# The Alan Turing Institute

The Turing Way
A how to guide for
reproducible research

Kirstie Whitaker



# An introduction to me





0	В	С		J	K	L	M
2							
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	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

0	В	С	1	J	K	L.	M			
2	-		Real GDP growth							
3			Debt/GDP							
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35	New Zealand	1948-2009	2.5	2.9	3.9	-7.9	2.6			
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The humans are the hardest part of reproducibility



Is not considered for promotion

Held to higher standards than others

Publication bias towards novel findings

Requires additional skills

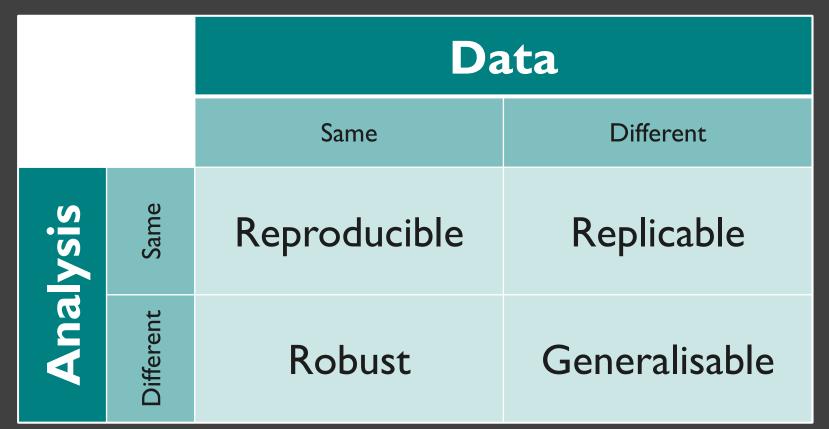
Barriers to reproducible research

Plead the 5th

Support additional users

Takes time

https://doi.org/10.6084/m9.figshare.5537101 #ORLancaster #TuringWay @kirstie\_j https://doi.org/10.5281/zenodo.3238189



https://the-turing-way.netlify.com/reproducibility/03/definitions.html #ORLancaster #TuringWay @kirstie\_j https://doi.org/10.5281/zenodo.3238189

# The Turing Institute



https://www.turing.ac.uk/news/enigma-machine-goes-display-alan-turing-institute #ORLancaster #TuringWay @kirstie\_j https://doi.org/10.5281/zenodo.3238189







## University network





























https://doi.org/10.5281/zenodo.3238189

# The Institute's partners and collaborators

























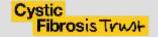






















# Challenges

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 #ORLancaster #TuringWay @kirstie\_j https://doi.org/10.5281/zenodo.3238189

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"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 can't do it at all."



https://www.turing.ac.uk/people/researchers/martin-oreilly #ORLancaster #TuringWay @kirstie\_j https://doi.org/10.5281/zenodo.3238189

# 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

https://the-turing-way.netlify.com/introduction/introduction #ORLancaster #TuringWay @kirstie\_j https://doi.org/10.5281/zenodo.3238189

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Is not considered for promotion

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https://doi.org/10.6084/m9.figshare.5537101 #ORLancaster #TuringWay @kirstie\_j https://doi.org/10.5281/zenodo.3238189

### **Catherine Lawrence**

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

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



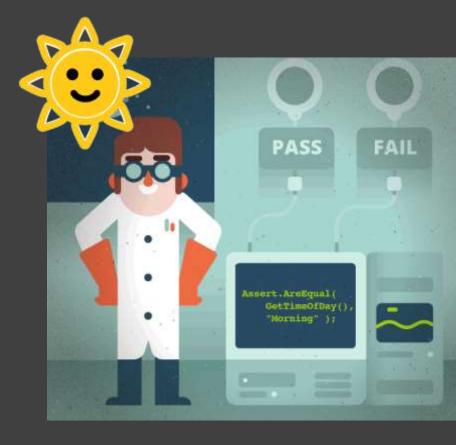
- Reusable (bus factor)" https://www.turing.ac.uk/people/business-team/catherine-lawrence #ORLancaster #TuringWay @kirstie\_j https://doi.org/10.5281/zenodo.3238189

