker images`. So if images A and B both use Ubuntu Jammy as a base, but image A has RStudio installed and B also RStudio but Python as well, most

## 14.6. Dockerizing development environments

of the space that A and B take up will be shared. The only difference will be that B will need a little bit more space for Python.

You can also list the running containers with `docker container ls` (or `docker ps`). If a container is running you should see something like this:

| CONTAINER ID | IMAGE                   | COMMAND       |
|--------------|-------------------------|---------------|
| 545e4538a28a | rocker/tidyverse        | "/init" 3     |
| STATUS       | PORTS                   |               |
| Up 3 minutes | 0.0.0.0:8787->8787/tcp, |               |
|              | :::8787->8787/tcp       | elastic_morse |

You can stop the container by running `docker stop CONTAINER_ID`. So, list the images again using `docker images`. Take note of the image id of the image you want to push to Docker Hub.

Now, log in to Docker Hub using `docker login` (yes, from your terminal). You will be asked for your credentials, and if log in is successful, you see a message `Log In Succeeded` in your terminal (of course, you need first to have an account on Docker Hub).

Now, you need to tag the image (this gives it a version number). So you would write something like:

```
owner@localhost $ docker tag IMAGE_ID
 ↵ your_username_on_docker_hub/your_image:version1
```

so in my case, it would be:

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```
owner@localhost $ docker tag 92fcf973ba42
↪ rap4all/dev_env_r:4.2.2
```

Next, I need to push it using `docker push`:

```
owner@localhost $ docker push
↪ rap4all/dev_env_r:4.2.2
```

You can go check your profile and your repositories, you should see your image there. In my case, you can find the image here<sup>18</sup>.

This image can now be used as a stable base for developing our pipelines. Here's how I can now use this base image for my housing pipeline:

```
FROM rap4all/dev_env_r:4.2.2

RUN mkdir /home/housing

RUN mkdir /home/housing/pipeline_output

RUN mkdir /home/housing/shared_folder

COPY renv.lock /home/housing/renv.lock

COPY functions /home/housing/functions

COPY analyse_data.Rmd /home/housing/analyse_data.Rmd

COPY _targets.R /home/housing/_targets.R
```

---

<sup>18</sup><https://is.gd/7eiz5L>

## 14.6. Dockerizing development environments

```
RUN R -e
"setwd('/home/housing');renv::init();renv::restore()"

RUN cd /home/housing && R -e "targets::tar_make()"

CMD mv /home/housing/pipeline_output/*
/home/housing/shared_folder/
```

Take a look at this Dockerfile's first line:

```
FROM rap4all/dev_env_r:4.2.2`
```

This is different from before, where I pulled from `ubuntu:jammy`. Now I'm re-using the image that defines the development environment, and I can do so for as many projects as necessary. In time, I could update to a newer version of R, if required. But R and (Ubuntu) being quite stable, as long as I can install the packages required for my projects, I can keep using it for years (and LTS versions of Ubuntu like Jammy get supported for 5 years).

If you want to test this, you could delete all images and containers from your system. This way, when you will build the image using the above Dockerfile, it will have to pull from Docker Hub. To delete all containers, start by using `docker system prune`. You can then delete all images using `docker rmi $(docker images -a -q)`. This should remove everything. Now, let's build the image using the above Dockerfile using `docker build -t housing_image .` (don't forget to add the necessary files for the build process to succeed, `renv.lock`, `_targets.R`, `analyse_data.Rmd` and the `functions` folder). You should see the image getting pulled from Docker Hub and then the build process resuming and the pipeline running.

## 14. Reproducible analytical pipelines with Docker

In the next section, I'll explain to you how you can re-use base images like we just did, but without using Docker Hub, in case you cannot, or do not want, to rely on it.

### 14.6.3. Sharing a compressed archive of your image

If you can't upload the image on Docker Hub, you can still "save it" into a file and share that file instead (internally to your institution/company).

Run `docker save` to save the image into a file:

```
owner@localhost $ docker save dev_env_r >
↪ dev_env_r.tar
```

This will create a `.tar` file of the image. You can then compress this file with an archiving tool if you want. If you're on Linux, you could do so in one go (this will take some time):

```
owner@localhost $ docker save dev_env_r | gzip >
↪ dev_env_r.tgz
```

If you want to load this image, use `docker load`:

```
owner@localhost $ docker load < dev_env_r.tar
```

you should see an output like this:

```
202fe64c3ce3: Loading layer
↪ [=====] 80.33MB/80.33MB
```

```
e7484d5519b7: Loading layer
↳ [=====] 6.144kB/6.144kB
a0f5608ee4a8: Loading layer
↳ [=====] 645.4MB/645.4MB
475d1d69813f: Loading layer
↳ [=====] 102.9kB/102.9kB
d7963749937d: Loading layer
↳ [=====] 108.9MB/108.9MB
224a0042a76f: Loading layer
↳ [=====] 600MB/600MB
a75e978c1654: Loading layer
↳ [=====] 605.7kB/605.7kB
7efc10233531: Loading layer
↳ [=====] 1.474MB/1.474MB
Loaded image: dev_env_r:latest
```

or if you compressed the file on Linux, you can also use:

```
owner@localhost $ docker load -i dev_env_r.tgz
```

to load the archive.

You can then use `dev_env_r` for a pipeline by using this `FROM` statement in your Dockerfile:

