The Alan Turing Institute

Kirstie Whitaker

The Turing Way
A how to guide for
reproducible research



#PyDataLDN #TuringWay @kirstie_j https://doi.org/10.5281/zenodo.3333760

The Turing Way is:

- -a book
- -a community
- -a global collaboration
- -a whole tonne of work



Rachael Ainsworth





Louise Bowler



Sarah Gibson





Patricia Herterich



James Hetherington



Rosie Higman



Anna Krystalli



Catherine Lawrence



Alex Morley



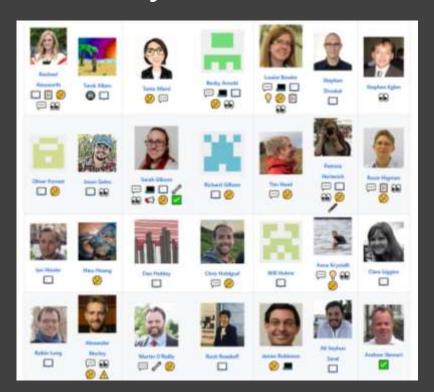
Martin O'Reilly

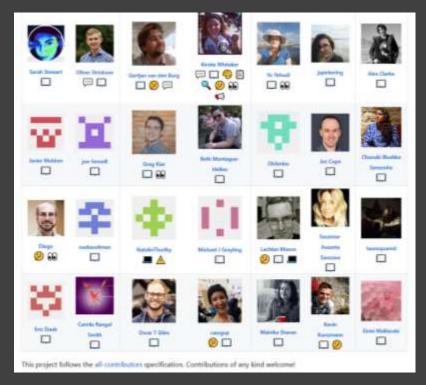


Binder Team

#PyDataLDN #TuringWay @kirstie i https://doi.org/10.5281/zenodo.3333760

Thank you to all our contributors





An introduction to me



#PyDataLDN #TuringWay @kirstie_j https://doi.org/10.5281/zenodo.3333760



Academic errors have real world effects

0	В	С	1	J	K	L	M	
2		-		Real GDP growth				
3								
4	Country	Coverage	30 or less	30 to 60	60 to 90	90 or above	30 or less	
26			3.7	3.0	3.5	1.7	5.5	
27	Minimum		1.6	0.3	1.3	-1.8	0.8	
28	Maximum		5.4	4.9	10.2	3.6	13.3	
29								
30	US	1946-2009	n.a.	3.4	3.3	-2.0	n.a.	
31	UK	1946-2009	n.a.	2.4	2.5	2.4	n.a.	
32	Sweden	1946-2009	3.6	2.9	2.7	n.a.	6.3	
33	Spain	1946-2009	1.5	3.4	4.2	n.a.	9.9	
34	Portugal	1952-2009	4.8	2.5	0.3	n.a.	7.9	
35	New Zealand	1948-2009	2.5	2.9	3.9	-7.9	2.6	
36	Netherlands	1956-2009	4.1	2.7	1.1	n.a.	6.4	
37	Norway	1947-2009	3.4	5.1	n.a.	n.a.	5.4	
38	Japan	1946-2009	7.0	4.0	1.0	0.7	7.0	
39	Italy	1951-2009	5.4	2.1	1.8	1.0	5.6	
40	Ireland	1948-2009	4.4	4.5	4.0	2.4	2.9	
41	Greece .	1970-2009	4.0	0.3	2.7	2.9	13.3	
42	Germany	1946-2009	3.9	0.9	n.a.	n.a.	3.2	
43	France	1949-2009	4.9	2.7	3.0	n.a.	5.2	
44	Finland	1946-2009	3.8	2.4	5.5	n.a.	7.0	
45	Denmark	1950-2009	3.5	1.7	2.4	n.a.	5.6	
46	Canada	1951-2009	1.9	3.6	4.1	n.a.	2.2	
47	Belgium	1947-2009	n.a.	4.2	3.1	2.6	n.a.	
48	Austria	1948-2009	5.2	3.3	-3.8	n.a.	5.7	
49	Australia	1951-2009	3.2	4.9	4.0	n.a.	5.9	
50								
51			4.1	2.8	2.8	=AVERAG	E(L30:L44)	

https://statmodeling.stat.columbia.edu/2013/04/16/memo-to-reinhart-and-rogoff-i-think-its-best-to-admit-your-errors-and-go-on-from-there https://www.bbc.co.uk/news/magazine-22223190

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29				-				
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The humans are the hardest part of reproducibility



		Data		
		Same	Different	
Analysis	Same	Reproducible	Replicable	
	Different	Robust	Generalisable	

https://the-turing-way.netlify.com/reproducibility/03/definitions.html #PyDataLDN #TuringWay @kirstie_j https://doi.org/10.5281/zenodo.3333760 Is not considered for promotion

Held to higher standards than others

Publication bias towards novel findings

Requires additional skills

Barriers to reproducible research

Plead the 5th

Support additional users

Takes time

https://doi.org/10.6084/m9.figshare.5537101 #PyDataLDN #TuringWay @kirstie_j https://doi.org/10.5281/zenodo.3333760

The Turing Institute



https://www.turing.ac.uk/news/enigma-machine-goes-display-alan-turing-institute #PyDataLDN #TuringWay @kirstie_j https://doi.org/10.5281/zenodo.3333760







University network





























https://doi.org/10.5281/zenodo.3333760

The Institute's partners and collaborators

























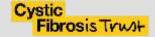






















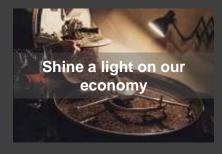
Challenges

Advance data science and artificial intelligence to...













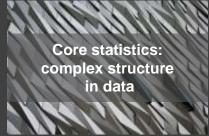




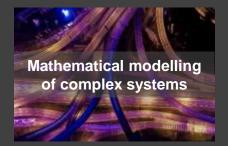
Core capabilities













Ethics of data science and artificial intelligence

Martin O'Reilly

"Make reproducible research too easy not to do."



https://www.turing.ac.uk/people/researchers/martin-oreilly #PyDataLDN #TuringWay @kirstie_j https://doi.org/10.5281/zenodo.3333760

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Martin O'Reilly

"Make reproducible research too easy not to do.

Do you need a biscuit?

If we can't do it here, we

can't do it at all."



https://www.turing.ac.uk/people/researchers/martin-oreilly #PyDataLDN #TuringWay @kirstie_j https://doi.org/10.5281/zenodo.3333760

The Turing Way



#PyDataLDN #TuringWay @kirstie_j https://doi.org/10.5281/zenodo.3333760

1. Introduction

- 2. Reproducibility
- 3. Open Research
- 4. Version Control
- 5. Collaborating on GitHub/GitLab
- 6. Research Data Management
- 7. Reproducible Environments
- 8. Testing
- 9. Reviewing
- 10. Continous Integration
- 11. Reproducible Research with Make
- 12. Risk Assessment

Welcome to the Turing Way

The Turing Way is a lightly opinionated guide to reproducible data science.

Our goal is to provide all the information that researchers need at the start of their projects to ensure that they are easy to reproduce at the end.

This also means making sure PhD students, postdocs, PIs and funding teams know which parts of the "responsibility of reproducibility" they can affect, and what they should do to nudge data science to being more efficient, effective and understandable.

