The Alan Turing Institute

Reproducible research is impossible without software (so why don't we reward it?)

Kirstie Whitaker



A beautiful example



NASA, https://flic.kr/p/tJbJf5 #CiteSoftware #TuringWay @kirstie_j https://doi.org/10.5281/zenodo.2783998

Focus on the First Event Horizon Telescope Results

Shep Doeleman (EHT Director) on behalf of the EHT Collaboration

April 2019

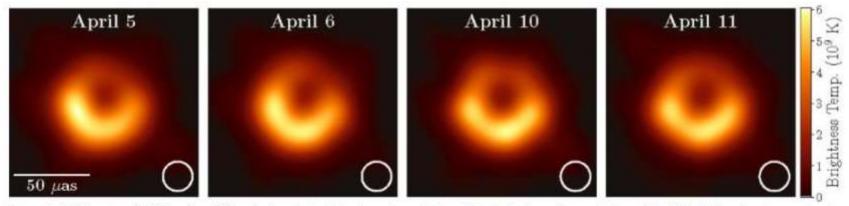


Figure 1. EHT images of M87 on four different observing nights. In each panel, the white circle shows the resolution of the EHT. All four images are dominated by a bright ring with enhanced emission in the south. From Paper IV (Figure 15).

We report the first image of a black hole.

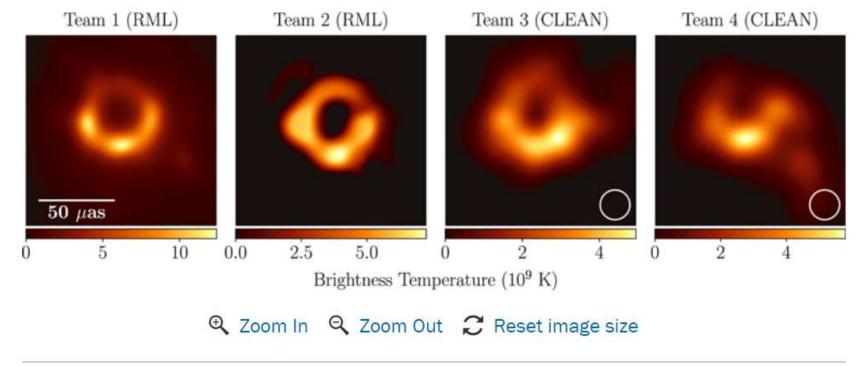
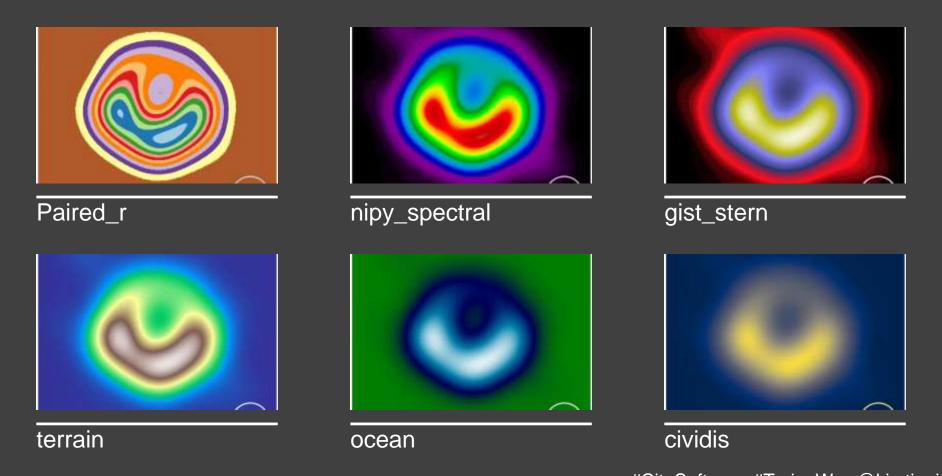


Figure 4. The first EHT images of M87, blindly reconstructed by four independent imaging teams using an early, engineering release of data from the April 11 observations.

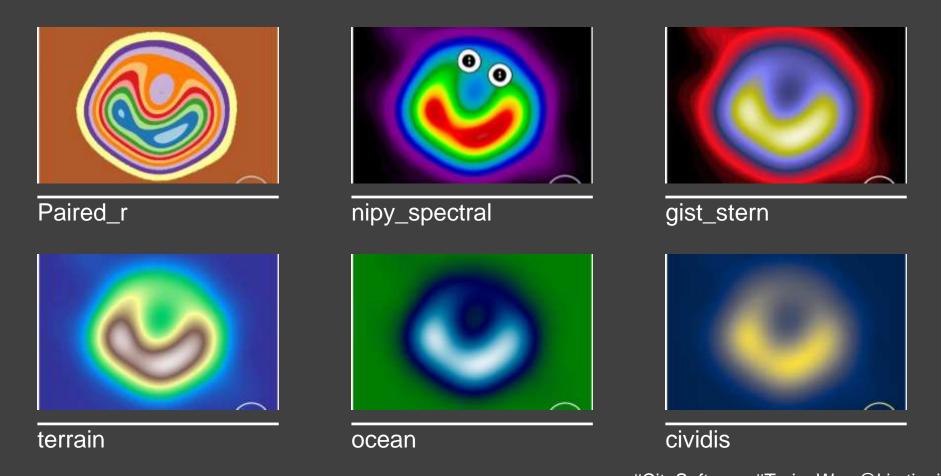
https://iopscience.iop.org/journal/2041-8205/page/Focus_on_EHT #CiteSoftware #TuringWay @kirstie_j https://doi.org/10.5281/zenodo.2783998



https://twitter.com/sweichwald/status/1116430285342695424 #CiteSoftware #TuringWay @kirstie_j https://doi.org/10.5281/zenodo.2783998



https://github.com/liamedeiros/ehtplot/blob/docs/docs/COLORMAPS.ipynb #CiteSoftware #TuringWay @kirstie_j https://twitter.com/sweichwald/status/1116430285342695424 https://doi.org/10.5281/zenodo.2783998



https://github.com/liamedeiros/ehtplot/blob/docs/docs/COLORMAPS.ipynb #CiteSoftware #TuringWay @kirstie_j https://twitter.com/sweichwald/status/1116430285342695424 https://doi.org/10.5281/zenodo.2783998

