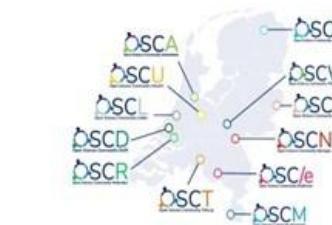


Organizing your data and software with a reproducible project workflow

DCC Spring Training Days 2023
June 22 2023

2023 DCC Spring Training Days

Stephanie van de Sandt, VU
Meron Vermaas, VU
Renate Mattiszik, Saxion UAS



UNIVERSITEIT VAN AMSTERDAM

What sport would you compete in if you were in the Olympics?



https://commons.wikimedia.org/wiki/File:Muggle_Quidditch_Game_in_Vancouver.jpg



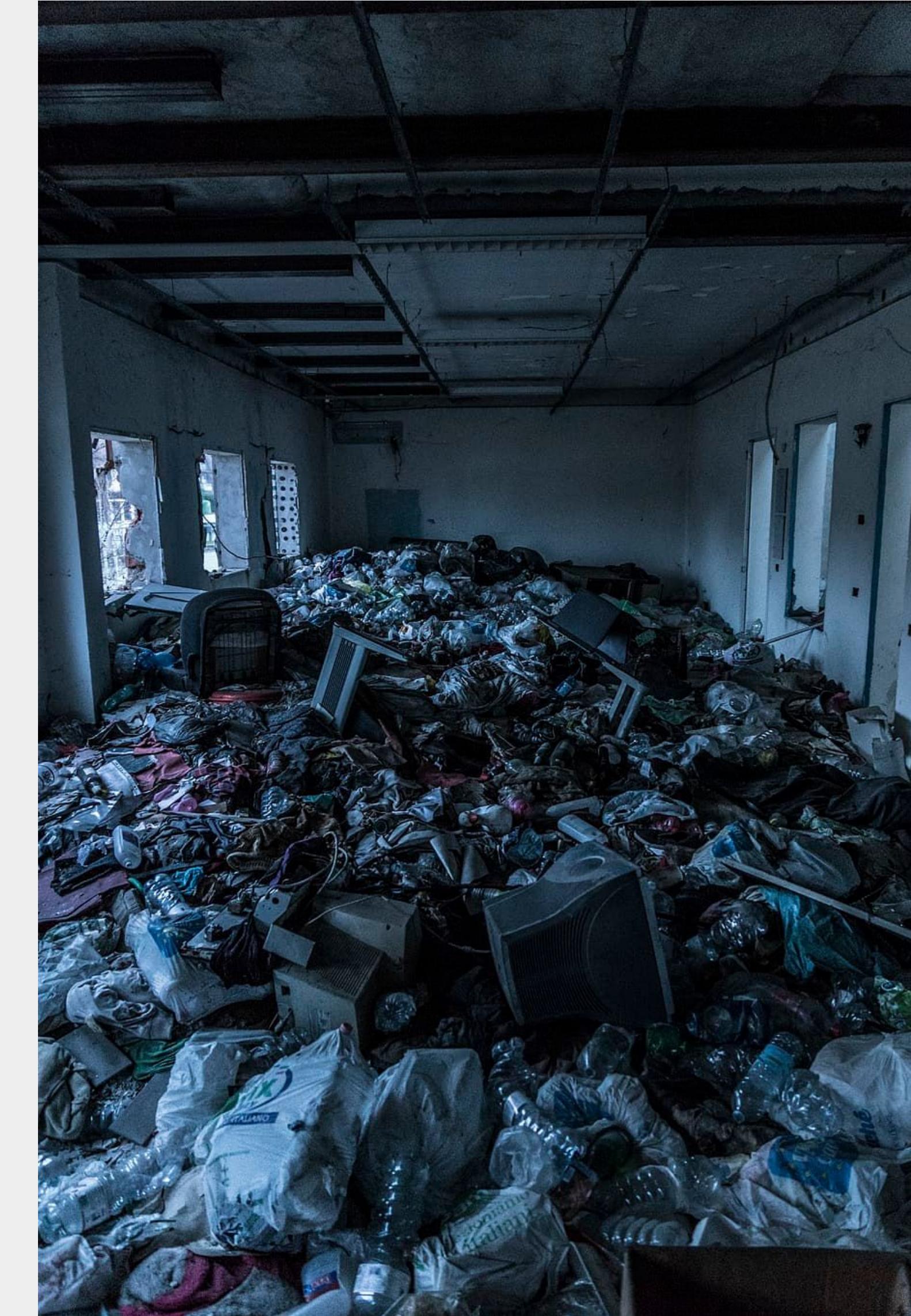
Pexels: Ron Lach

Pexels

What does your living room look like?



Forgemind ArchiMedia / CC BY 2.0 / Flickr



<https://www.wallpaperflare.com/garbage-inside-a-room-abandoned-abandoned-building-decay-dirty-wallpaper-arqkg>

How is your Desktop organized?



Ron Lach: Photo of an Untidy and Messy White Wooden Closet.
Pexels



Anastasia Shuraeva: A White Wooden Closet of a Woman.
Pexels

Planning our Workshop

How we will run the workshop today with you

PRESENT

Organizing and structuring a project

1. Save your project in a single folder.



my_project

- **description**
- **data**
- **tools**
- **manuscript**



Scriberia

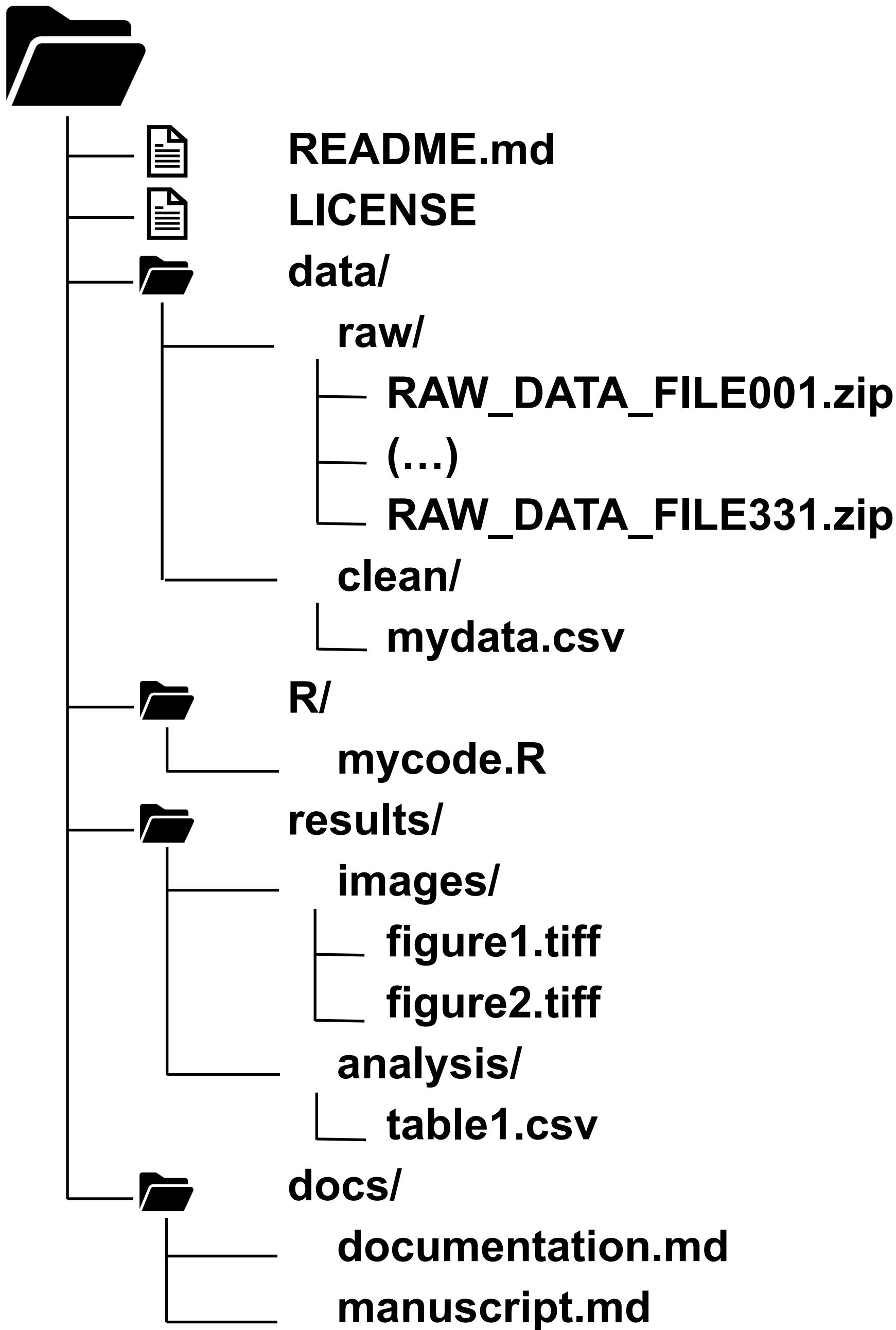
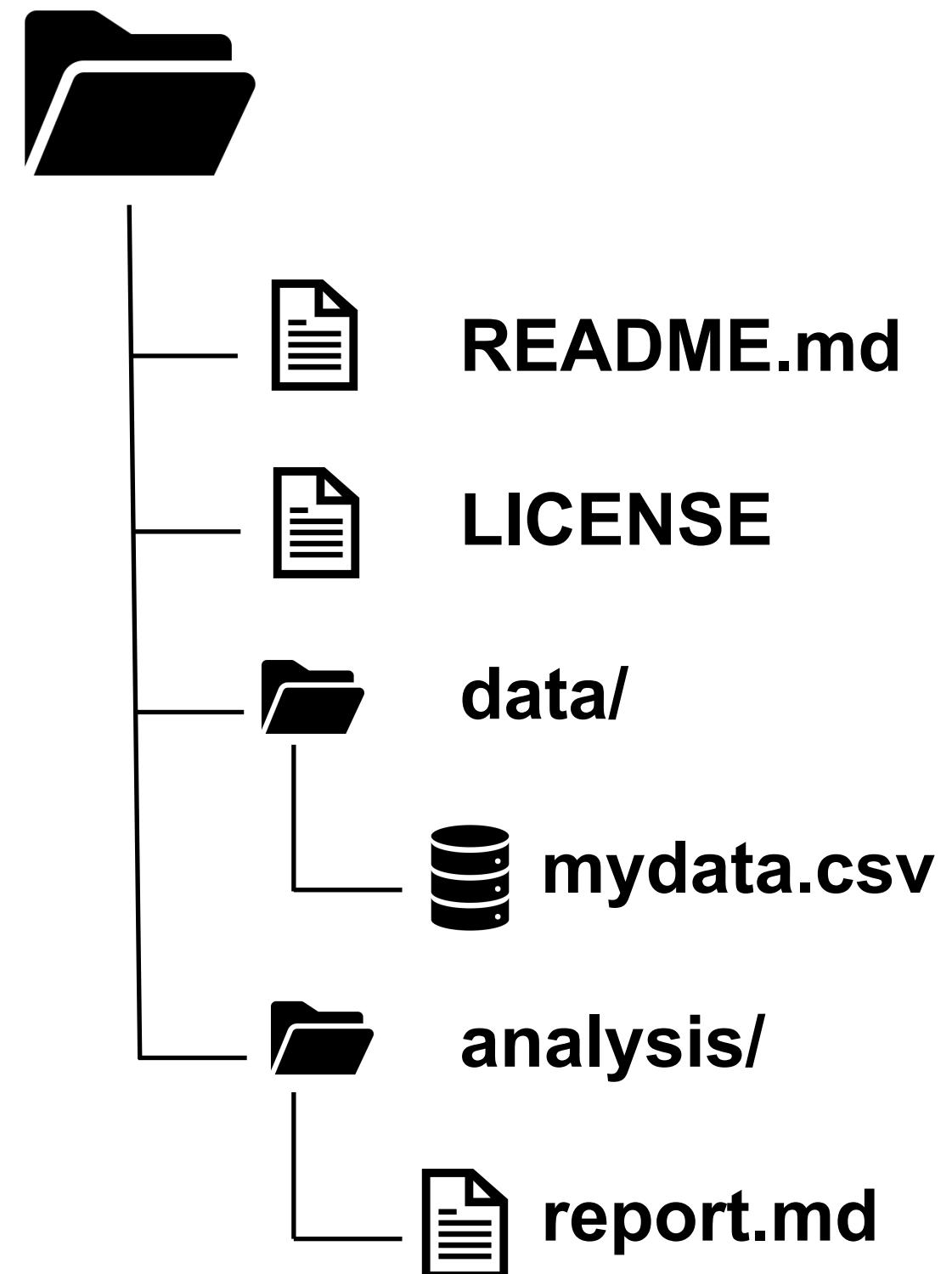
KÖMPENDIUM

