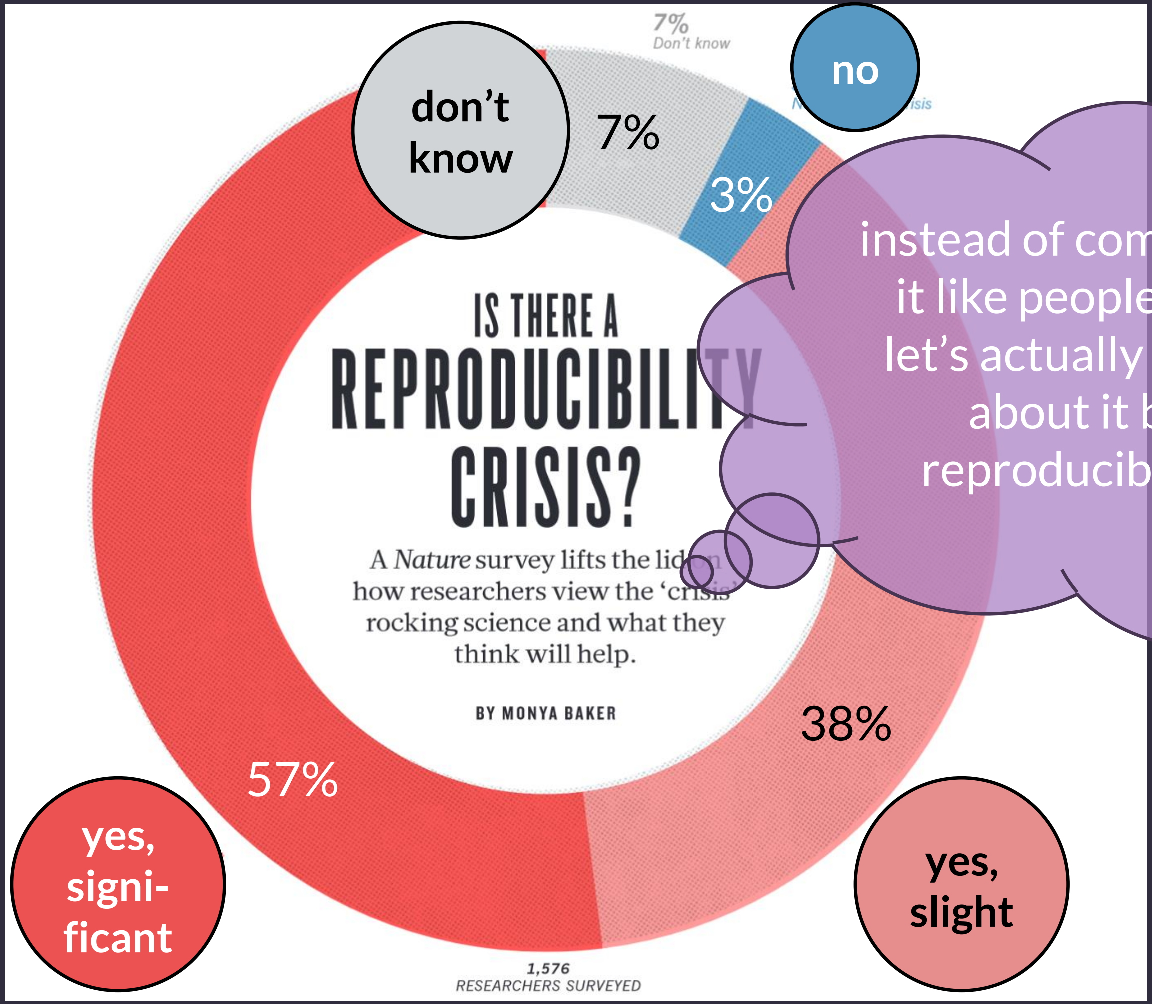