A bit more background

Reproducible research is necessary to ensure that scientific work can be trusted. Funders and publishers are beginning to require that publications include access to the underlying data and the analysis code. The goal is to ensure that all results can be independently verified and built upon in future work. This is sometimes easier said than done. Sharing these research outputs means understanding data management, library sciences, sofware development, and continuous integration techniques: skills that are not widely taught or expected of academic researchers and data scientists.

The Turing Way is a handbook to support students, their supervisors, funders and journal editors

https://the-turing-way.netlify.com/introduction/introduction #PyDataLDN #TuringWay @kirstie_j https://doi.org/10.5281/zenodo.3333760

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Catherine Lawrence

"We should ensure all our processes for running programmes are FAIR.

- Findable (intranet)
- Accessible (EDI)
- Interoperable across programmes and projects



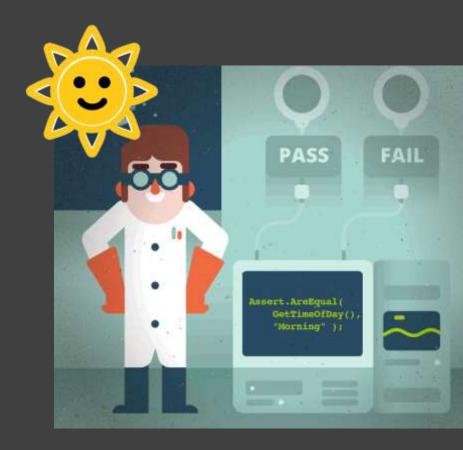
- Reusable (bus factor)" https://www.turing.ac.uk/people/business-team/catherine-lawrence #PyDataLDN #TuringWay @kirstie_j https://doi.org/10.5281/zenodo.3333760

Testing for research



#PyDataLDN #TuringWay @kirstie_j
https://doi.org/10.5281/zenodo.3333760

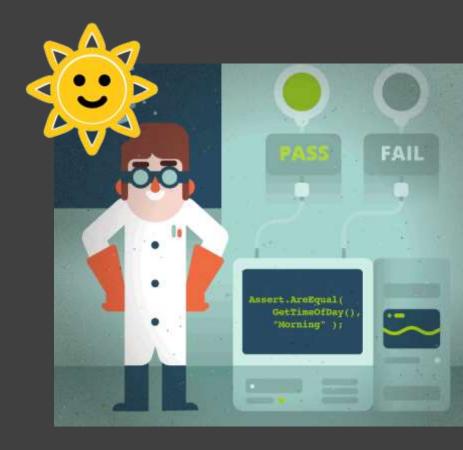




Assert.AreEqual(

GetTimeOfDay(),

"Morning")



Assert.AreEqual(

GetTimeOfDay(),

"Morning")



Louise Bowler

"Add a test before you change anything."



https://www.turing.ac.uk/people/researchers/louise-bowler #PyDataLDN #TuringWay @kirstie_j https://doi.org/10.5281/zenodo.3333760

Louise Bowler

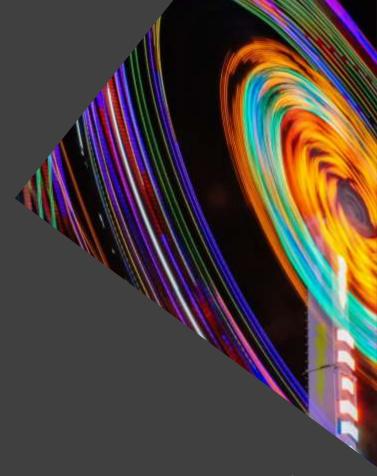
"Add a test before you change anything.

Particularly if you're just going to tidy up your code before sharing it."



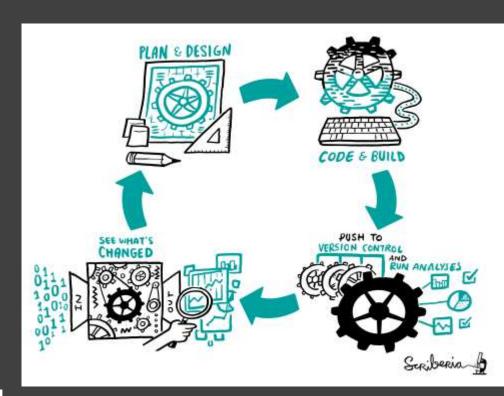
https://www.turing.ac.uk/people/researchers/louise-bowler #PyDataLDN #TuringWay @kirstie_j https://doi.org/10.5281/zenodo.3333760

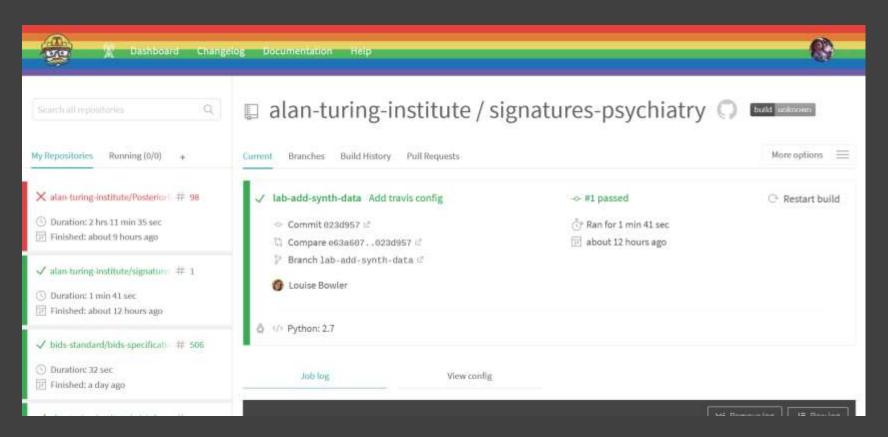
Continuous Analysis



#PyDataLDN #TuringWay @kirstie_j
https://doi.org/10.5281/zenodo.3333760

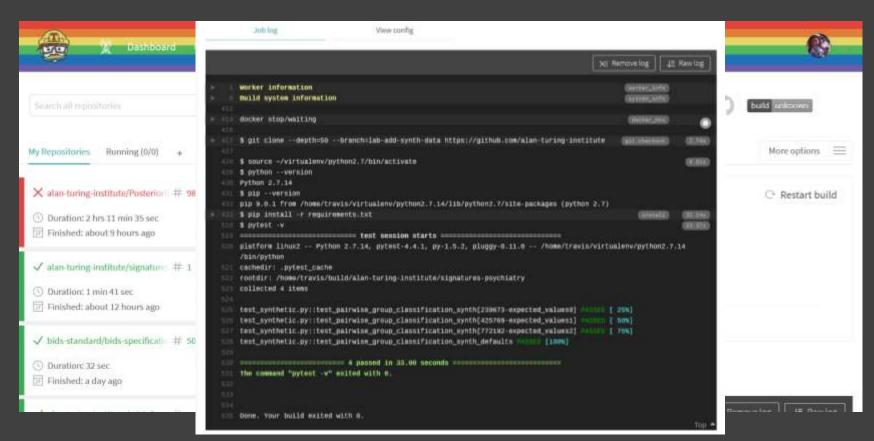
- Plan and design your experiment
- Write down those steps in code
- Push to version control and run the analyses
 - Traditionally done on the cloud,
 but the important part is that <u>all</u>
 <u>steps</u> are run <u>every time</u>
- Test to see what's changed





https://github.com/alan-turing-institute/signatures-psychiatry #PyDataLDN #TuringWay @kirstie_j

https://doi.org/10.5281/zenodo.3333760



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

https://the-turing-way.netlify.com/continuous_integration.html

- Run the analysis from start to finish as you work
- Many times tests will fail as expected: you're developing the analysis!
- Sometimes tests will fail unexpectedly
- CI makes you be explicit about what has changed