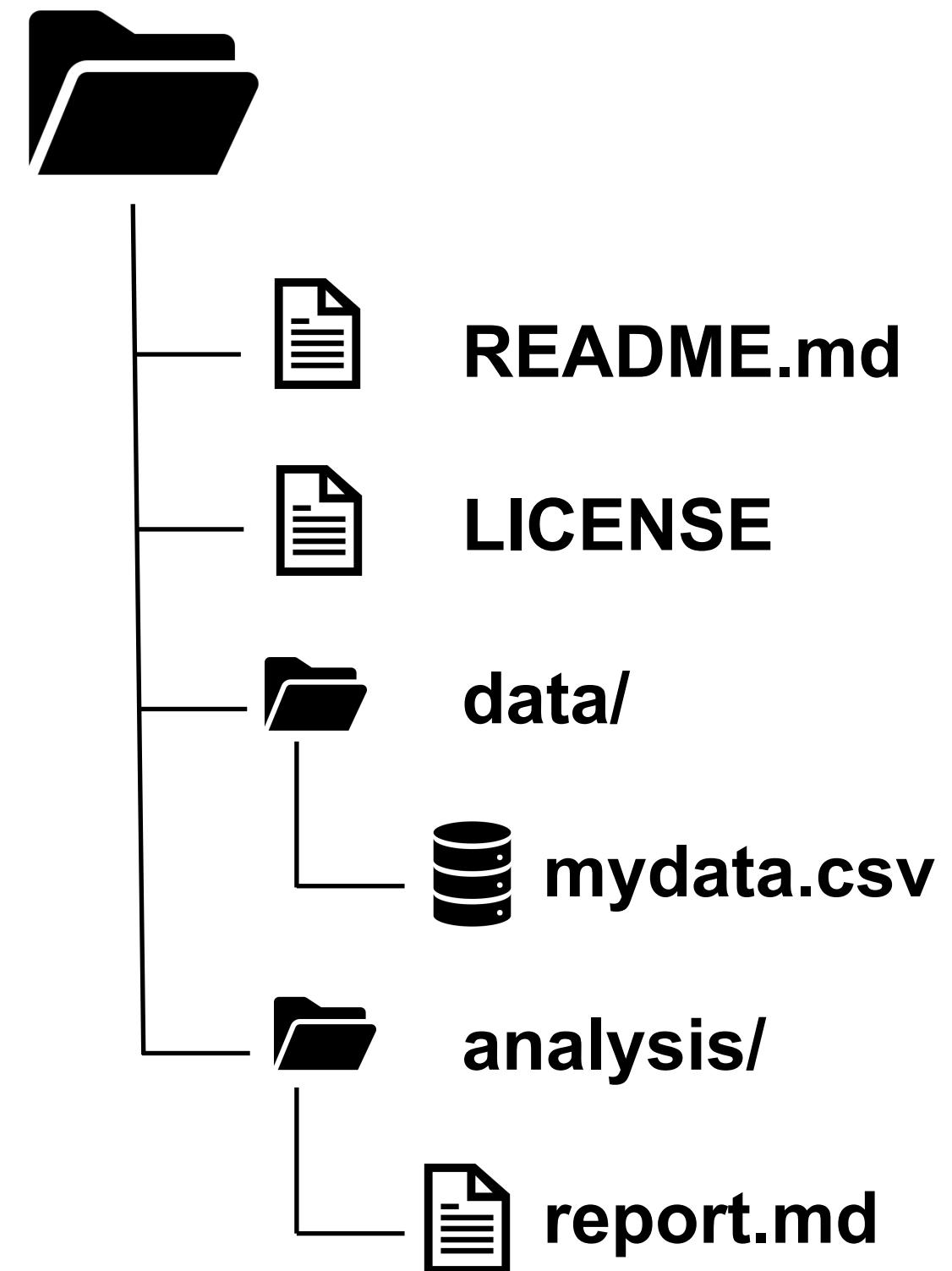
- 1.
- 2.
- 3.
- 4.
- 5.

Credit: Scriberia for The Turing Way

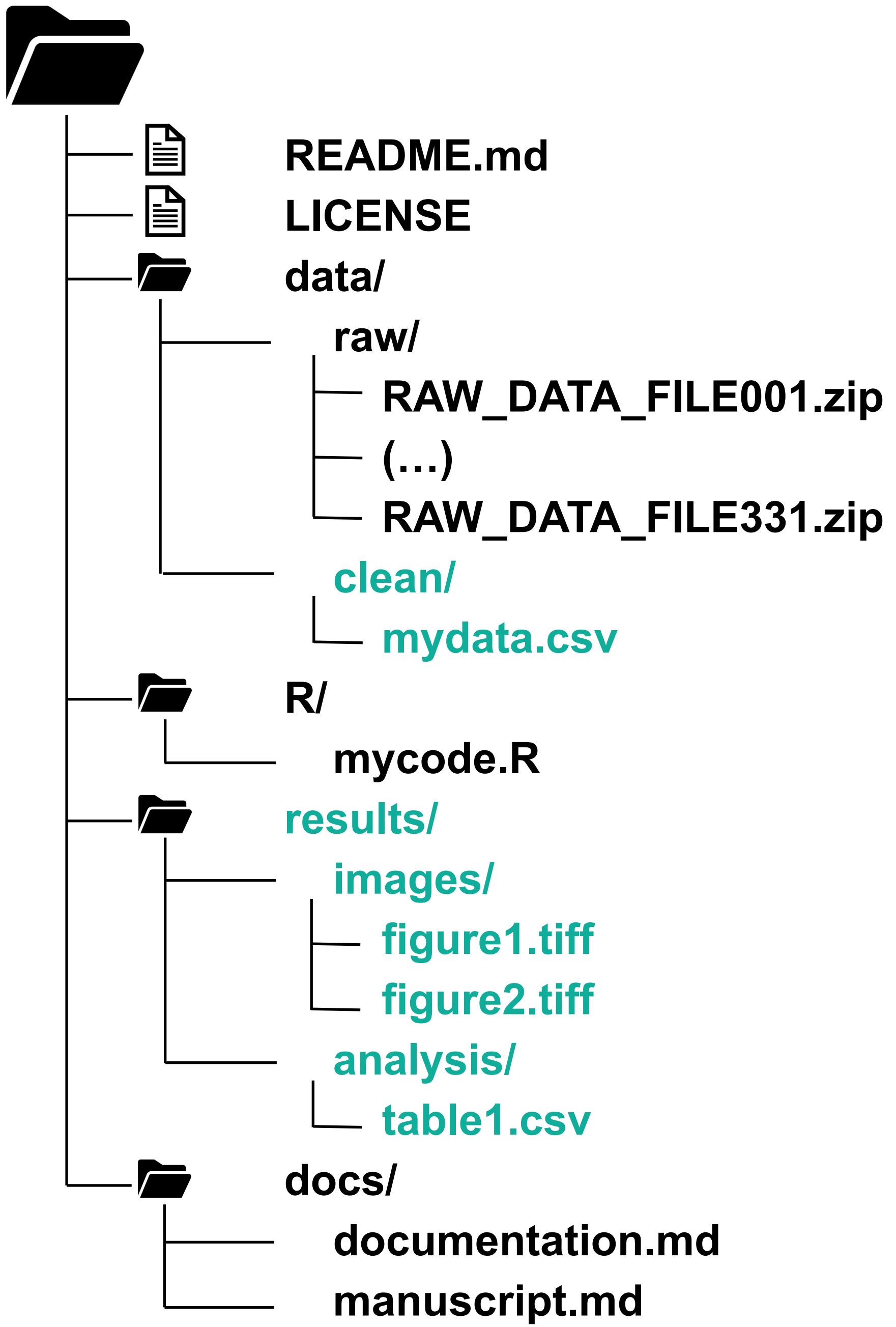
Credit: Karthik Ram

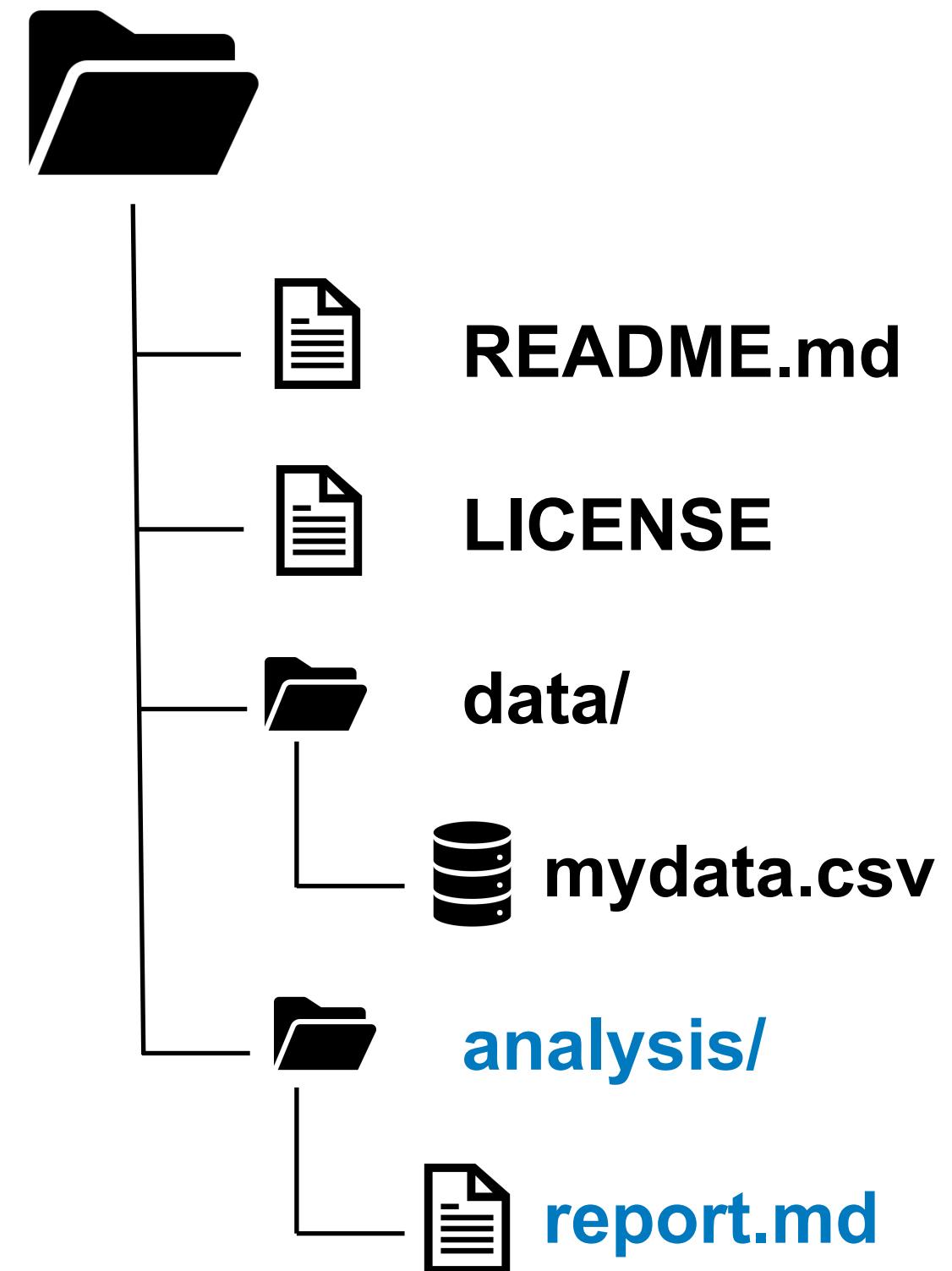
2. Devise a logical system of sub-folders.



