### Agenda

### Boost your reproducibility with Binder

- 13:30 Registration and introductions
- 13:40 Introduction to the workshop and The Turing Way
- 13:50 Presentation: Why you need a reproducible computing environment and how Binder can help
- 15:00 Coffee break
- 15:30 Code along demo: Zero to Binder, build a Binder resource
- 16:30 Build your own Binder
- 16:50 Feedback, group picture and close

#### The Alan Turing Institute

### Reproducible Computational Environments

Kirstie Whitaker

Pronouns: she/her



#### The science is the code

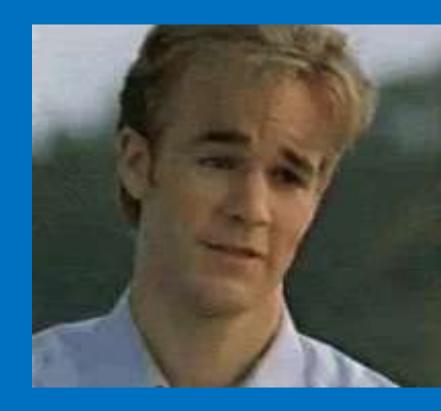
An article about computational science in a scientific publication is not the scholarship itself, it is merely advertising of the scholarship. The actual scholarship is the complete software development environment and the complete set of instructions which generated the figures.

Buckheit and Donoho (paraphrasing John Claerbout) WaveLab and Reproducible Research, 1995

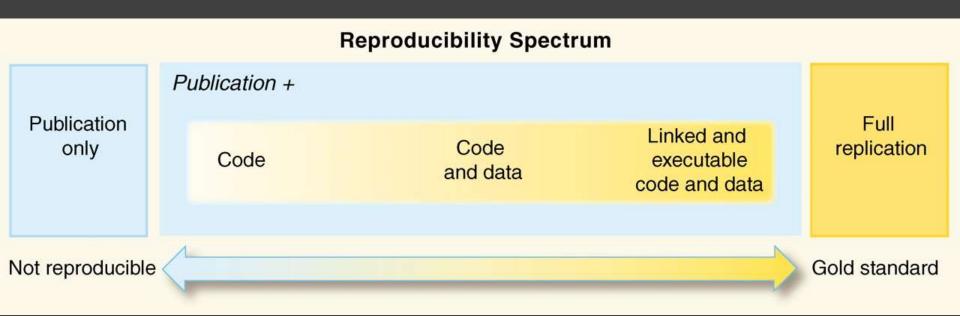
Slide courtesy of Chris Holdraf and the Jupyter Team

# **Upsetting take home message**

Sharing your code and data isn't enough



### You need the computational environment too



### You need the computational environment too



## The computational environment includes:

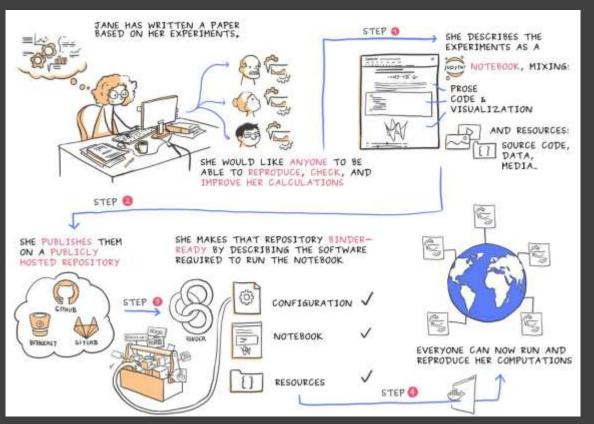
- Hardware (GPU, CPU)
- Operating system (mac, windows, linux)
- Software
  - Language version
  - Package version(s)

## And all the interactions between the layers



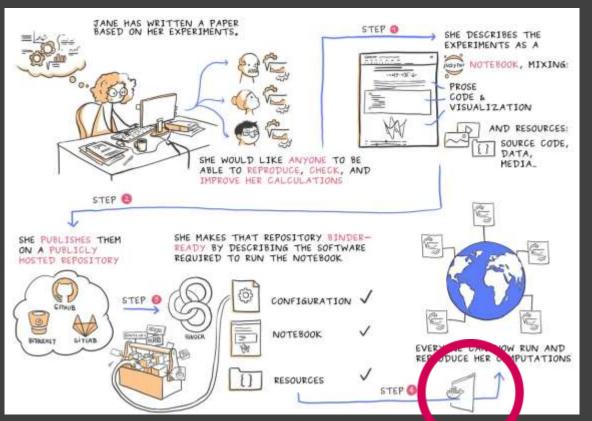
### What is Binder?





Courtesy of Juliette Taka: https://twitter.com/mybinderteam/status/1082556317842264064 #TuringWay @kirstie\_j @mybinderteam

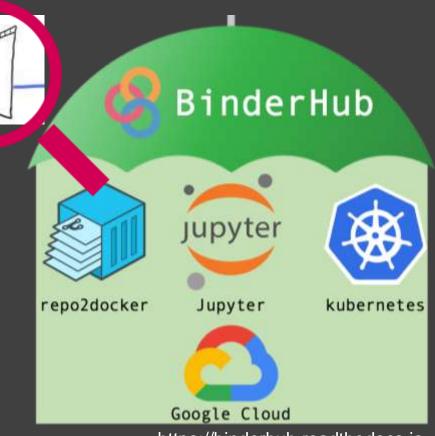
https://doi.org/10.5281/zenodo.3632913



Courtesy of Juliette Taka: https://twitter.com/mybinusrteem/catus/1082556317842264064 #TuringWay kirstie\_j @mybinderteam

https://doi.org/10.5281/zenodo.3632913

- Coordinate cloud
   computing resources
   with Kubernetes (k8s)
- Make it easy for users to access with a JupyterHub
- Set up the environment from your GitHub repository



https://binderhub.readthedocs.io #TuringWay @kirstie\_j @mybinderteam https://doi.org/10.5281/zenodo.3632913

