Building reproducible analytical pipelines with Python

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Table of contents

W	elcom	ie!	1	
	How	using a few ideas from software engineering can help data scientists, analysts and researchers		
		write reliable code	1	
Pr	eface		5	
1	Intro	oduction	9	
	1.1	Who is this book for?	9	
	1.2	What is the aim of this book?	10	
	1.3	Prerequisites	12	
	1.4	What actually is reproducibility?	13	
		1.4.1 Using open-source tools to build a RAP		
		is a hard requirement	14	
		1.4.2 There are hidden dependencies that can		
		hinder the reproducibility of a project	16	
		1.4.3 The requirements of a RAP	17	
	1.5	Are there different types of reproducibility?	19	
2	Sett	ing up a development environment	25	
	2.1	Why is installing Python such a hard problem? .	25	
	2.2	Creating a project-specific development environ-		
		ment	27	
	2.3	One last thing	33	
	2.4	A high-level description of how to set up a project	33	

Table of contents

3	Project start			
	3.1	The Polars package and why you should ditch		
		Pandas in its favour	35	
	3.2	Housing in Luxembourg	35	
	3.3	Saving trapped data from Excel		
	3.4	Analysing the data		
3.5 Your project is not done			52	
		3.5.1 How easy would it be for someone else to		
		rerun the analysis?	52	
		3.5.2 How easy would it be to update the project?	53	
		3.5.3 How easy would it be to reuse this code		
		for another project?	53	
		3.5.4 What guarantee do we have that the out-		
		put is stable through time?	54	
	3.6	Conclusion	55	
Re	ferer	nces	57	

Welcome!

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

This is the Python edition of the book "Building reproducible analytical pipelines", and it's a work-in-progress. If you're looking for the R version, visit this link.

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 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://b-rodrigues.github.io/raps_with_py/ and you'll be able buy a DRM-free Epub or PDF on Leanpub¹ once there's more content.

This is the *Python edition* of my book titled Building reproducible analytical pipelines with R². This means that a lot of text is copied over, but the all of the code and concepts are completely adapted to the Python programming language. This book is also shorter than the R version. Here's the topics that I will cover:

• Dependency management with pipenv;

¹https://leanpub.com/

 $^{^2}$ https://raps-with-r.dev

How using a few ideas from software engineering can help data scientists, a

- Some thoughts on functional programming with Python;
- Unit and assertive testing;
- Build automation with ploomber;
- Literate programming with Quarto;
- Reproducible environments with Docker;
- Continuous integration and delivery.

While this is not a book for beginners (you really should be familiar with Python before reading this), I will not assume that you have any knowledge of the tools discussed. 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 TO UPDATE

If you want to get to know me better, read my bio³.

You can submit issues, PRs and ask questions on the book's Github repository⁴.

³https://www.brodrigues.co/about/me/

 $^{^4} https://github.com/b-rodrigues/raps_with_py$

Preface

I don't like Python. Or rather, don't like using it to analyze data. I believe that certain design choices were made that make Python a subpar language for analyzing data. That being said, Python is currently the most popular general purpose programming language, and also the most popular language to analyze data, especially in machine learning and AI. As such, it is a good idea to at least know your way around it even if, like me, you prefer using the R programming language.

I state that I don't like Python because I want to make something very clear, right from the start. I am not an expert in Python. I know enough to get things done, but it is not a language that I know well. I consider myself an expert in R, but definitely not in Python. So why write a book on Python in that case? Well, in truth, this is not a book about Python.

This book is about building reproducible pipelines. And in order to build reproducible pipelines, you need to apply certain general ideas. This book will discuss these ideas, and illustrate them using the Python programming language. I wrote such a book already: you can read it here⁵. The book was well received: lots of people contacted me to thank me for having written it, I was invited to give talks several times on the book already, give some workshops and some people are already asking me for a second edition. I thought it would be an interesting challenge to write

 $^{^5 \}rm https://www.raps-with-r.dev$

a Python edition. It would be a good excuse to dive back into Python after having barely touched it since my Phd days, more than 10 years ago, where I used it alongside R for a project. It is also a good opportunity to see what is currently available in the Python programming language, and if it would be possible to reproduce the way I work with R.