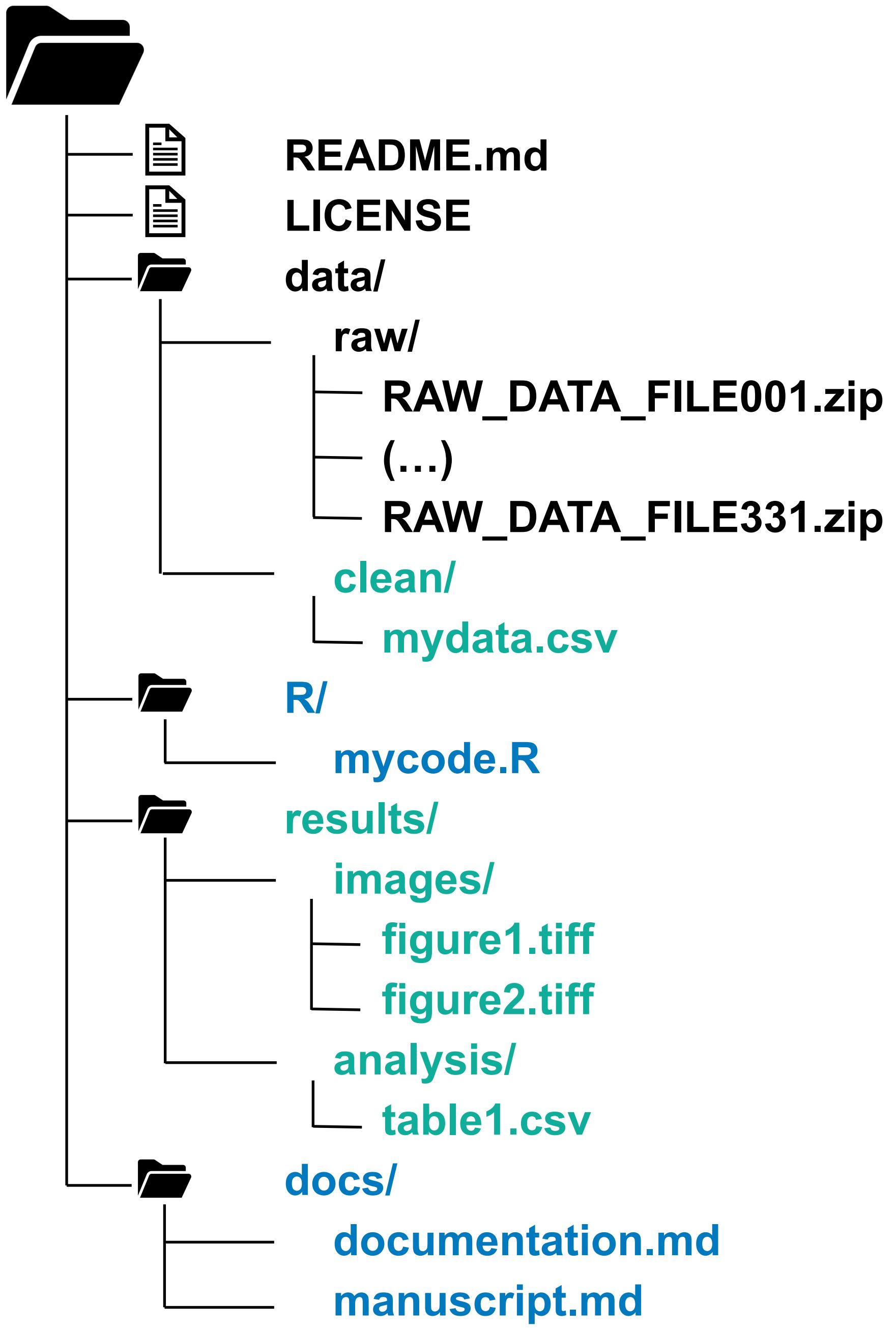


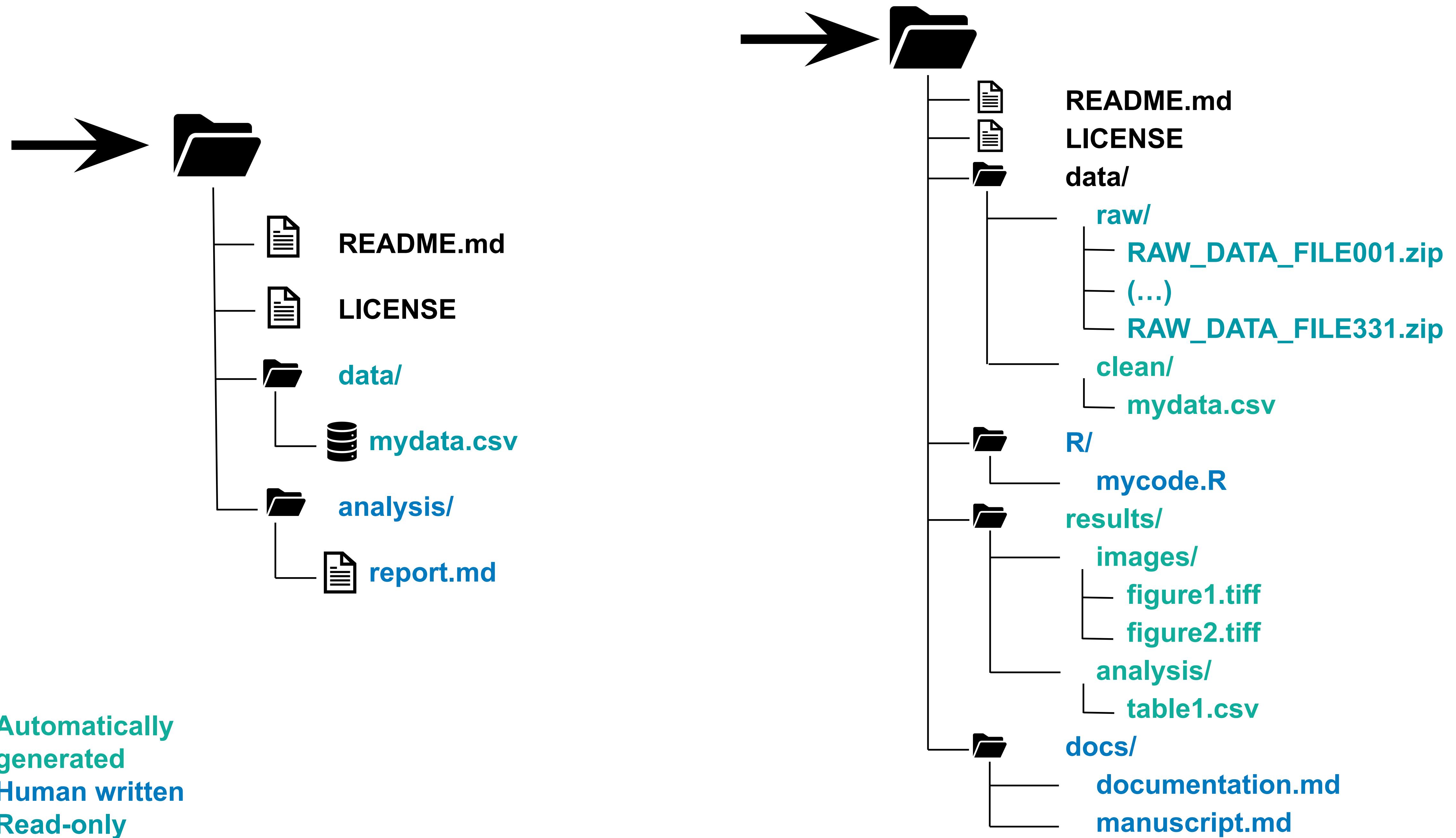
Automatically
generated
Human written
Read-only





Automatically
generated
Human written
Read-only







(CC0
)

3. Introduce the project (or sub-folder) in a README.

- **What** is the project about?
- **Who** are involved?
- **How** was the data collected?
- **When & where** is the research conducted?

Other inspiration...

- Abbreviations
- Folder structure
- File explanations
- References & links

4. Use interoperable file types.

	A	B	C
1	Letter	Number	
2	A	124	
3	B	125	
4	C	126	
5	A	127	
6	B	128	
7	C	129	
8	A	130	
9	B	131	
10	C	132	
11	A	133	

Bestandsnaam:

Opslaan als:

dataset.csv — Edited

Letter;Number
A;124
B;125
C;126
A;127
B;128
C;129
A;130
B;131
C;132
A;133
D;124
E;4005

