Snakemake

A framework for reproducible data analysis

Microbiome group
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Cristina Leal

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“The Snakemake workflow management system is a tool to create reproducible and scalable data analyses. Workflows are described via a human readable, Python based language.

They can be seamlessly scaled to server, cluster, grid and cloud environments without the need to modify the workflow definition.

Finally, Snakemake workflows can entail a description of required software, which will be automatically deployed to any execution environment.”

https://snakemake.readthedocs.io/

Reproducible because…

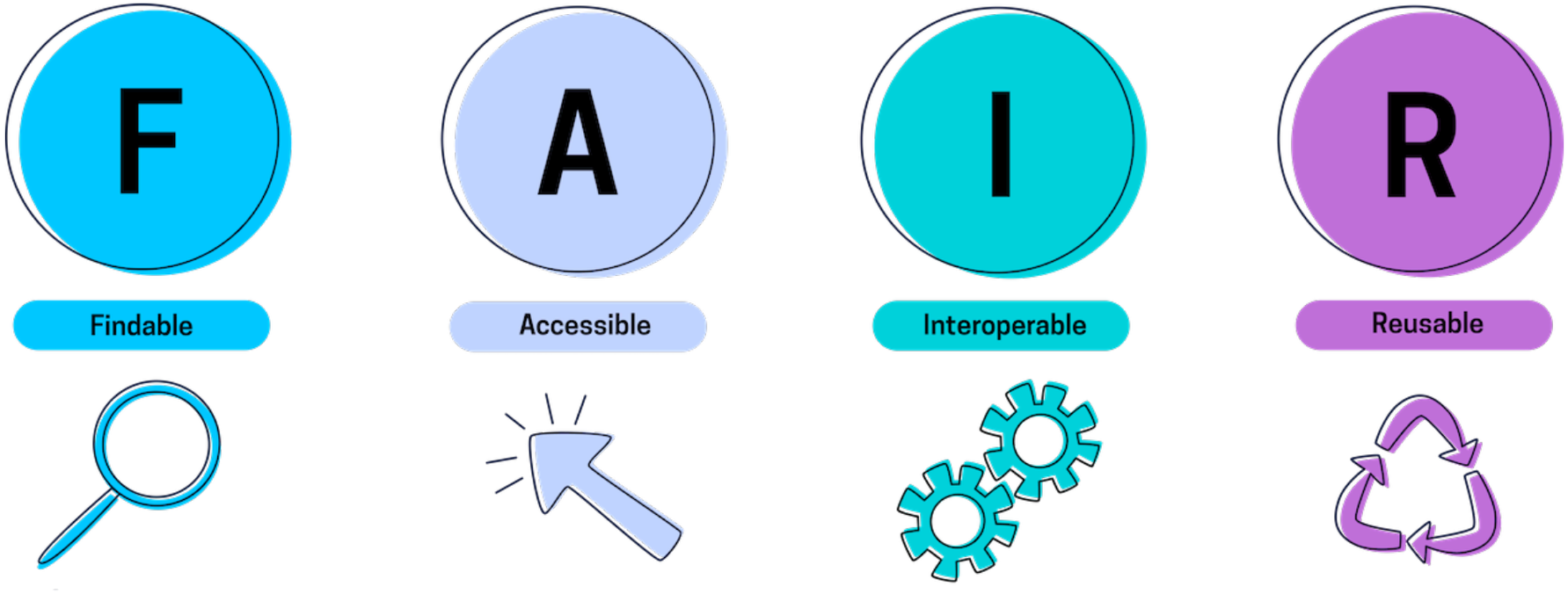
1. **Scalable**

   Optimizes the number of processes that can be run in parallel wrt CPU cores and needed threads

2. **Portable**

   Runs across many different platforms

3. **Automated**



Makes sure everything is **up-to-date**

Wilkinson, Mark D., et al. "The FAIR Guiding Principles for scientific data management and stewardship." *Scientific data* 3.1 (2016): 1-9.
https://flur.ee/2020/07/08/making-data-fair/

History of Snakemake

- Based on ideas from **UNIX make**…
  - Originally created by Stuart Feldman in 1976 at Bell Labs, now it is a standard build tool
- By Johannes Köster, University Hospital Essen
- V1.0 was released in 2012
- V7.8.2 was released two days ago, 08/06/2022
- Free software
- Works on Linux, Mac and Windows