#### Sarah Gibson

"It took me a while to feel like I knew enough to contribute to Binder. But the team are always so excited to have my input. Its really motivating to be part of such a welcoming community."



https://www.turing.ac.uk/people/researchers/sarah-gibson #TuringWay @kirstie\_j @mybinderteam https://doi.org/10.5281/zenodo.3632913

- Check analysis on my phone
- Share the responsibility with busy PIs
- Requires version
   control, capturing
   environment and new
   build for each change





#### Table of Contents

Getting started with Binder

Getting started with Binder Common usage patterns in Binder

#### How to ...

Choose languages for your environment Configure the user interface Generate custom launch badges for your Binder repository Track repository data on mybinder.org

#### What is mybinder.org?

mybinder.org is a single deployment of a BinderHub instance, managed by the Binder community. It serves as both a public service and a demonstration of the BinderHub technology, though it is by no means the only BinderHub in existence. If you're interested in deploying your own BinderHub for your own uses, please see the BinderHub documentation and don't hesitate to reach out to the Binder community.

For more information, check out About mybinder.org.

#### Is mybinder.org free to use?

Yes! Though note that it has relatively limited computational resources.

#### How much does running mybinder.org cost?

Great question! If you're interested in the technical costs of running mybinder.org, we publish a semi-up-to-date dataset of our costs at the binder-data repository. In addition, you can explore these costs with the binder link below!

launch binder

#### How can mybinder.org be free to use?

#### On this page

What is a Binder?
What is the Binder community?
What is BinderHub?
What is mybinder.org?
Is mybinder.org free to use?
How much does running
mybinder.org cost?
How can mybinder.org be free to
use?
How much memory am I given
when using Binder?
How long will my Binder session
last?

Can I use mybinder.org for a live demo or workshop?

How does mybinder.org ensure user privacy?

How secure is mybinder.org?

Where can I report a security issue? Can I push data from my Binder session back to my repository?

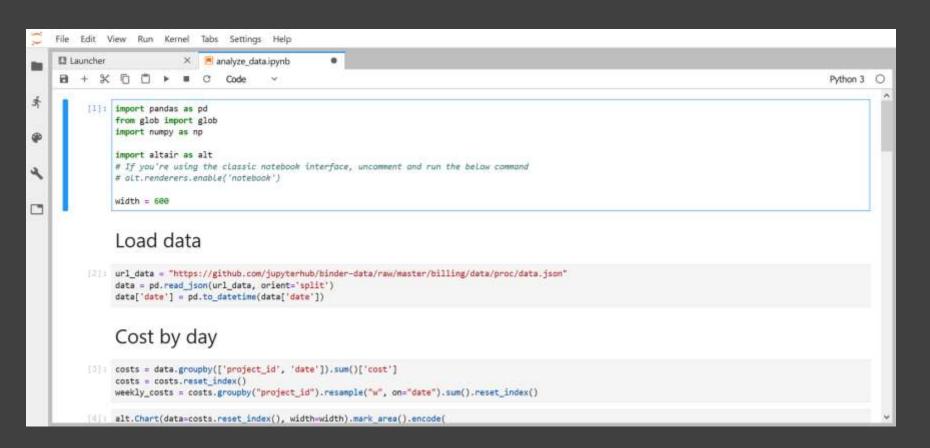
Can I put my configuration files outside the root of S v. lalest ▼

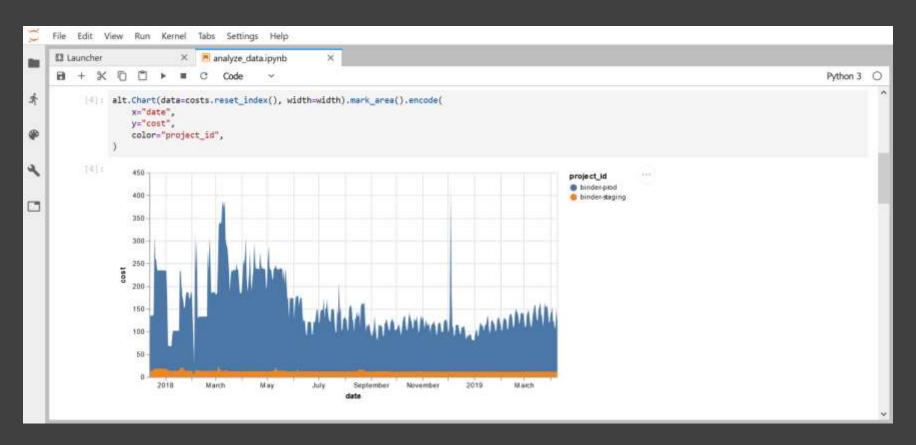
What factors influences takes a Binder session to start?