```
FROM dev_env_r
```

Since the image is available locally, it'll get used instead of pulling it from Docker Hub. So in case you cannot use Docker Hub, you could build the base images, compress them, and share them on your corporate network. Then, people can simply download them and load them and build new images on top of them.

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So in summary, here's how you can share images with the world, your colleagues, or future you:

- Only share the Dockerfiles. Users need to build the images.
- Share images on Docker Hub. It's up to you if you want to share a base image with the required development environment, and then separate, smaller images for the pipelines, or if you want to share a single image which contains everything.
- Share images but only within your workplace.

Whatever option you go for, I hope that I've convinced you that Docker is really convenient. It may look complicated at first, but it saves a lot of headaches in the long run. Let me finish this section by stating something plainly: up until now, I tried to sell to you the idea that reproducibility did not require any extra effort, if you simply used the tools and techniques discussed in this book right from the start, with the added benefit of improving the quality of the code of your pipeline. I truly believe this to be the case with everything that I've shown up until now, but Docker. Using Docker for reproducibility does require some extra effort. However, if your projects require reproducibility, and you really want to play it safe, I think that Docker is unavoidable. It takes time to set up, but once it's done, you do not have to think about the infrastructure anymore and can focus on developing. Also, if you need to maintain your pipeline and keep running it against newer and newer versions of R, you simply need to change one line (the `FROM` statement, for example, from Ubuntu Jammy to Ubuntu 24.04, the next LTS) in the Dockerfile to update everything to the latest version of R.

But, there is still a “little” issue, that I'm discussing in the next section.

## 14.7. Some issues of relying on Docker

### 14.7.1. The problems of relying so much on Docker

So we now know how to build truly reproducible analytical pipelines, but let's be blunt, relying entirely on one single tool, Docker, is a bit of an issue... it's a single point of failure. But the problem is not Docker itself, but the infrastructure.

Let me explain: Docker is based on many different open-source parts, and that's great. This means that even if the company behind Docker ruins it by taking some weird decisions, we have alternatives that build upon the open-source parts of Docker. There's Podman, which is a drop-in replacement (when combined with other tools) made by Red Hat, which is completely open-source as well. So the risk does not come from there, because even if for some reason Docker would disappear, or get abandoned or whatever, we could still work with Podman, and it would also be technically possible to create a fork from Docker.

But the issue is the infrastructure. For now, using Docker and more importantly hosting images is free for personal use, education, open-source communities and small businesses. So this means that a project like Rocker likely pays nothing for hosting all the images they produce (but who knows, I may be wrong on this). But in early 2023, Docker announced that they would abandon their *Docker Free Team subscription* plans that some open-source organisations use, meaning that these organisations had 30 days to switch to a paid subscription. Docker finally did not do this, but it is not unreasonable to think that they might change their minds once more and this time really go through with this plan. Don't get me wrong, I'm not saying that Docker is not allowed to make money. But it is something that you need

## 14. Reproducible analytical pipelines with Docker

to keep in mind in case you cannot afford a subscription (and who knows how much it's going to cost). This is definitely a risk that needs mitigation, and thus a plan B. This plan B could be to host the images yourself, by saving them using `docker save`. Or you could even self-host an image registry (or lobby your employer/institution/etc to host a registry for its developers/data scientists/researchers). In any case, it's good to have options and now what potential risks using this technology entail.

### 14.7.2. Is Docker enough?

I would say that for 99% of applications, yes, Docker is enough for building RAPs. But strictly speaking, using a Dockerfile which installs a specific version of R and uses `{renv}` to install specific versions of packages and use an LTS release of Ubuntu, we could end up with two different images. This is because Ubuntu gets updated, so if you build an image in the beginning of 2022 and then once again in 2023, the system-level libraries will be different. So strictly speaking, you end up with two different images, and it's not absolutely impossible that this may impact your pipeline. So ideally, we would also need a way to always install the same system-level dependencies, regardless of when we build the image. There is a package manager called Nix that makes this possible, but this is outside the scope of this book. The reason is that, again, in practice if you use an LTS release you should be fine. But if you really require *bitwise reproducibility* (i.e., two runs of the same pipeline will yield the same result to the last bit), then yes, you should definitely look into Nix (and who knows, I might write a book just about that titled *Building bitwise reproducible analytical pipelines (braps) using Nix*).

Another issue with Docker is that images can be quite opaque,

especially if you define images that pull from images that pull themselves from other images... Just look at our pipeline: it pulls from `dev_env_r`, which pulls from `rocker:4.2.2` which pulls itself from the official Ubuntu Jammy image. So to be fully transparent, we would need to link to all the Dockerfiles, or rewrite one big Dockerfile that pulls from Ubuntu Jammy only.

## 14.8. Conclusion

This book could stop here. We have learned the following things:

- version control;
- functional programming;
- literate programming;
- package development;
- testing;
- build automation;
- “basic” reproducibility using `{renv}`;
- “total” reproducibility using Docker.

It is now up to you to select the tools that are most relevant for your projects. You might not need to package code for example. Or maybe literate programming is irrelevant to your needs. But it is difficult to argue against Docker. If you need to keep re-running a pipeline for some years, Docker is (almost) the only option available (unless you dedicate an entire physical machine to running that pipeline and never, ever, again touch that machine).

In the next and final chapter, we will learn some basics about continuous integration with Github Actions, which will allow us

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to automate even the building of Docker images and running pipelines.

# 15. Continuous integration and continuous deployment

As I wrote in the conclusion of the previous chapter, the book could have stopped there. So consider this chapter as a bonus. What I'm going to show here is not the most important aspect of reproducibility, and you could even make the case that is not needed at all. However, I still think that it is worth showing you how to use CI/CD, even if only superficially, and then you decide whether this is a tool that you should add to your toolbox.

The CI/CD (*Continuous Integration and Continuous Deployment or Delivery*) platform I'll be discussing here is Github Actions, which should not surprise you since we've been using Github for version control. But maybe you're wondering what a "CI/CD platform" even is, so let me start there.

Let's go back to the first idea of this book: Don't Repeat Yourself. We have written functions and used tools such as `{renv}` to avoid having to repeat ourselves. And yet, when it comes to using Docker, we need to keep building and running containers, running `docker build` and `docker run` over and over again. It would be great if instead, we didn't need to do it. This is what a CI/CD platform essentially allows you to do. The idea is that

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building, running and, if applicable, deploying are also tasks that can be automated, so why not automate them and only take care of writing code? And as the size of your team grows, the need to automate these tasks grows as well. Using CI/CD is an essential part of the DevOps methodology for software engineering.

This chapter can be seen as a small introduction to DevOps for data science.

According to Atlassian<sup>1</sup>:

DevOps is a set of practices, tools, and a cultural philosophy that automate and integrate the processes between software development and IT teams. It emphasizes team empowerment, cross-team communication and collaboration, and technology automation.

Most of the tools and practices described in this book would make adopting DevOps in your day-to-day a breeze. Strictly speaking though, we will be using “GitOps”, because our Github repository will be the centre stage of our project. The Github repository will not only contain the code of our project but also the definition of the infrastructure the code will run on. This way, our Github repository will be a single source of truth.

Concretely this means that each time we will push code (or merge a pull request, or perform any other Git-related event) to our Github repository, we can define a certain set of arbitrary actions to get executed, like building a Docker image. This image can then be pushed to Docker Hub, or a container can be executed. This container in turn can run a pipeline and the output can then be downloaded from Github. All of this happens in the cloud, all you need to do is push code changes

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<sup>1</sup><https://www.atlassian.com/devops>

to Github. As stated in the chapter on Git, Github offers 2000 minutes of computation time a month for CI/CD, which should be really sufficient for a lot of purposes (but of course, if your RAP takes hours to complete, you might want to run it locally instead).

Github Actions is very flexible, and you could use it to perform many tasks, not just building Docker images or running containers. For example, this book gets built and published online automatically each time I push an update to the repository<sup>2</sup> holding the book's source code. If you're developing a package, you could run `R CMD check` each time you push code to the repository. `R CMD check` runs many tests, including the package's unit tests (when using `{fusen}`, `R CMD check` is run each time a flat file gets inflated.) and using Github Actions, it's possible to run `R CMD check` on Ubuntu (Linux), Windows and even macOS (see this documentation page<sup>3</sup> if you're interested).

In this chapter, I'm going to show you how to use Github Actions to:

- run some simple arbitrary code;
- run a `{targets}` pipeline without Docker;
- build a Docker image containing a development environment (dev env) and push it to Docker Hub when pushing changes to its Dockerfile on Github;
- run a Docker container that runs a RAP and builds some output that we can then download from Github.

Finally, what does *integration* and *deployment* or *delivery* even mean? Continuous integration means that changes get merged to the master or main branch continuously. Remember Trunk-based development? In TBD, the goal is achieving continuous

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<sup>2</sup><https://github.com/b-rodrigues/rap4all>

<sup>3</sup><https://is.gd/F9AOZI>

## *15. Continuous integration and continuous deployment*

integration, and Gitops is one efficient way of doing so. Now, what's the difference between deployment and delivery? Both obviously mean that we're shipping a product. The difference is only in how the project is managed. If the code gets pushed immediately to production, then we speak of deployment. If instead the code gets pushed to a test server, and final deployment to production needs to be approved by a manager, then it's delivery. For our purposes, this distinction doesn't really matter. Think of delivery or deployment simply as “shipping”.

### **15.1. CI/CD quickstart for R programmers (and others)**

Before defining a “Hello World” pipeline that gets executed in the cloud, I need to define some terms. A workflow that runs on Github Actions is defined as a Yaml file, and this file contains a succession of “actions”, and each action performs a specific task. Here is the simplest Github Actions workflow file that you could write (source: link<sup>4</sup>):