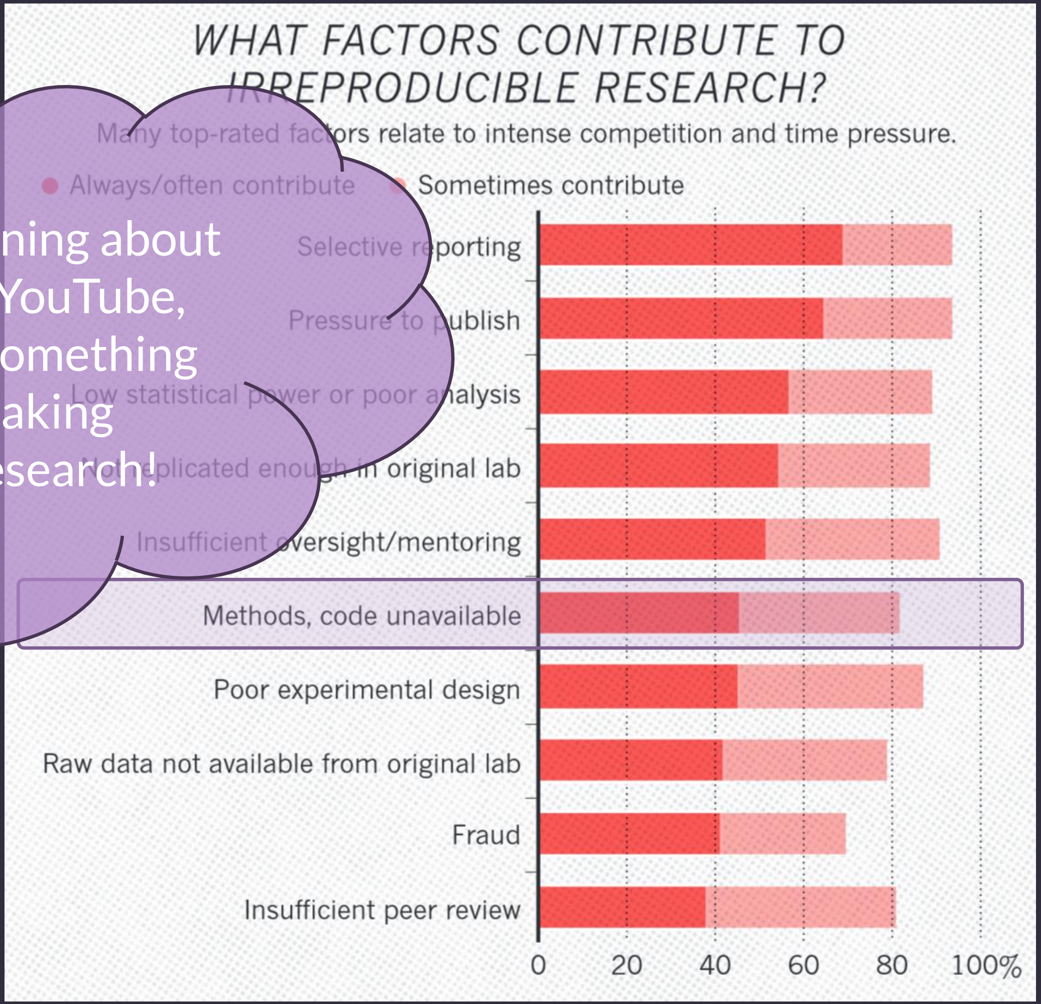
Scientific project reproducibility