Will repos with fewer notebooks launch faster? Should I split my









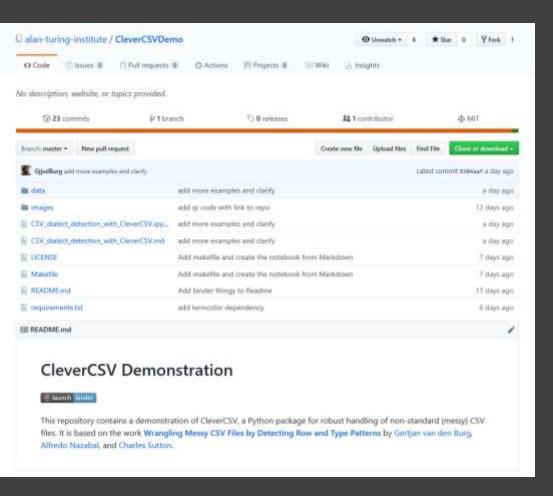
https://mybinder.readthedocs.io/en/latest/faq.html#how-much-does-running-mybinder-org-cost #TuringWay @kirstie\_j @mybinderteam https://doi.org/10.5281/zenodo.3632913

### Gertjan van den Burg

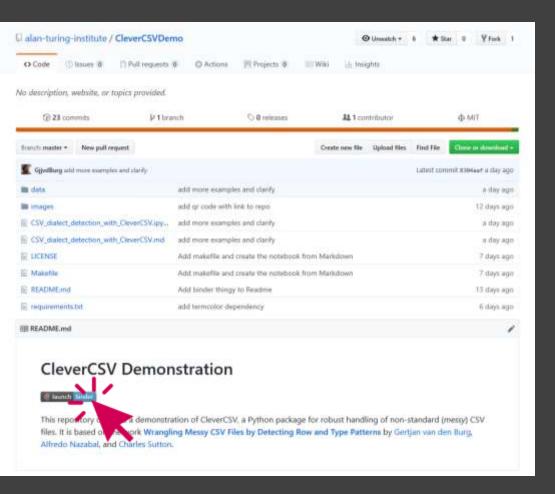
"The fun part of data science is the modelling. Being able to read in information from a csv file should not be the hardest part."



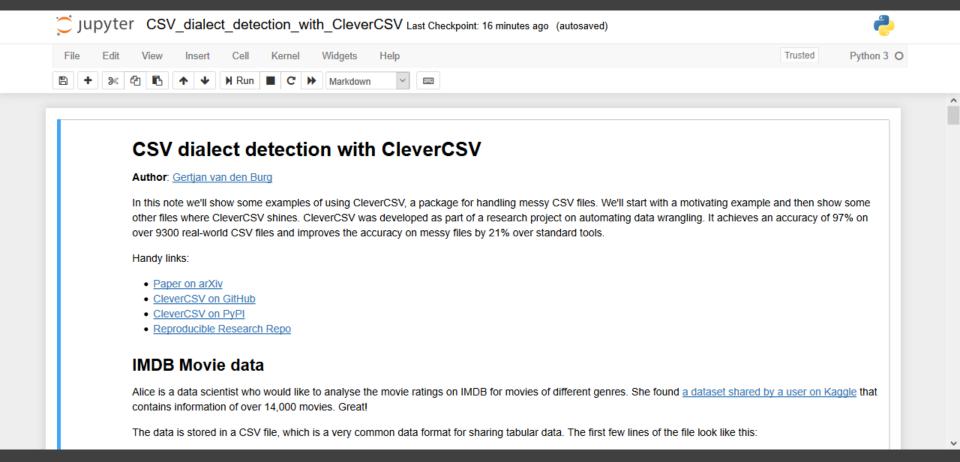
https://gertjanvandenburg.com #TuringWay @kirstie\_j @mybinderteam https://doi.org/10.5281/zenodo.3632913



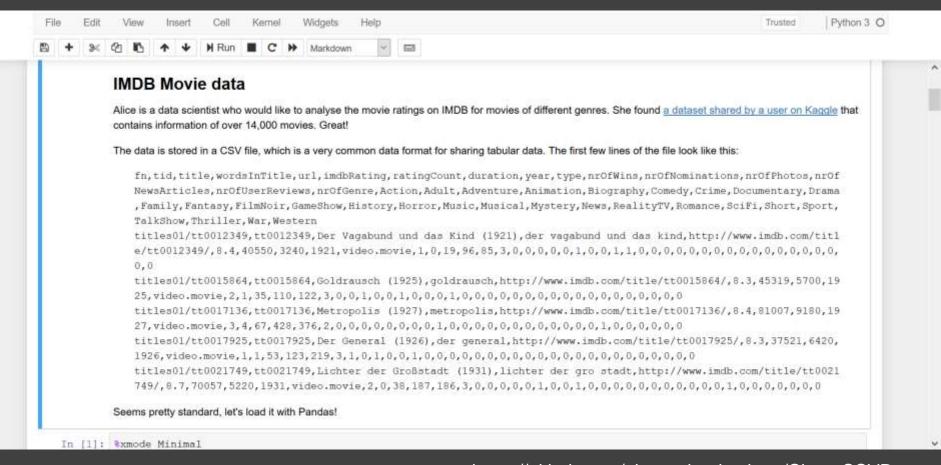
#### https://github.com/ alan-turing-institute/ CleverCSVDemo

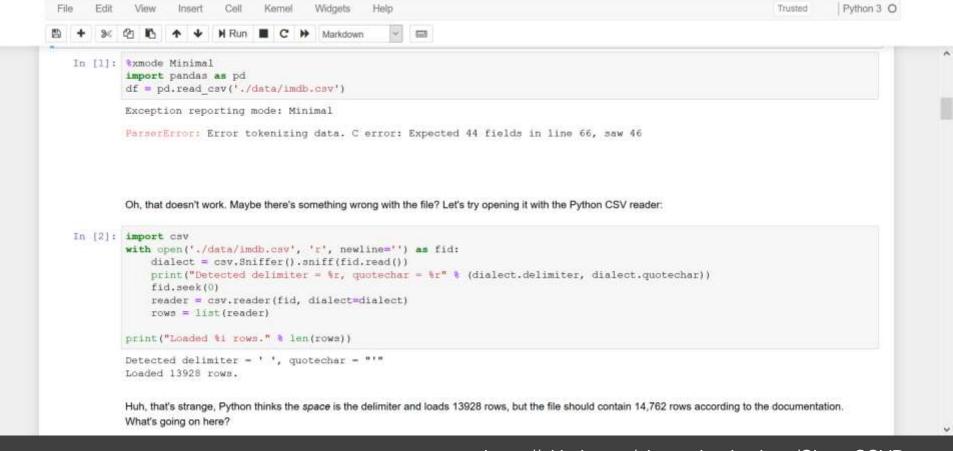


- https://github.com/alan-turing-institute/CleverCSVDemo
- "Wrangling Messy
   CSV Files by
   Detecting Row and
   Type Patterns"
   arXiv:1811.11242