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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 #PyDataLDN #TuringWay @kirstie_j https://doi.org/10.5281/zenodo.3333760

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Continuous integration

Notes	Importance	Prerequisite
A tutorial on working via the command line can be found here	Necessary	Experience with the command line
See the chapter on this for more information	Necessary	Version control
See the chapter on this for more information	Very helpful	Testing
See the chapter on this for more information, particularly the sections on YAML files and containers	Necessary	Reproducible computational environments

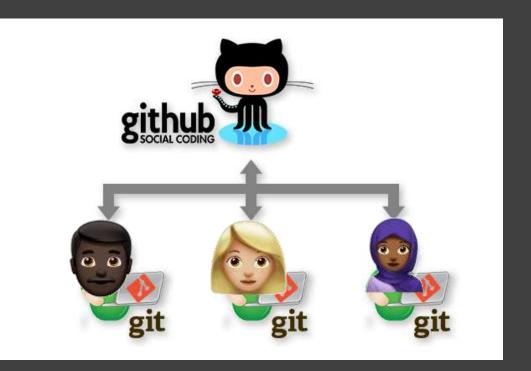
Table of contents

- Summary
- How this will help you/ why this is useful
 What are continuous delivery and continuous deployment?
- · What is Travis and how does it work?
- Setting up continuous integration with Travis
 - o Basic steps

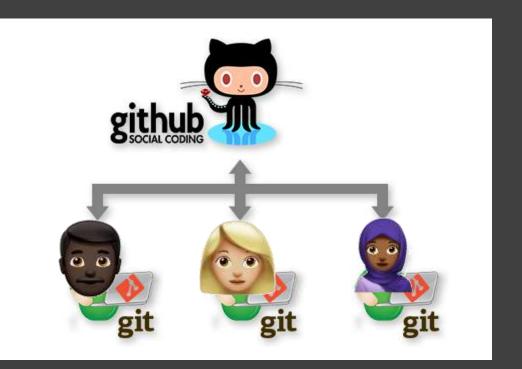
https://the-turing-way.netlify.com/continuous_integration/continuous_integration.html

Version control





https://the-turing-way.netlify.com/collaborating_github/collaborating_github.html
https://the-turing-way.netlify.com/version_control/version_control.html #OHBM2019 #OpenForAll @kirstie_j
https://doi.org/10.5281/zenodo.3333760





https://the-turing-way.netlify.com/collaborating_github/collaborating_github.html https://the-turing-way.netlify.com/version_control/version_control.html #C https://neurohackademy.org https://

#OHBM2019 #OpenForAll @kirstie_j https://doi.org/10.5281/zenodo<u>.3333760</u>

Neurohackademy

"Every hackathon should have a gong that you can ring when you complete your first pull request."



https://neurohackademy.org #PyDataLDN #TuringWay @kirstie_j https://doi.org/10.5281/zenodo.3333760

Workshops & trainings





https://github.com/alan-turing-institute/the-turing-way/tree/master/workshops #PyDataLDN #TuringWay @kirstie_j https://doi.org/10.5281/zenodo.3333760

Rosie Higman

"There's no point in running events when you're only preaching to the choir. We need to show researchers the selfish reasons to follow our recommendations."



https://rosiehigman.wordpress.com #PyDataLDN #TuringWay @kirstie_j https://doi.org/10.5281/zenodo.3333760

Book Dashes

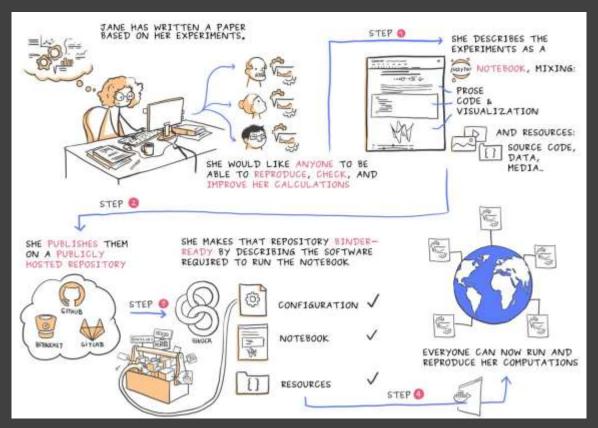
- Manchester and London
- 13 selected people to contribute to the book
- 1:3 support ratio: mentored support to contribute expertise



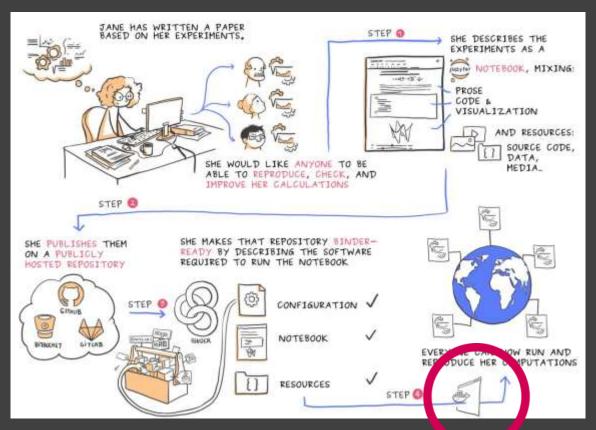
https://github.com/
alan-turing-institute/the-turing-way/
blob/master/
workshops/book-dash/
book-dash-[mcr|ldn]-report.md

Turing Way & Binder



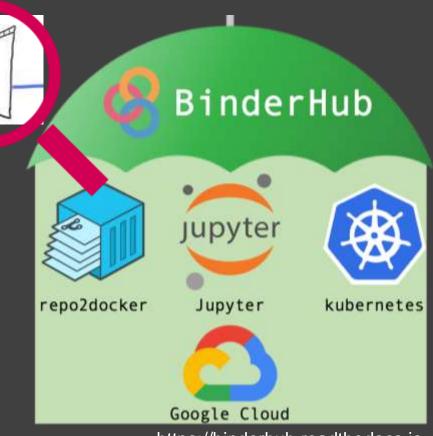


Courtesy of Juliette Taka: https://twitter.com/mybinderteam/status/1082556317842264064



Courtesy of Juliette Taka: https://twitter.com/mybinusrtee.il/catus/1082556317842264064

- 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 #PyDataLDN #TuringWay @kirstie_j https://doi.org/10.5281/zenodo.3333760

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 #PyDataLDN #TuringWay @kirstie_j https://doi.org/10.5281/zenodo.3333760

- 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!

of launch binder

How can mybinder.org be free to use?

On this page

What is a Rinder? 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 How much memory am I given when using Binder? How long will my Binder session

Can I use mybinder.org for a live

demo or workshop?

How does mybinder.org ensure user privacy?

How secure is mybinder.org?