PUBLISH REPRODUCIBLE PAPERS,
END THE CYCLE OF DESPAIR

Is there a reproducibility crisis…?

- 1,500 scientists lift the lid on reproducibility (Nature 533, 452–454 (2016))





instead of complaining about it like people on YouTube, let's actually do something about it by making reproducible research!

The key take-home messages for today…

1. Reproducibility is ***fundamentally important for trustworthy science***

2. Reproducibility is a ***matter of habit, not a time sink***
   - *"Reproducibility is like brushing your teeth, once you learn it, it becomes a habit"*

3. There are ***tools offering streamlined reproducible workflows***

it really is a matter of ***education***

- (clarification: these slides are about computational sciences)

We want trustworthy & confident science

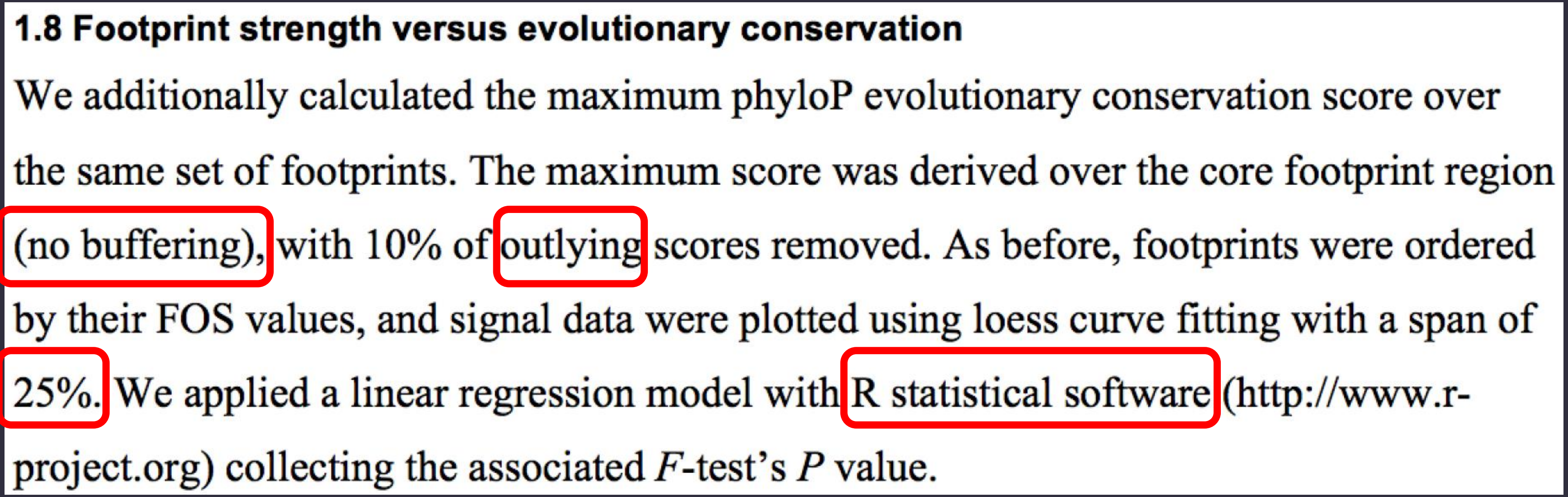
trust
hope that researchers do their stuff correctly but ***also*** allow us to examine their work openly nevertheless

confidence
the results are robust w.r.t. expected statistical variability, random number generation, computational algorithms, …

- ❑ Reproducibility is a pre-requisite for either! That's why it matters!
- ❑ Whole baggage of other reasons: accessibility, openness to public, accelerating follow-up research, fairness, education, future collaborations, …

Reproducibility == shared code

- The only way for 100%, absolutely true reproducibility is to share code
- A human-language based description of code is ***not precise enough***



1.8 Footprint strength versus evolutionary conservation

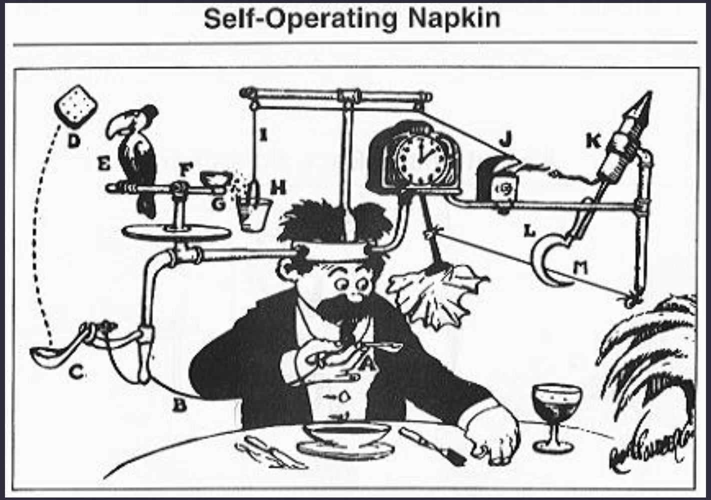
We additionally calculated the maximum phyloP evolutionary conservation score over the same set of footprints. The maximum score was derived over the core footprint region (no buffering), with 10% of outlying scores removed. As before, footprints were ordered by their FOS values, and signal data were plotted using loess curve fitting with a span of 25%. We applied a linear regression model with R statistical software (http://www.r-project.org) collecting the associated *F*-test's *P* value.

