Data analysis in R and Python

Programming and reproducible research

Ondrej Lexa Vojtěch Janoušek

Institute of Petrology and Structural Geology
Faculty of Science
Albertov 6

lexa@natur.cuni.cz

vojtech.janousek@natur.cuni.cz

2022

What this course is about

This practical course is aimed at undergraduate and postgraduate students. It is intended to:

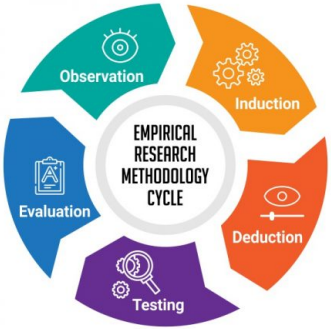
- explain fundamentals of data processing and visualization in geology as well as functioning of computing algorithms in general
- present basics of the R and Python programming languages
- illustrate the usability and versatility of both languages for everyday calculations, as well as for production of publication-quality graphics
- demonstrate examples of using both languages in reproducible research (with certain structural geology and whole-rock geochemistry bias).

An emphasis is on practical examples and exercises.

How to survive and perhaps even enjoy this course

I have been teaching this type of courses for several years now, and one reaction that I get quite often is **fear, panic, and even anger**. A common reaction is: Why do I have to learn all this? How can I do all this programming? And so on...

If you have such questions popping up in your mind, you have to stop and consider a few things before continuing with this course. Education and research at our department is strongly empirical (based on observed and measured phenomena and derives knowledge from actual experience). It is impossible to get through a master's degree without coming into contact with **data**. If you are at IPSG, you are automatically committed to an empirically driven education.



Fear, panic and anger...

In order to pass this course, you have to understand that you **have to read the lecture notes**, and that **it is not enough** to just passively read these lecture notes. You have to **play with the ideas** by asking yourself questions like "*what would happen if...*", and then check the answer right there using Python or R. That's the whole point of our approach to teaching data analysis, that you can verify what happens under repeated runs. There is no point in memorizing formulas; focus on developing understanding.

The ideas are not easy to understand, but simulation is a great way to develop a deeper understanding of the logic of theory.

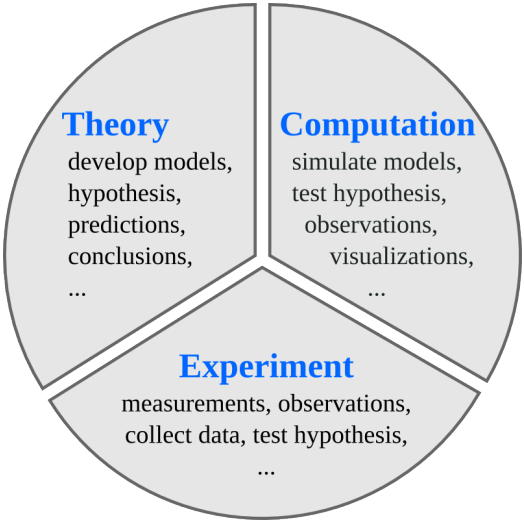
Outline

1. Reproducible Research
2. Big data
3. Why Python?
4. Python installation

The role of computing in science

Science has traditionally been divided into experimental and theoretical disciplines, but during the last several decades computing has emerged as a very important part of science.

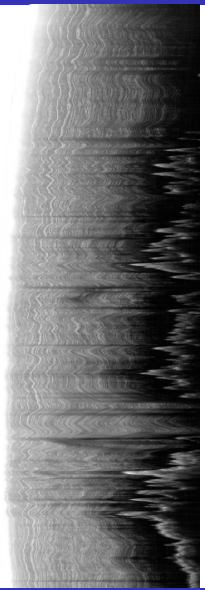
Scientific computing is often closely related to theory, but it also has many characteristics in common with experimental work. It is therefore often viewed as a new third branch of science.



Data Analysis in Earth Sciences

Earth scientists make observations and gather data about natural processes on Earth. They formulate and test hypotheses on the forces that have operated in a certain region to create its structure. They also make predictions about future changes of the planet. All these steps in exploring the system Earth include the acquisition and **analysis of numerical data**.

An earth scientist needs a solid knowledge in statistical and numerical methods to analyze these data, as well as the ability to use **suitable software packages** on a computer.