- First M87 Event Horizon
 Telescope Results. III.
 Data Processing and
 Calibration
- A series of 6 papers
 published in April 2019
- Incredible long term international collaboration (200+ scientists, 60 institutes, 18 countries, 6 continents)

Software: DiFX (Deller et al. 2011), CALC, PolConvert (Martí-Vidal et al. 2016), HOPS (Whitney et al. 2004), CASA (McMullin et al. 2007), AIPS (Greisen 2003), ParselTongue (Kettenis et al. 2006), GNU Parallel (Tange 2011), GILDAS, eht-imaging (Chael et al. 2016, 2018), Numpy (van der Walt et al. 2011), Scipy (Jones et al. 2001), Pandas (McKinney 2010), Astropy (The Astropy Collaboration et al. 2013, 2018), Jupyter (Kluyver et al. 2016), Matplotlib (Hunter 2007).

> doi: 10.3847/2041-8213/ab0c57 #CiteSoftware #TuringWay @kirstie_j https://doi.org/10.5281/zenodo.2783998

An introduction to me





0	В	C		J	K	L.	M
2	-			Real GD	P growth		
3			Debt/GDP				
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	п.а.	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

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The humans are the hardest part of reproducibility



The humans are the hardest part of reproducibility and of software citation



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

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		Data		
		Same	Different	
Analysis	Same	Reproducible	Replicable	
	Different	Robust	Generalisable	

https://the-turing-way.netlify.com/reproducibility/03/definitions.html #CiteSoftware #TuringWay @kirstie_j https://doi.org/10.5281/zenodo.2783998

The Turing Institute



https://www.turing.ac.uk/news/enigma-machine-goes-display-alan-turing-institute #CiteSoftware #TuringWay @kirstie_j https://doi.org/10.5281/zenodo.2783998







University network





























https://doi.org/10.5281/zenodo.2783998

The Institute's partners and collaborators

























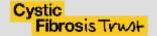






















Challenges

Advance data science and artificial intelligence to...













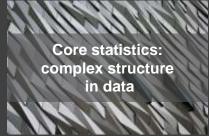




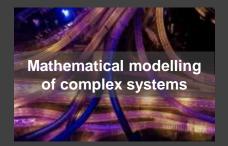
Core capabilities













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 #CiteSoftware #TuringWay @kirstie_j https://doi.org/10.5281/zenodo.2783998

Martin O'Reilly

"Make reproducible research too easy not to do.

Do you need a biscuit?"



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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

If we can't do it here, we can't do it at all."



https://www.turing.ac.uk/people/researchers/martin-oreilly #CiteSoftware #TuringWay @kirstie_j https://doi.org/10.5281/zenodo.2783998

The Turing Way



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

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https://the-turing-way.netlify.com/introduction/introduction #CiteSoftware #TuringWay @kirstie_j https://doi.org/10.5281/zenodo.2783998 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 #CiteSoftware #TuringWay @kirstie_j https://doi.org/10.5281/zenodo.2783998

Catherine Lawrence

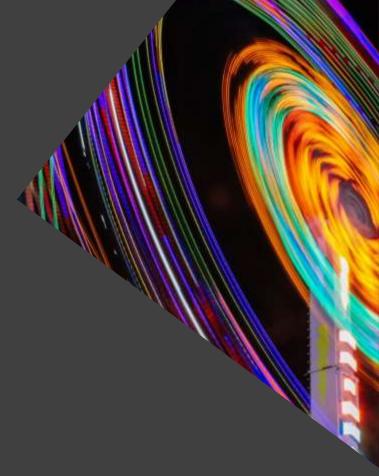
"We should ensure all our processes for running programmes are FAIR.

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

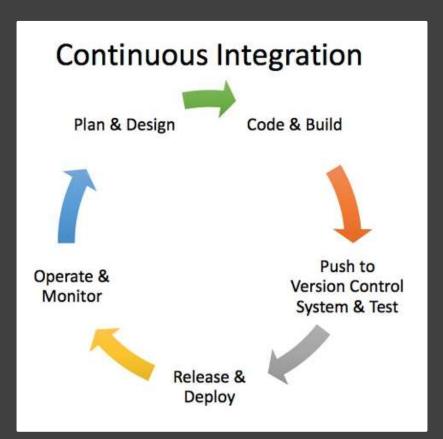


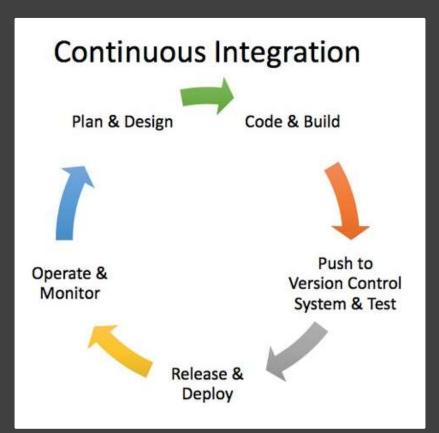
- Reusable (bus factor)" https://www.turing.ac.uk/people/business-team/catherine-lawrence #CiteSoftware #TuringWay @kirstie_j https://doi.org/10.5281/zenodo.2783998