Snakemake is popular

Volume 28, Issue 19
1 October 2012

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Snakemake—a scalable bioinformatics workflow engine FREE

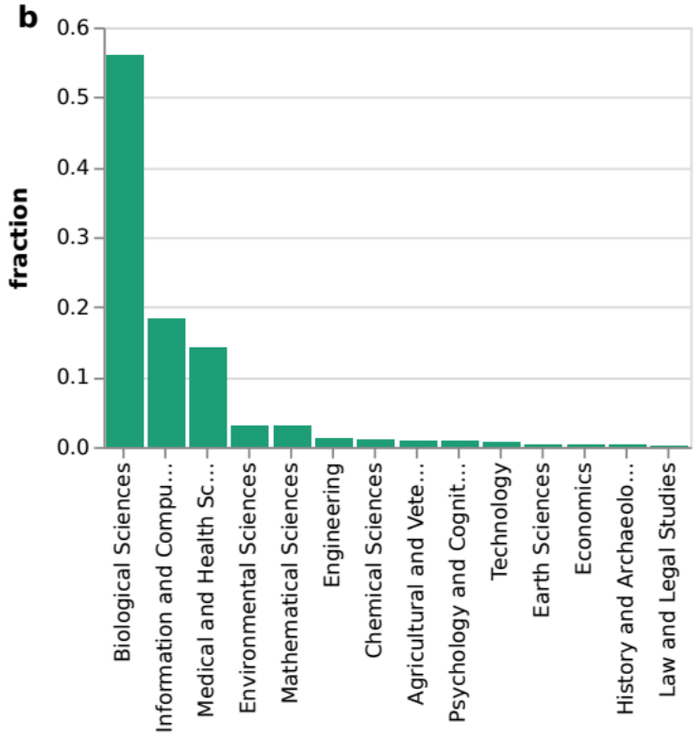
Johannes Köster, Sven Rahmann Author Notes

Bioinformatics, Volume 28, Issue 19, 1 October 2012, Pages 2520–2522,
https://doi.org/10.1093/bioinforma
Published: 20 August 2012 **Arti**

A correction has been published:
Bioinformatics, Volume 34, Issue
https://doi.org/10.1093/bioinfor

Accessed 10/08/2021

Snakemake—a scalable bioinformatics workflow engine
J Köster, S Rahmann - Bioinformatics, 2012 - academic.oup.com
Snakemake is a workflow engine that provides a readable Python-based workflow definition language and a powerful execution environment that scales from single-core workstations to compute clusters without modifying the workflow. It is the first system to support the use of …
☆ Citado por 1402 Artículos relacionados Las 16 versiones



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flow engine
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tions to compute clusters without modifying
m to support the use of automatically inferred
riables) in input and output filenames.
ooglecode.com.
·due.de
IS

Widely used and accepted for reproducible data science. On average, it has **6 new citations per week** !!

Köster, Johannes, and Sven Rahmann. "Snakemake—a scalable bioinformatics workflow engine." *Bioinformatics* 28.19 (2012): 2520-2522.

Snakemake

Like a script but not a script

- Snakemake reads a **Snakefile**
- A Snakefile defines a set of **rules**
- Rules have **inputs** and **outputs** and **actions**
- Snakemake works out the correct order of rules to reach a given **target**, then runs them

Rules: the lego pieces of your workflow

Snakemake defines workflows in terms of rules

Rule name

```
rule mytask:
        input:
                sample_data = "data/{sample}.txt"
        output:
                outfile = "outputs/{result}.txt"
    shell:
        "some-tool {input} > {output}"
```

Generalizable wildcard

Define

Input

Output

Log files

Parameters

Resources

…

How to create output from input

Rules: the lego pieces of your workflow

Snakemake defines workflows in terms of rules

Boilerplate-free integration of scripts

```
rule mytask:
        input:
                sample_data = "data/{sample}.txt"
        output:
                outfile = "outputs/{result}.txt"
        script:
                "script/myscript.R"
```

R/Python/Julia ←

Boilerplate-free integration of R and python scripts

R scripts

```r
for (p in c("data.table", "dplyr")) {
        library(p, character.only = TRUE)
}

data <- fread(snakemake@input$sample_data) %>%
        arrange(desc(id))
fwrite(data, snakemake@output$outfile)
```

Python scripts

```python
import pandas as pd

data = pd.read_table(snakemake.input["sample_file"])
data = data.sort_values("id")
data.to_csv(snakemake.output["outfile"], sep="\t")
```


Rules: the lego pieces of your workflow

Snakemake defines workflows in terms of rules

…and more!