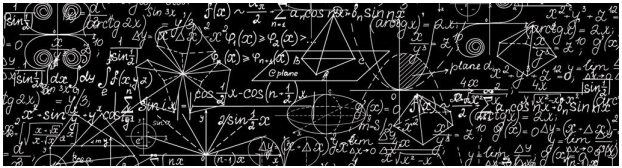


Access to results and methods

In experimental and theoretical sciences there are well established codes of conducts for how **results and methods are published and made available** to other scientists.

In theoretical sciences, derivations, proofs and other results are published in full detail, or made available upon request. Likewise, in experimental sciences, the methods used and the results are published, and all experimental data should be available upon request.

It is considered unscientific to withhold crucial details in a theoretical proof or experimental method, that would hinder other scientists from **replicating and reproducing** the results.

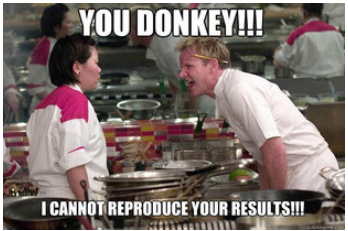


Computational sciences

In computational sciences there are not yet any well established guidelines for how source code and generated data should be handled. For example, it is relatively rare that source code used in simulations for published papers are provided to readers, in contrast to the open nature of experimental and theoretical work.

And it is not uncommon that source code for simulation software is withheld and considered a competitive advantage (or unnecessary to publish).

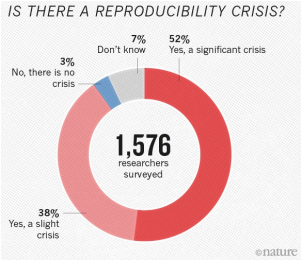
"**Replication is something scientists should be thinking about before they write the paper,**" says Ritu Dhand, the editorial director at Nature.



Reproducibility crisis

A 2016 poll of 1,500 scientists conducted by Nature reported that 70% of researchers have tried and failed to reproduce another scientist's experiments, and more than half have failed to reproduce their own experiments.

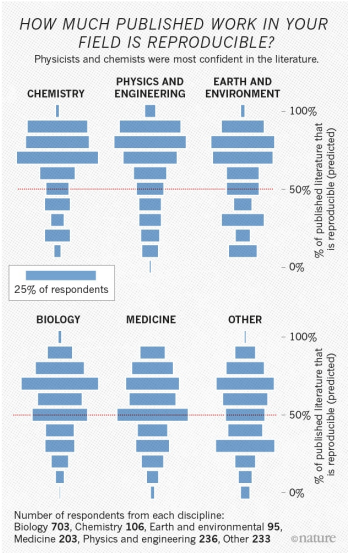
The data reveal sometimes-contradictory attitudes towards reproducibility. Although 52% of those surveyed agree that there is a *significant crisis* of reproducibility, less than 31% think that failure to reproduce published results means that the result is probably wrong, and most say that they still trust the published literature.



Reproducible Research I.

However, this issue has recently started to attract increasing attention, and a number of editorials in high-profile journals have called for **increased openness in computational sciences**. Some prestigious journals, including Science, have even started to demand of authors to **provide the source code** for simulation software used in publications to readers upon request.

Discussions are also ongoing on how to facilitate distribution of scientific software, for example as supplementary materials to scientific papers.



Reproducible Research II.

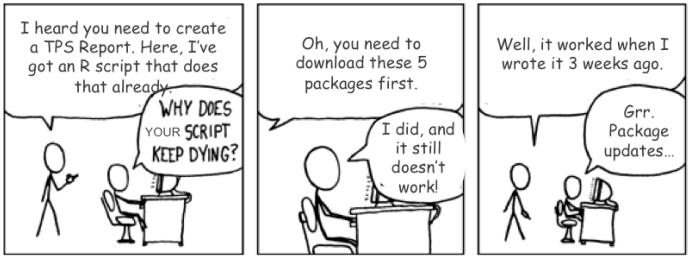
What makes science reliable? The ability to reproduce the results of an experiment, known as reproducibility, is one of the hallmarks of a valid scientific finding. But science is facing what many consider a reproducibility crisis, and the stakes are high. Many scientific claims cannot be replicated, and many clinical trials fail as a result.