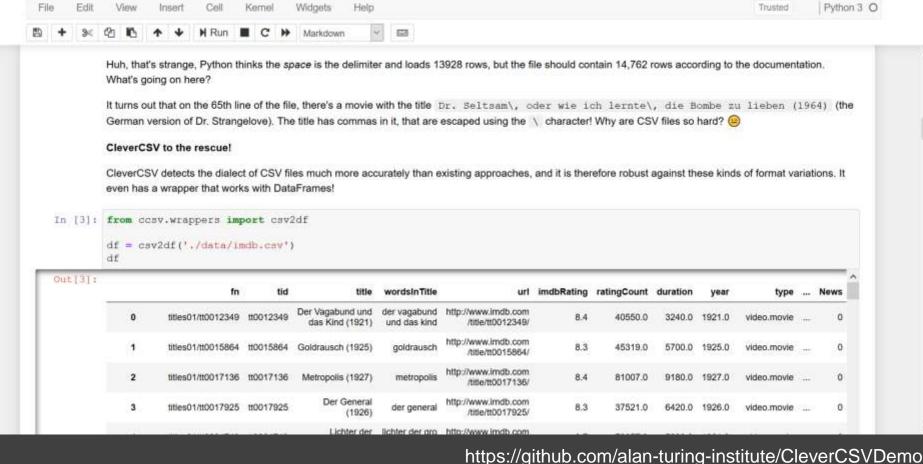


https://github.com/alan-turing-institute/CleverCSVDemo #TuringWay @kirstie\_j @mybinderteam https://doi.org/10.5281/zenodo.3632913

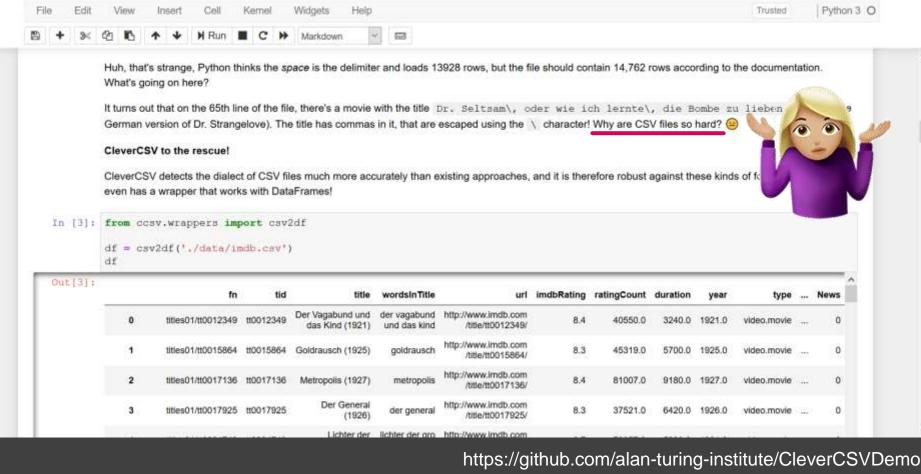




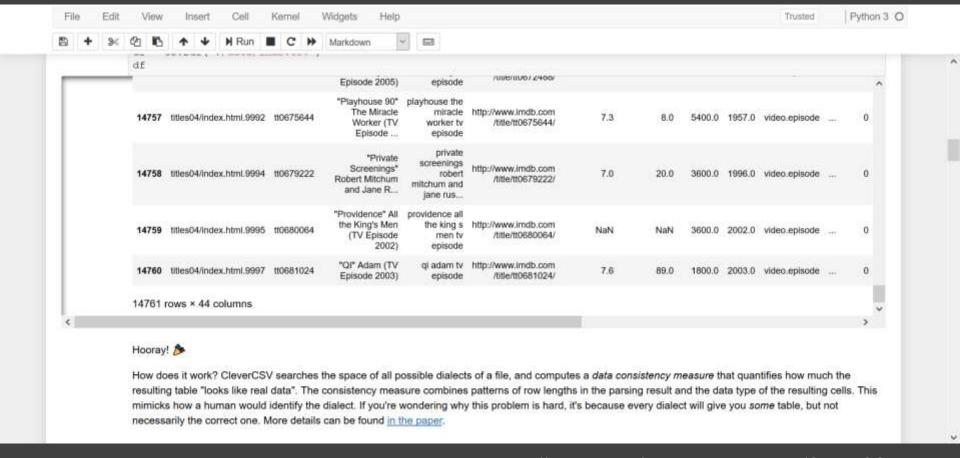
https://github.com/alan-turing-institute/CleverCSVDemo #TuringWay @kirstie\_j @mybinderteam https://doi.org/10.5281/zenodo.3632913



nttps://github.com/alan-turing-institute/CleverCSVDemo #TuringWay @kirstie\_j @mybinderteam https://doi.org/10.5281/zenodo.3632913



nttps://github.com/alan-turing-institute/CleverCSVDemo #TuringWay @kirstie\_j @mybinderteam https://doi.org/10.5281/zenodo.3632913



https://github.com/alan-turing-institute/CleverCSVDemo #TuringWay @kirstie\_j @mybinderteam https://doi.org/10.5281/zenodo.3632913 Defining your computational environment