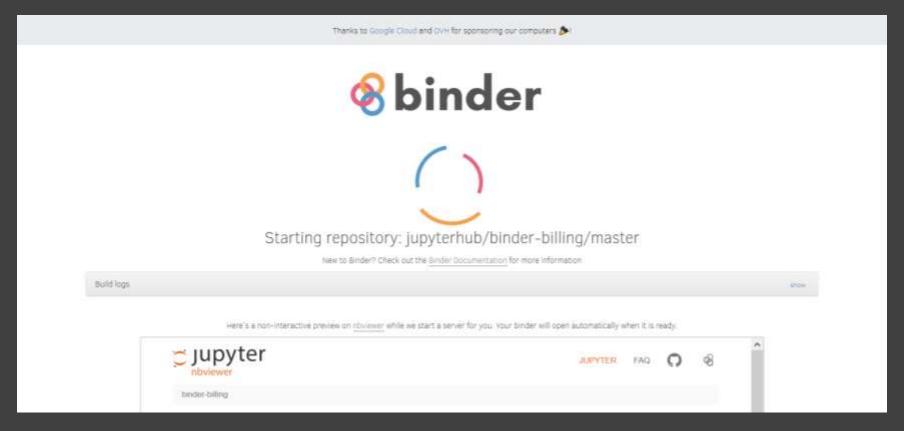
Where can I report a security issue? Can I push data from my Binder session back to my repository?

Can I put my configuration files outside the root of E v. latest .

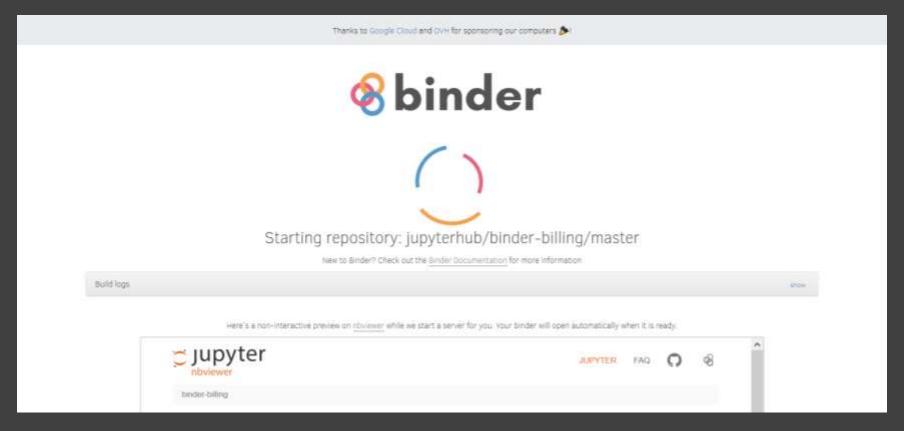
takes a Binder session to start?

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

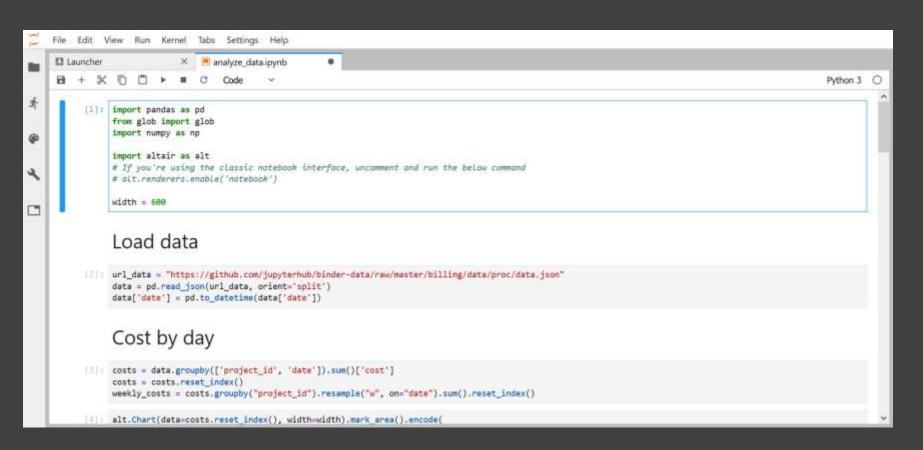
https://mybinder.readthedocs.io/en/latest/faq.html#how-much-does-running-mybinder-org-cost #PyDataLDN #TuringWay @kirstie i https://doi.org/10.5281/zenodo.3333760



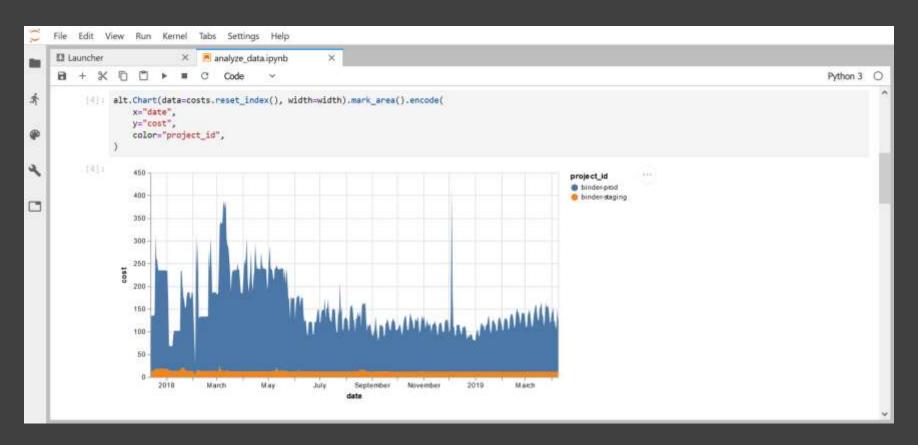
https://mybinder.readthedocs.io/en/latest/faq.html#how-much-does-running-mybinder-org-cost #PyDataLDN #TuringWay @kirstie_j https://doi.org/10.5281/zenodo.3333760



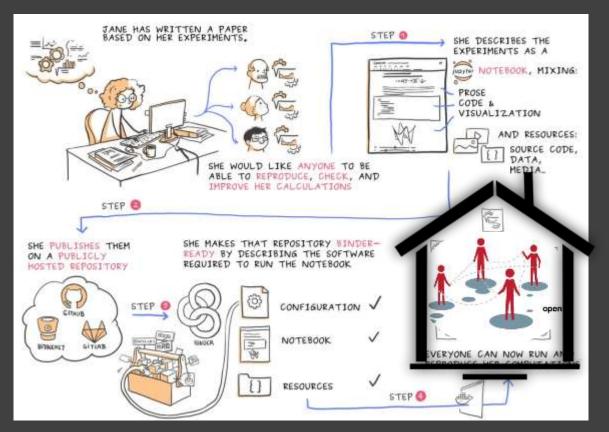
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Courtesy of Juliette Taka: https://twitter.com/mybinderteam/status/1082556317842264064