# Testing for research





https://www.toptal.com/qa/how-to-write-testable-code-and-why-it-matters #ORLancaster #TuringWay @kirstie\_j https://doi.org/10.5281/zenodo.3238189

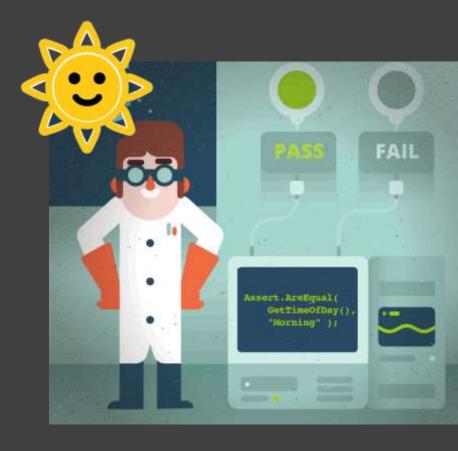


https://www.toptal.com/qa/how-to-write-testable-code-and-why-it-matters #ORLancaster #TuringWay @kirstie\_j https://doi.org/10.5281/zenodo.3238189

Assert.AreEqual(

GetTimeOfDay(),

"Morning" )



https://www.toptal.com/qa/how-to-write-testable-code-and-why-it-matters #ORLancaster #TuringWay @kirstie\_j https://doi.org/10.5281/zenodo.3238189

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### **Louise Bowler**

"Add a test before you change anything."



https://www.turing.ac.uk/people/researchers/louise-bowler #ORLancaster #TuringWay @kirstie\_j https://doi.org/10.5281/zenodo.3238189

### **Louise Bowler**

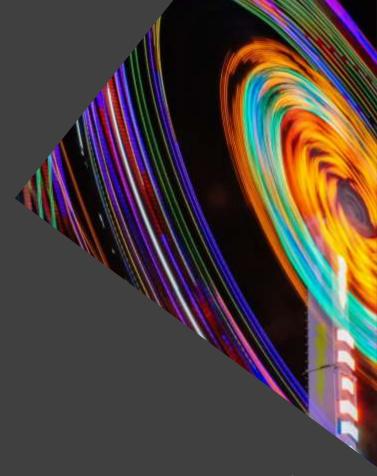
"Add a test before you change anything.

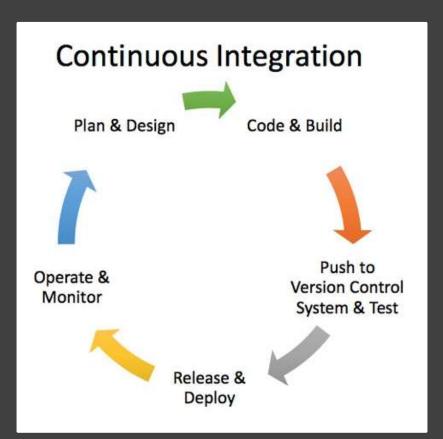
Particularly if you're just going to tidy up your code before sharing it."



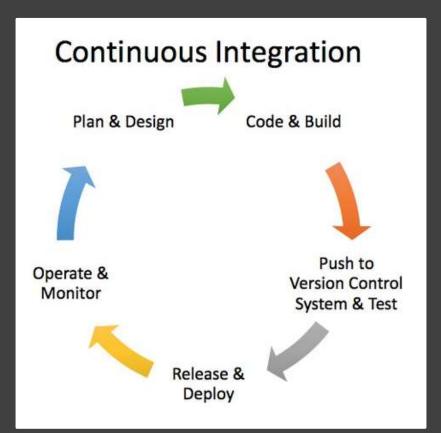
https://www.turing.ac.uk/people/researchers/louise-bowler #ORLancaster #TuringWay @kirstie\_j https://doi.org/10.5281/zenodo.3238189