5. Use descriptive and logical file names.

File names should be

- Machine readable
- Human readable
- Logically sortable

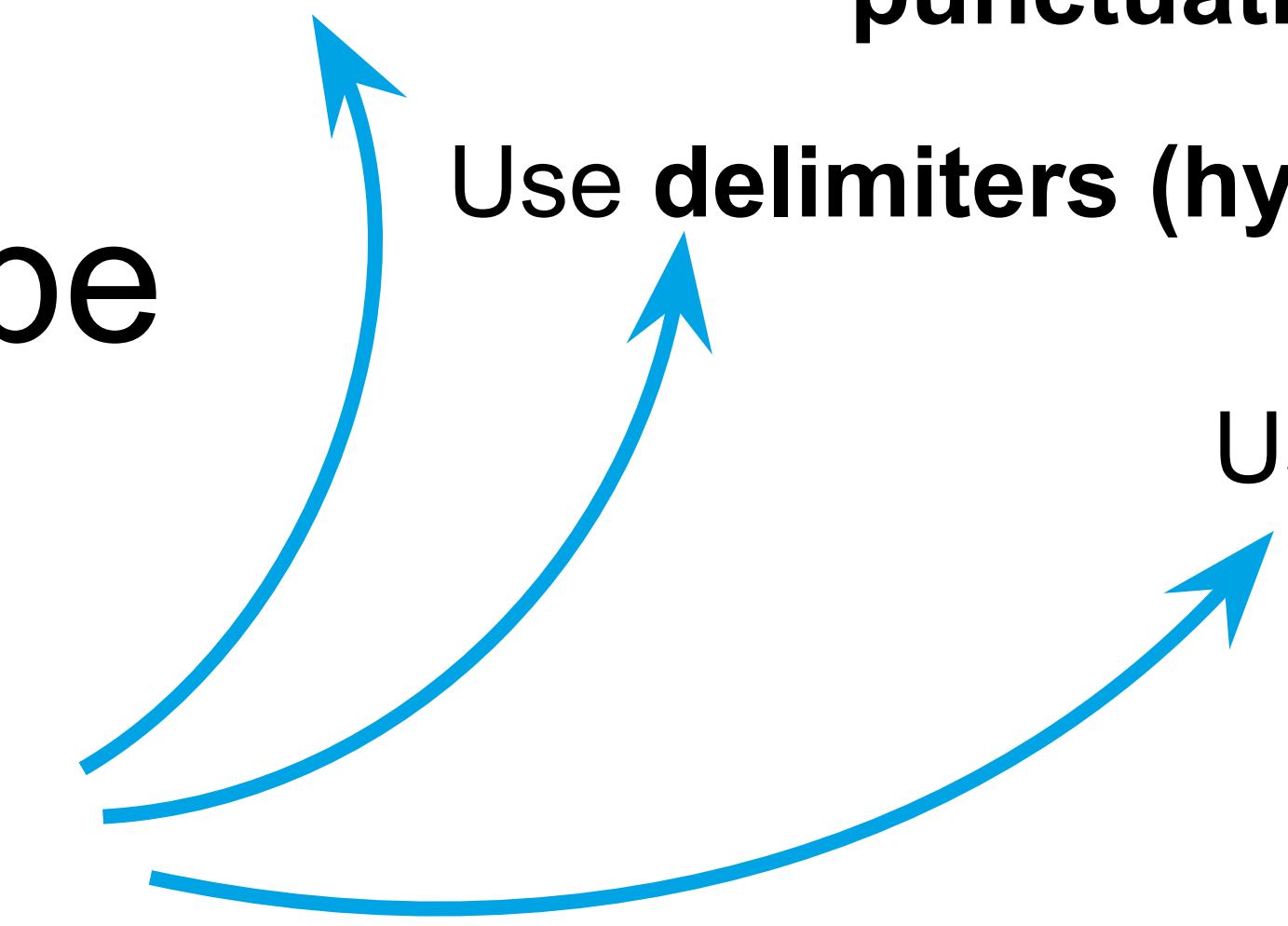
File names should be

- Machine readable
- Human readable
- Logically sortable

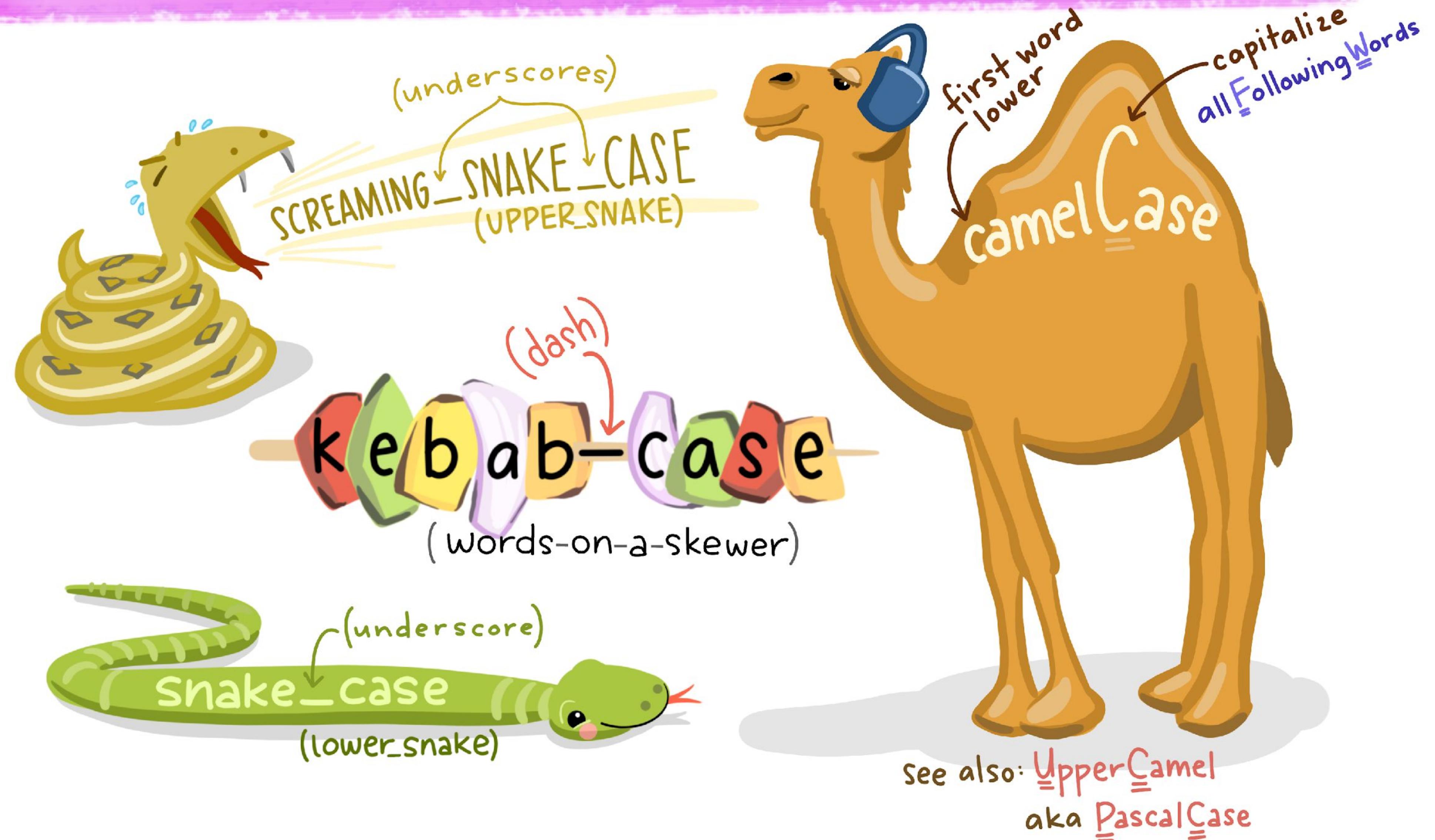
Avoid spaces, accents, odd punctuation...

Use delimiters (hyphens, underscores) for easy separation of elements

Use informative elements so that files can be easily found



in that case...



Which set of file(name)s do you want at
3 AM before a deadline?

File names should be

- Machine readable
- Human readable
- Logically sortable

Use informative elements

01_marshal-data.md	01.md
01_marshal-data.r	01.r
02_pre-dea-filtering.md	02.md
02_pre-dea-filtering.r	02.r
03_dea-with-limma-voom.md	03.md
03_dea-with-limma-voom.r	03.r
04_explore-dea-results.md	04.md
04_explore-dea-results.r	04.r
90_limma-model-term-name-fiasco.md	90.md
90_limma-model-term-name-fiasco.r	90.r
Makefile	Makefile
figure	figure
helper01_load-counts.r	helper01.r
helper02_load-exp-des.r	helper02.r
helper03_load-focus-statinf.r	helper03.r
helper04_extract-and-tidy.r	helper04.r
tmp.txt	tmp.txt

File names should be

- Machine readable
- Human readable
- Logically sortable

Name
LEICA_Dmelanogaster_dpp-RNAi_20200822_03.zip
LEICA_Dmelanogaster_dpp-RNAi_20200822_02.zip
LEICA_Dmelanogaster_dpp-RNAi_20200822_01.zip
LEICA_Dmelanogaster_dpp-RNAi_20200815_04.zip
LEICA_Dmelanogaster_dpp-RNAi_20200815_03.zip
LEICA_Dmelanogaster_dpp-RNAi_20200815_02.zip
LEICA_Dmelanogaster_dpp-RNAi_20200815_01.zip
LEICA_Dmelanogaster_ctrl_20200823_02.zip
LEICA_Dmelanogaster_ctrl_20200823_01.zip
LEICA_Dmelanogaster_ctrl_20200815_03.zip
LEICA_Dmelanogaster_ctrl_20200815_02.zip
LEICA_Dmelanogaster_ctrl_20200815_01.zip

6. Make your data tidy.

TIDY DATA

is a standard way of mapping the meaning of a dataset to its structure. ’’

—HADLEY WICKHAM

In tidy data:

- each variable forms a column
- each observation forms a row
- each cell is a single measurement

each column a variable

each row an observation

id	name	color
1	floof	gray
2	max	black
3	cat	orange
4	donut	gray
5	merlin	black
6	panda	calico

Wickham, H. (2014). Tidy Data. Journal of Statistical Software 59 (10). DOI: 10.18637/jss.v059.i10

An example of untidy data: plant measurements

Plant_no	Treatment	Stem length	Leaf width	Stem length	Leaf width	Stem length	Leaf width
		day 1	day 1	day 2	day 2	day 3	day 3
A1_14	control	120	21	122	23	124	25
A1_18	control	132	23	135	25	138	27
A1_21	control	131	18	133	20	135	21
A2_09	UV	109	29	114	31	115	31
A3_02	UV	125	25	127	27	129	28
A3_10	UV	130	12	133	14	136	16

An example of untidy data: plant measurements

Values in column
names

Plant_no	Treatment	Stem length	Leaf width	Stem length	Leaf width	Stem length	Leaf width
		day 1	day 1	day 2	day 2	day 3	day 3
A1_14	control	120	21	122	23	124	25
A1_18	control	132	23	135	25	138	27
A1_21	control	131	18	133	20	135	21
A2_09	UV	109	29	114	31	115	31
A3_02	UV	125	25	127	27	129	28
A3_10	UV	130	12	133	14	136	16

An example of untidy data: plant measurements

Multiple observations in a single row

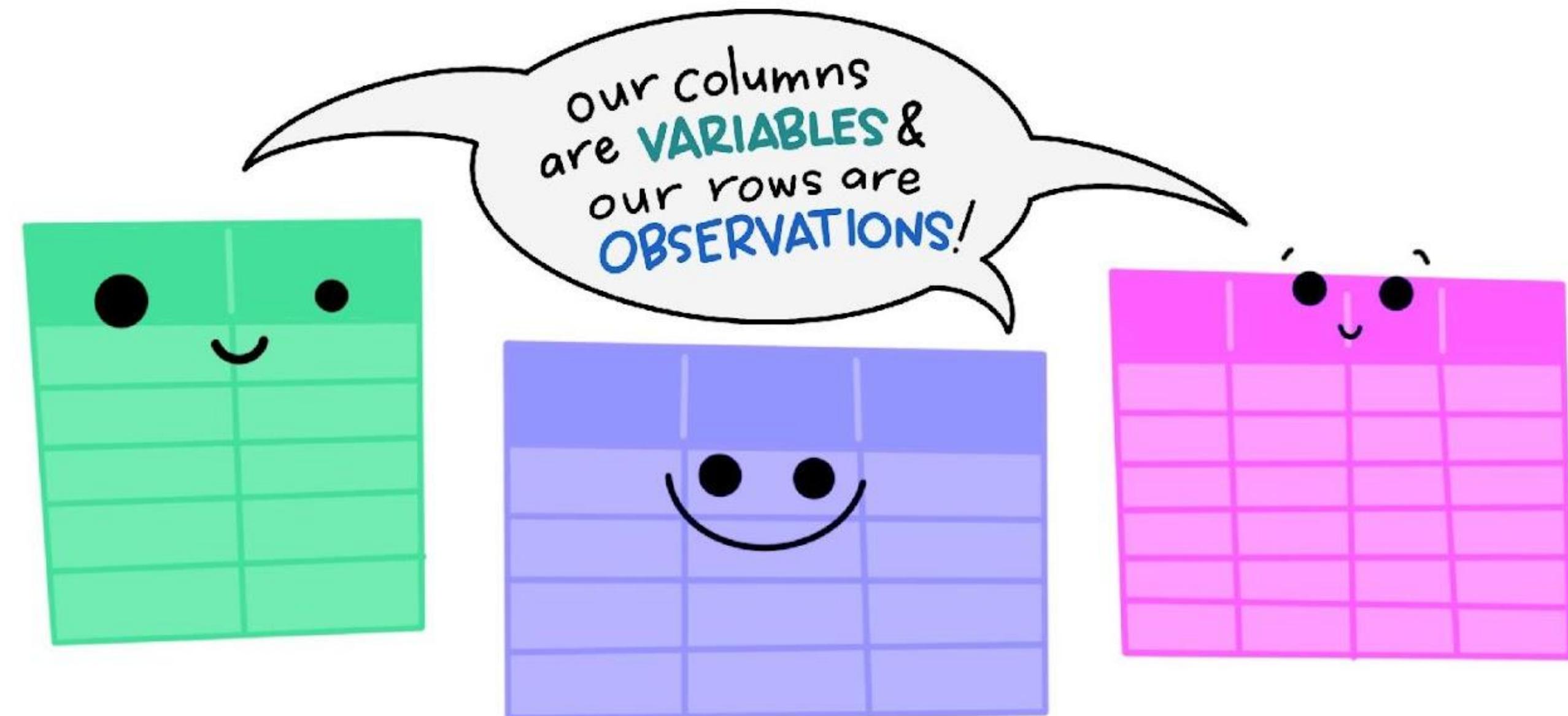
Plant_no	Treatment	Stem length	Leaf width	Stem length	Leaf width	Stem length	Leaf width
		day 1	day 1	day 2	day 2	day 3	day 3
A1_14	control	120	21	122	23	124	25
A1_18	control	132	23	135	25	138	27
A1_21	control	131	18	133	20	135	21
A2_09	UV	109	29	114	31	115	31
A3_02	UV	125	25	127	27	129	28
A3_10	UV	130	12	133	14	136	16

Same data, now in a tidy format

Plant_no	Treatment	Element	Day	Measurement
A1_14	control	Stem length	1	120
A1_14	control	Leaf width	1	21
A1_14	control	Stem length	2	122
A1_14	control	Leaf width	2	23
A1_14	control	Stem length	3	124
A1_14	control	Leaf width	3	25
A1_18	control	Stem length	1	132
A1_18	control	Leaf width	1	23
A1_18	control	Stem length	2	135
A1_18	control	Leaf width	2	25
A1_18	control	Stem length	3	138
A1_18	control	Leaf width	3	27
A1_21	control	Stem length	1	131

+ 23 more rows

The standard structure of
tidy data means that
“tidy datasets are all alike...”