from Neph, Shane, et al. "An expansive human regulatory lexicon encoded in transcription factor footprints." Nature 489.7414 (2012): 83. (Supplement)

Saying "we used Python to do our analysis" is as useful as saying "we run the analysis on a computer"

- Furthermore, some variable's value may be forgotten in text.
  But code, ***by definition, will not run unless all variables have a value!***
- Please, always share your code! Even if it isn't good code, ***it still makes a big difference***

Principle of least gears

- Bad: 

Good:

- Rule of thumb: ***minimize the different gears used in your project***
- If you can use a ***single*** programming language/environment for ***literally everything*** in your project, from submitting jobs to cluster to generating figures, ***then do it***
  - Bad: use bash to submit to cluster, a 1,000,000,000 l.o.c. FORTRAN code to simulate climate, a C command line tool to process output, Python to analyze the simulations, and some archaic library to plot Earth maps. ***This is a real workflow in some research institutes!***
  - Better: Just use Python! Reader has to (a) only read a single language and (b) only run a single language! (wrap the libraries, submit jobs to a cluster with Python, don't use bash)

Project structure

- Follow same structure for all projects => everything is more organized => more likely to be reproducible
- On the right: DrWatson suggestion, but no golden standard exists (many templates exist, pick your favorite).
- The important thing is to be consistent!

```
│projectdir          <- Project's main folder. It is initialized as a Git
│                       repository with a reasonable .gitignore file.
│
├── _research        <- WIP scripts, code, notes, comments,
│   │                   to-dos and anything in an alpha state.
│   └── tmp          <- Temporary data folder.
│
├── data             <- **Immutable and add-only!**
│   ├── sims         <- Data resulting directly from simulations.
│   ├── exp_pro      <- Data from processing experiments.
│   └── exp_raw      <- Raw experimental data.
│
├── plots            <- Self-explanatory.
├── notebooks        <- Jupyter, Weave or any other mixed media notebooks.
│
├── papers           <- Scientific papers resulting from the project.
│
├── scripts          <- Various scripts, e.g. simulations, plotting, analysis,
│   │                   The scripts use the `src` folder for their base code.
│   └── intro.jl     <- Simple file that uses DrWatson and uses its greeting.
│
├── src              <- Source code for use in this project. Contains functions,
│                       structures and modules that are used throughout
│                       the project and in multiple scripts.
│
├── test             <- Folder containing tests for `src`.
│   └── runtests.jl  <- Main test file, also run via continuous integration.
│
├── README.md        <- Optional top-level README for anyone using this project.
├── .gitignore       <- by default ignores _research, data, plots, videos,
│                       notebooks and latex-compilation related files.
│
├── Manifest.toml    <- Contains full list of exact package versions used currently.
└── Project.toml     <- Main project file, allows activation and installation.
                        Includes DrWatson by default.
```

Use notebooks appropriately

- Notebooks (Jupyter, Weave, Pluto) are a fancy new way to code that makes a mixed medium interlacing code, markdown, and produced figures
- ***Notebooks are good for presentation, but not for creating a codebase***
- Do not abuse Notebooks for doing research!
  - Notebooks (with the exception of Pluto) are full of hidden variables
  - Notebooks do not communicate well with each other
  - Notebooks are hard to update: you need to run them through their server
  - It is really difficult to version control notebooks
  - Scripts are cleaner and train you to use a source folder structure
- Suggestion: use notebooks for structuring reports/drafts, plotting scripts, or presentations (if you use a notebook for a week or so, drop it!)
- Use a high quality IDE like VSCode for day to day work and establish a code base
  - Modern IDEs are ***truly powerful***
  - ***In fact, you can create Jupyter notebooks entirely within VSCode***