```
name: hello-world
on: push
jobs:
 my-job:
 runs-on: ubuntu-latest
 steps:
 - name: my-step
 run: echo "Hello World!"
```

---

<sup>4</sup><https://is.gd/9mDykY>

## 15.1. CI/CD quickstart for R programmers (and others)

This needs to be saved in a `hello_world.yml` file, and placed inside the `.github/workflows/` directories in the Github repository you want this action to run each time something gets pushed to the repo.

Each time code gets pushed to the repository containing this workflow file, a *runner* runs the code `echo "Hello World!"` on the latest version of Ubuntu. A workflow file is thus defined as a series of steps, that can either run code, or an action (more on actions later) that get executed on a so-called runner (in essence, a container). This workflow gets executed when a specific event occurs, in the example above that event is pushing to the repo. To see the output of the workflow, click on “Actions” on your Github repository:

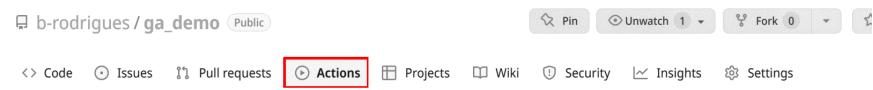


Figure 15.1.: Click on ‘Actions’ to monitor your workflows.

You should see a list of workflow runs, each corresponding to a commit. Click on the latest one and then click on the job named `my-job`. If your workflow has multiple jobs, they’ll all be listed here. Once you click on the job, you should see a list of steps. The step that interested us here is `my-step` which should simply print “Hello World!”. Click on it to see the output:

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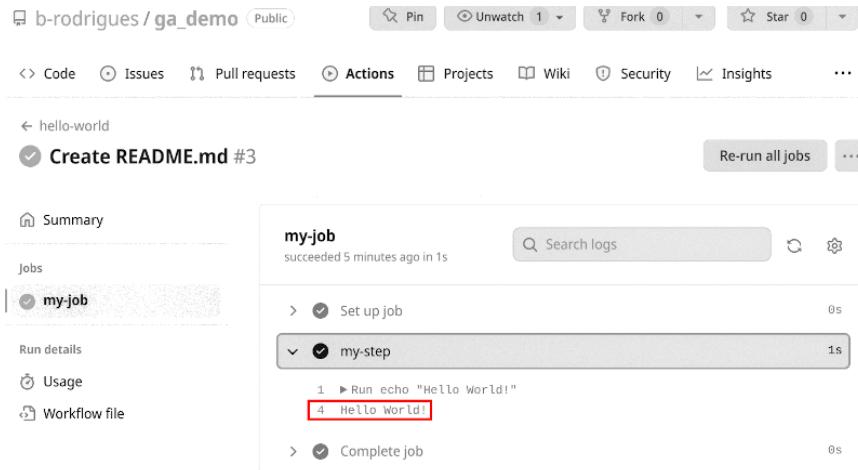


Figure 15.2.: Congrats, that's your first GA workflow.

To help you define complex workflows, you can use pre-defined actions that you can choose from to perform a series of common tasks. You can find them in the Github Actions Marketplace<sup>5</sup>.

We are not going to use any actions from the Github Actions Marketplace just yet though, but instead, we will be looking at a repository containing actions specifically made for R users (if you're using another programming language, it is quite likely that you might find a repository of actions for that programming language).

This repository<sup>6</sup> contains many actions for R users. For example, let's say that you want to install R and run some code using Github Actions. Simply take a look at the setup-r<sup>7</sup> and see how it's used. Let me edit my `hello_world.yml` from before, and

<sup>5</sup><https://github.com/marketplace>

<sup>6</sup><https://github.com/r-lib/actions>

<sup>7</sup><https://github.com/r-lib/actions/tree/v2/setup-r>

## 15.1. CI/CD quickstart for R programmers (and others)

add one step that downloads R and prints "Hello from R!" using R:

```
name: hello-from-R
on: push
jobs:
 my-job:
 runs-on: ubuntu-latest
 steps:
 - name: hello-from-bash
 run: echo "Hello from Bash!"

 - name: checkout-repo
 uses: actions/checkout@v3

 - name: install-r
 uses: r-lib/actions/setup-r@v2
 with:
 r-version: '3.5.3'