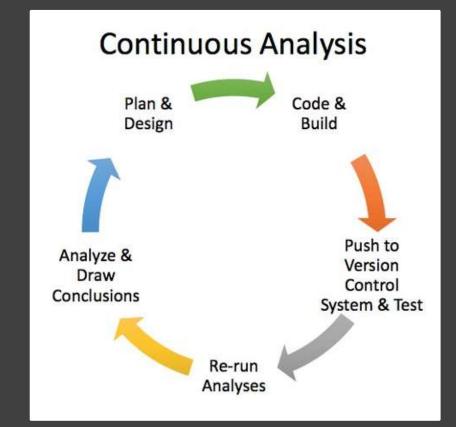
# Continuous Analysis



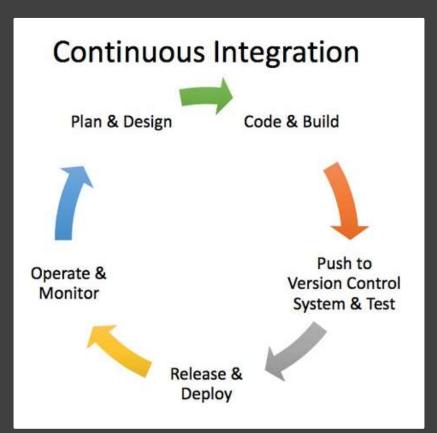


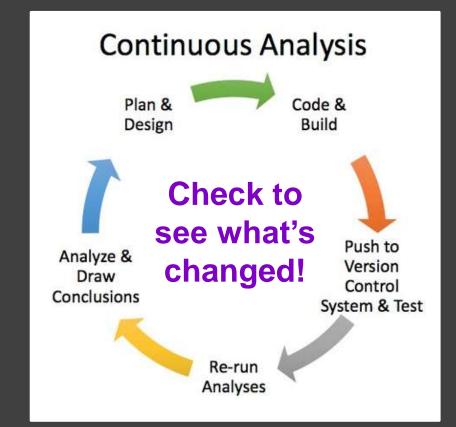
https://elifesciences.org/labs/e623676c/reproducibility-automated #ORLancaster #TuringWay @kirstie\_j https://doi.org/10.5281/zenodo.3238189





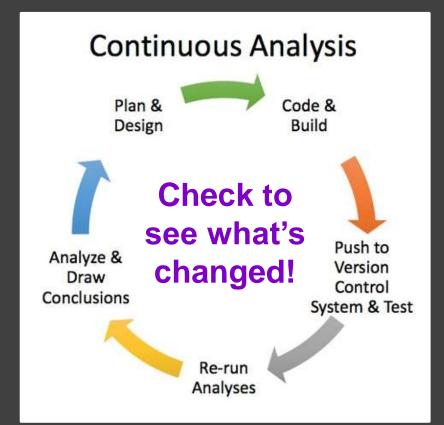
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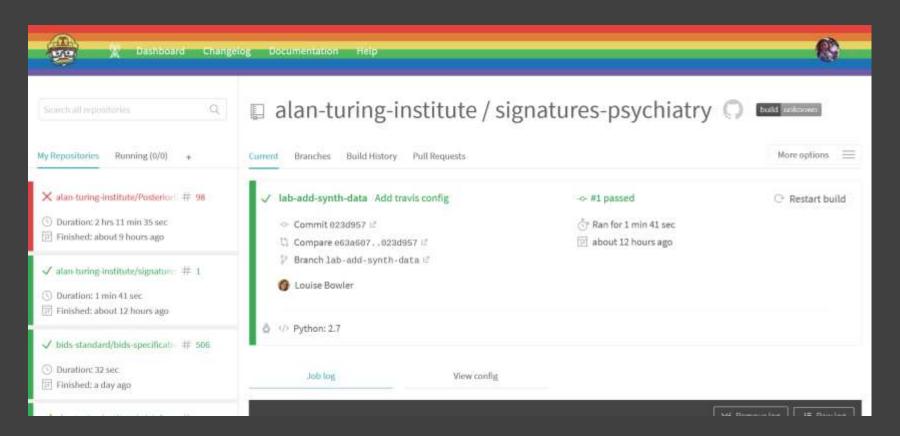