There are currently some interesting packages available for Python that are quite close to some available for R. But R and Python have some very fundamental differences in their design that make using Python feel awkward if you're used to R, especially if take full advantage of R's functional programming features. But it's not just these design choices that differentiate both languages, there are also differences in culture, in how people use them. For example, notebooks are very popular in the Python world, but it's quite rare to see someone share R code through a notebook. In general, R users tend to write code as plain-text scripts or in Markdown using Rmarkdown or Quarto. Throughout this book, I will be writing Python with a heavy R accent, mainly for two reasons: first, because I'm fluent in R, but not in Python, as I've stated above. Second, because I also think that some of R's idioms actually make it more readable than equivalent Python code, and thus we can make Python more readable if we make it look more like R.

If the previous sentence didn't scare you into continuing and you are actually curious to see what I mean, then read on, you're in the perfect state of mind to approach this book!

Let me finish this section by talking a little bit about the history of these books (the original R edition and this one). It all started when a former colleague of mine contacted me in the summer of 2022 to ask me if I was interested in teaching a course for the Data Science Master degree at the University of Luxembourg. Long story short, I've decide to teach students how to set up

data science projects in a way that they're reproducible. I wrote my course notes into a freely available bookdown⁶ that I used for teaching. When I started compiling my notes, I discovered the concept of Reproducible Analytical Pipelines as developed by the Office for National Statistics⁷ (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 ebook⁸ in 2019 already. Another big source of inspiration is Software Carpentry⁹ 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. This was also the project where I've used Python.

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) to users of the Python programming language, even if I'm not one.

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

Enjoy!

⁶https://rap4mads.eu/

 $^{^{7}} https://analysis function.civils ervice.gov.uk/support/reproducible-analytical-pipelines/$

 $^{^8} https://ukgov datascience.github.io/rap_companion/$

⁹https://software-carpentry.org/

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

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 Python programming language. As I've stated in the preface, I'm not a Python expert, but I'm comfortable enough with the language. In any case, this is not a book about programming itself, and bar a short discussion on the merits of the Polars package, I won't be teaching you programming.

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 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 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 Python programming language. This book will assume that you have been using Python for some projects already, and want to improve not only your knowledge 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 plotnine 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 VS Code, 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 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 reexecute 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 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.



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

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

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);

 $^{^{1} \}rm https://github.com/numpy/numpy/issues/9187$

- 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 Python 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. 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 Python, this could be as simple as providing a requirements.txt file that lists the dependencies of the project, and which could be easily install using pip:

pip install -r requirements.txt

Doing this ensures that others, or future you, will be able to install the required packages to reproduce a study. However, this is not enough, and I will be talking about pipenv to do this kind of thing instead of pip. In the next chapter I'll explain why.

You should also ensure that people run the same analysis on the same version of Python that was used to program it. Just installing the right packages is not enough. The same code can produce different results on different versions of Python, or not even work at all. If you've been using Python for some time, you certainly remember the switch from Python 2 to Python 3... and who knows, the switch to Python 4 might be just as painful!

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 and explicitly deal with versions of the language itself.

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;
- 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".

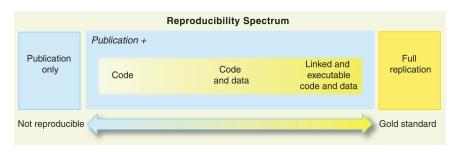


Figure 1.3: The reproducibility spectrum from Peng's 2011 paper.

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 (at least not without a compatibility layer). Which means that if you have a recent Apple Silicon Macbook and need to install old 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. 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 older Python and package 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 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!

2 Setting up a development environment

I have to start with on of the hardest chapters of the book, how to set up a development environment for Python.

If you are already using Python, you already have an environment set up and might be familiar with pyenv or other similar tools. I would still suggest you read this chapter and see if you agree with how I approach this issue. You may want to adapt your current workflow to it, or keep on doing what you've been doing up until now, it is up to. If you're completely new to Python, then you definitely need to read this chapter, but also, I need to remind you that this is not a book about Python per se. So I won't be teaching you any Python (I wouldn't really be competent to do so either) and you might want to complement reading this book with another that focuses on actually teaching Python. Remember, this book is about building reproducible analytical pipelines!

2.1 Why is installing Python such a hard problem?

If you google "how to install Python" you will find a surprising amount of articles explaining how to do it. I say "surprising amount" because one might expect to install Python like any other piece of software. If you're already familiar with R, you could think that installing Python would be done the same way: download the installer for your operating system, and then install it. And, actually, you can do just that for Python as well. So why are there 100s of articles online explaining how to install Python, and why aren't all of these articles simply telling you to download the installer to install Python? Why did I write this chapter on installing Python?