The Alan Turing Institute

8 binder



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

New to Binder? Check out the Binder Documentation for more information

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

JUPYTER FAQ 0 8

branchLSTM sgibson91python-runtime-patch

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

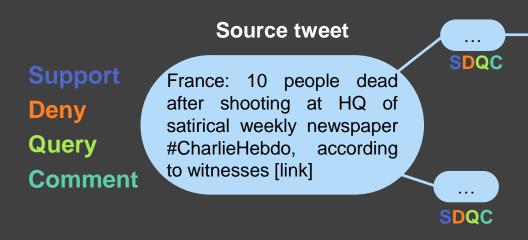
https://doi.org/10.5281/zenodo.3333760

Champion: Elena Kochkina

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

Elena Kochkina, Maria Liakata, Isabelle Augenstein

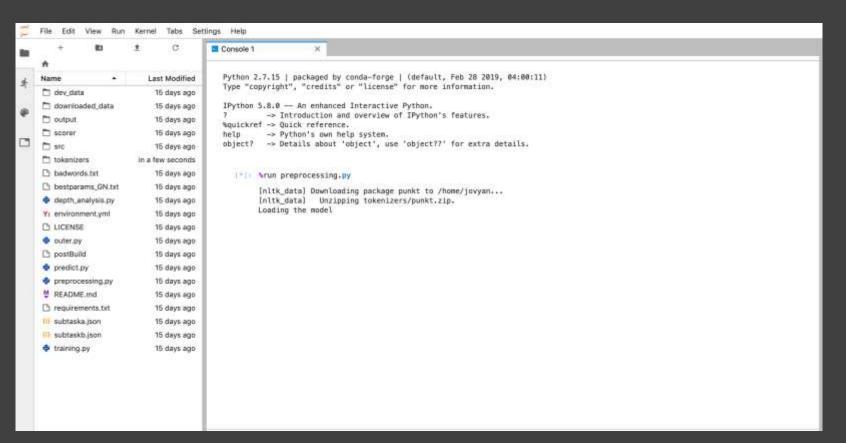
SDQC

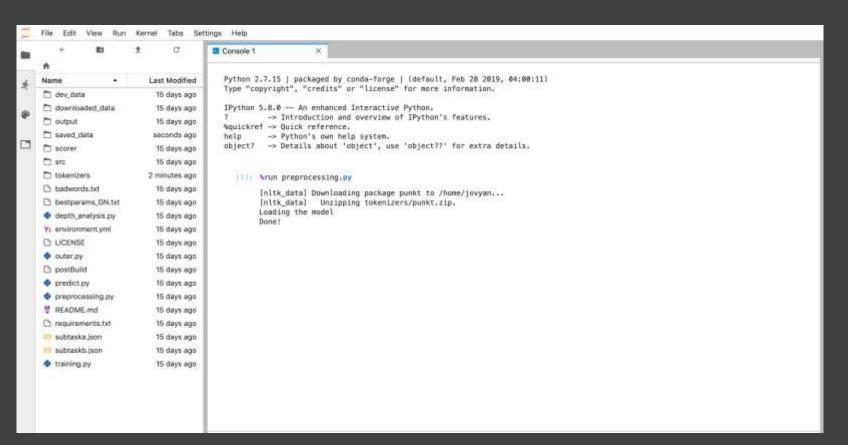


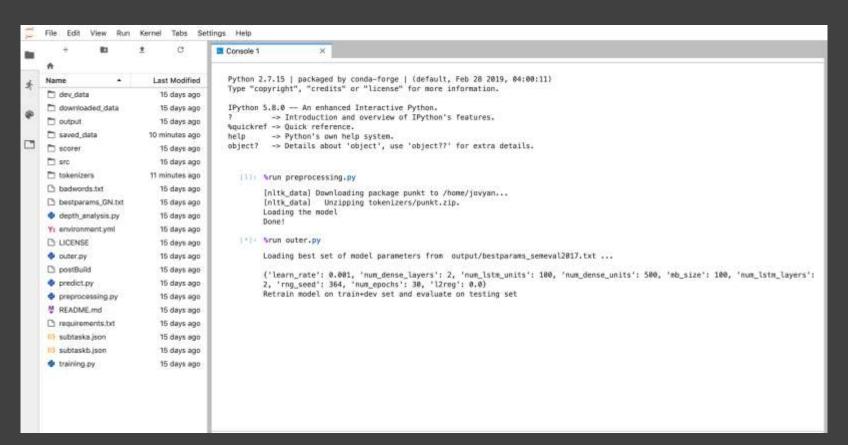
Prediction	С	D	Q	S
Commenting	760	0	12	6
Denying	68	0	1	2
Querying	69	0	36	1
Supporting	67	0	1	26

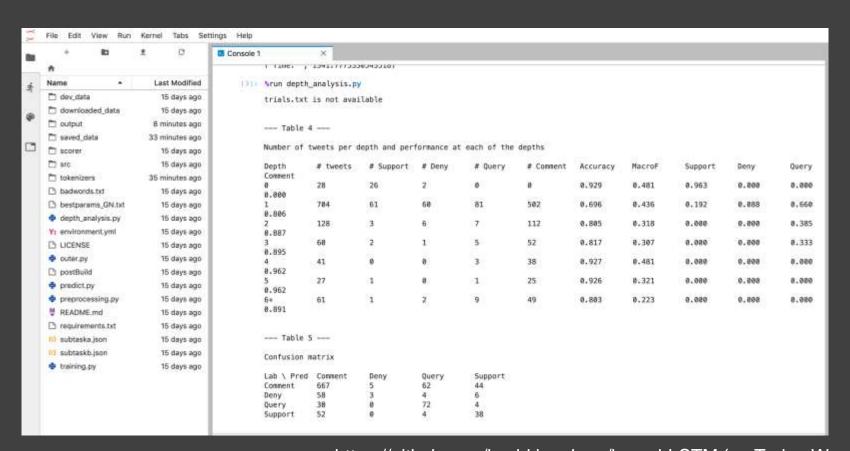
Table 5: Confusion matrix for testing set predictions

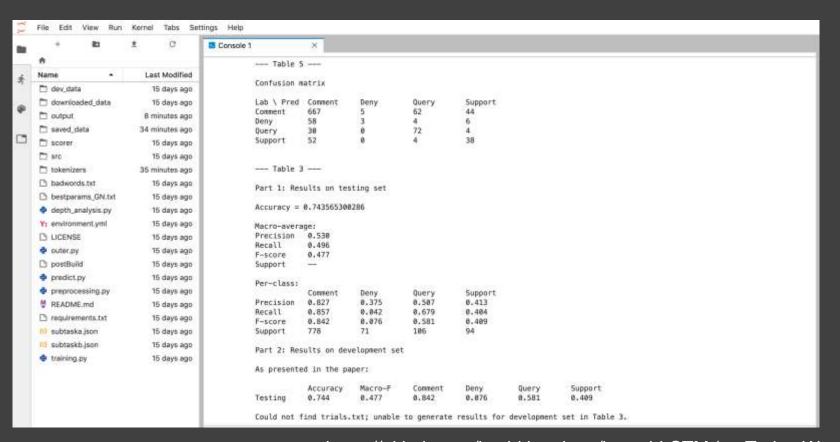
https://github.com/kochkinaelena/branchLSTM https://doi.org/10.18653/v1/S17-2083











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

https://doi.org/10.5281/zenodo.3333760

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."