### pip freeze

- Python Package Index (PyPI)
- Pip is a recursive
   acronym that can
   stand for either "Pip
   Installs Packages" or
   "Pip Installs Python"

#### pip freeze

#### Contents

- pip freeze
  - Usage
  - Description
  - Options
  - Examples

#### Usage

pip freeze [options]

### pip freeze

- pip freeze
   captures the versions
   of all packages that
   you're currently using
- Can print to screen or save in a file called requirements.txt

#### Examples

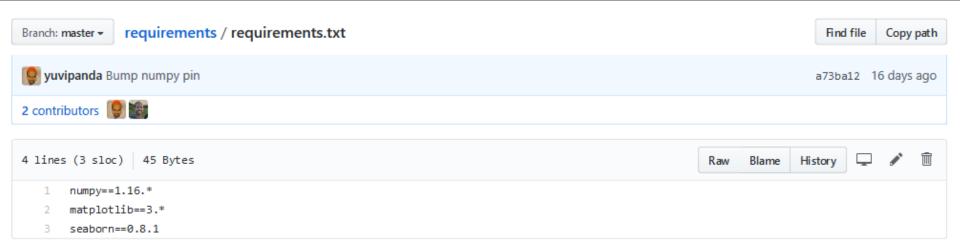
Generate output suitable for a requirements file.

```
$ pip freeze
docutils==0.11
Jinja2==2.7.2
MarkupSafe==0.19
Pygments==1.6
Sphinx==1.2.2
```

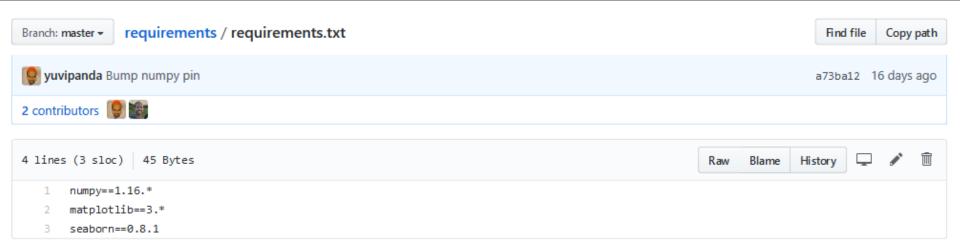
2. Generate a requirements file and then install from it in another

```
$ env1/bin/pip freeze > requirements.txt
$ env2/bin/pip install -r requirements.txt
```

### Binder example: requirements.txt



### Binder example: requirements.txt



#### Conda env create

- Package manager for multiple languages
- Information about installed software saved in file called environment.yml

#### Creating an environment from an environment.yml file

Use the terminal or an Anaconda Prompt for the following steps:

1. Create the environment from the environment.yml file:

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

The first line of the yml file sets the new environment's name. For details see Creating

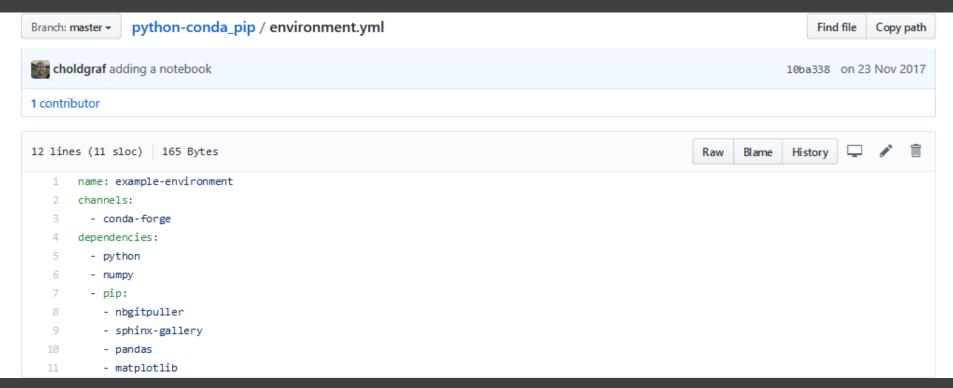
- 2. Activate the new environment: conda activate syeny
- 3. Verify that the new environment was installed correctly:

```
conda env list
```

You can also use conda info --enva -

```
https://docs.conda.io/projects/conda/en/latest/user-guide/tasks/manage-environments.html
https://the-turing-way.netlify.com/
reproducible_environments/02/package-management.html
```

### Binder example: environment.yml



### install.R

- Binder interface includes Rstudio
- install.R contains required packages
- runtime.txt sets
  the version on MRAN

#### Specifying an R environment with a runtime.txt file

Jupyter+R: @ tourich binder

RStudio: Studio: Ilirober

RShiny: Raunds beating

Binder supports using R and RStudio, with libraries pinned to a specific snapshot on MRAN.

You need to have a runtime, txt file that is formatted like:

P--(YYYY)--(MH)--(DD)-

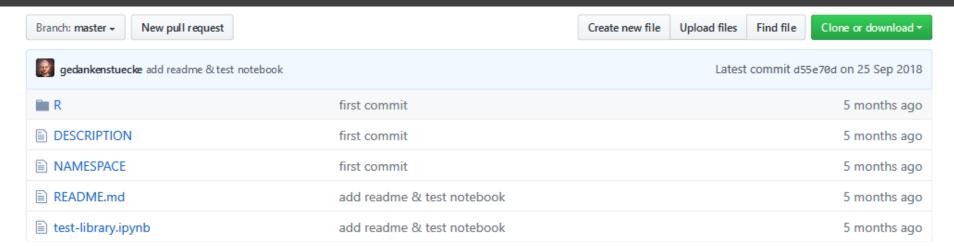
where YYYY-MM-DD is a snapshot at MRAN that will be used for installing libraries.

