# Reproducibility and Snakemake

*ANF Workflow et reproductibilité en Bioinformatique*

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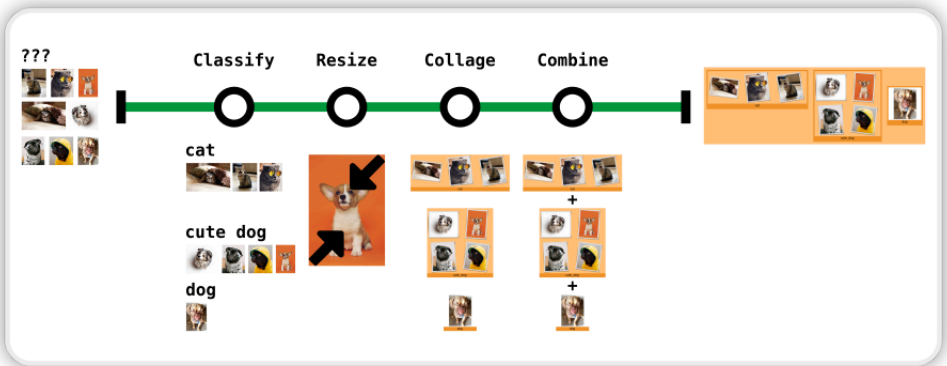
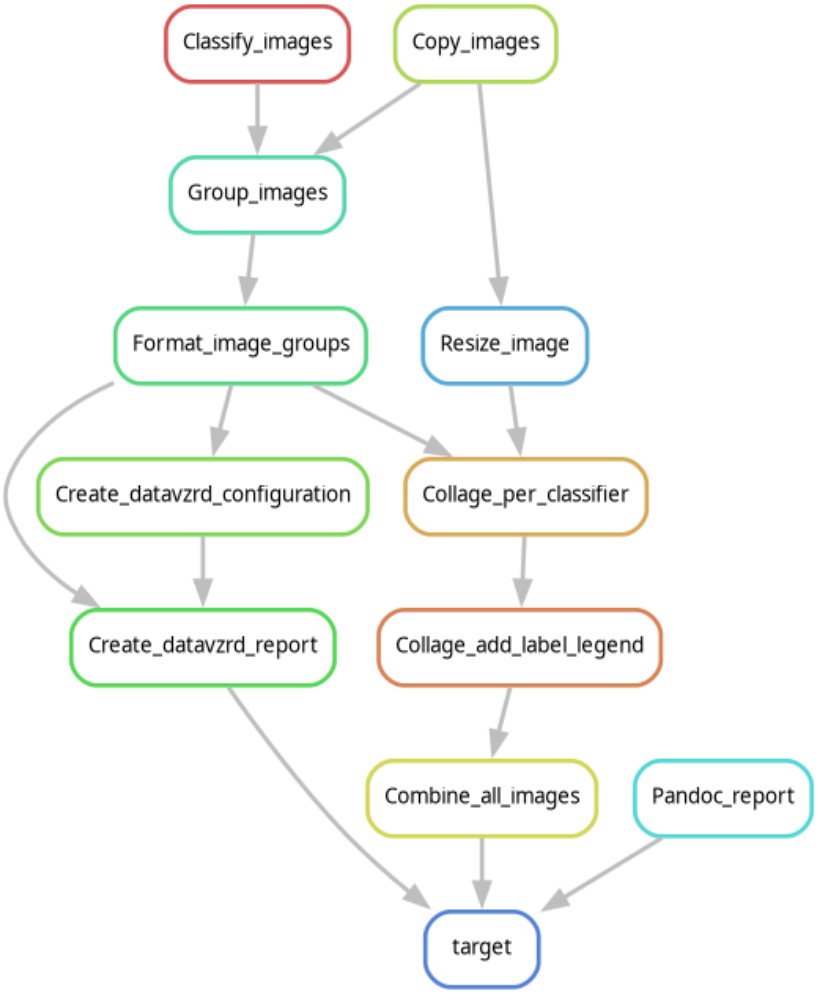
# Translate from the initial main.nf




Classify -> Classify_images (red)
Resize -> Resize_images (blue) on Copy_images (green)
Collage -> Collage_per_classifier (maron)
Collage -> Collage_add_label_legend (red)
Combine -> Combine_all_images (yellow)
+ associate: Group_images & Format_image_groups
+ report: Create_datavzrd* & Pandoc_report (blue)
+ snakemake convention: Target (blue)