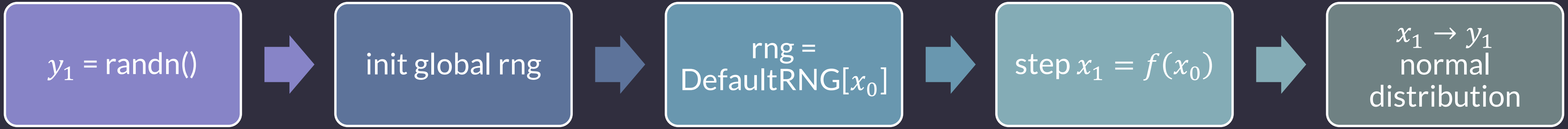
Datastructures: keep em’ simple

- ***Avoid creating new data structures, use native ones as much as possible.***
  - You want a named parameter container? Use a dictionary
  - Use the simplest possible data structure that does what you need
  - Favor existing data structures from existing packages than rolling your own
  - ***I.e., don’t reinvent the wheel please!***
- Similarly: don’t create new classes for 1 task that could be a function instead!
- Use special/new data structures for:
  - performance optimization
  - multiple dispatch
  - algorithm deciding arguments (e.g. sort(x; alg = QuickSort())
  - name space establishment when developing a software
  - developing interfaces for a new API

Deterministic code

- Computers are deterministic → you should write ***deterministic code***
  - For this, you need to understand random number generators (RNGs)

- RNGs, with the exception of true entropy sources, are not actually random
  - Some of them are chaotic maps, $x_{n+1} = f(x_n)$ with f the RNG function
  - RNGs generate sequences $X = \{x_0, x_1, \dots, x_n\}$ which are (typically) distributed uniformly and sufficiently randomly in the unit interval [0, 1).
  - X can be transformed to any distribution Y via the inverse of the cumulative density function



- If you use randomness, you should explicitly use RNG objects
  - E.g., Julia, instead of `x = rand()`, do `using Random; rng = Random.Xoshiro(seed); x = rand(rng)`.
  - This is transparent, and better performance, and allows checking for valid results by changing the seed, while it also allows reproducing the randomness using the same seed

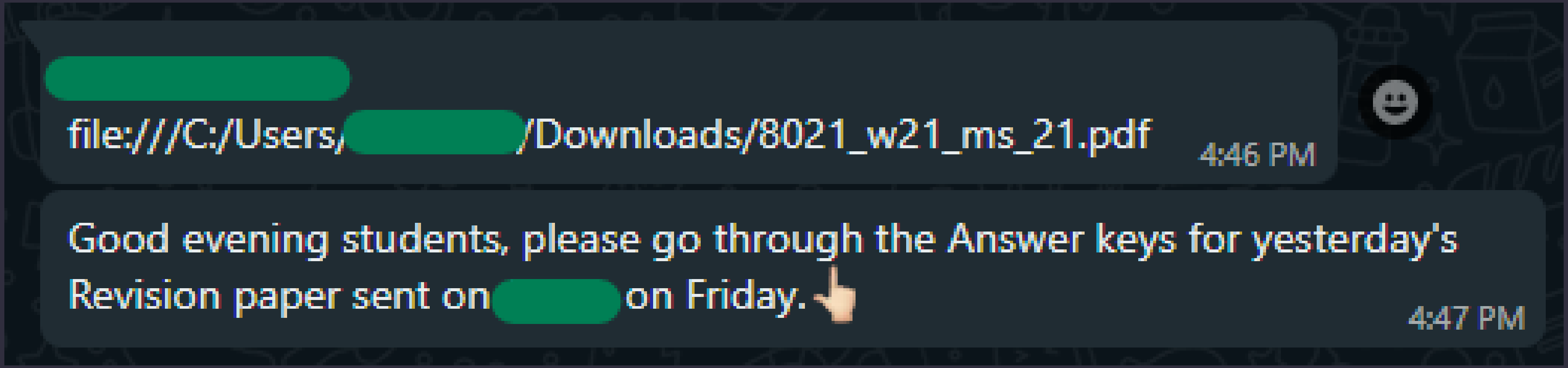
Make it work on other machines

- Often: share a project and then “nothing works”
- You want to detach your project from your machine as much as possible… but how?
- 1) Bundle project with a list of ***versions*** of every package you have used (and their dependencies)
  - How to do this? Only language-specific solutions, see next slide
- (yes, your own code should be versioned as well)

you want to absolutely avoid this hell-hole

- 2) Avoid using absolute paths
  - Try to get to root folder and use relative from there
  - Or, use e.g. `DrWatson.srcdir` instead

Next level of “but it works on my computer!”