Well, there are several thing that we need to deal with if we want to install and use Python the "right way". First of all, Python is pre-installed on Linux distributions and older versions of macOS. So if you're using one of these operating systems, you could use the built-in Python interpreter, but this is not recommended. The reason being that these bundled versions are generally older, and that you don't control their upgrade process, as these get updated alongside the operating system. On Windows and newer versions of macOS, Python is, as far as I know, never bundled, so you'd need to install it anyways.

Another thing that you need to consider is that newer Python versions can introduce breaking changes, making code written for an earlier version of Python not run on a newer version of Python. This is not a Python-specific issue: it happens with any programming language. So this means that ideally you would want to bundle a Python version with your project's code.

The same holds true for individual packages: newer versions of packages might not even work with older releases of Python, so to avoid any issues, an analysis would get bundled with a Python release and Python packages. This bundle is what I call a development environment, and in order to build such development environment, specific tools have to be used. And there's a lot of these tools in the Python ecosystem... so much so that when

you're first starting, you might get lost. So here is he two tools that I use for this, and that I think work quite well: micromamba and pipenv.

The workflow is as follows:

- Install micromamba, a lightweight package manager
- Using micromamba, create an environment that contains a Python interpreter and pipenv
- Using this environment, install the required packages using pipenv
- pipenv will automatically generate two very useful files, Pipfile and Pipfile.lock

In the following sections I detail this process.

2.2 Creating a project-specific development environment

What we want is to have project-specific development environments that should include a specific Python version, specific versions of Python packages and all the code to actually run the project.

I'm going to assume that you don't have any Python version available on your computer and need to get one. Let's suppose that Python version 3.12.1 is the latest released version, and let's also suppose that you would like to use that version to start working on a project. To first get the right Python interpreter ready, you should install micromamba. Please refer to the micromamba documentation here¹ but on Linux, macOS and

 $^{^{1}} https://mamba.readthedocs.io/en/latest/installation/micromamba-installation.html\#automatic-install$

2 Setting up a development environment

Git Bash on Windows (there's also instructions for Powershell, if you don't have Git Bash installed on Windows), it should be as easy as:

```
"${SHELL}" <(curl -L micro.mamba.pm/install.sh)
```

for Poweshell use instead Invoke-Expression ((Invoke-WebRequest -Uri https://micro.mamba.pm/install.ps1).Content)

We can now use micromamba to create an environment that will contain a Python interpreter for our project and pipenv. Type the following command to create this environment:

```
micromamba create -n housing python=3.11.9 pipenv
```

This will create an environment named "pipenv_env" that includes pipenv and the version 3.11.9 of Python. If you're just starting a project, you can safely choose the very latest released version (check the releases pages on Python's website).

We can now use pipenv to install the packages for our project. But why don't we just the more common pip instead of pipenv, or even micromamba which can also install any other Python package that we require for our projects? Why introduce yet another tool? In my opinion, pipenv has one absolutely crucial feature for reproducibility: pipenv enables deterministic builds, which means that when using pipenv, we will always get exactly the same packages installed.

"But isn't that exctaly what using requirements.txt file does?" you wonder. You are not entirely wrong. After all, if you make the effort to specify the packages you need, and their versions, wouldn't running pip install -r requirements.txt also install exactly the same packages?

Well, not quite. Imagine for example that you need a package called hello and you put it into your requirements.txt like so:

hello==1.0.1

Suppose that hello depends on another package called ciao. If you run pip install -r requirements.txt today, you'll get hello at version 1.0.1 and ciao, say, at version 0.3.2. But if you run pip install -r requirements.txt in 6 months, you would still get hello at version 1.0.1 but you might get a newer version of ciao. This is because ciao itself is not specified in the requirements.txt, unless you made sure to add it (and then also add its dependencies, and their dependencies...). pipenv takes care of this for you by generating a so-called lock file automatically, and adds further security checks by comparing sha256 hashes from the lock file to the ones from the downloaded packages, making sure that you are actually installing what you believe you are.

What about using micromamba? micromamba could indeed be used to install the project's dependencies, but would required another tool called conda-lock to generate lock files, and in my experience, using conda-lock doesn't always work. I have 0 issues with pipenv on the other hand.