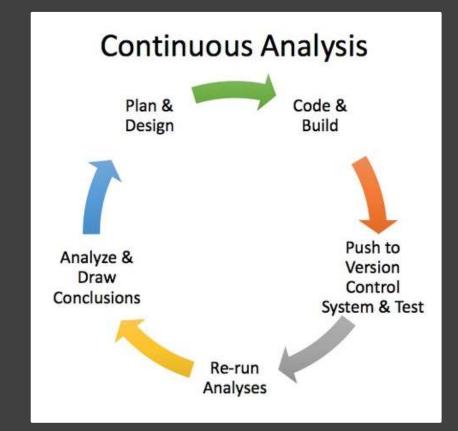
Continuous Analysis

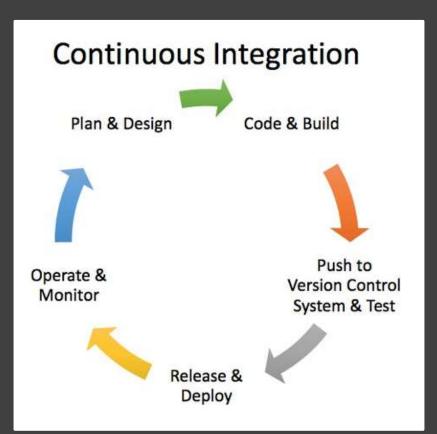


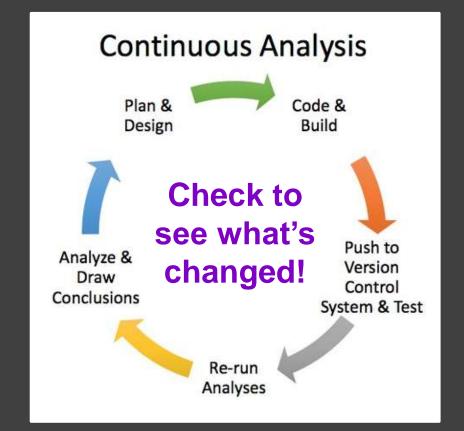
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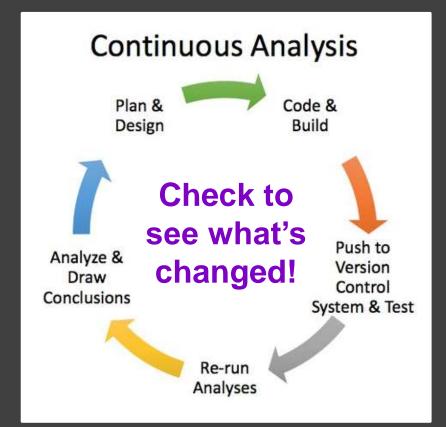


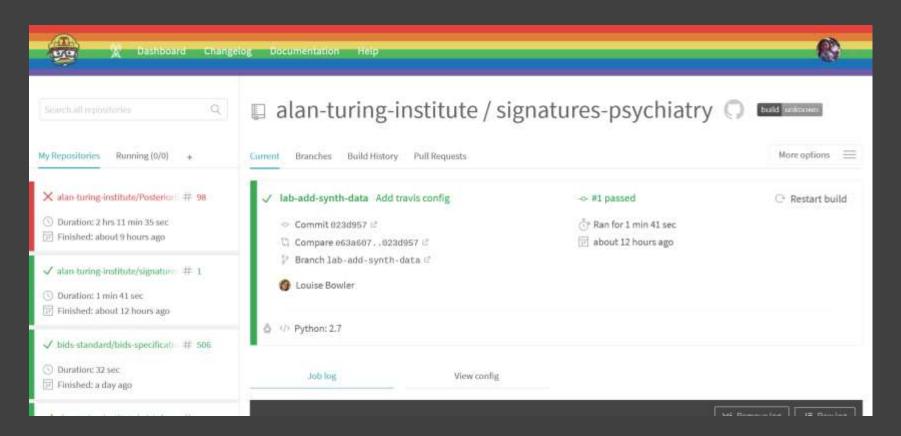




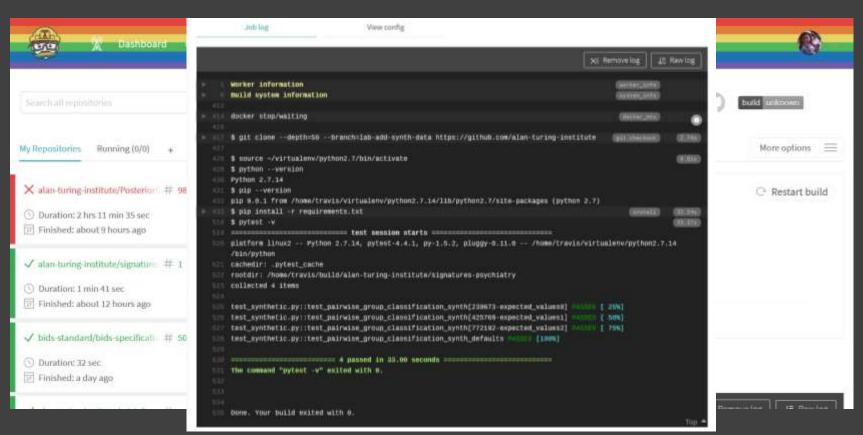








https://github.com/alan-turing-institute/signatures-psychiatry #CiteSoftware #TuringWay @kirstie_j https://doi.org/10.5281/zenodo.2783998



https://github.com/alan-turing-institute/signatures-psychiatry #CiteSoftware #TuringWay @kirstie_j https://doi.org/10.5281/zenodo.2783998