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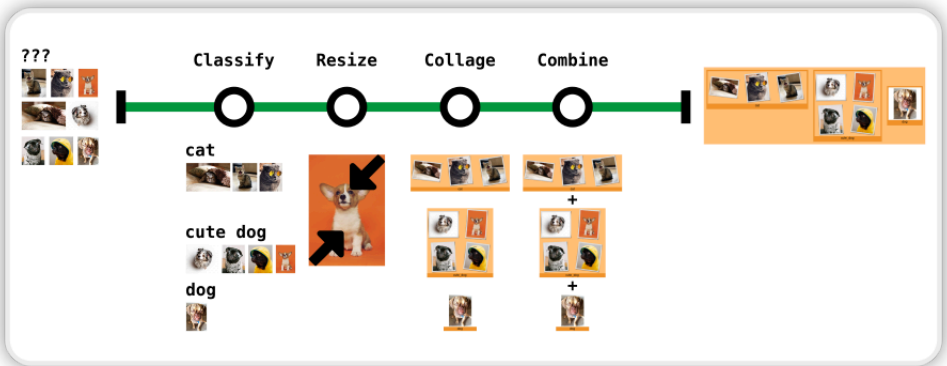


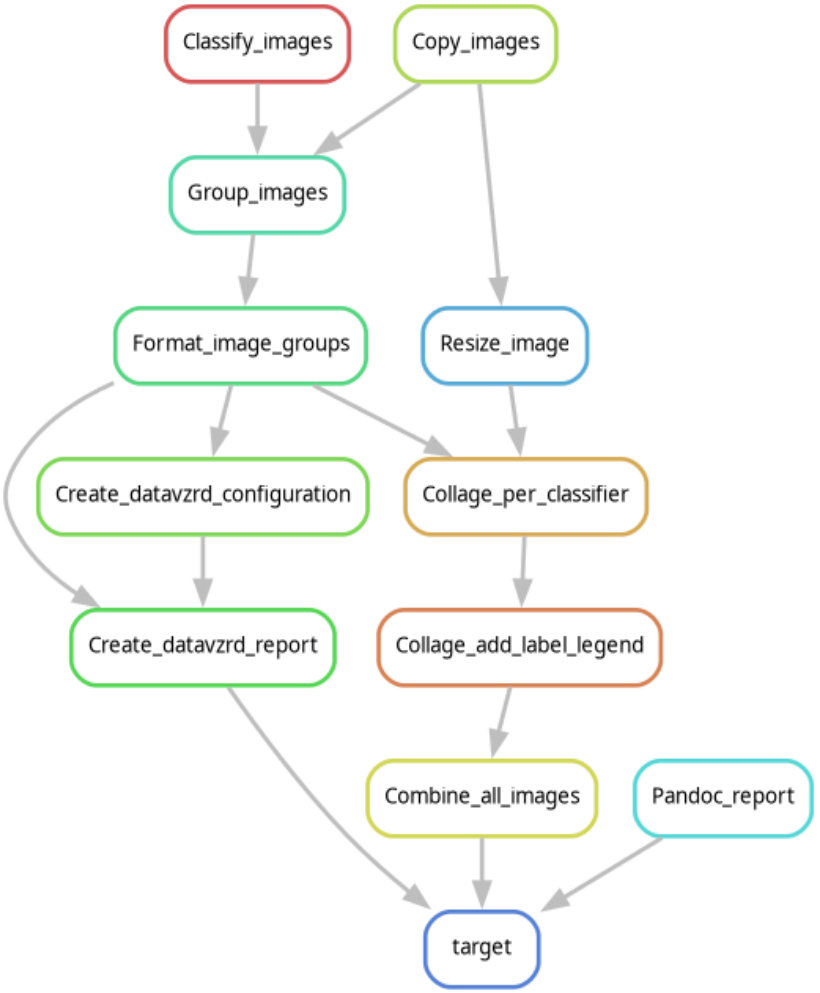


## How to get the rulegraph?

```
snakemake --rulegraph > smk_rlgraph.dot
# create a pixi.toml with graphviz (v.14.0.4)
pixi shell
dot smk_rlgraph.dot -Tpng > smk_rlgraph.png
```

# The standardized folder structure of Snakemake

1st item of the distribution-and-reproducibility section in doc (v.9.13.7)

```
Smk_translate/ # before run
├── config/
│   └── style.css
├── pyproject.toml
├── README.md
└── workflow/
    ├── ...
    └── Snakefile
```

```
pyproject.toml:
      - dependencies list (chanels)
      - test.tasks: linting, activ. env., ...
      - dev.tasks: run, clean, report fmt, ...
```

# Example of a pyproject.toml usage

```
module load pixi

pixi shell
# activate the project environment: add "(pixi shell)" upstream the promt

pixi run
# Available tasks:
#       format-all
#       format-environments
#       format-markdown
#       format-snakemake
#       snakemake-clean
#       snakemake-lint
#       snakemake-run
#       test-environments
#       test-rules
#       test-snakemake-formatting
```