Jupyter notebook integration

```
rule mytask:
        input:
                sample_data = "data/{sample}.txt"
        output:
                outfile = "outputs/{result}.txt"
        notebook:
                "notebooks/mynotebook.ipynb"
```

Reusable wrappers from central snakemake repo

```
rule sort_reads:
        input:
                sample_data = "data/{sample}.bam"
        output:
                outfile = "outputs/{sample}.sorted.bam"
        wrapper:
                "0.22.0/bio/samtools/sort"
```

e.g. DADA2

https://snakemake-wrappers.readthedocs.io/en/stable/

The snakefile

The file that rules them all

```
configfile: config.yaml

rule all:
        input:
                "a.tsv"
                "b.tsv"
                "b.png"

rule mytask_1:
        input: config["input_data"]
        output: "a.tsv"
        threads: 1
        script: "scripts/01_mytask.py"

rule mytask_2:
        input: config["input_data"]
        output:
                outfile = "b.tsv",
                fig = "b.png"
        threads: 1
        script: "scripts/02_mytask.R"
```


Run your workflow

Portability and flexibility in many different platforms

Perform a dry-run

```
snakemake -n
```

Execute workflow locally with 16 CPU cores

```
snakemake --cores 16
```

Execute on cluster

```
snakemake --cluster qsub --jobs 100
```

Execute in the cloud

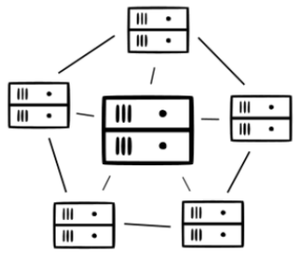
```
snakemake --k
```

workstation

compute server

cluster

grid computing



cloud computing

kubernetes

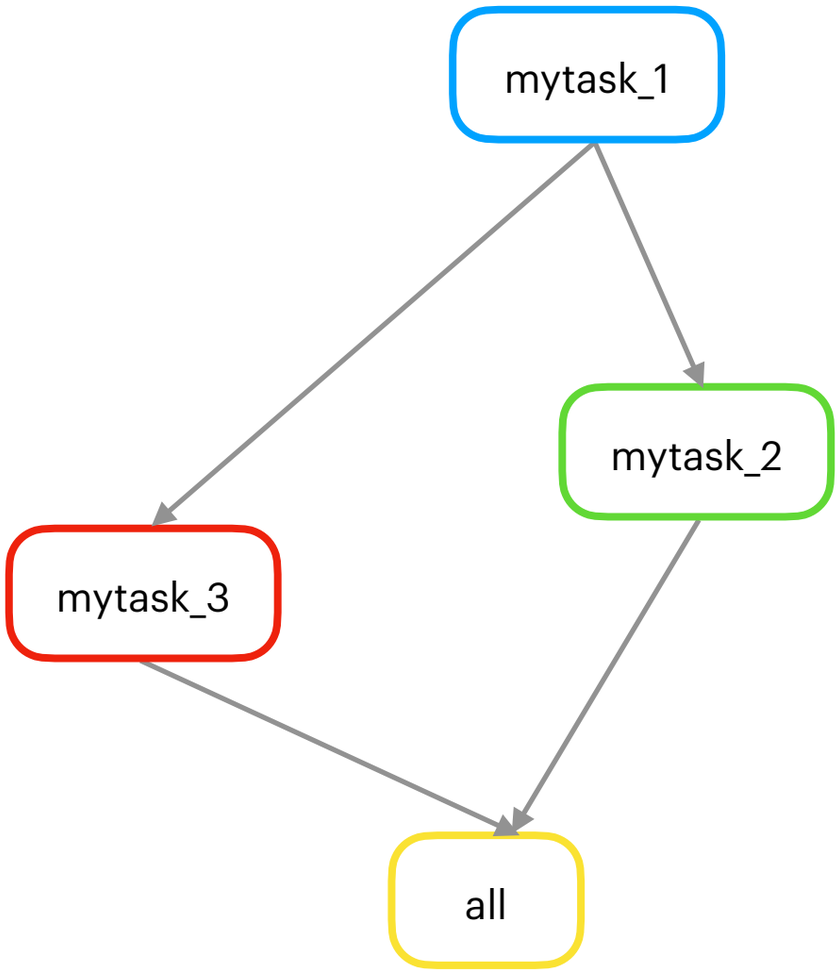
Google Cloud Platform

amazon web services

Visualise your workflow

The **rulegraph** diagram

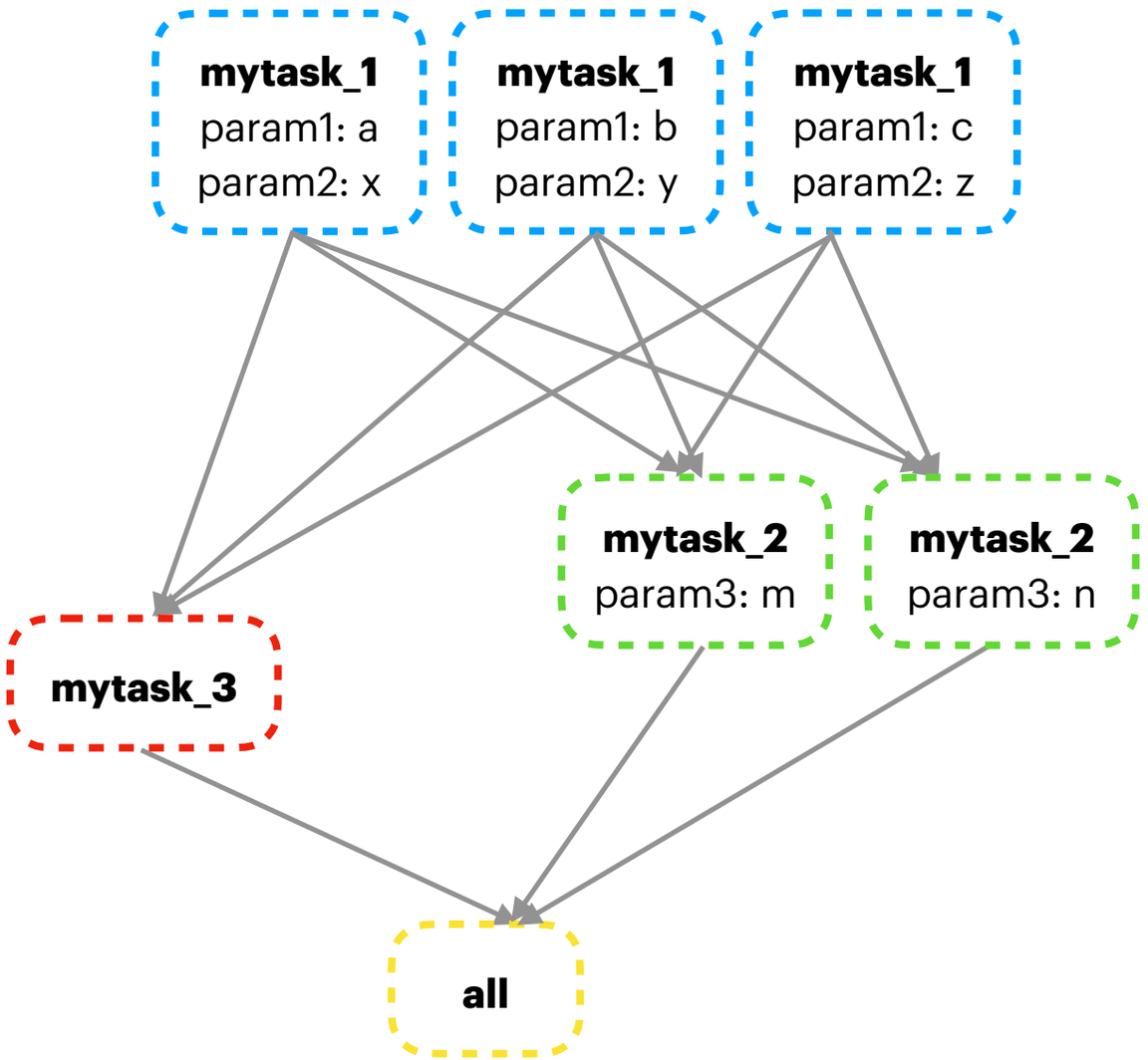
```
snakemake --rulegraph | dot -Tpng > workflow/rulegraph.png
```



Visualise your workflow

The **dag** diagram

```
snakemake --dag | dot -Tpng > workflow/dag.png
```



Workflow benchmarking and report

Workflow statistics, runtime, params, etc.