 - name: hello-r
 run: Rscript -e 'print("Hello from R!")'
```

So now my job performs two tasks, one that prints "Hello from Bash!" and another that prints "Hello from R!". There are several steps involved, the second step, called `checkout-repo` runs the action `actions/checkout@v3` and the third step, called `install-r` uses the action `r-lib/actions/setup-r@v2`. The first action, `actions/checkout@v3` is an action that you will see on almost any Github Actions workflow file, even though it is likely superfluous in this case. You can read about it here<sup>8</sup> and it essentially makes the files inside the repository available to the runner. Sometimes I think that it would have made more

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<sup>8</sup><https://github.com/actions/checkout>

## 15. Continuous integration and continuous deployment

sense to call this action `clone`, like the `git clone` command. But I'm sure there's a very good reason that this is not the case. The next action is `setup-r@v2` which downloads and installs, in our example here, R version 3.5.3. The final step then runs the command `Rscript -e 'print("Hello from R!")'`. If you check out the “Actions” tab on Github, you should now see this:

The screenshot shows a GitHub repository page for 'b-rodrigues/ga\_demo'. The 'Actions' tab is selected. A pipeline named 'my-job' is shown, which succeeded 3 minutes ago in 1m 13s. The steps are: Set up job (13s), hello-from-bash (0s), checkout-repo (1s), install-r (57s), and hello-r (0s). The 'hello-r' step is expanded, showing the command 'Run Rscript -e 'print("Hello from R!")'' and its output '[1] "Hello from R!"'.

Figure 15.3.: This time it's R that's waving hello.

We could have installed any other version of R by the way. We can keep adding steps, for example, let's add one to install `{renv}` and install packages from an `renv.lock` file (the file needs to be in our repository, and becomes available to the workflow thanks to `actions/checkout@v3`):

```
name: my-pipeline
on: push
jobs:
```

## 15.1. CI/CD quickstart for R programmers (and others)

```
my-job:
 runs-on: ubuntu-22.04
 steps:

 - name: checkout-repo
 uses: actions/checkout@v3

 - name: install-r
 uses: r-lib/actions/setup-r@v2
 with:
 r-version: '4.2.2'

 - name: install-renv
 uses: r-lib/actions/setup-renv@v2
```

I think you’re starting to see where this is going. This workflow runs on Ubuntu 22.04, installs R version 4.2.2 and installs all the packages defined in the `renv.lock` file stored in our repository (and if you don’t have an `renv.lock` file, only `{renv}` will get installed). So to have our RAP running in the cloud, we would simply need to add the other required files and finish writing the workflow. One note of warning though: if you’re running pipelines defined like the above, each time you push, every step will run from scratch (apart from package installation using `r-lib/actions/setup-renv@v2` because packages will be cached for future runs of the workflow), and this may take some time to run.

## 15.2. Running a RAP using Github Actions

Because running `{targets}` pipelines on Github Actions is a common task, there is of course a way to do it very easily, without the need to write our own workflow file. Simply go to the folder that contains your pipeline (which, I hope, is versioned using Git, right?), open an R session and run `targets::tar_github_actions()`. This will automatically create a folder called `.github/` in the root of your pipeline’s folder, with inside a `workflows/` folder, and inside a `targets.yaml` workflow file. This file is ready to use, but you may adapt it to your needs. For example, this workflow file runs on `ubuntu-latest` and installs the latest version of R. You may want to change the version of Ubuntu to `ubuntu-22.04` (this way, Ubuntu 22.04 will keep getting used even when the next LTS, 24.04, will be released) and install R version 4.2.2 (or whichever version you used for your pipeline). Also, don’t forget to install the Ubuntu dependencies under the “Install Linux System dependencies” step. There’s already some dependencies there, but you should add the others that we’ve listed in the Dockerfile (the syntax is slightly different from the Dockerfile, so pay attention to it). This workflow file also runs some other useful actions, like caching packages, so they don’t need to get re-downloaded each time you push a change to the repository!

You can see the repository with the workflow file here<sup>9</sup>. The workflow file is inside the `.github/workflows/` folder here<sup>10</sup>. As I explained before, pay attention to line 29 (where I stated that the action should trigger when a change gets pushed to the branch `gitops-pipeline`), to line 35 where I changed the

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<sup>9</sup><https://github.com/rap4all/housing/tree/gitops-pipeline>

<sup>10</sup><https://is.gd/iIJwuG>

## 15.2. Running a RAP using Github Actions

runner from `ubuntu-latest` to `ubuntu-22.04`, line 43 where I install R version 4.2.2 and finally lines 53 to 74 where I install the required Ubuntu dependencies (the same as for the Dockerfile). Don't hesitate to use this repository as a template for your projects! The rendered HTML file is in the newly created `targets-runs` branch of the repository. This branch gets created automatically by the workflow and the output gets saved in there automatically.

So it turns out that running a RAP on Github Actions is quite easy, you only need to use `targets::tar_github_actions()`, and adapt the `targets.yaml` file a little bit to install the right version of R and run it on the right version of Ubuntu (or Windows or macOS, but careful, you only have 2000 free minutes and Windows and macOS are more expensive than Ubuntu, 1 minute of CPU time on Ubuntu is equal to 2 minutes of run-time on macOS). By using `{renv}` and the generated `renv.lock` file, the pipeline dependencies get installed seamlessly as well. You can now focus on coding, each time you push to this branch, you will see the output get generated (and because caching is being used, runs will be executed rather quickly).

But, and yes there is a but, you should think about the following, potential, issues:

- you are limited to 2000 minutes of free run-time. If your pipeline takes several hours to run, you might need to upgrade to a paid account, or run it locally (but this is mitigated thanks to caching on Github and by using `{targets}` that caches results as well);
- Github Actions does not keep old versions of operating systems for too long. For example, as of writing, only versions 20.04 and 22.04 of Ubuntu are available. Ubuntu 18.04 was removed in August 2022. If your RAP absolutely needs a specific version of Ubuntu for a very long time, Github

## 15. Continuous integration and continuous deployment

Actions might not be the right solution. The same is true for Windows or macOS as well. However, what you might want to do instead is migrate the pipeline to newer versions of Ubuntu when these become available. Generally speaking, this should not be a very painful process.

So you need to think about what it is you really need. Does your pipeline run relatively quickly, and you don't need to keep it running forever on the same operating system? Then Github Actions is for you. Or perhaps you are writing a book using Rmarkdown, or Quarto, and don't want to bother building it and deploying it manually? Then Github Actions is for you as well (and take a look at this book's workflow file here<sup>11</sup> for an example of exactly this). But if you are working on a pipeline that may take several hours to run, and you want it to stay reproducible for a very long time, then using Docker might be a better option. Thankfully, you can also use Github Actions to build Docker images and upload them to Docker Hub. You can even then run a Docker container that runs your RAP (but here again, if your pipeline takes several hours to run, you may not want to do that).

### 15.3. Craft a dockerized dev env with GA

This section and the next are going to mirror the sections on dockerizing projects and dockerizing dev envs (development environments) from the previous chapter. The only difference is that all the heavy lifting will happen on Github Actions, instead of our own computer.

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<sup>11</sup><https://is.gd/6nhYaf>

### 15.3. Craft a dockerized dev env with GA

I'm going to describe the following repository<sup>12</sup>. This repository contains a Dockerfile, and a `.github/workflows/` folder with a Github Actions workflow file. Each time I push any change to any file from this repository, a new Docker image gets built automatically and pushed to Docker Hub. The image that gets built defines a dev env that we will then use for our RAPs.

As stated before, the advantage of using Docker images for your RAPs instead of simply running them directly inside Github Actions (as in the previous section), is that you don't rely on Github to have the base image (in our example, `ubuntu-22.04`), forever available, which they won't.

The idea is the same as before: work on the code of your project, define a Dockerfile and get an updated image each time you push your changes to the repository.

Let's start with the Github Actions workflow file that we need. Here it is:

```
name: build_docker

on:
 push:
 branches:
 - master
 - main

jobs:
 docker:
 runs-on: ubuntu-latest
 env:
 IMAGE_NAME: r_4.2.2
 steps:
```

---

<sup>12</sup>[https://github.com/b-rodrigues/ga\\_demo/tree/main](https://github.com/b-rodrigues/ga_demo/tree/main)

## 15. Continuous integration and continuous deployment

```
- name: Setup
 uses: docker/setup-buildx-action@v2
- name: Login to Docker Hub
 uses: docker/login-action@v2
 with:
 username: ${{ secrets.DOCKERHUB_USERNAME }}
 password: ${{ secrets.DOCKERHUB_TOKEN }}
- name: Build image and push to Docker Hub
 uses: docker/build-push-action@v4
 with:
 tags: ${{ secrets.DOCKERHUB_USERNAME }}/{{ env.IMAGE_NAME }}:
 ${{ github.ref_name }}-${{ github.sha }}
 push: true
```

Just one remark: I had to split the `tags:` line into two lines. When copying this line into the yaml file, put the two lines back into one line. Click here<sup>13</sup> for the actual file.

I believe that this file is the simplest one you could have for this. Let's study it in detail.

The start of the file is pretty standard: we give the workflow a name, and state that it should run on `ubuntu-latest` whenever anything gets pushed to either `main` or `master`. We define an environment variable called `r_4.2.2`. This is the name of the image that we are going to build. We will build an image that comes with R 4.2.2 pre-installed as well as many required Ubuntu packages; it's the same image as we built in the previous chapter on top of which we will then build RAPs. This image is based on the one from the Rocker project. We

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<sup>13</sup><https://is.gd/0xqH22>

### 15.3. Craft a dockerized dev env with GA

will take a look at the Dockerfile afterwards. Then, the action `docker/setup-buildx-action@v2` simply sets up everything for `buildx` to run smoothly (`buildx` will build the Docker image using the `docker buildx` command an alternative to `docker build`). Honestly, I don't even know exactly what it sets up. I guess it may at least checkout the repository to make the files available to the next actions and maybe set some other variables for `docker buildx`.

Then we use the `docker/login-action@v2` to login from Github Actions to Docker Hub. Essentially, we need to be able to tell our Github Actions runner how to login to Docker Hub, and of course we want to do so in a secure manner (and it must run non-interactively). To login to Docker Hub from Github Actions, you need first to create an access token from your Docker Hub account. Login to your Docker Hub account, go to your account settings and then to the “Security” tab:

## 15. Continuous integration and continuous deployment

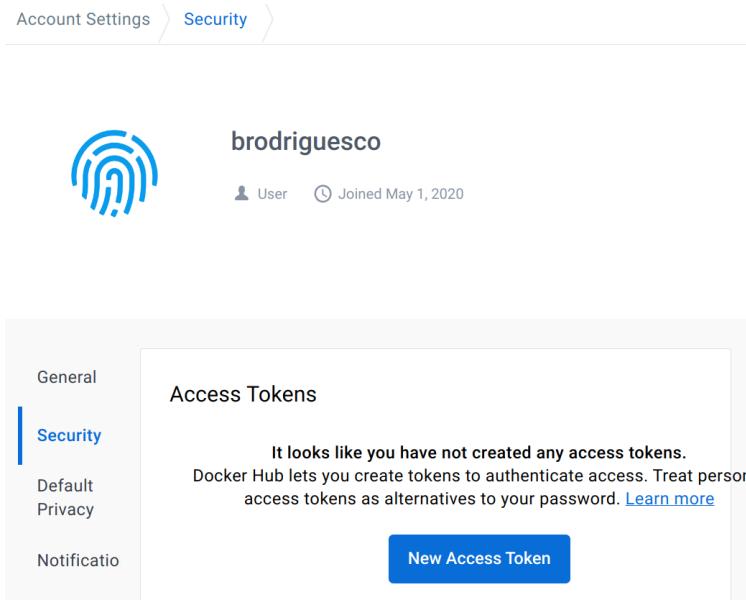


Figure 15.4.: Create your access token.

Name it `github_actions` for example, and set its permissions to “Read, Write, Delete”. On the next window that pops up, make sure to save your access token:

### 15.3. Craft a dockerized dev env with GA

#### Copy Access Token

When logging in from your Docker CLI client, use this token as a password. [Learn more](#)

ACCESS TOKEN DESCRIPTION

github\_action

ACCESS PERMISSIONS

Read, Write, Delete

To use the access token from your Docker CLI client:

1. Run `docker login -u brodriguesco`
2. At the password prompt, enter the personal access token.

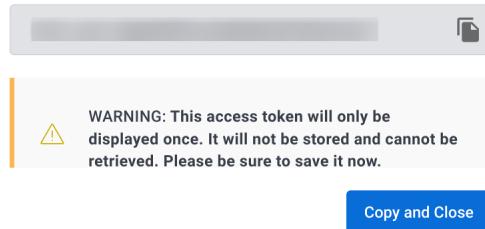


Figure 15.5.: Make sure to write it down!

You then need to go to the settings area of the repository. Under “Security”, “Secrets and variables” and finally “Actions” you can create a secret called DOCKERHUB\_TOKEN and copy the value of the token in the free text area:

## 15. Continuous integration and continuous deployment

### Copy Access Token

When logging in from your Docker CLI client, use this token as a password. [Learn more](#)

ACCESS TOKEN DESCRIPTION

github\_action

ACCESS PERMISSIONS

Read, Write, Delete

To use the access token from your Docker CLI client:

1. Run `docker login -u brodriguesco`
2. At the password prompt, enter the personal access token.

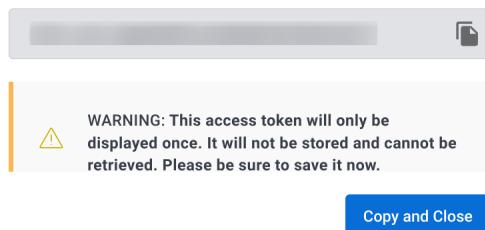


Figure 15.6.: Copy the token in your repo's secrets.

Create a second secret with your Docker Hub username called `DOCKERHUB_USERNAME`. These can now be used in the workflow file using so-called *contexts*. Your Docker Hub username will get replaced wherever you write `${{ secrets.DOCKERHUB_USERNAME }}` in the workflow file, same for your Docker Hub token with `${{ secrets.DOCKERHUB_TOKEN }}`.

Finally, we build and push the image to Docker Hub. This is done using the action called `docker/build-push-action@v4`. We use the `tags` option to tag our image. The tag needs to start with your username, followed by a `/`, then the image name, and then a version, so something like `bob/r_4.2.2:latest` where `latest` would be the latest version of the image that is available. Getting `bob/r_4.2.2` is quite easy: simply use your Docker Hub

### 15.3. Craft a dockerized dev env with GA

username that you defined as a secret, then literally type / and then use the image name that you've defined in the beginning of the workflow file. Careful though: `bob/r_4.2.2` needs to exist on Docker Hub as well. `bob` is easy, that's your Docker Hub username as already stated, but `r_4.2.2` is a repository that you need to create on Docker Hub. So both your image name and the repository name on Docker Hub will be `r_4.2.2`. If you don't create a repository on Docker Hub that is exactly named like that, your image will not get pushed, because Github Actions will not know where to push the image. So if this is not already the case, go back to Docker Hub and create a repository named `r_4.2.2`. For the version, you can do whatever you want, but I suggest to use the context `github.ref_name` and `github.sha`. `github.ref_name` gives the name of the branch that starts the workflow, and `github.sha` returns the hash number of the commit that starts the workflow. This way, your image will be named something like `bob/r_4.2.2:master-65ai9besta65948`. This allows you to see which commit generated which image, which is really useful. We then also set `push` to `true`, so that the image gets pushed.

With this workflow file in hand, I can now build a Docker image and push it to Docker Hub simply by pushing code to my repository. Here are two commits that generated two images:



Figure 15.7.: Two successful runs of Github Actions.

and here are the two corresponding images on Docker Hub:

## 15. Continuous integration and continuous deployment

| Tags                                 |                                                                                   |       |        |           |
|--------------------------------------|-----------------------------------------------------------------------------------|-------|--------|-----------|
| This repository contains 2 tag(s).   |                                                                                   |       |        |           |
| Tag                                  | OS                                                                                | Type  | Pulled | Pushed    |
| <a href="#">main-b1950d55ccbd...</a> |  | Image | ---    | a day ago |
| <a href="#">main-6b7bba10b9ce...</a> |  | Image | ---    | a day ago |

Figure 15.8.: The corresponding images on Docker Hub.

I noticed a typo in my Dockerfile: originally, I was basing my image on R version 4.2.1. So I changed this and pushed. This is the commit that starts with b1950. The image then got built, tagged, and pushed to Docker Hub without any manual intervention on my part. You can see that the tag is of the form `repo-hash`, in this case, `main-b1950d`. Clicking on this tag on Docker Hub shows you some useful information:

### 15.3. Craft a dockerized dev env with GA

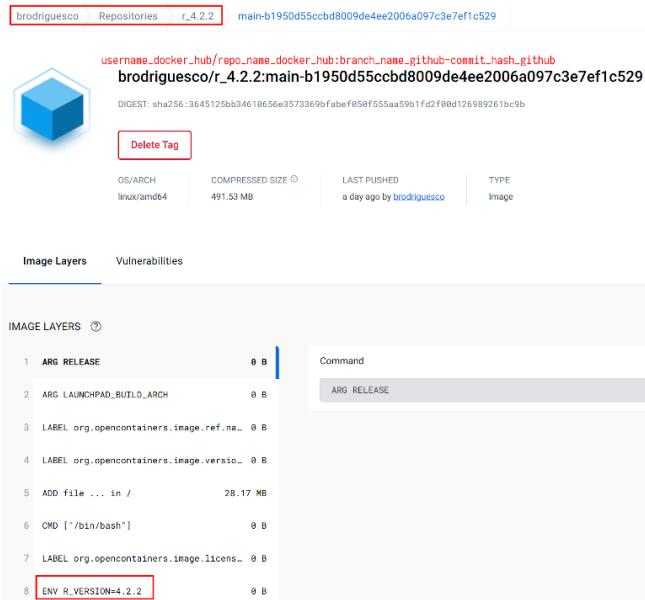


Figure 15.9.: This is the image with the correct R version.

## 15.4. Run a RAP using a dockerized dev env on GA

Now that we have a dockerized dev env that gets built by pushing changes to a Github repo, it is now time to use it for our RAPs. As I wrote in the beginning, this will mirror the section on running a RAP that uses a dockerized environment, so we can start from that repository. This<sup>14</sup> was the repository that we used at the time. You can create a new repository with the same content (but you can remove the `.gitignore` file, it won't be needed here). This is what my repository<sup>15</sup> looks like. The only difference with the first repository is the Dockerfile and the Github Actions workflow file that is inside `.github/workflows`. Let's take a look at the Dockerfile first:

```
FROM brodriguesco/r_4.2.2:main-b1950d55ccbd8009de4ee
2006a097c3e7ef1c529

RUN mkdir /home/housing

RUN mkdir /home/housing/pipeline_output

RUN mkdir /home/housing/shared_folder

COPY renv.lock /home/housing/renv.lock

COPY functions /home/housing/functions

COPY analyse_data.Rmd /home/housing/analyse_data.Rmd

COPY _targets.R /home/housing/_targets.R
```

---

<sup>14</sup><https://github.com/rap4all/housing/tree/docker>

<sup>15</sup>[https://github.com/b-rodrigues/ga\\_demo\\_rap](https://github.com/b-rodrigues/ga_demo_rap)

## 15.4. Run a RAP using a dockerized dev env on GA

```
RUN R -e
"setwd('/home/housing');renv::init();renv::restore()"

RUN cd /home/housing && R -e "targets::tar_make()"

CMD mv /home/housing/pipeline_output/*
/home/housing/shared_folder/
```

It is almost exactly the same as the one from the dockerized pipeline from the previous chapter. The only difference is the very first statement, where we pull the base image. Now I'm using the image from the dockerized environment that I built in the previous section. Apart from that, everything's the same.

The magic happens with the workflow file. Here it is:

```
name: Reproducible pipeline

on:
 push:
 branches:
 - main
 - master

 jobs:

 build:
 runs-on: ubuntu-latest

 steps:
 - name: Checkout repository
 uses: actions/checkout@v3

 - name: Build the Docker image
```

## 15. Continuous integration and continuous deployment

```
run: docker build -t housing_image .