- Run the analysis from start to finish as you're developing
- 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



https://www.youtube.com/watch?v=3GwjfUFyY6M #CiteSoftware #TuringWay @kirstie_j https://doi.org/10.5281/zenodo.2783998

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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 #CiteSoftware #TuringWay @kirstie_j https://doi.org/10.5281/zenodo.2783998

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Continuous integration

Note	Importance	Prerequisite
A tutorial on working via the command line ca be found her	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 an container	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 #CiteSoftware #TuringWay @kirstie_j

"FINAL".doc













FINAL_rev.6.COMMENTS.doc

FINAL_rev.8.comments5. CORRECTIONS.doc

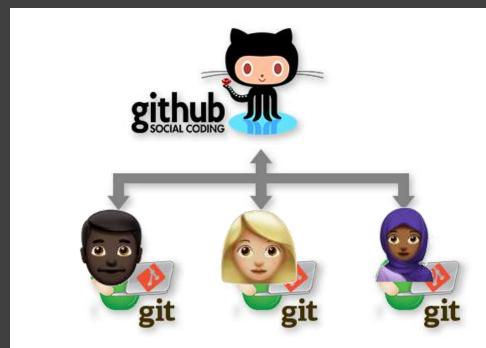






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FINAL_rev.22.comments49. corrections.10.#@\$%WHYDID ICOMETOGRADSCHOOL????.doc



http://phdcomics.com/comics/archive.php?comicid=1531 #CiteSoftware #TuringWay @kirstie_j https://doi.org/10.5281/zenodo.2783998

Neurohackademy

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



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https://www.youtube.com/watch?v=hSsjxbRxgqY #CiteSoftware #TuringWay @kirstie_j https://doi.org/10.5281/zenodo.2783998

Workshops & trainings



#CiteSoftware #TuringWay @kirstie_j https://doi.org/10.5281/zenodo.2783998



https://github.com/alan-turing-institute/the-turing-way/tree/master/workshops #CiteSoftware #TuringWay @kirstie_j https://doi.org/10.5281/zenodo.2783998

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 #CiteSoftware #TuringWay @kirstie_j https://doi.org/10.5281/zenodo.2783998



https://www.software.ac.uk/cw19 #CiteSoftware #TuringWay @kirstie_j https://doi.org/10.5281/zenodo.2783998

A Good Checklist

- ✓ Adds value
- ✓ Modular
- Customisable
- Guides & encourages communication



Checklist Manifesto

- Codify best practice: distil and collate community knowledge.
- Level the team: Spread responsibility and level authority.
- Create awareness: Bring focus to the routine, prepare for the unexpected.
- Bring teams together: Act of reviewing fosters feeling of teamwork and shared ownership.

G GitHub issue templates as checklists for Open Reproducible Research

- Library of customisable templates for common tasks + infrastructure for domain specific variations
- Ability to programmatically create domain/task specific issue sets
- Open for contribution Community ownership and sense of value imperative!

Part of the Turing Way project - https://github.com/alan-turins-institute/the-turing-way

@annakrystalli

https://checklib.github.io/checklib #CiteSoftware #TuringWay @kirstie_j https://doi.org/10.5281/zenodo.2783998

Anna Krystalli

"Checklists are a great way to make it really easy for busy people to do reproducible research. They can catch easily forgotten steps."



https://alexmorley.me #CiteSoftware #TuringWay @kirstie_j https://doi.org/10.5281/zenodo.2783998

Anna Krystalli

"Checklists are a great way to make it really easy for busy people to do reproducible research. They can catch easily forgotten steps..... like citing software!"

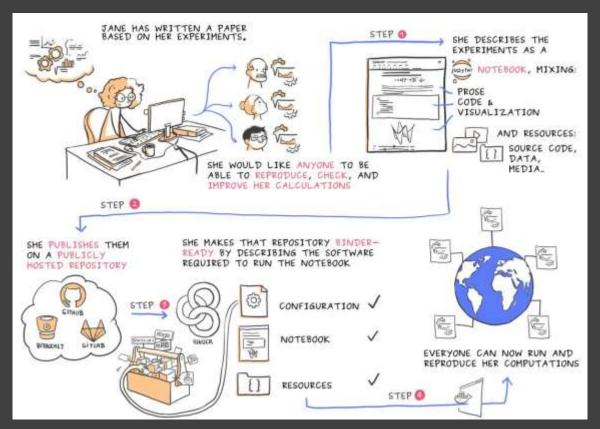


https://alexmorley.me #CiteSoftware #TuringWay @kirstie_j https://doi.org/10.5281/zenodo.2783998

Turing Way & Binder

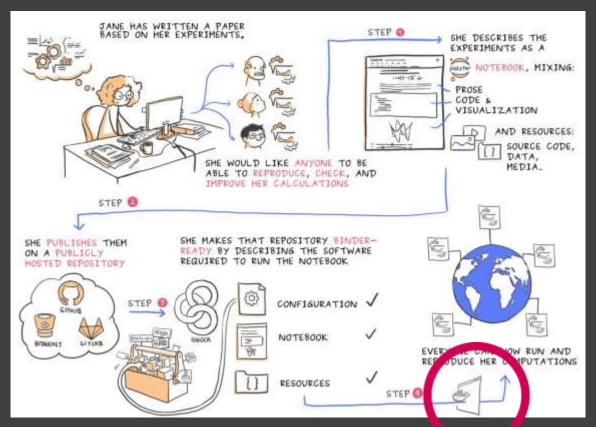


#CiteSoftware #TuringWay @kirstie_j https://doi.org/10.5281/zenodo.2783998



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

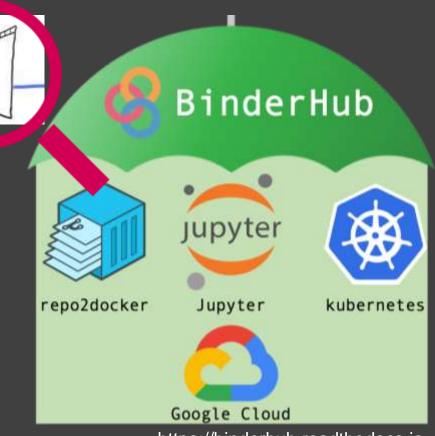
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- Coordinate cloud
 computing resources
 with Kubernetes (k8s)
- Make it easy for users to access with a JupyterHub
- Set up the environment from your GitHub repository