# Example of a pyproject.toml usage

```
pixi run test-environments
# Using profile workflow/profiles/local for setting default command line arguments.
# To get started with GitHub CLI, please run:  gh auth login
# Alternatively, populate the GH_TOKEN environment variable with a GitHub API
authentication token.
gh auth login  # answer to questions

pixi run test-environments
# ✨ Pixi task (test-environments in test): prettier --check --parser yaml workflow/
envs/*.yaml:
# (Verify proper environment YAML formatting)
# Checking formatting...
# All matched files use Prettier code style!

pixi run snakemake-run
# ✨ Pixi task (...

exit
```

# The standardized folder structure of Snakemake

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```
pyproject.toml:
      - dependencies list (chanels)
      - test.tasks: linting, activ. env., ...
      - dev.tasks: run, clean, report fmt, ...
```

# Zoom on the workflow repository

```
Smk_translate/workflow/
├── envs/
│   ├── classify.{linux-64.pin.txt|yaml}
│   ├── datavzrd.{linux-64.pin.txt|yaml}
│   ├── grep.{linux-64.pin.txt|yaml}
│   ├── imagemagick.{linux-64.pin.txt|yaml}
│   ├── pandoc.{linux-64.pin.txt|yaml}
│   ├── README.md
│   ├── rsync.{linux-64.pin.txt|yaml}
│   └── sed.{linux-64.pin.txt|yaml}
├── profiles/
│   ├── google/
│   │   └── config.yaml
│   ├── local/
│   │   └── config.yaml
│   ├── README.md
│   └── workflow-local/
│       └── config.yaml
├── report/
│   ├── Classification_html.rst
│   ├── Classification.rst
│   ├── Collage.rst
│   ├── README.md
│   └── Thoughts.rst
├── rules/
│   ├── classify_each_image.smk
│   ├── common.smk
│   ├── datavzrd.smk
│   ├── imagemagick.smk
│   ├── pandoc_report.smk
│   └── README.md
├── scripts/
│   ├── pipeline_explanation.md
│   └── README.md
└── Snakefile
```

# How create the envs files?

```
snakedeploy pin-conda-envs <environement>.yaml
```

creates `<environnement>.{os}.pin.txt` with os standing for the runnning distribution (linux-64 bits in the project)

# Snakemake repository before and after run

1st item of the distribution-and-reproducibility section in doc (v.9.13.7)

```
Smk_translate/ # before run
├── config/
│   └── style.css
├── pyproject.toml
├── README.md
└── workflow/
    ├── ...
    └── Snakefile
```

```
# Snakefile:
include: "rules/common.smk"
include: "rules/classify_each_image.smk"
include: "rules/imagemagick.smk"
include: ...
rule target:
    input:
        "collage_all.png",
        "Thoughts.html",
        "datavzrd/Classification_table",
```

```
Smk_translate/ # after run
├── benchmark/
├── classification_table.csv
├── collage_all.png
├── config/
│   └── style.css
├── pixi.lock
├── pyproject.toml
├── README.md
├── report/
├── Thoughts.html
└── workflow/
    ├── ...
    └── Snakefile
```

# Benchmark?

Creation of tsv files with resource consumption for each rule

- snakemake run option `--benchmark-extended`
- `benchark:` directive in rule

```
rule Resize_image:
    """Part1-cli, Step3: Resize all images for each classifier"""
    input:
        "pics/{image}.png",
    output:
        temp("resized/{image}.png"),
    log:
        "logs/Resize_image/{image}.log",
    benchmark:
        "benchmark/Resize_image/{image}.benchmark"
    params:
        extra="-resize 100x100 -format png",
        outpath=lambda wildcards, output: subpath(output[0], parent=True),
    conda:
        "../envs/imagemagick.yaml"
    shell:
        "mogrify {params.extra} -path {params.outpath:q} {input:q} > {log:q} 2>&1"
```

# Report?

Creation of a self-contained HTML report with default statistics (benchmark), provenance information and user-specified results. Caption for results stands in rst (restructured text format) files

Snakemake run option `--report`

⟶ report demo: see moodle

⟶ repository of the snakemake project: `/shared/projects/2557_anf_workflow/Smk_translate`

# Bonus: conditional flows and *snakemaking* a Nextflow

- best practice for conditional flows: branch function
- best practice for unknown input/output numbers: checkpoint keyword

To resume:
Data dependent ⟶ checkpoint
Logic dependent ⟶ branch

- best practice to *snakemaking* a Nextflow workflow: handover 🤩