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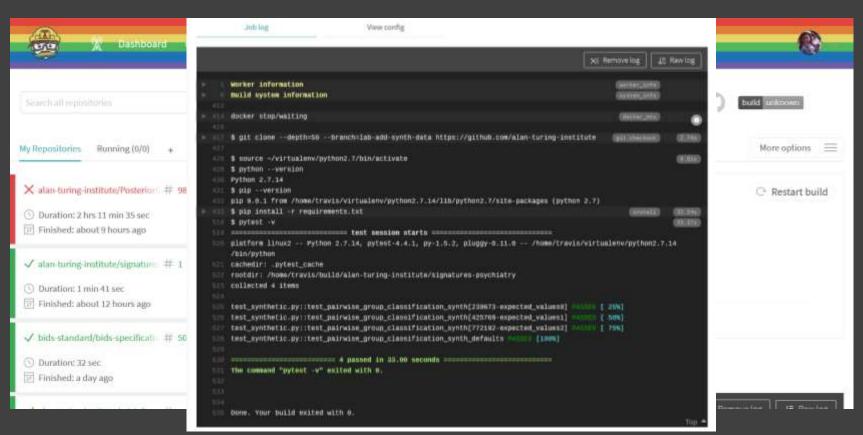




https://elifesciences.org/labs/e623676c/reproducibility-automated #ORLancaster #TuringWay @kirstie\_j https://doi.org/10.5281/zenodo.3238189



https://github.com/alan-turing-institute/signatures-psychiatry #ORLancaster #TuringWay @kirstie\_j https://doi.org/10.5281/zenodo.3238189



https://github.com/alan-turing-institute/signatures-psychiatry #ORLancaster #TuringWay @kirstie\_j https://doi.org/10.5281/zenodo.3238189

- 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 #ORLancaster #TuringWay @kirstie\_j https://doi.org/10.5281/zenodo.3238189

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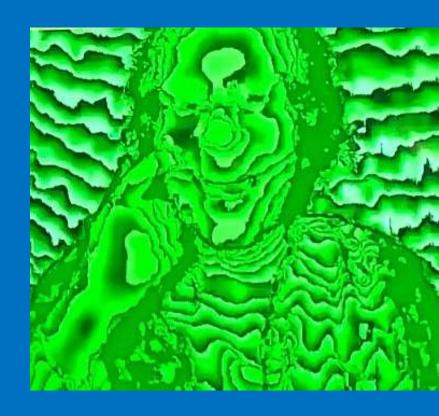
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https://the-turing-way.netlify.com/introduction/introduction #ORLancaster #TuringWay @kirstie\_j https://doi.org/10.5281/zenodo.3238189

# **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/ #ORLancaster #TuringWay @kirstie\_j https://doi.org/10.5281/zenodo.3238189

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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 #ORLancaster #TuringWay @kirstie\_j

## Version control



### "FINAL".doc







FINAL.doc!







FINAL\_rev.6.COMMENTS.doc

FINAL\_rev.8.comments5. CORRECTIONS.doc

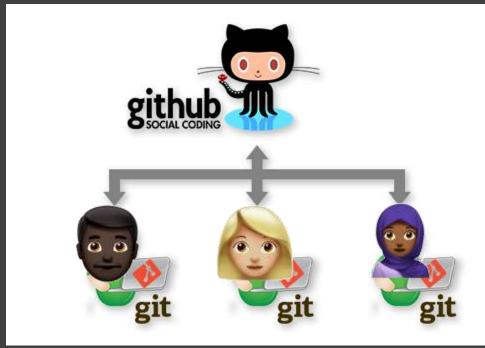






FINAL\_rev.18.comments7. corrections9.MORE.30.doc

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



http://phdcomics.com/comics/archive.php?comicid=1531 #ORLancaster #TuringWay @kirstie\_j https://doi.org/10.5281/zenodo.3238189