Keep **control** of the time and resources used, parameters, and the outputs

- Benchmarks: define it within your rules
- A beautiful and interactive report

```
snakemake --report workflow/report.html
```

https://snakemake.readthedocs.io/en/stable/snakefiles/reporting.html

Distribution and reproducibility

Your workflow folder structure

tutorial/structure.md

```
my_project
├── .gitignore
├── README.md
├── config
│   ├── config.yaml
├── workflow
│   ├── envs
│   │   ├── environment.yaml
│   ├── benchmarks
│   ├── scripts
│   │   ├── script1.py
│   │   └── script2.R
│   ├── notebooks
│   │   ├── notebook1.py.ipynb
│   │   └── notebook2.r.ipynb
│   ├── report
│   │   ├── report.html
│   └── Snakefile
├── results
├── logs
└── resources
```


Snakemake

In summary

- Applies rules based on file name patterns
- {wildcard} placeholders
- Starts with a target output filename and looks for rules with a matching output
- Repeats until it runs out of rules
- Nothing is actually run until a full plan is made
- Order of rules in the Snakefile is unimportant

Hands-on

https://github.com/crlero/snakemake-tutorial

Then, download this repository to your favourite local computer. If you already have `git` installed, you can download it with:

```
git clone https://github.com/crlero/snakemake-tutorial.git
# or
git clone git@github.com:crlero/snakemake-tutorial.git
```

... otherwise download the `ZIP` repository from the `Code` button on the up-right side of this page.

First, we start by creating our project environment

tutorial/create_your_environment.md

Install miniconda3

If you don't have conda (miniconda, conda or Anaconda) yet, install miniconda3.

```
bash Miniconda3-latest-MacOSX-x86_64.sh
```

Follow the prompts on the installer screens and test the installation with:

```
conda list
```

Set up your conda channels

```
conda config --add channels defaults
conda config --add channels bioconda
conda config --add channels conda-forge
```


First, we start by creating our project environment

tutorial/create_your_environment.md

Create a new environment

```
conda create -n tutorial -c conda-forge mamba
conda activate tutorial
```

Installing needed packages and dependencies

From conda (recommended)

```
conda install snakemake
conda install r-essentials
conda install bioconductor-microbiome
conda install bioconductor-phyloseq
conda install bioconductor-metagenomeseq
conda install r-vegan
conda install r-cowplot
conda install r-ggthemes
conda install r-ggsci
```

First, we start by creating our project environment

tutorial/create_your_environment.md

Installing needed packages and dependencies

From R (not recommended, and if so add a rule to your workflow to download the packages)

```
$ R
>> if (!requireNamespace("BiocManager", quietly = TRUE))
    install.packages("BiocManager")

>> BiocManager::install("phyloseq")
>> BiocManager::install("microbiome")
>> install.packages("vegan")
```

When your project env is ready, you are ready to start writing your scripts

tutorial/create_your_environment.md

Testing and scripting using RStudio with your environment

Open a `tmux` screen, activate your environment and launch your RStudio. Now you are all set up for start writing testing your own code.

```
tmux new-session -s rstudio
conda activate tutorial
/Applications/RStudio.app/Contents/MacOS/RStudio
```


Recreate this tutorial environment

In order to be able to run this workflow example, we must ensure we are running it within a defined environment. To do so, you can either create a new conda environment using the `yaml` file and download the specific dependencies defined in it or you can activate the environment from the zipped folder that I have placed in the NAS server to speed up the slow stuff :-).