[redacted]

file:///C:/Users/[redacted]/Downloads/8021_w21_ms_21.pdf 4:46 PM

Good evening students, please go through the Answer keys for yesterday's Revision paper sent on [redacted] on Friday.👆 4:47 PM

The SemVer2.0 versioning system

- A version is a ***unique, unchangeable*** identifier of a code base's contents
  - Establishes reproducibility, compatibility, and (tries to) eliminate dependency hell
  - Any software used in published research must have an associated published version. If not, it is like citing "the conversation you had at the bar with that dude".

- ***Semantic Versioning 2.0.0*** is a well-established standard for versioning software. Given a version number vMAJOR.MINOR.PATCH, increment the:
  1. MAJOR version when you make backwards-incompatible API changes,
  2. MINOR version when you add new functionality in a backwards compatible manner, and
  3. PATCH version when you make backwards compatible bug fixes.
  - Example: code using v1.2.1 is compatible with versions [1.2.1, 2)
  - Example: code using v1.4.2 is NOT compatible with v1.3 because of (potentially) new API

- All software should have a CHANGELOG.md with noteworthy changes!

One science project = one environment

- Most programming languages allow the concept of “environments”
  - They are self-contained “spaces” where one can add packages and track package versions and specify compatibility bounds to packages
  - Once “activated”, the packages loaded on `import` statements are the versions specified
  - They can be shared with other users and instantiated in other computers
  - They allow for reproducible code by ensuring everyone runs the same versions
  - By default, there is the “global environment” which is what is activated when the language starts, but you shouldn’t be using this for scientific work
- ***Each project should have its own environment!***
  - This allows confidence that each project doesn’t break over time due to updates elsewhere
- To create or activate an environment and add packages to it:

Julia

```julia
using Pkg; Pkg.activate("path")
Pkg.add("PackageName")
```

Python

```
conda env create -n <NAME>  # create a new environment
conda activate <NAME>  # switch to an existing environment
conda install <PKGNAME>   # add a package
```

Bundling project with package versions

- Julia: a file `Project.toml`:

```
name = "ScienceProjectTemplate"
[deps] # Specifies dependencies (no compat bounds)
Documenter = "e30172f5-a6a5-5a46-863b-614d45cd2de4"
DrWatson = "634d3b9d-ee7a-5ddf-bec9-22491ea816e1"
[compat] # Specifies versions
DrWatson = "2.9.1"     # Default: SemVer compatible
Documenter = "≥ 0.27" # 0.27 or upper, any
julia = "1.7.0"
```

- Julia's package manager generates a `Manifest.toml` file based on the above with exact versions of all dependencies
- To reproduce an environment: get the Project.toml containing folder, and then run:

```
using Pkg; Pkg.activate("path/to/Project.toml")
Pkg.instantiate()
```

- Python: a file `environment.yml`:

```
name: my-awesome-environment
dependencies:
    - python >= 3.9
    - matplotlib >= 3.0.0
    - numpy >= 1.21.6
    - pytest
```

- A machine file with all exact versions can be made with `conda list -e`
- To reproduce an environment from the `environment.yml` run:

```
conda env create -f environment.yml
```