### Neurohackademy

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



https://neurohackademy.org #ORLancaster #TuringWay @kirstie\_j https://doi.org/10.5281/zenodo.3238189



https://www.youtube.com/watch?v=hSsjxbRxgqY #ORLancaster #TuringWay @kirstie\_j https://doi.org/10.5281/zenodo.3238189

# Workshops & trainings





https://github.com/alan-turing-institute/the-turing-way/tree/master/workshops #ORLancaster #TuringWay @kirstie\_j https://doi.org/10.5281/zenodo.3238189

# **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 #ORLancaster #TuringWay @kirstie\_j https://doi.org/10.5281/zenodo.3238189



https://www.software.ac.uk/cw19 #ORLancaster #TuringWay @kirstie\_j https://doi.org/10.5281/zenodo.3238189

#### 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 #ORLancaster #TuringWay @kirstie\_j https://doi.org/10.5281/zenodo.3238189

### **Anna Krystalli**

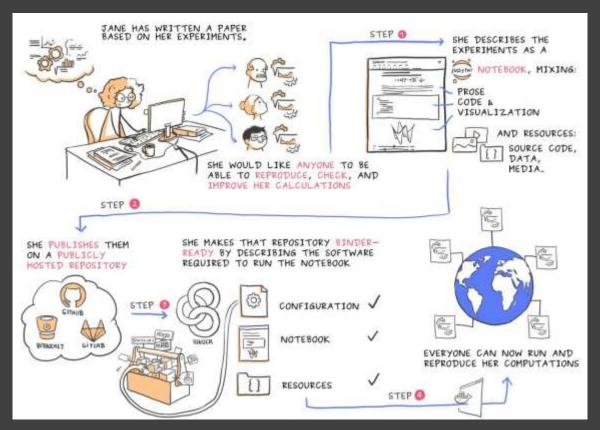
"Checklists are a great way to make it really easy for busy people to do reproducible research. They can catch easily forgotten steps."



https://alexmorley.me #ORLancaster #TuringWay @kirstie\_j https://doi.org/10.5281/zenodo.3238189

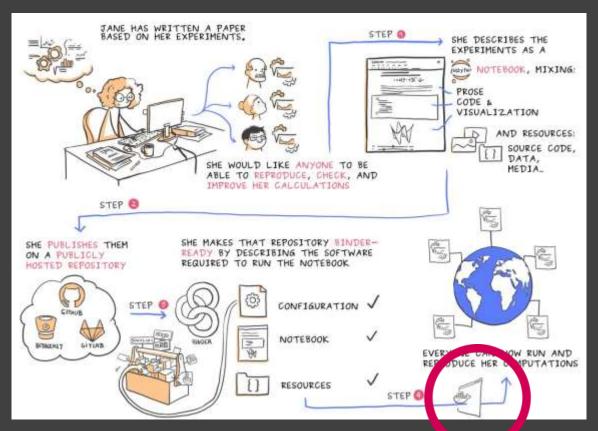
# Turing Way & Binder





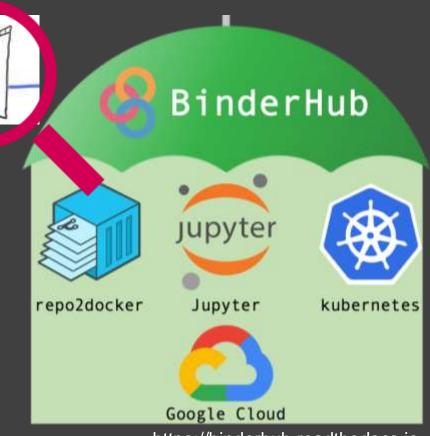
Courtesy of Juliette Taka: https://twitter.com/mybinderteam/status/1082556317842264064 #ORLancaster #TuringWay @kirstie\_j

https://doi.org/10.5281/zenodo.3238189



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 #ORLancaster #TuringWay @kirstie\_j https://doi.org/10.5281/zenodo.3238189