Create conda environment from the .yaml file

```
cd snakemake-tutorial/handson/
conda env create --name tutorial --file=workflow/environment.yaml
conda activate tutorial
```

Activate folder with the environment

```
mkdir environment_tutorial
tar xzvf /Volumes/UserFolders/cristina.leal/snakemake-tutorial/environment_tutorial.tar.gz -C enviro
source environment_tutorial/bin/activate # activates the environment
source environment_tutorial/bin/deactivate # deactivates the environment
```


Hands-on

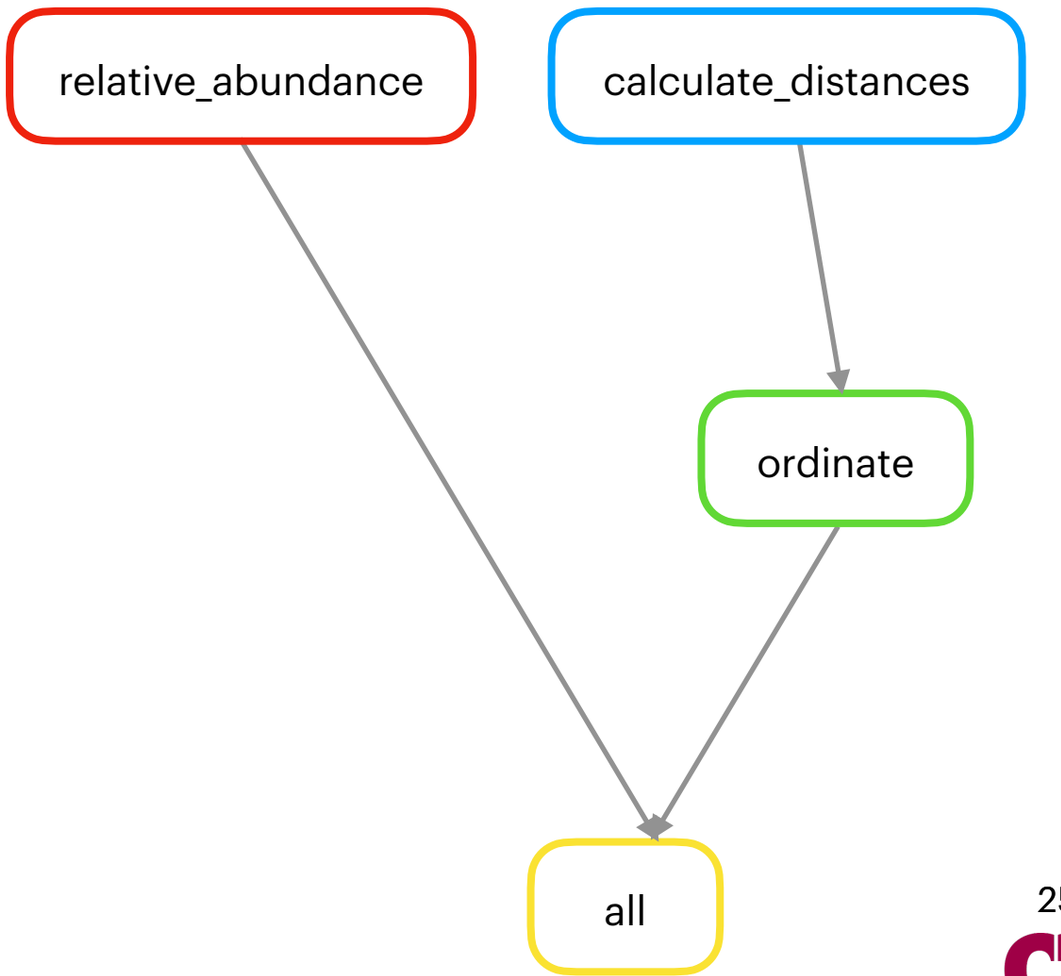
- Activate the environment
- Open the **handson/** folder in your preferred editor (mine is visual studio code)
- Look at the folder structure
- Open the Snakefile
- First rule: **relative_abundances**
  - Try a dry run
  - The config.yaml file
- Second rule: **calculate distances**
  - Wildcards and the expand function
- Third rule: **ordinate**
- Run it all
- Check logs, benchmarks
- Create a report

```
snakemake -n # dry-run
snakemake -j # run jobs in parallel
Snakemake -p # print shell commands
snakemake -F # force running all rules
```

```
snakemake --rulegraph | dot -Tpng >
workflow/rulegraph.png
```

```
snakemake --dag | dot -Tpng > workflow/
dag.png
```

```
snakemake --report workflow/repport.html
```



Try yourself!