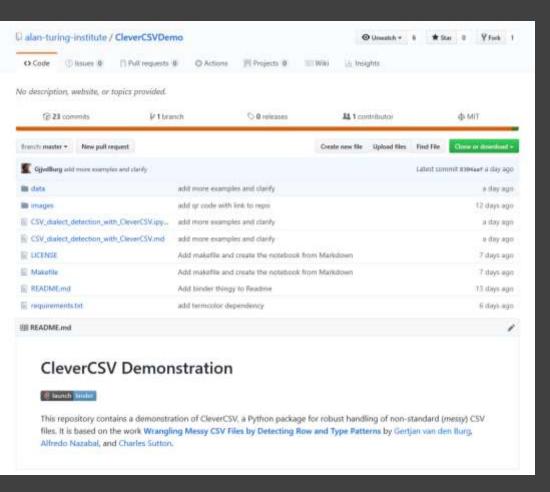
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Gertjan van den Burg

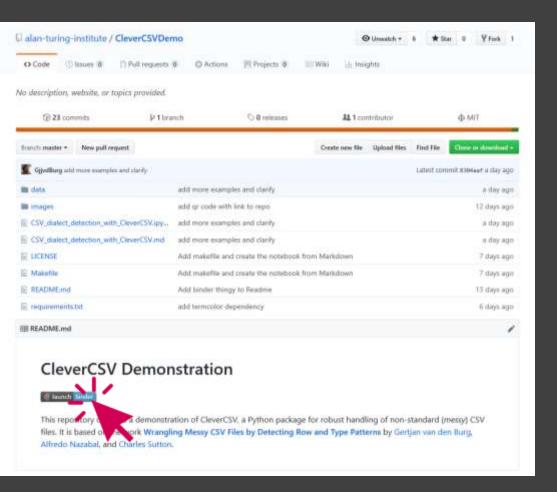
"The fun part of data science is the modelling. Being able to read in information from a csv file should not be the hardest part."



https://gertjanvandenburg.com #CiteSoftware #TuringWay @kirstie_j https://doi.org/10.5281/zenodo.2783998

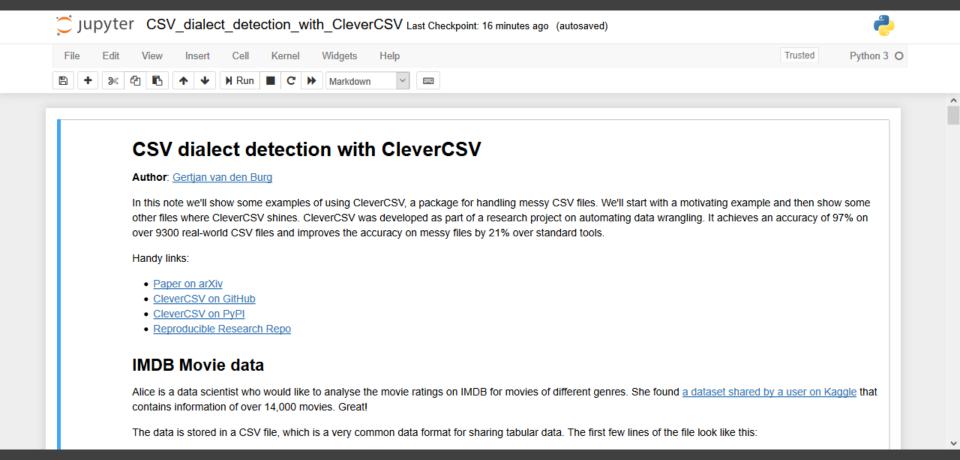


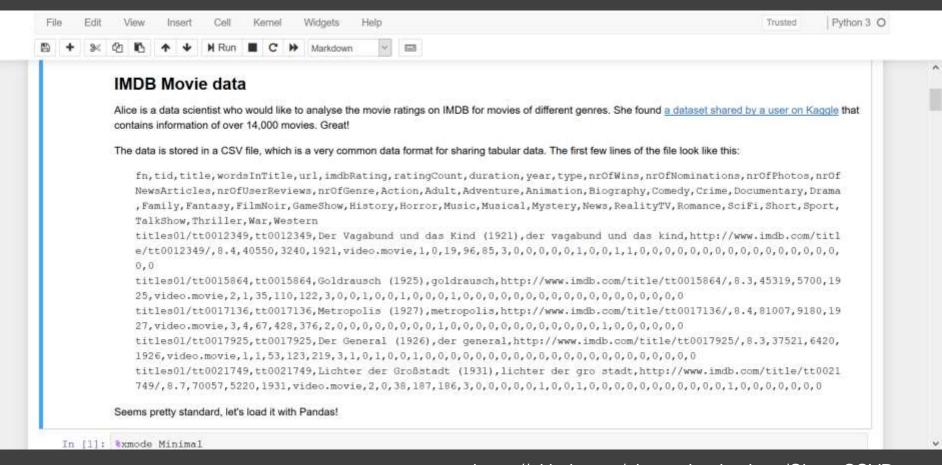
https://github.com/ alan-turing-institute/ CleverCSVDemo