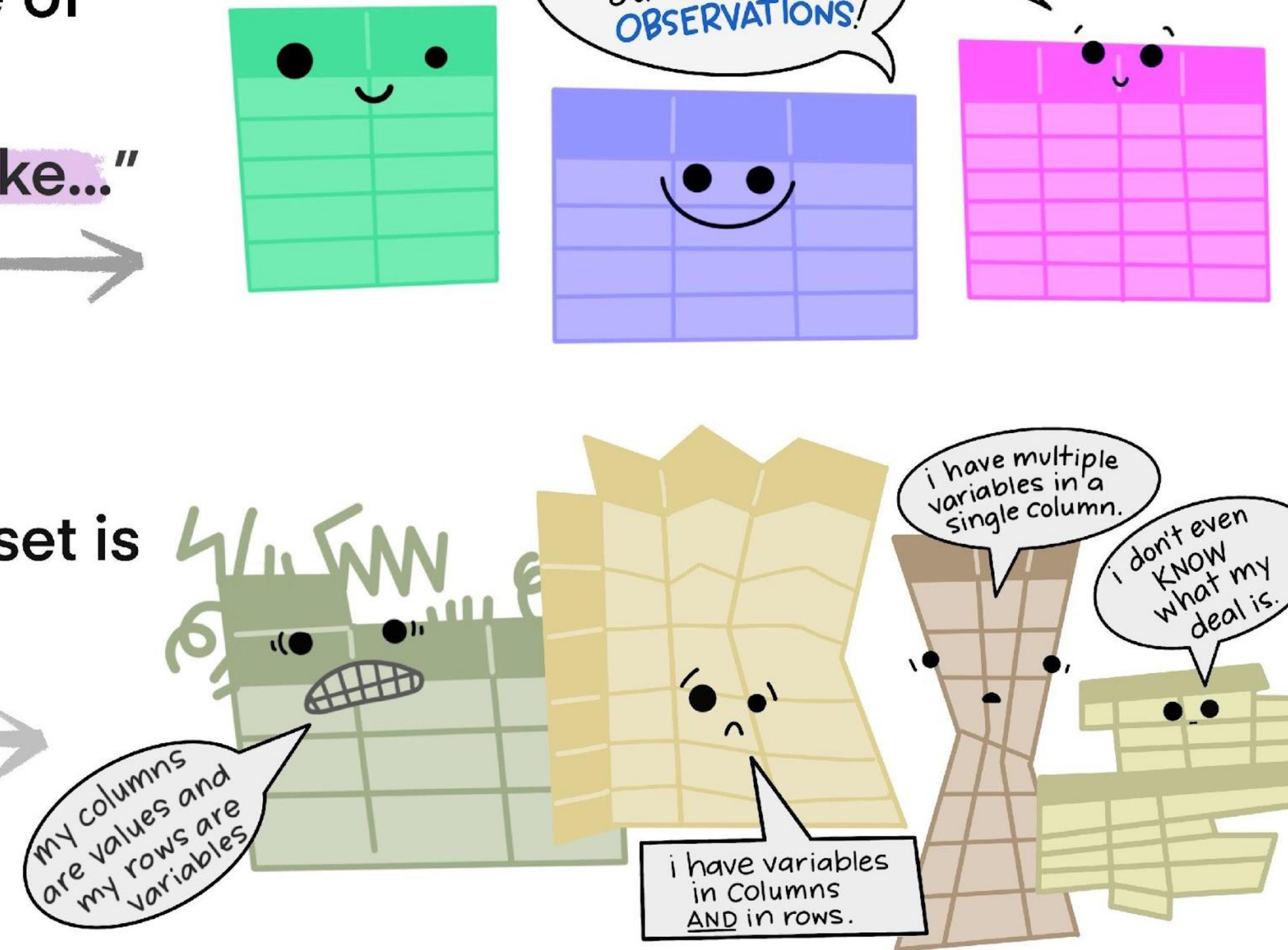


“...but every messy dataset is
messy in its own way.”

—HADLEY WICKHAM



my columns
are values
my rows are
variables



1. Save your project in a single folder
2. Devise a logical system of sub-folders
3. Introduce the project in a README
4. Use interoperable file types
5. Use descriptive and logical file names
6. Make your data tidy

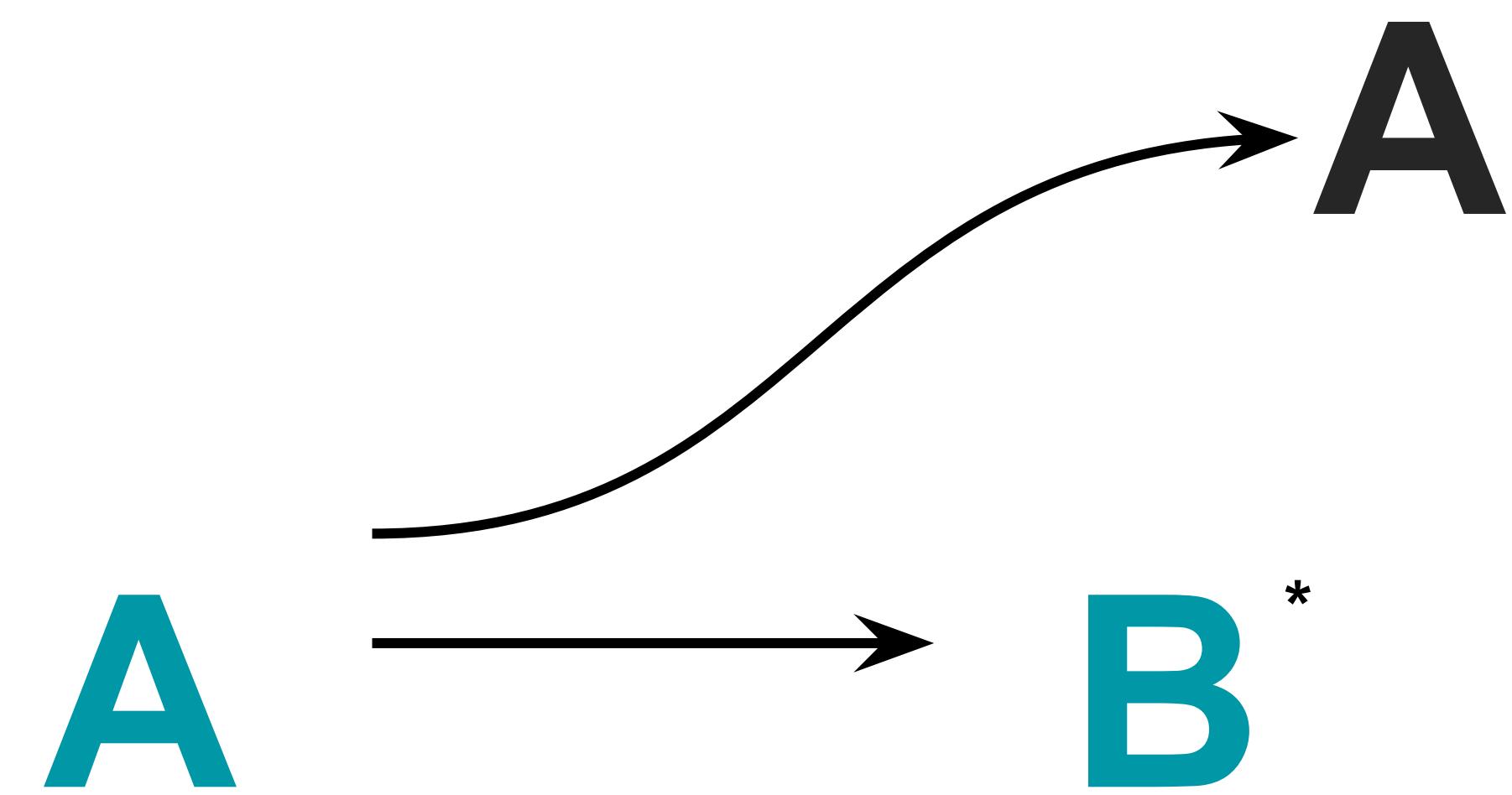
Exercise Present:

<https://dcc-training-lab.github.io/project-management/lessons/present.html>

A photograph of a man in a flight suit and headset, looking down at a computer monitor in what appears to be a flight control room. He is wearing a flight helmet with a communication system. In front of him is a large computer console with multiple screens and a keyboard. One screen displays the number '21'. The room has other people in similar gear in the background.

PAST

Recording project history



) Thanks to: **A , but not **A***

*time goes
on...*



git

1. Keep a changelog

Changelog: an example from keepachangelog.com

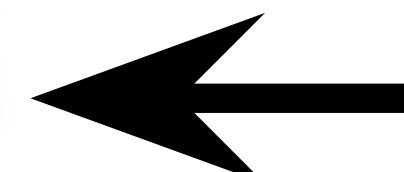
Changelog

All notable changes to this project will be documented in this file.

The format is based on [Keep a Changelog] (<https://keepachangelog.com/en/1.0.0/>)
and this project adheres to [Semantic Versioning] (<https://semver.org/spec/v2.0.0.html>)

[Unreleased]

[1.0.0] - 2017-06-20



Added

- New visual identity by [@tylerfortune8](https://github.com/tylerfortune8).
- Version navigation.
- Links to latest released version in previous versions.
- "Why keep a changelog?" section.
- "Who needs a changelog?" section.
- "How do I make a changelog?" section.

∞ How do I make a good changelog?