- Can we shorten the script for the rule relative abundances that takes a list of outcomes of interest? How?
- Add a new outcome parameter to the ordination plots
- Change the threshold_prevalence parameter and rerun snakemake. Which rules are affected?
- Generate a rulegraph
- Generate a dag
- Generate a report with all the outputs

```
snakemake -n # dry-run
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```
snakemake --rulegraph | dot -Tpng >
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```
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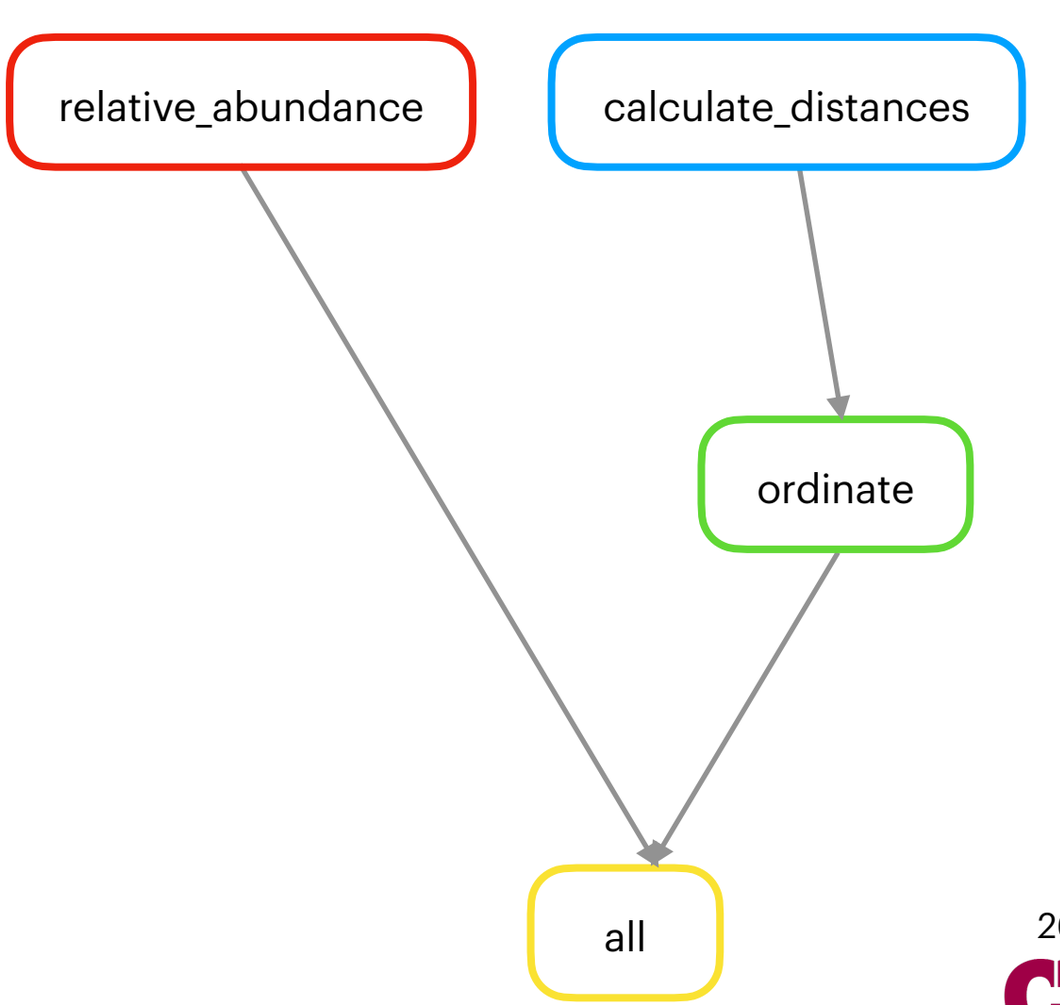

References

This introduction https://github.com/crlero/snakemake-tutorial

These slides in NAS /Volumes/UserFolders/cristina.leal/snakemake-tutorial/

Paper Köster, Johannes, and Sven Rahmann. "Snakemake—a scalable bioinformatics workflow engine." Bioinformatics 28.19 (2012): 2520-2522.

Snakemake official docs https://snakemake.readthedocs.io/

Snakemake official tutorial https://snakemake.readthedocs.io/en/stable/tutorial/tutorial.html#tutorial

Best practices https://snakemake.readthedocs.io/en/stable/snakefiles/best_practices.html#snakefiles-best-practices

YOUTUBE

https://www.youtube.com/watch?v=_dG9b3a9zkk

https://www.youtube.com/watch?v=NNPBDOBHlxo&t=655s