Now that pipenv is installed, let's start using it to install the packages we need for our project. Because the Python interpreter was installed using micromamba, we either need to activate the environment to get access to it, or we should use micromamba run to run the Python interpreter from this environment. First, create a folder called housing, which will contain our analysis scripts. Then, from that folder, run the following command:

```
micromamba run -n housing pipenv install

→ polars==1.1.0 plotnine beautifulsoup4 pandas

→ plotnine skimpy
```

(Little sidenote: in Chapter 2, we will be working together on a project using real data with polars instead of pandas. But for now, let's get pandas installed: I'll do a short comparison of the two, and then we'll keep on using polars for the remainder of the book.)

As you can see, I chose to install specific versions of polars. This is because I want you to follow along with the same versions as in the book. You could remove the ==x.y.z string from the command above to install the latest versions of polars available if you prefer, but then there would be no guarantee that you would find the same results as I do in the remainder of the book. You could also specify versions for the other packages if you wish.

You should see now two new files in the housing folder, Pipfile and Pipfile.lock. Start by opening Pipfile, it should look like this:

```
[[source]]
url = "https://pypi.org/simple"
verify_ssl = true
name = "pypi"

[packages]
polars = "==1.1.0"
plotnine = "*"
beautifulsoup4 = "*"
pandas = "*"
skimpy = "*"
```

[dev-packages]

```
[requires]
python version = "3.11"
```

I think that this file is pretty self-evident: the packages being used for this project are listed alongside their versions. The Python version is also listed. Sometimes, depending on how you set up the project, it could happen that the Python version listed is not the one you want for your project. In this case, I highly recommend you change the version to the right one. Also, you'll notice that here the Python version is "3.11", but we specified version "3.11.9" with micromamba when we created the environment. I would recommend that you add the missing ".9" for maximum reproducibility. If you edited the Pipfile then you need to run pipenv lock to regenerate the Pipfile.lock file as well:

micromamba run -n housing pipenv lock

this will make sure to also set the required/correct Python version in there.

If you open the Pipfile.lock in a text editor, you will see that it is a json file and that is also lists the dependencies of your project, but also the dependencies' dependencies. You will also notice several fields called hashes. These are there for security reasons: whenever someone, (or you in the future) will regenerate this environment, the packages will get downloaded and their hashes will get compared to the ones listed in the Pipfile.lock. If they don't match, then something very wrong is happening

2 Setting up a development environment

and packages won't get installed. These two files are very important, because they will make sure that it will be possible to regenerate the same environment on another machine.

To check whether everything installed correctly, drop into the development shell using:

```
\hbox{micromamba run $-r$ housing pipenv shell}
```

and check that the right version of Python is being used:

```
python --version
```

This should print Python 3.11.9 in the terminal. Start the Python interpreter and let's check polars's version:

```
python
```

Then check that the correct versions of the packages were installed:

```
import polars as pl
pl.__version__
```

```
'0.20.15'
```

You should see 1.1.0 as the listed version. Quite the shell, and then quite the environment with exit.

2.3 One last thing

Before continuing, it would be nice if we would automatically drop into the environment each time we are in the right folder; so for example, each time we navigate to the housing folder, the housing environment starts. We can achieve this by using a tool called direny.

- Install direnv
- Take note of the command when you run micromamba run
 -n housing pipenv shell in my case. /home/b-rodrigues/.log
- put that in a .envrc file in your folder
- direnv allow
- profit

2.4 A high-level description of how to set up a project

Ok, so to summarise, we install micromamba which will make it easy to install any version of Python that we require, and we also installed pipenv, which we use to install packages. The advantage of using pipenv is that we get deterministic builds, and pipenv works well with micromamba to build project-specific environments.

The way I would suggest you use these tools now, is that for each project, you install the latest available version of Python and then install packages by specyifing their versions, like so:

```
\begin{array}{ll} \texttt{micromamba} & \texttt{create} & \textbf{-n} \\ & \texttt{project\_name} \\ & \texttt{python=X.YY.Z} \\ & \texttt{pipenv} \end{array}
```

2 Setting up a development environment

then, use this environment in a fresh folder to install the packages you need:

```
micromamba run -n housing pipenv install
beautifulsoup4==4.12.2 pandas==2.1.4
plotnine==0.12.4 skimpy==0.0.11
```

(Replace the versions of Python and packages by the latest, or those you need.)