Credit: keepachangelog.com



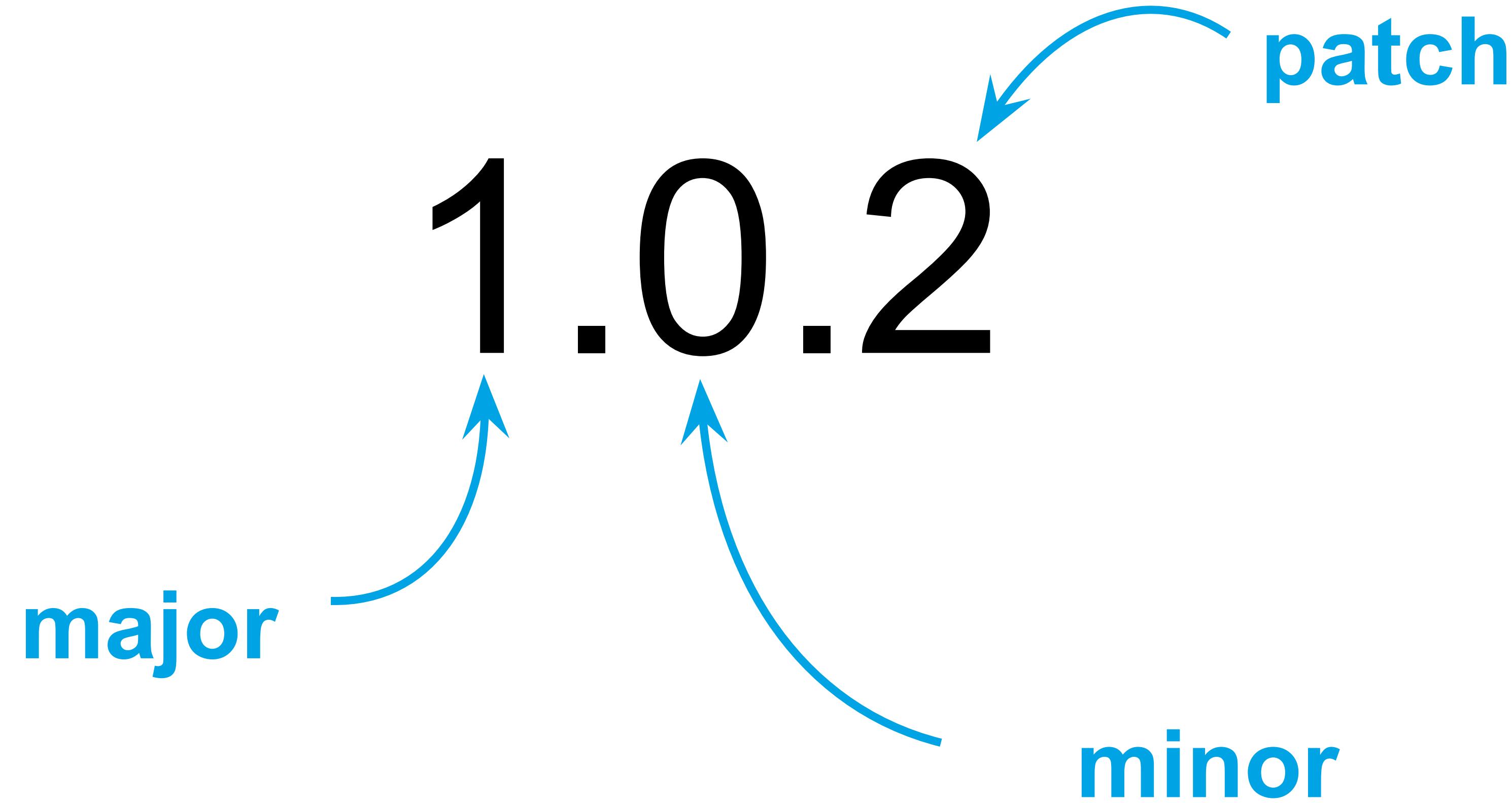
Guiding Principles

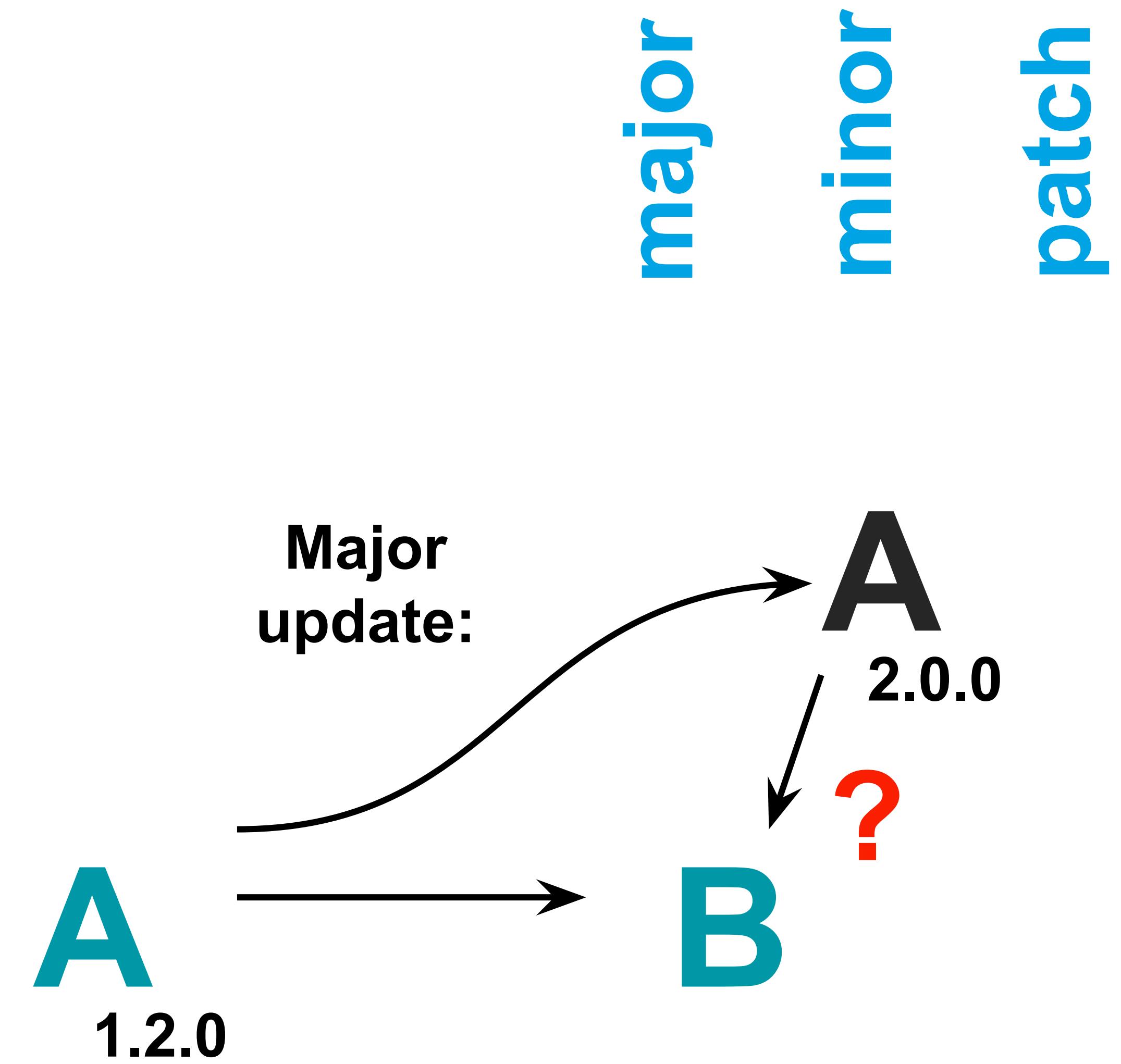
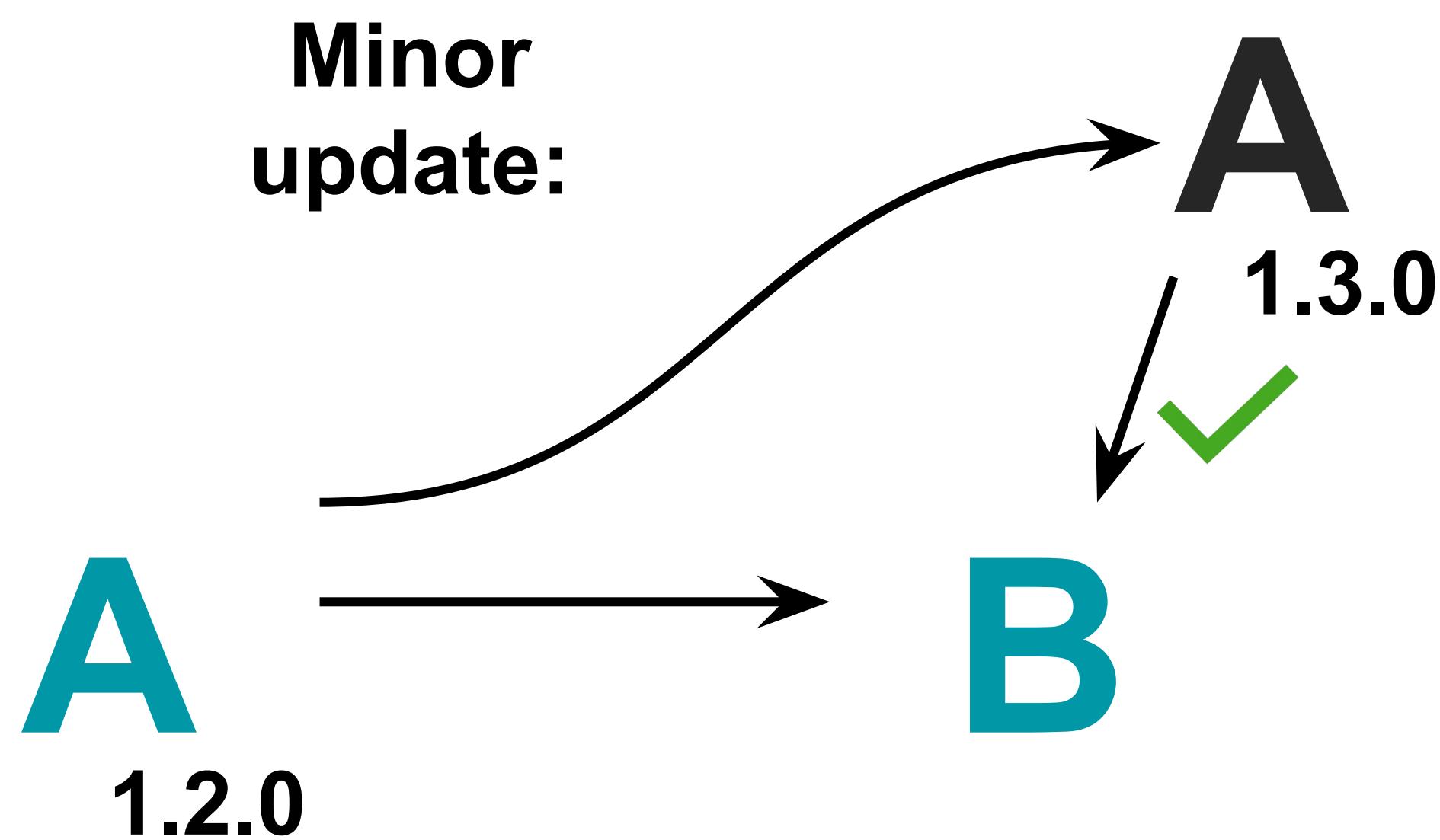
- Changelogs are *for humans*, not machines.
- There should be an entry for every single version.
- The same types of changes should be grouped.
- Versions and sections should be linkable.
- The latest version comes first.
- The release date of each version is displayed.
- Mention whether you follow [Semantic Versioning](#).