Check this 15-minute video ▸ YouTube examining the reproducibility crisis and reports on the outcome of five experiments designed to test the reproducibility of cancer biology studies.

Reproducible Research II.

A minimal standard for data analysis and other scientific computations is that they be **reproducible**: that the code and data are assembled in a way so that another group can re-create all of the results (e.g., the figures in a paper).

Our goal is that the students leave the course ready and willing to ensure that all aspects of their computational research (software, data analyses, papers, presentations, posters) are reproducible.



Benefits of Open Reproducible Science

Benefits of openness and reproducibility in science include:

- Transparency in the scientific process, as anyone including the general public can access the data, methods, and results.
- Ease of replication and extension of your work by others, which further supports peer review and collaborative learning in the scientific community.
- It supports you! You can easily understand and re-run your own analyses as often as needed and after time has passed.

How do you make your work reproducible?

The list below are things that you can begin to do to make your work more open and reproducible. It can be overwhelming to think about doing everything at once. However, each item is something that you could work towards.

- Use scientific programming to process data
- Use expressive names for files and directories to organize your work
- Follow FAIR principles to enhance the reproducibility of projects
- Protect your raw data
- Use version control and share your code (if you can)
- Document your workflows
- Design workflows that can be easily recreated

Use scientific programming to process data

Scientific programming allows you to automate tasks, which facilitates your workflows to be quickly run and replicated.

In contrast, graphical user interface (GUI) based workflows require interactive manual steps for processing, which become more difficult and time consuming to reproduce.

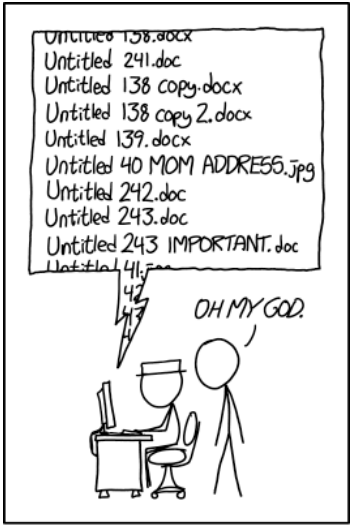
If you use an open source programming language like **Python or R**, then anyone has access to your methods.

However, if you use a tool that requires a license, then people without the resources to purchase that tool are excluded from fully reproducing your workflow.

Use expressive names for files and directories

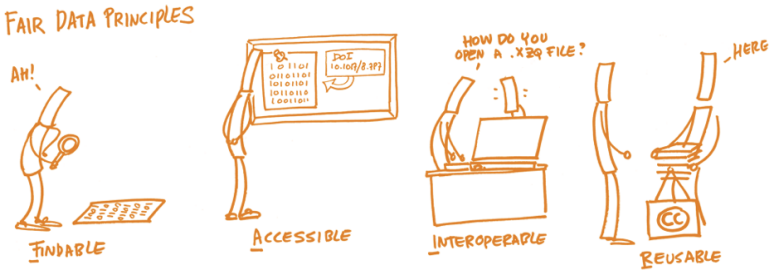
Expressive file and directory names allow you to quickly find what you need and also support reproducibility by facilitating others' understanding of your files and workflows (e.g. names can tell others what the file or directory contains and its purpose).

Be sure to organize related files into directories (i.e. folders) that can help you easily categorize and find what you need (e.g. raw-data, scripts, results).



Use FAIR data to enhance the reproducibility of projects

Make sure that the data used in your project adhere to the FAIR principles (*Wilkinson et al. 2016*), so that they are **Findable, Accessible, Interoperable, and Re-usable**, and there is documentation on how to access them and what they contain. FAIR principles also extend beyond the raw data to apply to the tools and workflows that are used to process and create new data. FAIR principles enhance the reproducibility of projects by supporting the reuse and expansion of your data and workflows, which contributes to greater discovery within the scientific community.