This will ensure that your project uses the correct software stack, and that collaborators or future you will be able to regenerate this environment by calling pipenv sync. pipenv sync differs from pipenv install because it will not touch the Pipfile.lock file, and will just download the packages as listed in the lock file. This is also the command that we will use later, in the chapter on CI/CD.

If you need to add packages to an environment, run: micromamba run -n housing pipenv install great_tables (or simply if pipenv install great_tables if you're already in the activated housing environment).

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 (well, not beyond what was done in the previous chapter to set up our development environment). We are going to download some data, and analyse it, that's it. But before all of that, I will present the Polars package. In the preface, I said that this wasn't supposed to be a book about Python, so why am I talking about a specific package? It's because I think that Polars, unlike Pandas, has some features and design choices that actually improve reproducibility.

3.1 The Polars package and why you should ditch Pandas in its favour

3.2 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 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.

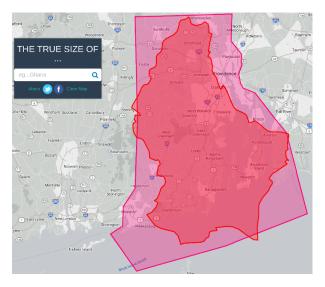


Figure 3.1: Luxembourg is about as big as the US State of Rhode Island.

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, 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 here¹.

 $^{^{1}\}rm https://is.gd/AET0ir$

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, 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

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

 $^{^3}$ https://archive.org/download/note-29/note-29.pdf

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. 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 \in). 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.

3.3 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:

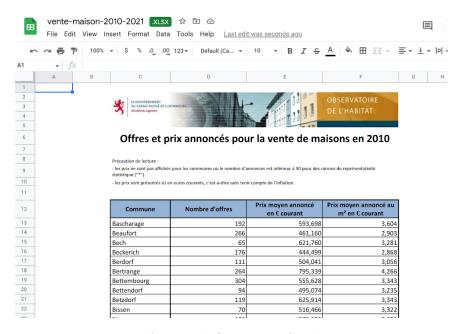


Figure 3.2: An Excel file meant for human eyes.

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

- 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 luxembourguish 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);
- \bullet 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.

⁴https://is.gd/1vvBAc

 $^{^5 \}rm https://data.public.lu/en/datasets/prix-annonces-des-logements-parcommune/$

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:

```
import polars as pl
import polars.selectors as cs
import re
```

I will be using the polars package to manipulate data.

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

```
~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"))
```

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
```

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)
```

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)
```

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

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

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

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 m² 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_prince_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:

```
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")
```

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 a list 6 .

An issue with scraping tables off the web is that they might change in the future. It is therefore a good idea to save the page by right clicking on it and then selecting save as, and then re-hosting it. I use Github pages to re-host the Wikipedia page above here⁷. I now have full control of this page, and won't

⁶https://w.wiki/6nPu

⁷https://is.gd/lux communes

get any bad surprises if someone decides to eventually update it. Instead of re-hosting it, you could simply save it as any other file of your project.

So let's scrape and save this list:

```
current_communes <- "https://is.gd/lux_communes" |>
  rvest::read_html() |>
  rvest::html_table() |>
  purrr::pluck(2) |>
  janitor::clean_names() |>
  dplyr::filter(name_2 != "Name") |>
  dplyr::rename(commune = name_2) |>
  dplyr::mutate(commune =
    stringr::str_remove(commune, " .$"))
```

We scrape the table from the re-hosted 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 second 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) and then I use the {dplyr} package for some further cleaning and renaming; the very last step removes a dagger symbol next to certain communes names, in other words it turns "Commune †" into "Commune".

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

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, and here again, I decide to re-host it on Github pages to avoid problems in the future:

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

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:

Let's run our test again:

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 here⁸ 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.

 $^{^8 \}rm https://is.gd/7 PhUjd$

3.4 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 here⁹. For 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 Area¹⁰) 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?

 $^{^9 \}mathrm{https://is.gd/qCJEbi}$

 $^{^{10} \}rm https://en.wikipedia.org/wiki/Schengen_Area$

3 Project start

• 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.

3.5 Your project is not done

3.5.1 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 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.

3.5.2 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 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.

3.5.3 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.

3.5.4 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.

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

References

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