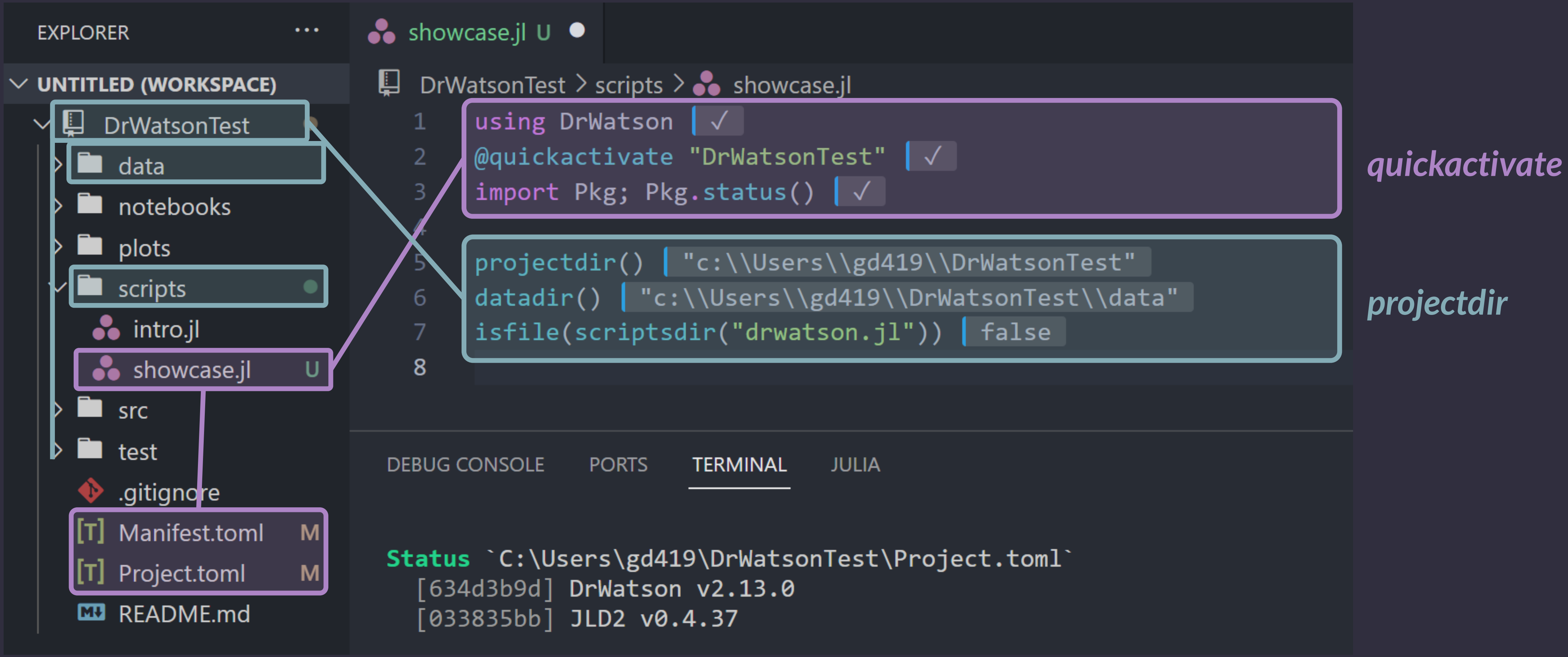
DrWatson

The perfect sidekick to your scientific inquiries

- DrWatson is a ***scientific project assistant*** software.
  - Full disclaimer, I’m a developer, so this is partly an advertisement
- It is a package for Julia, that is used within the language (no external tooling)
- Among other things, it helps you with:
  - *making self-contained reproducible projects; activating projects on run-time and enabling local pathing from root; automatic encapsulation of git status in saved output files; automating project input-to-output pipelines using configuration files; preparing ensemble simulations collecting and filtering simulation output files*
- Last time we checked, no real alternatives, but similar packages in other languages:
  - Cookiecutter (Python), Sumatra (Python/R/Matlab), ReproZip, explore (Matlab), recipy (Python)

Project activation and directories linkage

- Stressed importance of self-contained environments and versioning…
- DrWatson wraps a science project around two functionalities:



```julia
using DrWatson ✓
@quickactivate "DrWatsonTest" ✓
import Pkg; Pkg.status() ✓

projectdir() "c:\\Users\\gd419\\DrWatsonTest"
datadir() "c:\\Users\\gd419\\DrWatsonTest\\data"
isfile(scriptsdir("drwatson.jl")) false
```

```
Status `C:\Users\gd419\DrWatsonTest\Project.toml`
  [634d3b9d] DrWatson v2.13.0
  [033835bb] JLD2 v0.4.37
```