You can also have an install. R file that will be executed during build, and can be used to install

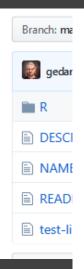
Both RStudio and IRKernel are installed by default, so you can use either the Jupyter notebool the RStudio interface.

This repository also contains an example of a Shiny app.

### Binder example: install.R



### Binder example: install.R



#### Specifying an R environment by having a DESCRIPTION file

Jupyter+R: launch binder

RStudio: launch binder

Binder supports using R and RStudio, with libraries pinned to a specific snapshot on MRAN.

If you specify a runtime.txt file that is formatted like:

r-<YYYY>-<MM>-<DD>

where YYYY-MM-DD it will use the MRAN snapshot of that day for setting up the R runtime.

Without specifying a runtime.txt it will use a 2-day old snapshot of MRAN.

Both RStudio and IRKernel are installed by default, so you can use either the Jupyter notebook interface or the RStudio interface.

Sep 2018
onths ago
onths ago
onths ago

onths ago

#### **Becky Arnold**

"There are a lot of things you need to know before you can jump into continuous integration.

Version control is a prerequisite for pretty much everything."



https://software.ac.uk/about/fellows/becky-arnold #TuringWay @kirstie\_j @mybinderteam https://doi.org/10.5281/zenodo.3632913

# Distributed and remote version control



#### "FINAL".doc

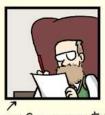












FINAL\_rev.6.COMMENTS.doc

FINAL\_rev.8.comments5. CORRECTIONS.doc

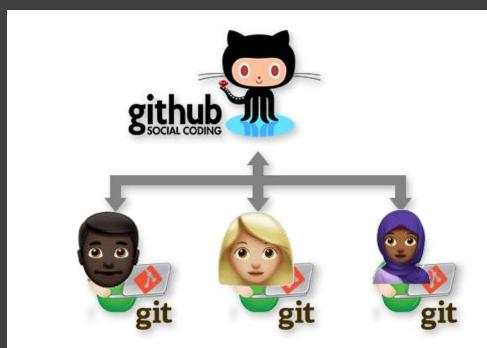






FINAL\_rev.18.comments7. corrections9.MORE.30.doc

FINAL\_rev.22.comments49. corrections.10.#@\$%WHYDID ICOMETOGRADSCHOOL????.doc



http://phdcomics.com/comics/archive.php?comicid=1531 #TuringWay @kirstie\_j @mybinderteam https://doi.org/10.5281/zenodo.3632913

## The cloud is just someone else's computer



Solutions

Pricina

Documentation Learn

Partner Network

AWS Marketplace

Explore More Q

**Our Data Centers** 

AWS pioneered cloud computing in 2006, creating cloud infrastructure that allows you to securely build and innovate faster. We are continuously innovating the design and systems of our data centers to protect them from manmade and natural risks. Then we implement controls, build automated systems, and undergo third-party audits to confirm security and compliance. As a result, the most highly-regulated organizations in the world trust AWS every day. Take a virtual tour of one of our data centers to learn about our security approach to protect the data of millions of active monthly customers.



#TuringWay @kirstie\_j @mybinderteam https://doi.org/10.5281/zenodo.3632913

https://aws.amazon.com/compliance/data-center/data-centers



Solutions

Pricina

AWS data center physical security begins at the Perimeter Layer. This

facation, such as security quants, fencing, security feeds, intrusion

layer includes a number of security features depending on the

detection technology, and other security measures.

EXPLORE \*

the only area that holds comoner data. Protection begins by

protocols, further safeguarding this layer.

Documentation Learn Partner Network AWS Marketplace

Explore More

#### **Our Data Centers** AWS pioneered cloud computing in 2006, creating cloud infrastructure that allows you to securely build and innovate faster. We are continuously innovating the design and systems of our data centers to protect them from man-PERIMETER LAYER DATA LAYER