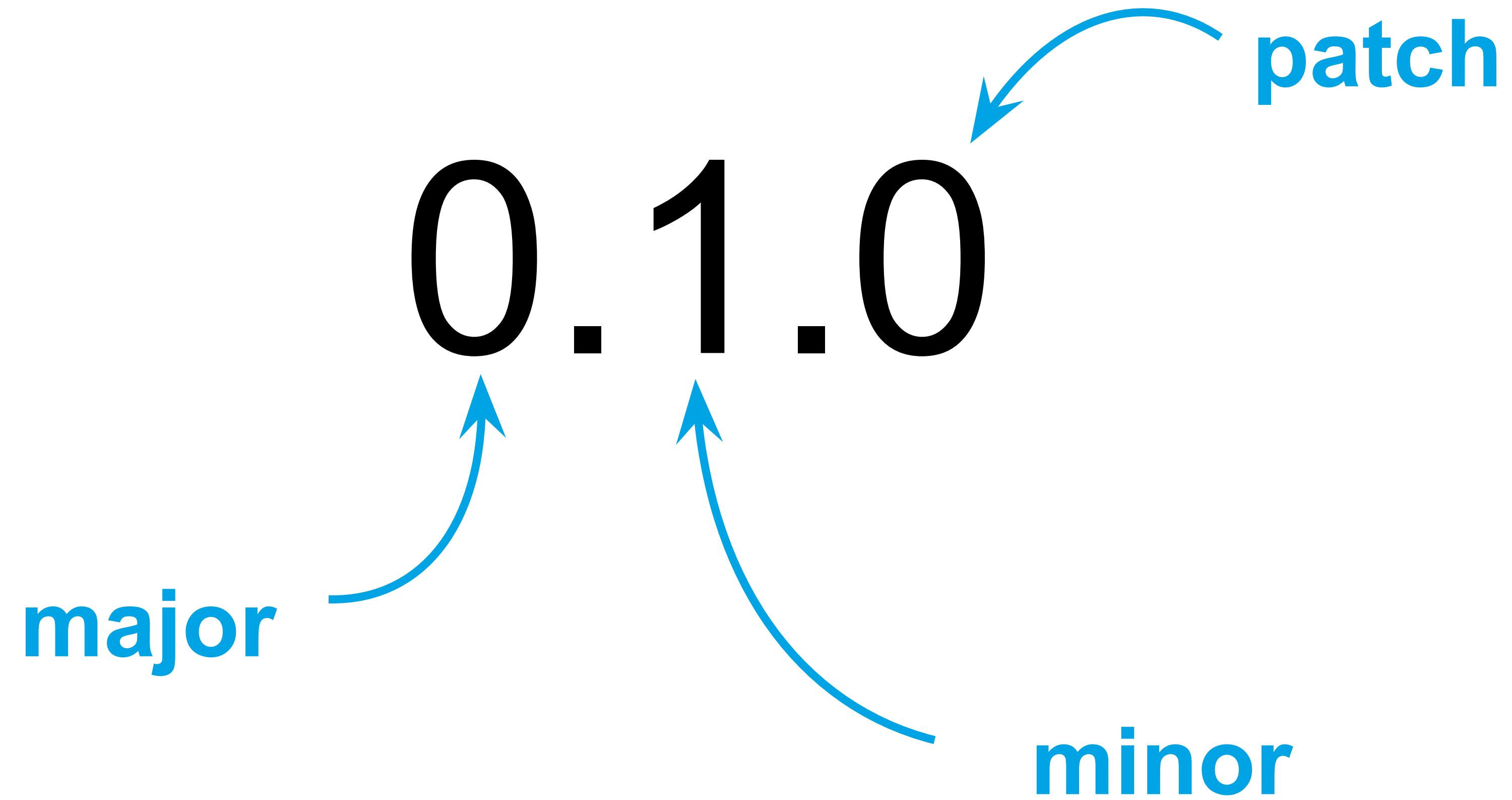
Types of changes

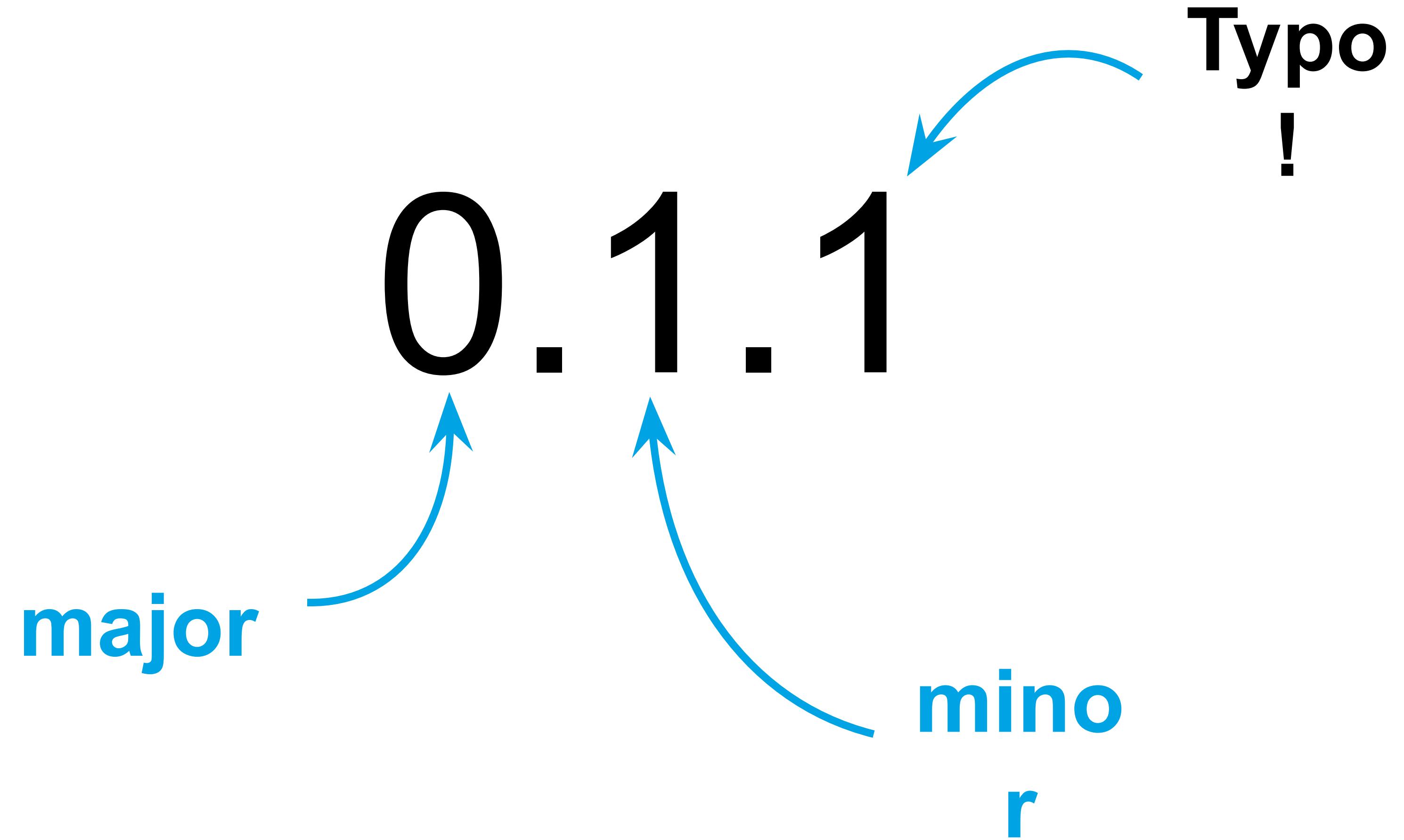
- **Added** for new features.
- **Changed** for changes in existing functionality.
- **Deprecated** for soon-to-be removed features.
- **Removed** for now removed features.
- **Fixed** for any bug fixes.
- **Security** in case of vulnerabilities.

2. Formalize updates using semantic versioning









Changelog

All notable changes to this project will be documented in this file.

The format is based on [Keep a Changelog] (<https://keepachangelog.com/en/1.0.0/>)
and this project adheres to [Semantic Versioning] (<https://semver.org/spec/v2.0.0.html>)

[Unreleased]

[1.0.0] - 2017-06-20

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- Version navigation.
- Links to latest released version in previous versions.
- "Why keep a changelog?" section.
- "Who needs a changelog?" section.
- "How do I make a changelog?" section.

"FINAL".doc



FINAL.doc!



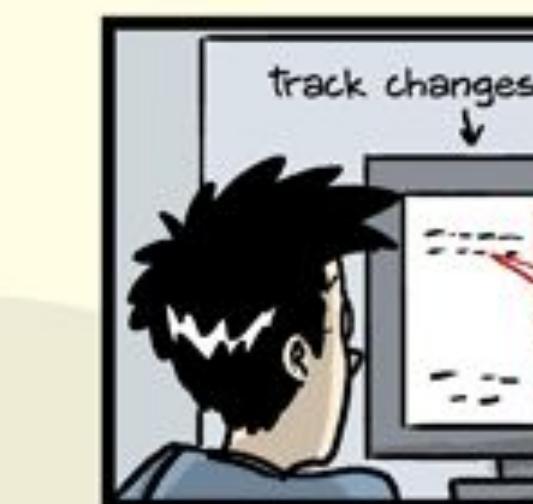
FINAL_rev.2.doc



FINAL_rev.6.COMMENTS.doc



FINAL_rev.8.comments5.
CORRECTIONS.doc



FINAL_rev.18.comments7.
corrections9.MORE.30.doc



FINAL_rev.22.comments49.
corrections.10.#@\$%WHYDID
ICOMETOGRAD SCHOOL?????.doc

Exercise Past

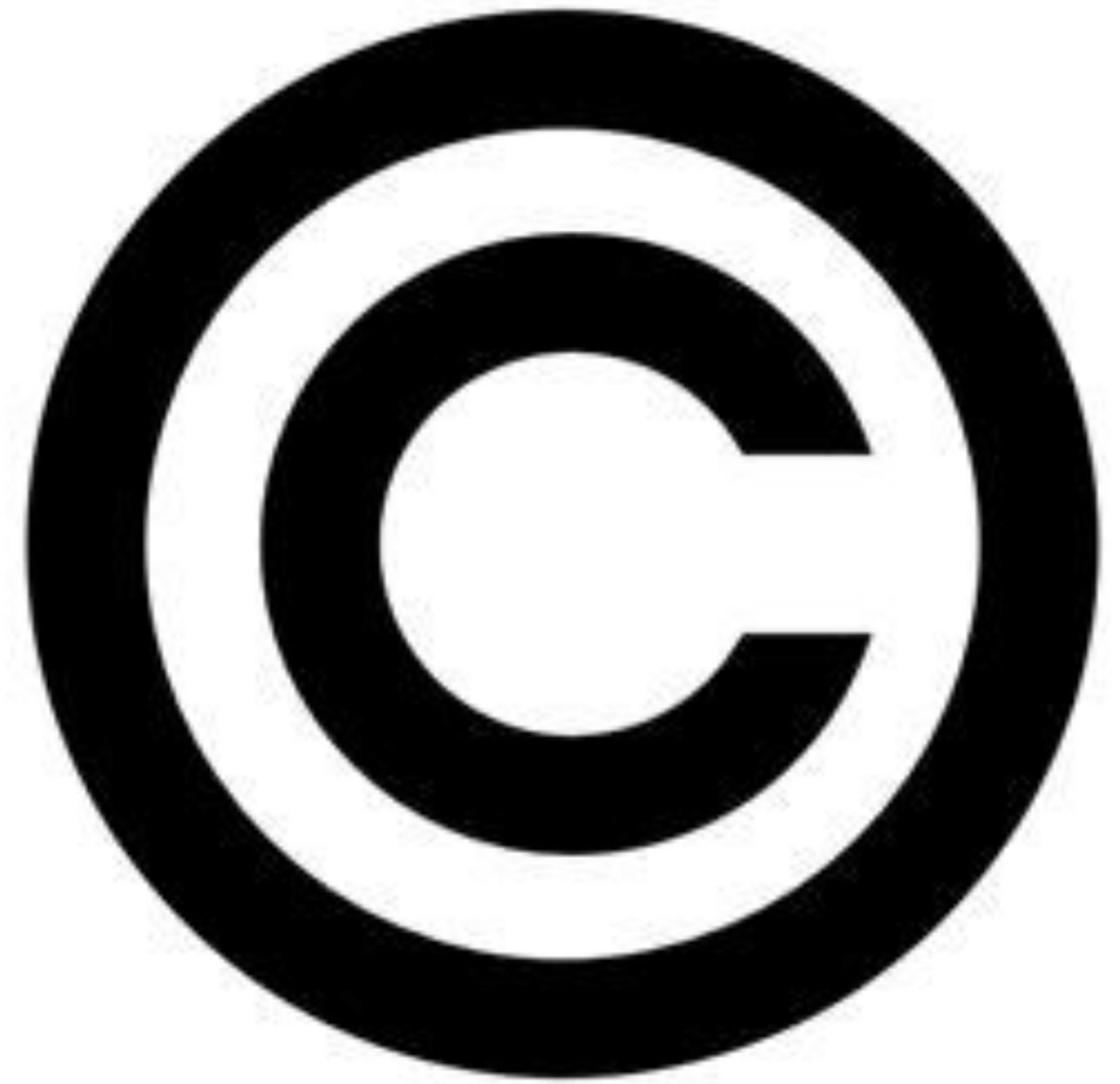
[https://dcc-training-lab.github.io/project-
management/lessons/past.html](https://dcc-training-lab.github.io/project-management/lessons/past.html)

A photograph of a person's hand holding a blue pen over a world map. The hand is positioned as if writing, with the pen tip pointing towards the bottom right. The map shows continents in light green and oceans in shades of blue. Overlaid on the upper left portion of the map is the word "FUTURE" in large, bold, white capital letters.

FUTURE

Publishing and archiving your project for future use

1. Choose a license.



Create Commons Licenses



Attribution

Others can copy, distribute, display, perform and remix your work if they credit your name as requested by you



No Derivative Works

Others can only copy, distribute, display or perform verbatim copies of your work



Share Alike

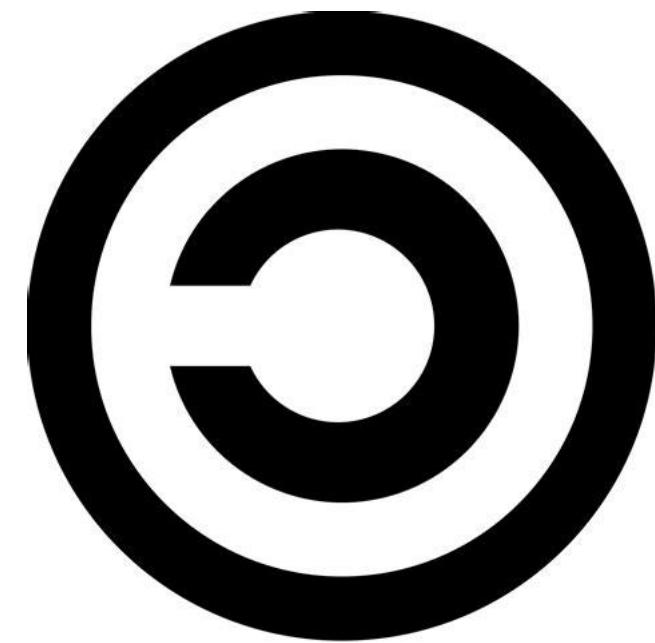
Others can distribute your work only under a license identical to the one you have chosen for your work



Non-Commercial

Others can copy, distribute, display, perform or remix your work but for non-commercial purposes only.

Copyleft vs Permissive



What open licenses do not imply

- You will not be forgotten.
- You are not forbidden from making money!

2. Maintain your living project on GitHub.

GitHub Repository

DCC-training-lab / [project-management](#) Public
Forked from [meronvermaas/2022-06-23-DCC-project-management](#)

> [Code](#) [Pull requests](#) [Actions](#) [Projects](#) [Wiki](#) [Security](#) [Insights](#) [Settings](#)

[main](#) [branches](#) [tags](#) [Go to file](#) [Add file](#) [Code](#)

This branch is [12 commits ahead](#) of meronvermaas:main. [Contribute](#) [Sync fork](#)

File	Description	Time
data	Add data source info	2 years ago
lessons	Update future.md	5 days ago
presentations	add pptx presentation used in movie	last year
transcripts	project archive transcript first draft	2 years ago
.gitignore	Create .gitignore	2 years ago
LICENSE.md	fix typo	2 years ago
README.md	Update README.md	yesterday
preparation.md	Update preparation.md	5 days ago

[README.md](#) [Edit](#)

DOI [10.5281/zenodo.8047483](#)

Organizing your data and software with a reproducible project workflow

DCC Spring Training Days

In this Spring Training workshop, we will take you through the life cycle of a project, teaching good habits along the way, and using familiar tools as much as possible.