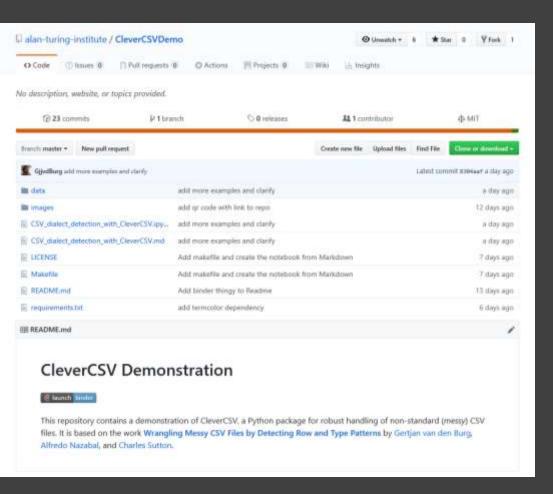
https://warwick.ac.uk/fac/sci/dcs/people/research/mapmbc #PyDataLDN #TuringWay @kirstie_j https://doi.org/10.5281/zenodo.3333760

Gertjan van den Burg

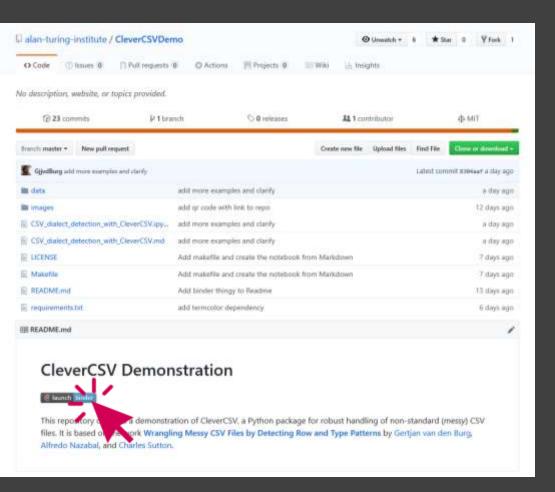
"The fun part of data science is the modelling. Being able to read in information from a csv file should not be the hardest part."



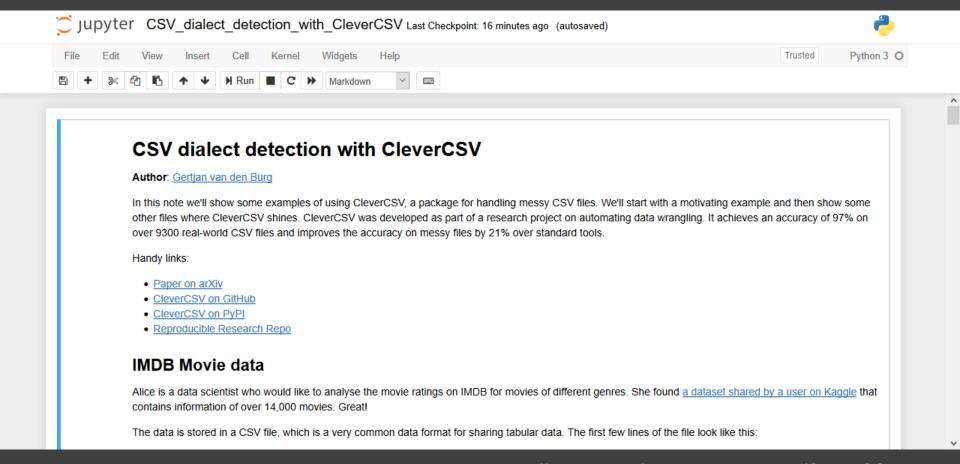
https://gertjanvandenburg.com #PyDataLDN #TuringWay @kirstie_j https://doi.org/10.5281/zenodo.3333760

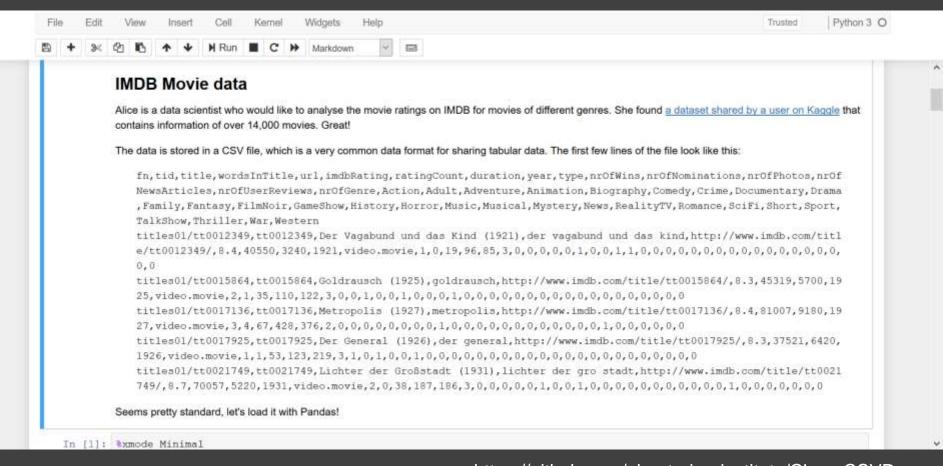


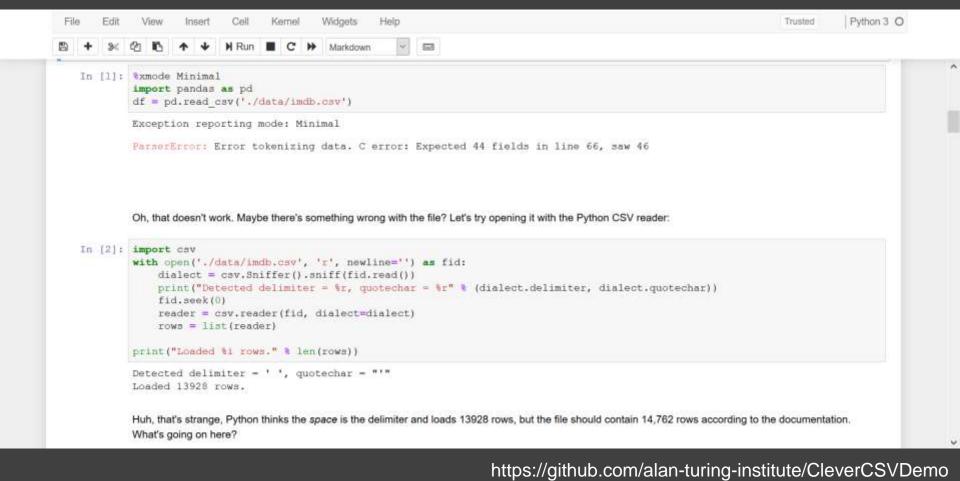
https://github.com/ alan-turing-institute/ CleverCSVDemo

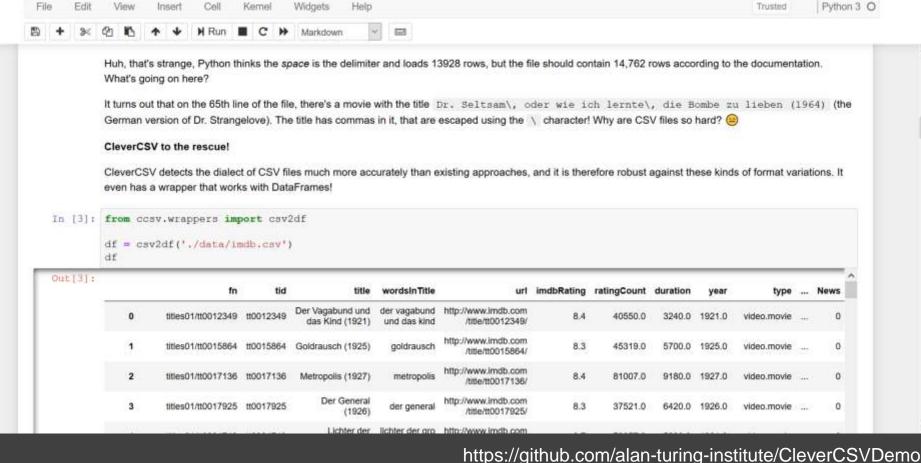


- https://github.com/alan-turing-institute/CleverCSVDemo
- "Wrangling Messy
 CSV Files by
 Detecting Row and
 Type Patterns"
 arXiv:1811.11242