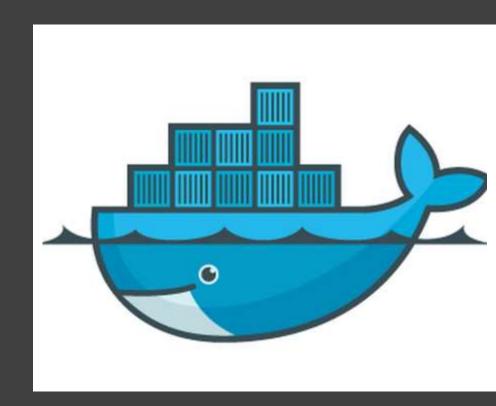
DIPLOSE +

## Containers

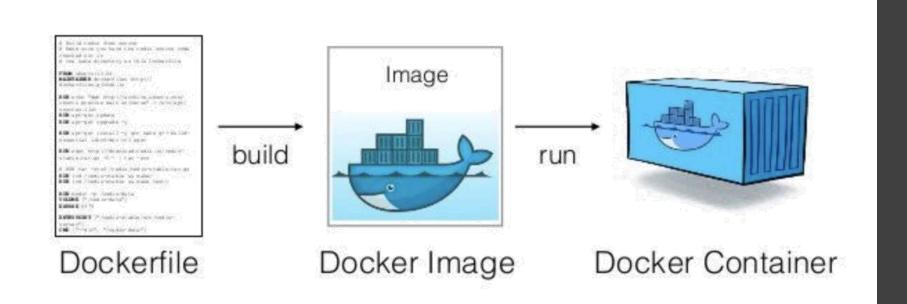


#### Docker

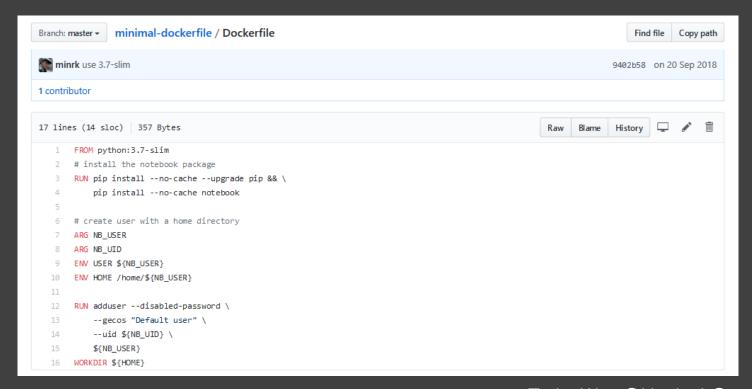
 A container that bundles all the infrastructure and software together.



#### Human and machine readable files



### Binder example: docker



## Small group exercise



## Small group exercise Get into groups of 2-3 and explore these examples

- Are there differences between different branches?
- Does that give different results?
- Did you get what you'd expect?

https://github.com/alan-turing-institute/

the-turing-way/blob/master/

workshops/

boost-research-reproducibility-binder/

paired\_examples.md

#### Zero to Binder

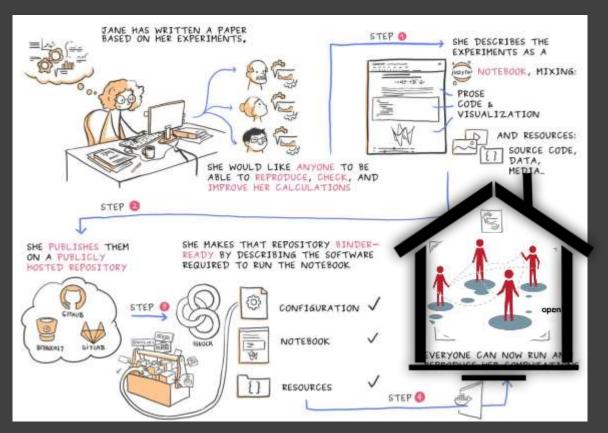
#### Please open these instructions in your browser

```
https://github.com/alan-turing-institute/
the-turing-way/blob/master/
workshops/
boost-research-reproducibility-binder/
workshop-presentations/
zero-to-binder.md
```

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Courtesy of Juliette Taka: https://twitter.com/mybinderteam/status/1082556317842264064

# The Alan Turing Institute

8 binder



Loading repository (can take 30s or more to load): sgibson91/branchLSTM/sgibson91python-runtime-patch

Build logs

Here's a non-interactive preview on noviewer while we start a server for you. Your binder will open automatically when it is ready.

JUPYTER FAQ O 8

branch/LSTM sighbour91python-runtime-patch

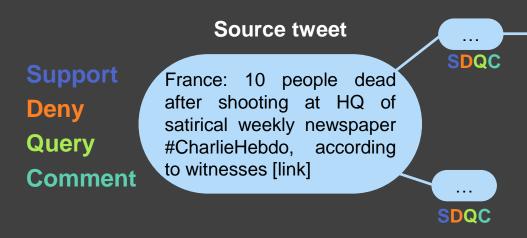
https://github.com/kochkinaelena/branchLSTM (on Turing Way Hub)
#PyDataLDN #TuringWay @kirstie j

https://doi.org/10.5281/zenodo.3632913

## Champion: Elena Kochkina

Turing at SemEval-2017 Task 8: Sequential Approach to Rumour Stance Classification with Branch-LSTM