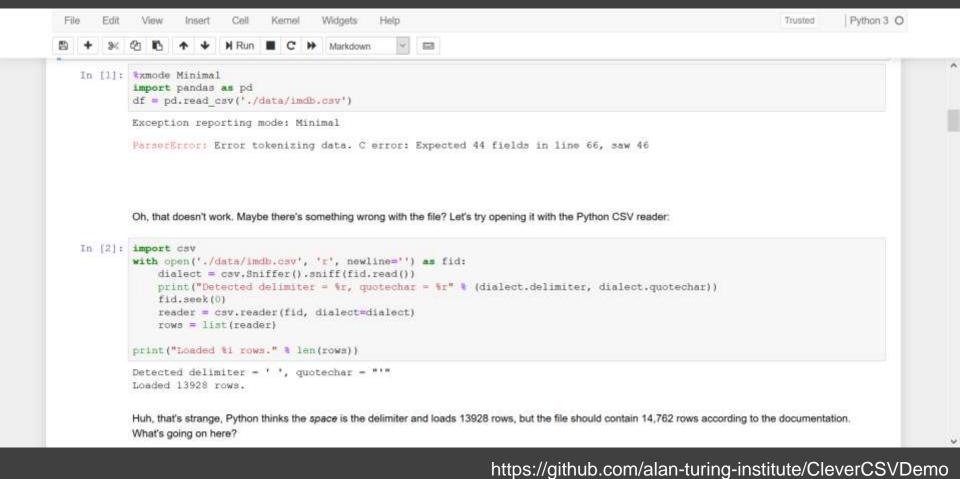


- https://github.com/ alan-turing-institute/ CleverCSVDemo
- "Wrangling Messy
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 arXiv:1811.11242

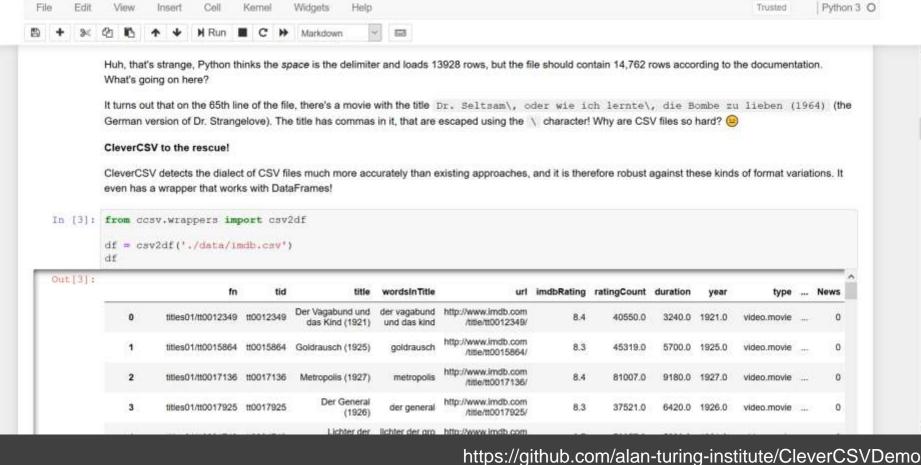
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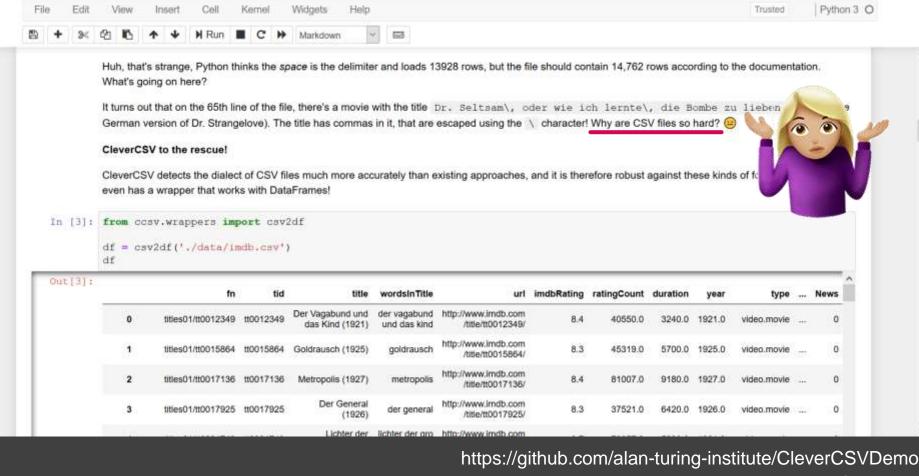