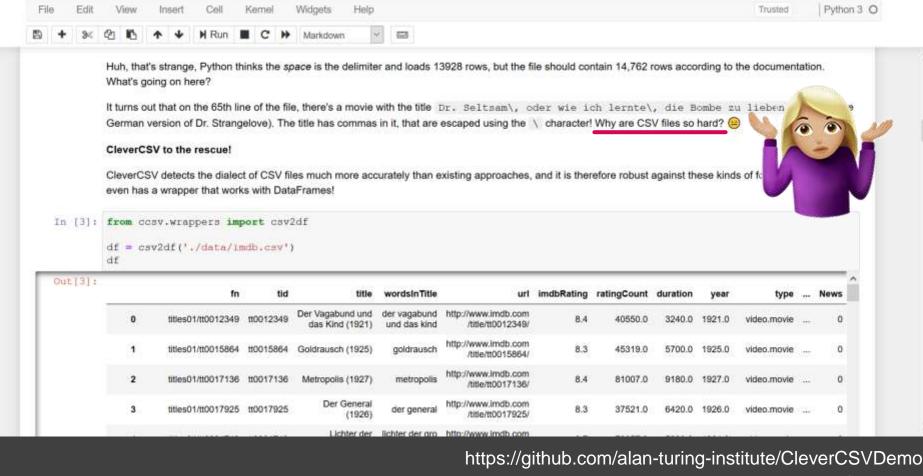


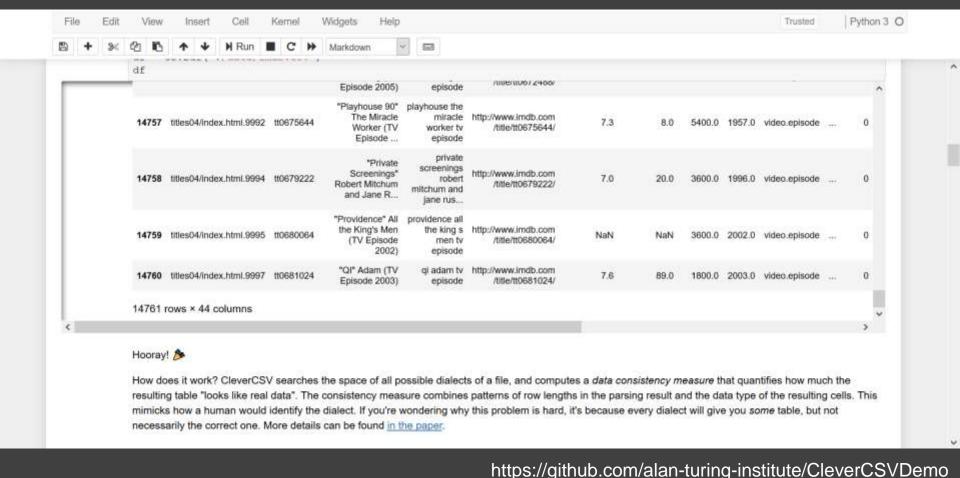






#PyDataLDN #TuringWay @kirstie_j





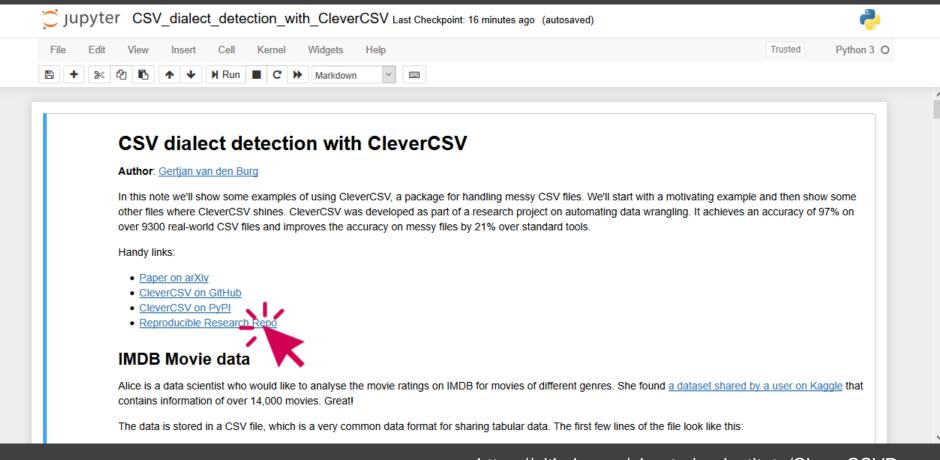
Gertjan van den Burg

"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.

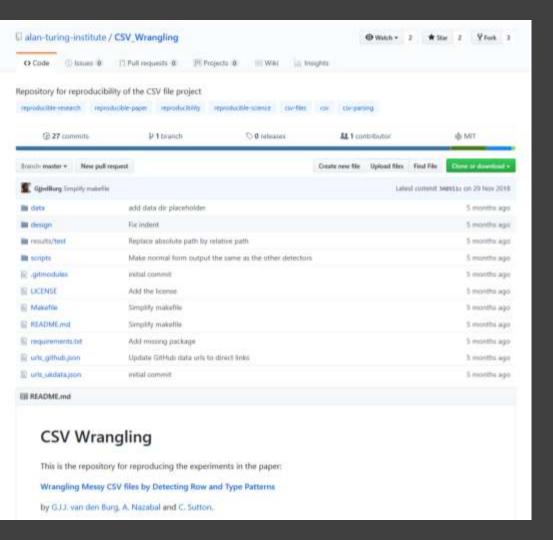
There is no Al. I am the Al."