We will start at the **PRESENT**, where you will create your project. From a few data files (adapted from [Hope et al.](#),

About
[dcc-training-lab.github.io/project-ma...](#)
[Readme](#) [View license](#) [Activity](#) [0 stars](#) [0 watching](#) [4 forks](#)
[Report repository](#)

Releases 4
[2023-DCC-Spring-Training-...](#) [Latest](#) 5 days ago
[+ 3 releases](#)

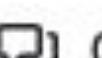
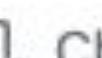
Packages
No packages published [Publish your first package](#)

Environments 1
[github-pages](#) [Active](#)

A pull request

Update session-05.md #6

Open XinyanFan-hub wants to merge 1 commit into `DCC-training-lab:main` from `XinyanFan-hub:main` 

 Conversation 0  Commits 1  Checks 0  Files changed 1

 XinyanFan-hub commented on Apr 20 First-time contributor ...

update the instructor 

 [Update session-05.md](#) ... Verified c075715

Add more commits by pushing to the `main` branch on [XinyanFan-hub/2023-spring-training-days](#).

 **This branch has not been deployed**
No deployments

Inviting collaborators in ‘settings’ > ‘collaborators’

The screenshot shows the GitHub repository settings page for a public repository. The left sidebar has sections for General, Access (Collaborators selected), Code and automation, Security, and Deployment keys. The main area shows 'Who has access' with a PUBLIC REPOSITORY section (visible to anyone) and a DIRECT ACCESS section (3 have access). The DIRECT ACCESS section lists two collaborators: 'meronvermaas' and 'Max Paulus'. A green 'Add people' button is visible.

General

Access

- Collaborators** (selected)
- Moderation options

Code and automation

- Branches
- Tags
- Rules (Beta)
- Actions
- Webhooks
- Environments
- Codespaces
- Pages

Security

- Code security and analysis
- Deployment keys

Who has access

PUBLIC REPOSITORY This repository is public and visible to anyone.
[Manage](#)

DIRECT ACCESS 3 have access to this repository. [2 collaborators](#). [1 invitation](#).

Manage access

Select all Type ▾

Find a collaborator...

<input type="checkbox"/>	meronvermaas Collaborator	
<input type="checkbox"/>	Max Paulus paulmaxus • Collaborator	

Add people

Showcasing

README right on
the
front page!

A screenshot of a GitHub repository page for 'meronvermaas/project-management'. The page features a prominent 'README' file at the top, with the text 'Organizing your data and software with a reproducible project workflow' and 'DCC Spring Training Days'. A blue arrow points from the text 'README right on the front page!' to the 'README' file in the commit list. The commit list shows several recent changes, including updates to README.md, preparation.md, and future.md, along with other files like data, lessons, presentations, and transcripts.

This branch is 12 commits ahead of meronvermaas:main.

Go to file Add file > Code About

Contribute Sync fork

meronvermaas Update README.md ... ✓ 2c66984 yesterday 76 commits

data Add data source info 2 years ago

lessons Update future.md 5 days ago

presentations add ptx presentation used in movie last year

transcripts project archive transcript first draft 2 years ago

.gitignore Create .gitignore 2 years ago

LICENSE.md fix typo 2 years ago

README.md Update README.md yesterday

preparation.md Update preparation.md 5 days ago

Releases 4

2023-DCC-Spring-Training-... Latest 5 days ago + 3 releases

Packages

No packages published Publish your first package

Environments 1

github-pages Active

main 2 branches 4 tags

DOI 10.5281/zenodo.8047483

Organizing your data and software with a reproducible project workflow

DCC Spring Training Days

3. Archive the project for posterity on Zenodo.

A release in GitHub

The screenshot shows a GitHub releases page with two entries:

- 2023-DCC-Spring-Training-Days** (Latest)
This is the material as used in our 2023 edition of this DCC spring training
- Zenodo Release of 2022 training material**
This is the material of the DCC spring trainings days in 2022

Both releases were made by user `vansteph` on April 17, 2023. Each release has two assets: "Source code (zip)" and "Source code (tar.gz)".

Release	Assets	Published
2023-DCC-Spring-Training-Days	Source code (zip), Source code (tar.gz)	Apr 17
Zenodo Release of 2022 training material	Source code (zip), Source code (tar.gz)	Apr 17

... can be automatically archived in Zenodo!

The screenshot shows the Zenodo homepage with a blue header bar. The header includes the Zenodo logo, a search bar with a magnifying glass icon, an "Upload" button, a "Communities" link, and "Log in" and "Sign up" buttons. Below the header, the text "Featured communities" is displayed, followed by a section for the "Transform to Open Science" (TOPS) community. This section features a shield-shaped logo for TOPS NASA, a brief description of the mission, and buttons for "Browse" and "New upload". A "Curated by: nasatransformtoopen" link is also present. Navigation arrows are visible on either side of the featured community section.

zenodo

Search

Upload

Communities

Log in

Sign up

Featured communities

Need help uploading? Contact us

Transform to Open Science

Browse

New upload

Curated by: nasatransformtoopen

TOPS NASA

Recent uploads

June 20, 2023 (v14) Dataset Open Access

View

Binary black-hole surrogate waveform catalog

Scott E. Field; Chad R. Galley; Jan S. Hesthaven; Jason Kaye; Manuel Tiglio; Jonathan Blackman; Béla Szilágyi; Mark A. Scheel; Daniel A. Hemberger; Patricia Schmidt; Rory Smith; Christian D. Ott; Michael Boyle; Lawrence E. Kidder; Harald P. Pfeiffer; Vijay Varma

This repository contains all publicly available numerical relativity surrogate data for waveforms produced by the Spectral Einstein Code. The base method for building surrogate models can be found in Field et al., PRX 4, 031006 (2014). Several numerical relativity surrogate models are currently...

Uploaded on June 20, 2023

13 more version(s) exist for this record

Why use Zenodo?

- **Safe** – your research is stored safely for the future in CERN's Data Centre for as long as CERN exists.
- **Trusted** – built and operated by CERN and OpenAIRE to ensure that everyone can join in Open Science.
- **Citeable** – every upload is assigned a Digital Object Identifier (DOI), to make them citable and trackable.
- **No waiting time** – Uploads are made available online as soon as you hit publish, and your DOI is registered within seconds.
- **Open or closed** – Share e.g. anonymized

Obtain a DOI for your software for every release

The screenshot shows the Zenodo GitHub integration interface. At the top, there's a navigation bar with 'Home' and 'Account'. Below it, a sidebar titled 'Settings' lists options like 'Profile', 'Change password', 'Security', 'Linked accounts', 'Applications', 'Shared links', and 'GitHub'. The 'GitHub' option is highlighted with a blue background. The main area is titled 'GitHub Repositories' and shows a 'Get started' section with three steps: 1. Flip the switch (with a note about selecting a repository and turning on automatic preservation), 2. Create a release (with a note about Zenodo automatically downloading .zip-balls and registering DOIs), and 3. Get the badge (with a note about a badge appearing in GitHub READMEs). A 'Sync now...' button is at the top right. Below this, an 'Enabled Repositories' section shows 'DCC-training-lab/2021-spring-training-days' with an 'ON' switch. At the bottom, a screenshot of a GitHub README.md file shows a 'DOI 10.5281/zenodo.8047483' badge, which is also highlighted with a red box.

Home / Account / GitHub

Settings

- Profile
- Change password
- Security
- Linked accounts
- Applications
- Shared links
- GitHub**

(updated now) Sync now ...

GitHub Repositories

Get started

- 1 Flip the switch**
Select the repository you want to preserve, and toggle the switch below to turn on automatic preservation of your software.
- 2 Create a release**
Go to GitHub and [create a release](#). Zenodo will automatically download a .zip-ball of each new release and register a DOI.
- 3 Get the badge**
After your first release, a DOI badge that you can include in GitHub README will appear next to your repository below.

DOI 10.5281/zenodo.8475
(example)

Enabled Repositories

DCC-training-lab/2021-spring-training-days

ON

README.md

DOI 10.5281/zenodo.8047483

ON

Organizing your data and software with a reproducible project workflow

Digital Object Identifier (DOI)

June 16, 2023

Software Open Access

DCC-training-lab/project-management: 2023-
DCC-Spring-Training-Days

Barbara Vreede; Stephanie van de Sandt; meronvermaas

This is the material as used in our 2023 edition of this DCC spring training

Preview

project-management-2023.zip

DCC-training-lab-project-management-c19735b

- .gitignore
- LICENSE.md
- README.md
- data**
 - README.md
 - datafile_1.xlsx
 - datafile_10.xlsx
 - datafile_11.xlsx
 - datafile_2.xlsx
 - datafile_3.xlsx
 - datafile_4.xlsx
 - datafile_5.xlsx
 - datafile_6.xlsx
 - datafile_7.xlsx
 - datafile_8.xlsx
 - datafile_9.xlsx
 - datafiles.zip
- lessons

12 Bytes
114 Bytes
3.5 kB

712 Bytes
9.1 kB
9.2 kB
9.2 kB
9.1 kB
9.1 kB
9.1 kB
9.1 kB
9.1 kB
9.2 kB
9.2 kB
9.3 kB
9.3 kB
9.2 kB
79.6 kB

Files (9.7 MB)

Name	Size
DCC-training-lab/project-management-2023.zip	9.7 MB

md5:773d16e0a5d99d9251def8e64f2fd43 ↗

Citations 0.0

Show only: Literature (0) Dataset (0) Software (0) Unknown (0)
 Citations to this version

No citations.

Older versions

License

Publication date:
May 12, 2021

DOI:
DOI 10.5281/zenodo.4753914

Keyword(s):
R package Natura 2000 habitat environment
data Flanders Belgium

Related identifiers:
Supplement to
<https://github.com/inbo/n2khab/tree/v0.5.0>

Communities:
Research Institute for Nature and Forest (INBO)
Zenodo

License (for files):
 GNU General Public License v3.0 only

Versions

Version 0.5.0	May 12, 2021
10.5281/zenodo.4753914	
Version 0.4.0	Feb 10, 2021
10.5281/zenodo.4531807	
Version 0.3.1	Oct 26, 2020
10.5281/zenodo.4133524	
Version 0.3.0	Oct 16, 2020
10.5281/zenodo.4096139	
Version 0.2.0	May 8, 2020
10.5281/zenodo.3817690	
View all 8 versions	

Exercise

1. Make a new public repository on GitHub.
2. Click on 'uploading an existing file'
 - a. Drag and drop the contents of your folder to the repository.
 - b. Click on 'commit changes' to complete the upload.
3. Add a license to the project:
 - a. Click 'Add file' > 'Create new file', and name your new file LICENSE
4. Connect your GitHub page to Zenodo SANDBOX.
 - a. Click 'log in with GitHub' and authorize Zenodo Sandbox to connect to your GitHub account.
 - b. Click on the triangle next to your name, and choose 'GitHub'.
 - c. Find the repository you just created, and enable Zenodo's access by toggling the switch to 'on'.
5. Make a release from the GitHub main page:
 - a. Click 'create a new release'
 - b. Click 'Publish release'.
6. Return to the GitHub page in your Zenodo profile and see what happened.

Discussion



Answer these questions for yourself and share the answers with the group

What is the main take-away from
this workshop?

What experience in your past has
taught you an important lesson
about project management?



Thank you!

3. Collaboration

- a. Create an overview of your project.
- b. Create a shared "to-do" list for the project.
- c. Decide on communication strategies.
- d. Make the license explicit.
- e. Make the project citable.

3. Collaboration

- a. Create an overview of your project.
- b. Create a shared "to-do" list for the project.
- c. Decide on communication strategies.
- d. Make the license explicit.
- e. Make the project citable.

1. Data management
 - a. Save the raw data.
 - b. Ensure that raw data are backed up in more than one location.
 - c. Create the data you wish to see in the world.
 - d. Create analysis-friendly data.
 - e. Record all the steps used to process data.
 - f. Anticipate the need to use multiple tables, and use a unique identifier for every record.
 - g. Submit data to a reputable DOI-issuing repository so that others can access and cite it.

3. Collaboration

- a. Create an overview of your project.
- b. Create a shared "to-do" list for the project.
- c. Decide on communication strategies.
- d. Make the license explicit.
- e. Make the project citable.