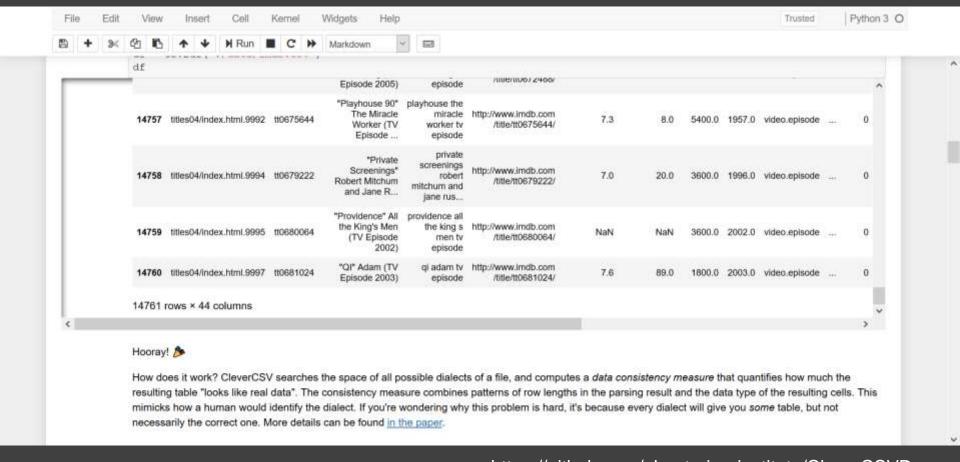


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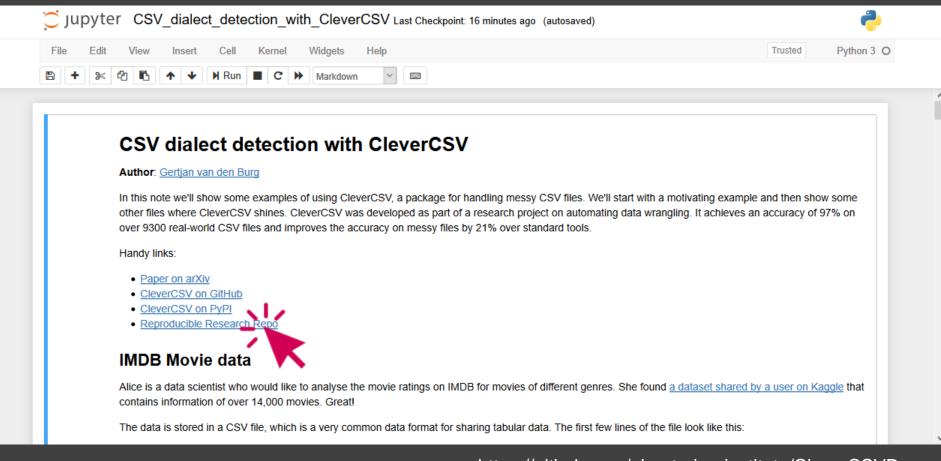


#CiteSoftware #TuringWay @kirstie_j

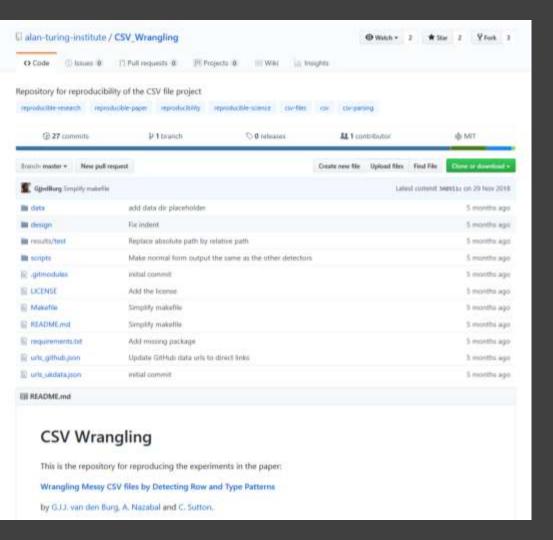




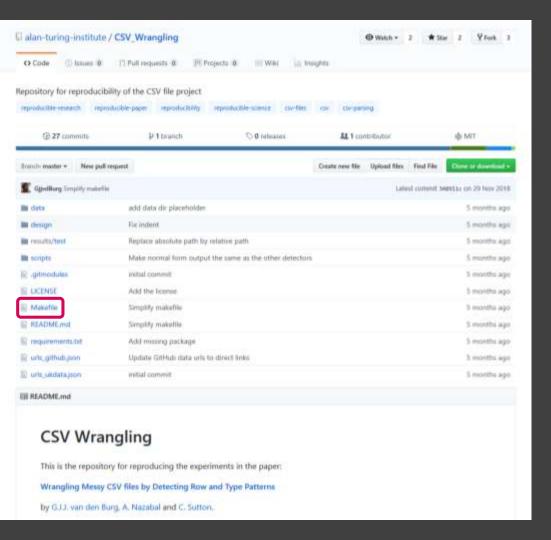
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The Turing Way

- 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 directed acyclic graph). 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

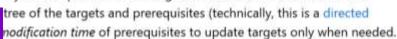
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No chapter on citing software....



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https://the-turing-way.netlify.com/make/make.html #CiteSoftware #TuringWay @kirstie_j https://doi.org/10.5281/zenodo.2783998

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

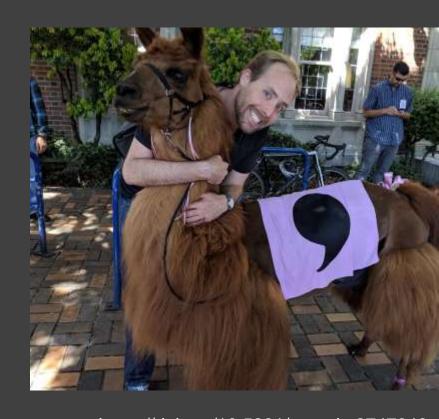


Software as infrastructure



Project Jupyter

- A community of people and an ecosystem of open tools and standards for interactive computing.
- Empower people to use other open tools.
- Slides by Chris Holdgraf (thank you!)



https://doi.org/10.5281/zenodo.2747640 #CiteSoftware #TuringWay @kirstie_j https://doi.org/10.5281/zenodo.2783998

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





code

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> https://doi.org/10.5281/zenodo.2747640 #CiteSoftware #TuringWay @kirstie_j https://doi.org/10.5281/zenodo.2783998



You Coffee!