Including git information in saved output

- Git = time travel of coding
- science repo == git repo => time travel of scientific results

```
using DrWatson
@quickactivate "MyProject"

~~save(datadir("test.jld2"), data)~~

@tagsave(datadir("test.jld2"), data)

Dict{String, Any} with 5 entries:
  "v"           => [0.396466, 0.218657, 0.582683, 0.542067, 0.0671513]
  "method"      => "linear"
  "gitcommit"   => "28057cec9331a17965e0fbad63cf9b26d937e5ab"
  "script"      => "docs/build/string#3"
  "b"           => 3
```

QoL for simulation input-output

Easily create input combinations

```
julia> d = Dict(:a => [1, 2], :b => 4,
    :c => @onlyif(:a == 1, [10, 11]));

julia> dict_list(d)
3-element Array{Dict{Symbol,Int64},1}:
 Dict(:a => 1,:b => 4,:c => 10)
 Dict(:a => 1,:b => 4,:c => 11)
 Dict(:a => 2,:b => 4)

 julia> d = Dict(:a => [1, 2], :b => 4,
    :c => [10, @onlyif(:a == 1, 11)]);

 julia> dict_list(d)
 3-element Array{Dict{Symbol,Int64},1}:
 Dict(:a => 1,:b => 4,:c => 10)
 Dict(:a => 1,:b => 4,:c => 11)
 Dict(:a => 2,:b => 4,:c => 10)
```

Collect saved simulations into a dataframe

```
res = collect_results(datadir("test"); ...)

8×4 DataFrame
 Row │ model     N       x          noise
     │ String?   Int64?  Float64?   Float64?
─────┼─────────────────────────────────────────
   1 │ kuramoto     100  0.188024   missing
   2 │ barkley      100  0.034592   missing
   3 │ kuramoto     100  0.72311          0.075
   4 │ barkley      100  0.0658607        0.075
   5 │ kuramoto     100  0.723048   missing
   6 │ barkley      100  0.588487         0.075
   7 │ kuramoto     100  0.524076         0.075
   8 │ barkley      100  0.961053   missing
```

Files that don't have parameters existing in other files get the `missing` value!

Recap of the tips for reproducible science

1. Share code. Please. The most ugly code on the planet is better than no code.
2. Principle of least gears
3. Follow the same folder layout in all your science projects
4. Use RNG objects for reproducible randomness
5. Datastructures: keep em' simple and use native ones as much as possible!
6. Use notebooks (Jupyter) appropriately
7. Ensure your project works on other machines as well
8. Use a self-contained environment for each different science project
9. Use tools that help you do clean & reproducible science like DrWatson

How I make a 100% reproducible project

1. Initialize a DrWatson project and add all packages I foresee using
2. Open three columns in my IDE: source, script, console
3. Start doing the analysis on middle column, the script, which uses DrWatson
4. Functionality of general purpose goes to the source file after creation in script
5. Periodically the code base is reorganized to more script and source files
6. When ready to publish:
   - Make one script per paper figure or table that needs numbers
   - Publish the entire code repository (+ README, Project.toml, Manifest.toml) on GitHub
   - Assign a DOI to the GitHub repo via Zenodo.org. Then, cite the DOI in the paper!
   - Example: Minimal recipes for global cloudiness (latest paper with code base)

Your code → reproducible project

- Ensure you have an intuitive folder structure (source, scripts, plots, data, …)
- Ensure you only use local/relative directories in the codebase

- Bundle your project with the appropriate environment
  - How does your language stores which package versions you used?
  - How do you bundle this information with your project?
  - How does someone that wants to reproduce your figure “instantiate” this environment?
  - Have this info in your README!

- Your exercise partner pulls latest version from GitHub and tries to reproduce it
  - Do not upload large datasets on GitHub. Instruct in the README where to find it.

Your code → released and citable with DOI!

- You are ready to release the first version of your code!
- Hell, you can even attach a Digital Object Identifier to it!
- Here's how! (I'll show steps online as well)

- Create a Zenodo account at Zenodo.org and link your GitHub account there!
- Navigate to the repository of interest and "turn on" the DOI badge button!
- Go back to GitHub and create a new "Release"!
  - Typically first running release has version 0.1.0
- Go back to Zenodo, and you'll see you now have an associated DOI with this release!
- Transform it into BibTeX with https://www.bibtex.com/c/doi-to-bibtex-converter/ !
- Cite it in your paper! MUCH SUCCESS MUCH WOW!!!!