- name: Docker Run Action
 run: >
 docker run --rm --name housing_container -v
 /github/workspace/shared_folder:
 /home/housing/shared_folder:rw
 housing_image

- uses: actions/upload-artifact@v3
 with:
 name: housing_output_${{ github.sha }}
 path: /github/workspace/shared_folder/
```

By now, you should certainly understand this workflow file without much trouble. First we checkout the contents of the repository to make the files available to the other steps. Then we build the Docker image. For this, I'm doing this the "old-school" way by using the actual command that we would use on our local machine. Then we run the container. Once again I use the command that I would use locally. But you'll notice that I use `/github/workspace/shared_folder` as the path to the shared folder. You likely guessed it, `/github/workspace/` is the "local" path inside the Github Actions runner. This is equivalent to the `/home/` directory on a Linux machine. The command is also on multiple lines (to write a command over multiple lines on github actions, you need to start by `>` and then use as many lines as you need).

The final action, `actions/upload-artifact@v3` is used to upload the contents of the shared folder and name them `housing_output_${{ github.sha }}`, where `${{ github.sha }}` will get replaced by the hash from the commit that triggered the action. This will be a zip file that you can then download.

## 15.4. Run a RAP using a dockerized dev env on GA

But download from where?

Simply click on the “Actions” tab on the Github repository, and then click on the run that you want the artifact from (pipeline outputs are called artifacts):

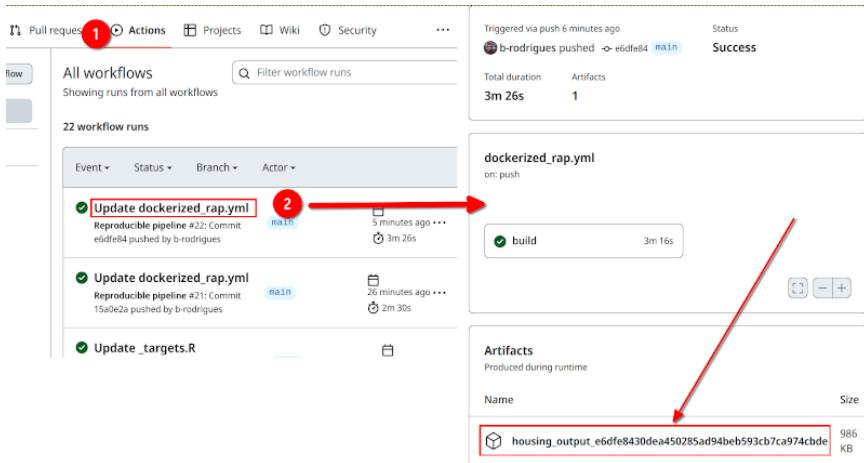


Figure 15.10.: Artifacts (pipeline outputs) can be found by going into a run’s details.

And that’s it! You could tweak the workflow file to instead push the files to a new branch in the repository, like the workflow file that `targets::tar_github_actions()` generates. But I think that this solution is easier to use, and also, if you need to download the artifact from a previous run, it’s all right there. Simply select a previous run and download the artifact. If instead, you push the outputs to a new branch, you’d need to revert to that commit to get past outputs.

## 15.5. Conclusion

At the start of this chapter, I stated that this chapter was optional, because it is not necessary to use a CI/CD service to ensure that your projects are reproducible. However, I believe that setting up your project to make it run on Github Actions (or any other CI/CD service) truly forces you to master all the topics presented in this book. In the conclusion of part 1 of the book, I wrote that it seemed as if functional programming was only about putting restrictions on our code, for very little gain. In some ways, forcing yourself to use a CI/CD service can feel similar. But here's the thing: if your project builds successfully on a CI/CD service, and if the results remain stable over time, then your project is reproducible. Someone else could then run it locally by simply following the same steps as in the workflow file, which would consist of the very same basic steps: clone the repository, build a Docker image and run a container (or set up the required R package library using `{renv}` and then run the pipeline with `{targets}` if you're not using Docker).

If you work in research, but cannot push the data to Github, you could always work on the code and the infrastructure using synthetic data for instance. The repository alongside the synthetic data could then be a nice complement to the paper (but again, only in case the data cannot be published).

# 16. Conclusion of part 2

Congratulations, we are done going down the reproducibility iceberg. Our project should now be entirely reproducible. I showed you how to reuse the same R version and the same package library as the one that was used to develop the pipeline originally. If in addition you've used the software engineering best practices from part 1, your project is also well tested and documented.

This part of the book focused on the operating system your pipeline runs on. It's a bit trickier to "freeze" an operating system, like we froze the R version and the packages library. Strictly speaking, we should develop and deploy our pipeline on the same operating system. If you're using Ubuntu as your daily driver, that is not an issue, but if you're a Windows or a macOS user, then this *could* potentially be a problem. After all, Docker images are based on Ubuntu (or other Linux distributions), so the best we can do is either start developing with the end in mind from the beginning; which means that we develop our project from inside a Docker environment, or we must ensure that running the pipeline inside Docker returns the same results as on your operating system of choice. This should most of the time not be an issue, but as already mentioned in this book, running the same code on Linux or Windows does sometimes return different results (this is rarer, at least in my experience, when comparing Linux to macOS).

But there is yet another, potential, issue. Let's assume the best

## 16. Conclusion of part 2

case scenario: the pipeline returns the same result inside Docker as on your development machine (which should be the case most of the time anyways). Is using Docker truly the best we can do? Is the pipeline truly reproducible? Well, *strictly* speaking, not quite. Indeed, the base operating system inside Docker also gets updated. So if you build an image based on Ubuntu 22.04 today, and then again in 6 months, the operating system is not the same anymore, because the software it ships got updated. So even if the R package library and R version remain fixed, the operating system does not. Now, I realize that this is really pushing it, but I want to be as thorough as possible. So there are two ways around this, if you really, absolutely, need also Ubuntu to remain frozen.

The first solution is the simplest and is explained in the reproducibility page<sup>1</sup> of the Rocker project. The idea is to use a digest, which is the equivalent of a commit hash on Github but for Docker images instead. As the example in the linked page above shows, instead of this:

```
FROM rocker/r-ver:4.2.0
```

which would base your Docker image on the latest Ubuntu 22.04 shipping R version 4.2.0, you would use this:

```
FROM rocker/r-ver@sha256:b343df137d83b0701e0...
```

which is the digest of the latest rebuild of that image. You can find digests on the Docker Hub page:

---

<sup>1</sup><https://is.gd/YKL0T4>



Figure 16.1.: You can find Docker image digests on Docker Hub.

If you use a digest instead of a tag, it doesn't matter when the image gets built, you'll be using the exact same Ubuntu version under the hood that was current *at that time*.

The second way around this is to use a functional package manager like Guix or Nix. As I stated in the reproducibility iceberg, this is outside the scope of this book, but the idea of these package managers is that they allow users to reproduce the entirety of a project (so including the operating system libraries) to the exact same byte. If you want to know more, take a look at Vallet, Michonneau, and Tournier (2022) (open access article<sup>2</sup>) which shows how Guix works by reproducing the results from another paper.

<sup>2</sup><https://www.nature.com/articles/s41597-022-01720-9#Abs1>



# 17. The end

Congratulations, you're done with the book and I hope you learned a thing or two.

Part 1 focused on teaching you best practices, tools and techniques to make your code as clean as possible. In part 2, I taught you how to turn your project into a pipeline, and then how to make this pipeline reproducible using `{renv}` and Docker. To summarise, here are all the things that we need to think about to write a RAP:

- Write code that is as clean as possible: keep it DRY, document and test it well;
- Record package dependencies of the project;
- Record the R version that you use;
- Use a tool that builds the project for you;
- Record the computational environment.

If you tick all these boxes, you, or anyone else, should not have any problems reproducing the results of your project. While it may seem that ticking these boxes takes up valuable time from other tasks, if you use the techniques and tools that I've showed you in part 1, this should not be the case, and you might end up even gaining time. The only exception to this will be preparing a Docker image, but if you supply at the very least an `renv.lock` file, creating a Docker image to run a project could even be done much later, and only if it's really needed (and maybe even by someone else).



# “So what?”

If you’ve reached this conclusion and are still thinking “meh, yeah, reproducibility is nice and all, but... so what?” I hope that this last attempt of mine to convince you that RAPs are important will be successful.

So, why bother building RAPs? Firstly, there are purely technical considerations. It is not impossible that in quite a near future, we will work on ever thinner clients while the heavy-duty computations will run on the cloud. Should this be the case, being comfortable with the topics discussed in this book will be valuable. Also, in this very near future, large language models will be able to set up most, if not all, of the required boilerplate code to set up a RAP. This means that you will be able to focus on analysis, but you still need to understand what are the different pieces of a RAP, and how they fit together, in order to understand the code that the large language model prepared for you, but also to revise it if needed. And it is not a stretch to imagine that simple analyses could be taken over by large language models as well. So you might very soon find yourself in a position where you will not be the one doing an analysis and setting up a RAP, but instead check, verify and adjust an analysis and a RAP built by an AI. Being familiar with the concepts laid out in this book will help you successfully perform these tasks in a world where every data scientist will have AI assistants.

## “So what?”

But more importantly, the following factors are inherently part of data analysis:

- transparency;
- sustainability;
- scalability.

It doesn’t matter if you’re working in research, for a public institution or a private sector company: the three points above are incredibly important and it’s impossible to perform data analysis without taking these into consideration, regardless of whether AIs take over some, or most, of the tasks you perform today. In the case of research, the *publish or perish* model has distorted incentives so much that unfortunately a lot of researchers are focused on getting published as quickly as possible, and see the three factors listed above as hurdles to getting published quickly. Herculean efforts have to be made to reproduce studies that are not reproducible, and more often than not, people that try to reproduce the results are unsuccessful. Thankfully, things are changing and there are more and more efforts being made to make research reproducible by design, and not as an afterthought. In the private sector, tight deadlines lead to the same problem: analysts think that making the project reproducible is an hindrance to being able to deliver on time. But here as well, taking the time to make the project reproducible will help with making sure that what is delivered is of high quality, and it will also help with making reusing existing code for future projects much easier, even further accelerating development.

Data analysis, at whatever level and for whatever field, is not just about getting to a result, the way to get to the result is part of it! This is true for science, this is true for industry, this is true everywhere. You get to decide where on the iceberg of reproducibility you want to settle, but the lower, the better.

*“So what?”*

So why build RAPs? Well, because there's no alternative if you want to perform your work seriously.



# References

- Arel-Bundock, Vincent. 2022. “modelsummary: Data and Model Summaries in R.” *Journal of Statistical Software* 103 (1): 1–23.
- Bhandari Neupane, Jayanti, Ram P. Neupane, Yuheng Luo, Wesley Y. Yoshida, Rui Sun, and Philip G. Williams. 2019. “Characterization of Leptazolines a–d, Polar Oxazolines from the Cyanobacterium *Leptolyngbya* Sp., Reveals a Glitch with the ‘Willoughby–Hoye’ Scripts for Calculating NMR Chemical Shifts.” *Organic Letters* 21 (20): 8449–53.
- Chambers, John M. 2014. “Object-Oriented Programming, Functional Programming and R.” *Statistical Science* 29 (2): 167–80.
- Chan, Chung-hong, and David Schoch. 2023. “RANG: Reconstructing Reproducible r Computational Environments.” arXiv.
- Firke, Sam. 2023. *Janitor: Simple Tools for Examining and Cleaning Dirty Data*.
- Gohel, David, and Panagiotis Skintzos. 2023. *Flextable: Functions for Tabular Reporting*.
- Hammant, Paul. 2020. *Trunk-Based Development and Branch by Abstraction*. Leanpub.
- Landau, William Michael. 2021. “The Targets r Package: A Dynamic Make-Like Function-Oriented Pipeline Toolkit for Reproducibility and High-Performance Computing.” *Journal of Open Source Software* 6 (57): 2959.
- Leisch, Friedrich. 2002. “Sweave: Dynamic Generation of Sta-

## References

- tistical Reports Using Literate Data Analysis.” In *Compstat*, edited by Wolfgang Härdle and Bernd Rönz, 575–80. Physica-Verlag HD.
- Peng, Roger D. 2011. “Reproducible Research in Computational Science.” *Science* 334 (6060): 1226–27.
- Rochette, Sébastien. 2022. *Fusen: Build a Package from Rmarkdown Files*.
- Trisovic, Ana, Matthew K Lau, Thomas Pasquier, and Mercè Crosas. 2022. “A Large-Scale Study on Research Code Quality and Execution.” *Scientific Data* 9 (1): 60.
- Vallet, Nicolas, David Michonneau, and Simon Tournier. 2022. “Toward Practical Transparent Verifiable and Long-Term Reproducible Research Using Guix.” *Scientific Data* 9 (1): 597.
- Wickham, Hadley. 2019. *Advanced r*. CRC press. <https://adv-r.hadley.nz/>.
- Wickham, Hadley, Mara Averick, Jennifer Bryan, Winston Chang, Lucy D’Agostino McGowan, Romain François, Garrett Grolemund, et al. 2019. “Welcome to the tidyverse.” *Journal of Open Source Software* 4 (43): 1686.
- Wickham, Hadley, and Jenny Bryan. 2023. *R Packages (2e)*. <https://r-pkgs.org/>.
- Xie, Yihui. 2014. “Knitr: A Comprehensive Tool for Reproducible Research in R.” In *Implementing Reproducible Computational Research*, edited by Victoria Stodden, Friedrich Leisch, and Roger D. Peng. Chapman; Hall/CRC.
- Xie, Yihui, Christophe Dervieux, and Emily Riederer. 2020. *R Markdown Cookbook*. Chapman; Hall/CRC.