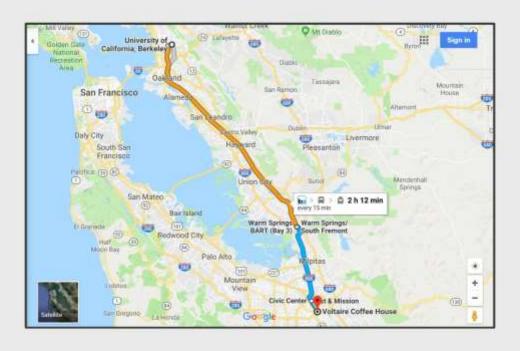
One option: walk there by myself

Another option: pay somebody to drive me

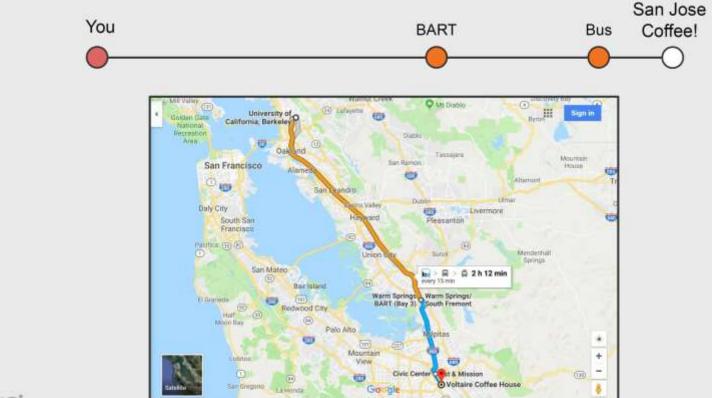
My favorite option: use public infrastructure





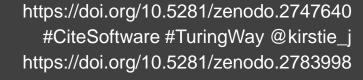










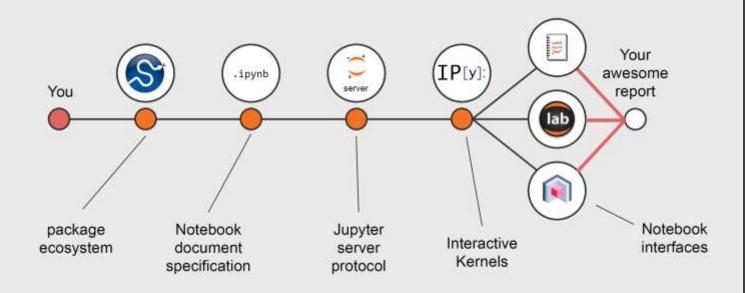


Public infrastructure gets us closer to our goal.

It makes the last mile shorter.



Jupyter shortens the last mile by creating and leveraging public infrastructure





Public infrastructure gets us closer to our goal.

It makes the last mile shorter.



Public infrastructure gets us closer to our goal.

It makes the last mile shorter.



Paying taxes is good

- We benefit from shared resources
- Some are so fundamental that we take them for granted
- We need them to get our jobs done

Tax summery description	Description of PESA source (See PESA Tobio 5.2)	Public Senter Expenditure (Ebn)	
thefure	Social Protector' excluding state persons	174.4	
Health.	Pealth.	965.8	
Stute Parasses	1004 Social Protection*	93.8	
Education	Elecation	618	
National Debt interest	VITTIS General Public Services, but shown in more series in Japan 5.2	44.5	
Defence	Defence	367	
Public Order & Selvey	Public Order & Safety	31.6	
Transport	Economic Affairs, without Studiess and Industry Sult alreads in Horse datalf in Table 5.2	31.3	
Business & Industry	Economic Affairs, without Transport	21.4	
Government Administration	Captured under General Public Services, but shown in more detail in table 5.2	0.2	
Endocement	Environment production	11.4	
Culture (n.g. sports, (director, museums)	Recreation, Culture & Religion	11.0	
Housing and utilities (e.g. street lights)	Housing & Community Amerities	19.1	
Overturas Atd	Captured under General Public Services, but shown in more dehalf in fable 5.2	8.6	
UK Contributions to EU footset	D/ Sussactions	5.4	

https://www.gov.uk/government/publications/how-public-spending-was-calculated-in-your-tax-summary/how-public-spending-was-calculated-in-your-tax-summary

Academi-coin



- Citations are academic currency (whether they should be or not!)
- They're the best way we have to endorse good work.
- We should be citing the software we use.



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 #CiteSoftware #TuringWay @kirstie_j https://doi.org/10.5281/zenodo.2783998

Next steps



The humans are the hardest part of reproducibility and of software citation



How can we change researchers' behaviour?

- Handbook, a place to capture knowledge easily, no excuse that they didn't know to/how
- Checklists, for researchers, Pls, funders and business team members
- Technology, to make it easy to cite the work
- Case studies, to show that it can be done
- Community, to advocate for change

It takes a village

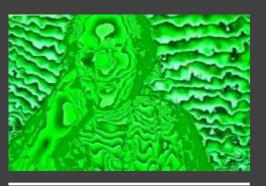




Rachael Ainsworth



Sarah Gibson



Becky Arnold



Patricia Herterich



Louise Bowler



James Hetherington



Rosie Higman



Alex Morley



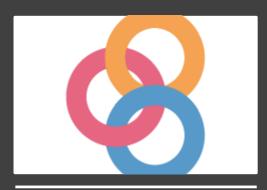
Anna Krystalli



Martin O'Reilly



Catherine Lawrence



Binder Team

Thank you

- https://the-turing-way.netlify.com
- https://tinyletter.com/TuringWay
- https://github.com/alan-turing-institute/the-turing-way
- https://gitter.im/alan-turing-institute/the-turing-way
- Unsplash photos by Freddy Castro, James Pond, Kinson Leung,
 Mateo Vrbnjak, Mimi Thian, Omar Albeik, Perry Grone, Toa Heftiba,
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