Elena Kochkina, Maria Liakata, Isabelle Augenstein

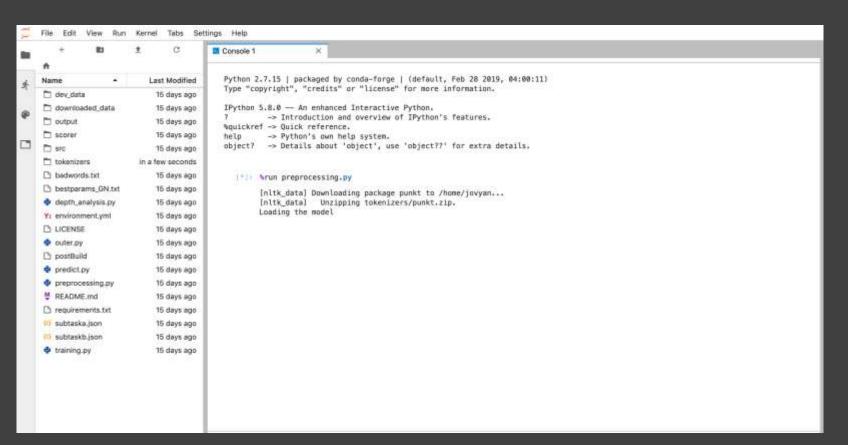


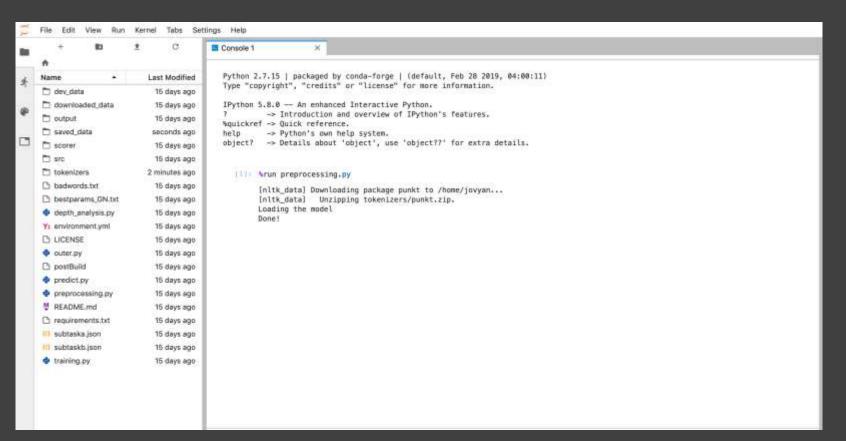
Prediction Label	С	D	Q	S
Commenting	760	0	12	6
Denying	68	0	1	2
Querying	69	0	36	1
Supporting	67	0	1	26

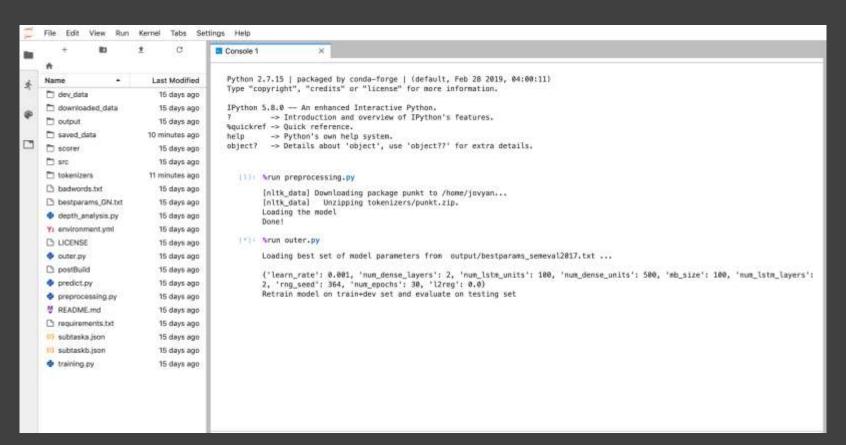
SDQC

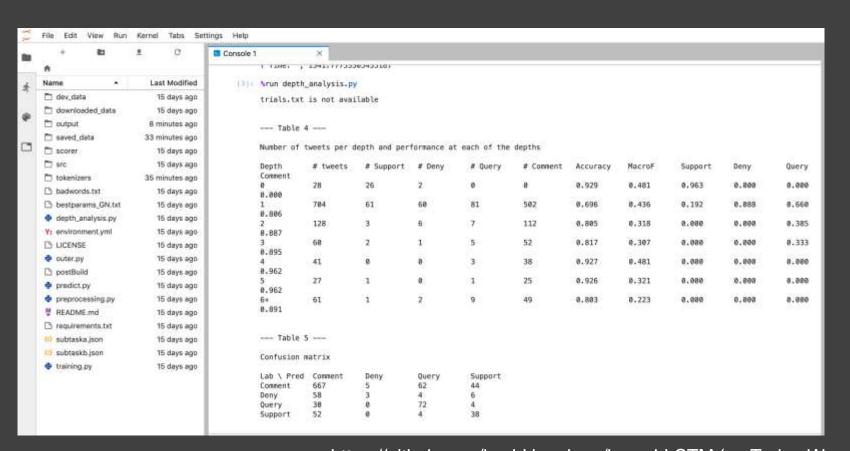
Table 5: Confusion matrix for testing set predictions

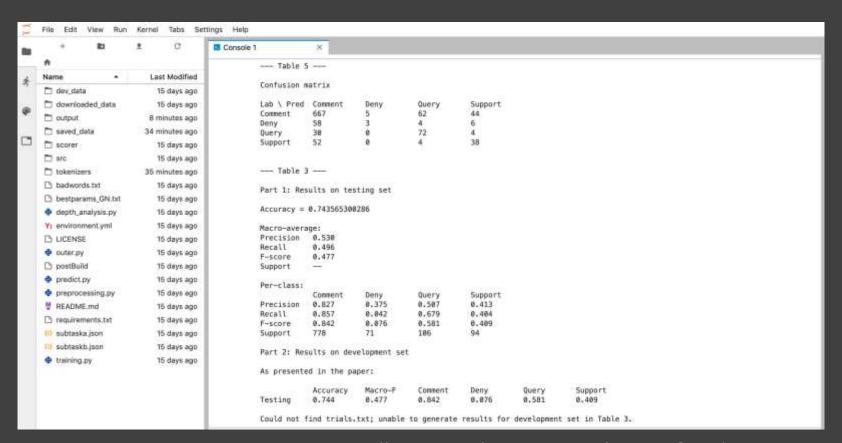
https://github.com/kochkinaelena/branchLSTM https://doi.org/10.18653/v1/S17-2083











https://github.com/kochkinaelena/branchLSTM (on Turing Way Hub) #PyDataLDN #TuringWay @kirstie\_i

https://doi.org/10.5281/zenodo.3632913

#### Elena Kochkina

"How would I have known that it would be different on a different machine?! I only have access to the university HPC to run deep learning analyses."



https://warwick.ac.uk/fac/sci/dcs/people/research/mapmbc #PyDataLDN #TuringWay @kirstie\_j https://doi.org/10.5281/zenodo.3632913