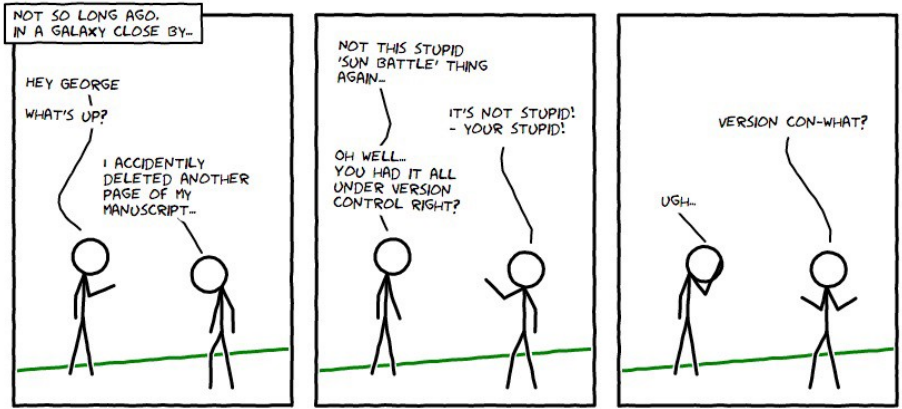


Protect your raw data

Don't modify (or overwrite) the raw data. Keep data outputs separate from inputs, so that you can easily re-run your workflow as needed. This is easily done if you organize your data into directories that separate the raw data from your results, etc.

Use version control and share your code (if you can)

Version control allows you to manage and track changes to your files (and even undo them!). If you can openly share your code, implement version control and then publish your code and workflows on the cloud. There are many free tools to do this including **Git** and **GitHub**.



Document your workflows

Documentation can mean many different things. It can be as basic as including (carefully crafted and to the point) comments throughout your code to explain the specific steps of your workflow. Documentation can also mean using tools such as Jupyter Notebooks to include a text narrative that is interspersed with code to provide high level explanation of a workflow. Documentation can also include docstrings, which provide standardized documentation of Python functions, or even README files that describe the bigger picture of your workflow, directory structure, data, processing, and outputs.

Design workflows that can be easily recreated

You can design workflows that can be easily recreated and reproduced by others by:

- listing all packages and dependencies required to run a workflow at the top of the code file (e.g. Jupyter Notebook).
- organizing your code into sections, or code blocks, of related code and include comments to explain the code.
- creating reusuable environments for Python workflows using tools like docker containers, conda environments, and interactive notebooks with binder.

Reproducible Research III.

In this course we will introduces the **Jupyter** project in the context of programming in both **Python and R** for reproducible research and knowledge transfer. After this course a students will have insights into why and how one would use Jupyter notebooks for research, training and/or instruction.

Jupyter notebooks

- have "live" code, which is interactive/modifiable
- allow for easy collaboration on a notebook system
- serve as a scratchpad for both code and notes

Outline

1. Reproducible Research
2. Big data
3. Why Python?
4. Python installation

Big Data Analysis in Earth Sciences

The term **Big Data** refers to various forms of large amount of data, which requires specific computing platforms for their analysis. The challenges include:

- capturing
- storage
- searching
- **analysis**
- **visualization**

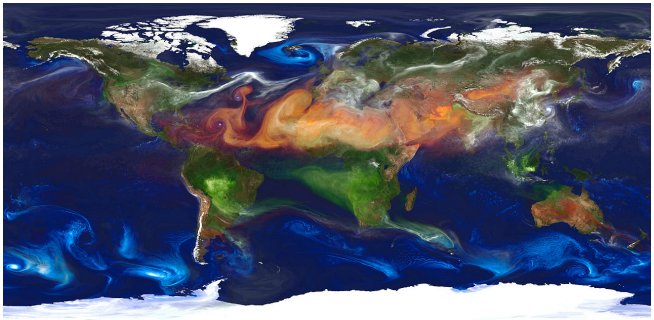
Why Learn To Code?

Earth Scientists Deal with Large Datasets

- Processing and Visualization should be automated

Can make your own tools

- Research is new, so no tools may exist



What Language Should I Learn?

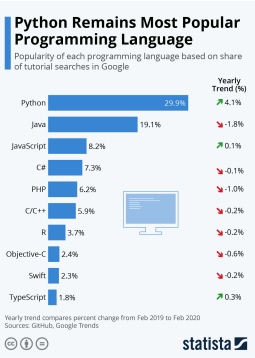
It doesn't really matter

- Once you know one language, you can learn new ones
- Most languages are more similar than different

Commonly used programming languages in Earth sciences

- MATLAB / Octave
- Python
- R
- C / C++
- Fortran
- Java
- Perl
- Mathematica / Maple

All have strengths and weaknesses



Progamming popularity evolution

PYPL - PopularitY of Programming Language Index Link is created by analyzing how often language tutorials are searched on Google.