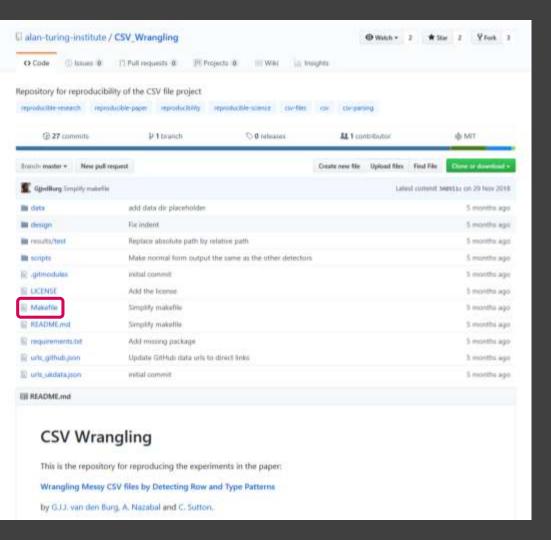
https://gertjanvandenburg.com #PyDataLDN #TuringWay @kirstie_j https://doi.org/10.5281/zenodo.3333760



https://github.com/alan-turing-institute/CleverCSVDemo #PyDataLDN #TuringWay @kirstie_j https://doi.org/10.5281/zenodo.3333760



- https://github.com/alan-turing-institute/CSV_Wrangling
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- "Wrangling Messy
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The Turing Way

- 1. Introduction
- 2. Reproducibility
- 3. Open Research
- 4. Version Control
- 5. Reproducible Environments
- 6. Testing
- 7. Reviewing
- 8. Continous Integration
- 9. Research Data Management
- Reproducible Research with Make

What is Make

Make is a build automation tool. It uses a configuration file called a Makefile that contains the *rules* for what to build. Make builds *targets* using *recipes*. Targets can optionally have *prerequisites*. Prerequisites can be files on your computer or other targets. Make determines what to build based on the dependency tree of the targets and prerequisites (technically, this is a <u>directed acyclic graph</u>). It uses the *modification time* of prerequisites to update targets only when needed.

Why use Make for Reproducible Research?

There are several reasons why Make is a good tool to use for reproducible research:

- 1. Make is available on many platforms
- 2. Make is easy to learn
- 3. Makefiles are text files, which makes them easy share and keep in version control.
- 4. Many people are already familiar with Make
- 5. Using Make doesn't exclude using other tools such as Travis, Docker, etc.

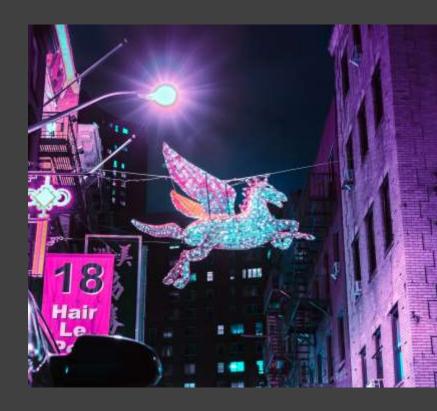
Learn Make by Example

One of the things that might scare people off from using Make is that existing Makefiles can seem daunting and it may seem difficult to tailor to your own needs. In this hands-on tutorial we will

https://the-turing-way.netlify.com/make/make.html

Case studies

- Show that it can be done
- Provide templates and starting points
- Inspire



A global collaboration



Patricia Herterich

"What really sets The Turing Way apart is HOW we're writing the book. The focus on community, the commitment to transparency and working open right from the beginning is an exciting (and terrifying) new way of working."



https://rd-alliance.org/users/patricia-herterich #PyDataLDN #TuringWay @kirstie_j https://doi.org/10.5281/zenodo.3333760

Open Leadership Principles



Understanding

You make the work accessible and clear

Read more

https://mozilla.github.io/olm-whitepaper





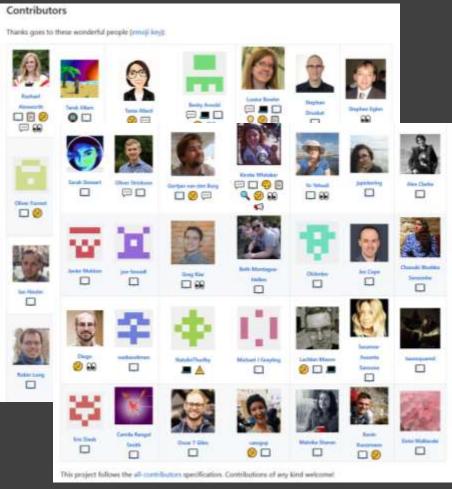
Sharing

You make the work easy to adapt, reproduce, and spread



Participation & Inclusion

You build shared ownership and agency to make the work inviting and sustainable for all.



eventOrganizing review question financial security bug fundingFinding tool blog translation ideas business infra test code tutorial content maintenance 6 talk doc platform userTesting design 8 plugin video examples projectManagement

88

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

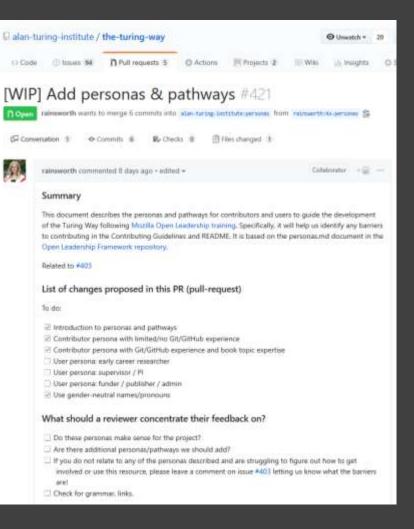
https://github.com/alan-turing-institute/the-turing-way#contributors https://allcontributors.org/docs/en/emoji-key

Rachael Ainsworth

"Personas and pathways exercises let me reflect on what people are finding difficult about contributing to The Turing Way. The project can only reach its potential if it is easy for a diverse constellation of contributions."



https://rainsworth.github.io #PyDataLDN #TuringWay @kirstie_j https://doi.org/10.5281/zenodo.3333760



- Sam, who has no GitHub experience
- Alex, who has a lot of GitHub experience
- Amal, who knows they want to contribute, and does
- Noor, who doesn't know they want to contribute, but does

https://github.com/alan-turing-institute/the-turing-way/pull/421 #PyDataLDN #TuringWay @kirstie_j https://doi.org/10.5281/zenodo.3333760



The future



Funding extension

- Expand scope to all data science practices
 - Ethics, model selection, project management, collaborative working
- Full time community
 manager, contributions
 from Turing & beyond



https://github.com/
alan-turing-institute/the-turing-way/
blob/master/project_management/
tps-funding-application-20190429.md
#PyDataLDN #TuringWay @kirstie i

https://doi.org/10.5281/zenodo.3333760

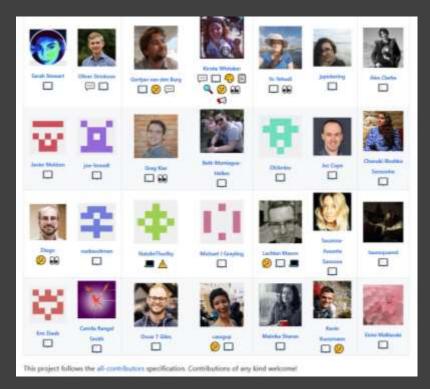
Metrics for success

- 20 new chapters
- 100 authors
- 200 contributors
- 1000 mailing list subscribers
- 50 first pull requests
- 20 new contributors to other open source projects



Thank you to current (& future) contributors





Thank you

- Book: https://the-turing-way.netlify.com
- Newsletter: https://tinyletter.com/TuringWay

- The Alan Turing Institute
- moz://a



- GitHub: https://github.com/alan-turing-institute/the-turing-way
- Chat: https://gitter.im/alan-turing-institute/the-turing-way
- This work was supported by The UKRI Strategic Priorities Fund under the EPSRC Grant EP/T001569/1, particularly the "Tools, Practices and Systems" theme within that grant, and by The Alan Turing Institute under the EPSRC grant EP/N510129/1
- Unsplash photos by Adolfo Felix, James Pond, Jose Alejandro Cuffia, Kinson Leung, Mateo Vrbnjak,
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