The more a language tutorial is searched, the more popular the language is assumed to be. It is a leading indicator. The raw data comes from Google Trends.

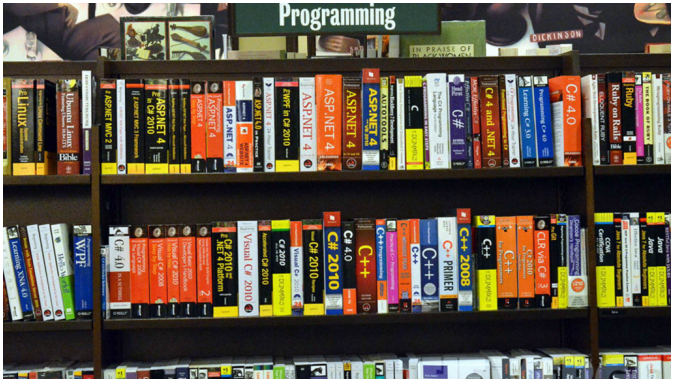
Check this video YouTube to see how top 10 most popular programming languages evolved during 1965 - 2019

Outline

1. Reproducible Research
2. Big data
3. Why Python?
4. Python installation

Why Python?

So, why all the fuss about Python? Perhaps you have heard about Python from a friends, heard a reference to this programming language at a conference, or followed a link from a page on scientific computing, but wonder **what extra benefits** the Python language provides given the suite of powerful computational tools the Earth sciences already has.



Python is beautiful

The chief reason is that it's just a **beautiful** programming language. And it's **versatile**. And it has an **extensive standard library**. And a sheer unimaginably humongous number of third-party libraries and extensions.

The Python Package Index PyPI is a repository of software for the Python programming language. There are currently **403,210** packages available.

Python is modern

Python is a modern, general-purpose, object-oriented, high-level programming language. It is the programming language of choice for many scientists to a large degree because it offers a great deal of power to analyze and model scientific data with relatively little overhead in terms of learning, installation or development time. Though it has been around for two decades, it exploded into use in the earth sciences after the development community converged upon the **standard scientific packages** needed for earth sciences work.

Python is easy

Python is a robust integration platform for all kinds of earth sciences work, from data analysis to distributed computing, and graphical user interfaces to geographical information systems.

Clean, simple and expressive

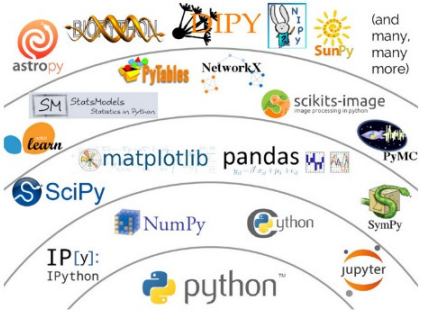
- Easy-to-read minimalistic syntax and intuitive code
- Fewer lines of code, fewer bugs, easier to maintain

It is a language you can pick up in a weekend, and use for the rest of one's life.

Python is open

Finally, **Python's open-source pedigree**, aided by a large user and developer base in sciences, means that your programs can take advantage of the **tens of thousands of Python packages** that exist. These include visualization, numerical libraries, Web services, mobile and desktop graphical user interface programming, and others.

You are not limited to only what one vendor can provide or even what only the scientific community can provide!



Outline

1 Reproducible Research

2 Big data

3 Why Python?

4 Python installation

Miniconda/Anaconda Python

Configuration of Python for scientific computing has historically been a huge pain, but recently has gotten a whole lot easier with the advent of Miniconda and other similar package managers like Miniforge or Mamba:

- it stays in a separate folder
- doesn't touch the system Python
- doesn't require administrator access to install or modify packages
- it uses a package manager called **conda** that is extremely easy to use
- Comes either in full-meal-deal version (anaconda), with numpy, scipy, PyQt, spyder IDE, etc. or in minimal version (miniconda) where you can install what you want, when you need it.

We suggest to install the Miniforge installer Link, that includes conda with conda-forge set as the default (and only) channel. We will use the conda install command to install needed packages in separate environment.

Follow instructions posted in Google Classroom to install software...