### 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 #ORLancaster #TuringWay @kirstie\_j https://doi.org/10.5281/zenodo.3238189

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



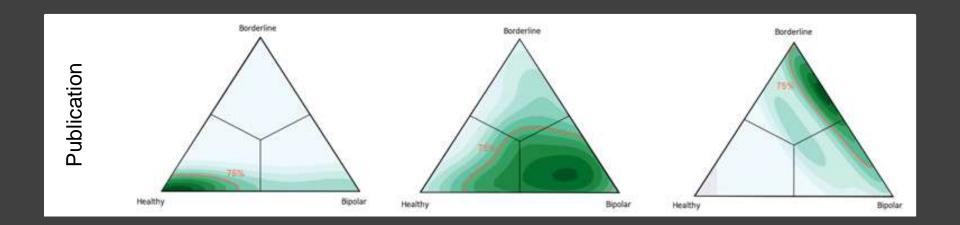
# **Champion: Terry Lyons**

A signature-based machine learning model for bipolar disorder and borderline personality disorder

Imanol Perez Arribas, Guy Goodwin, John Geddes, Terry Lyons, Kate Saunders



https://github.com/alan-turing-institute/signatures-psychiatry https://doi.org/10.1038/s41398-018-0334-0



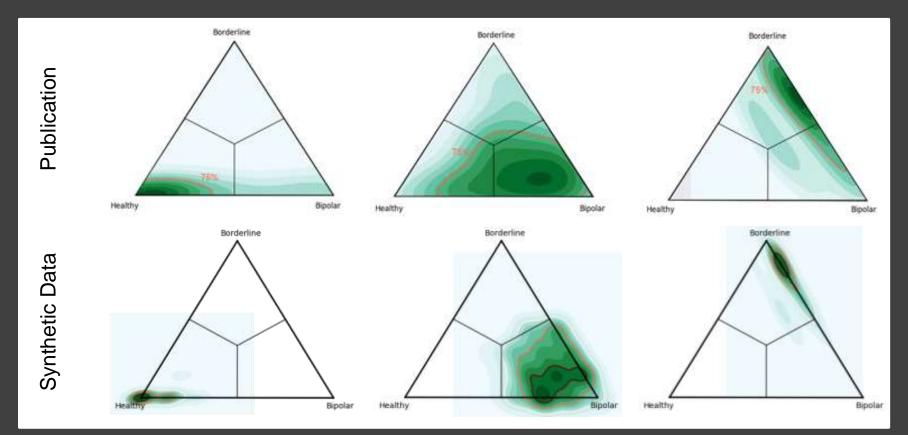
### **Imanol Pérez Arribas**

"We can't share the data. The original researchers did not ask for consent to do so.

We can share simulated and synthetic data so that researchers can feel confident in applying our method to their own data."



https://www.maths.ox.ac.uk/people/imanol.perez #ORLancaster #TuringWay @kirstie\_j https://doi.org/10.5281/zenodo.3238189



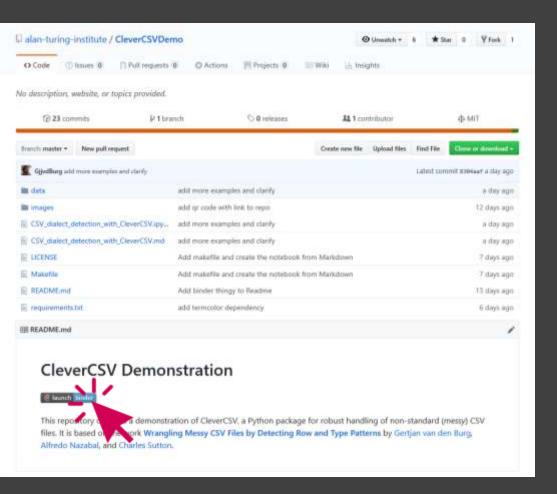
https://github.com/alan-turing-institute/signatures-psychiatry #ORLancaster #TuringWay @kirstie\_j https://doi.org/10.5281/zenodo.3238189

## Gertjan van den Burg

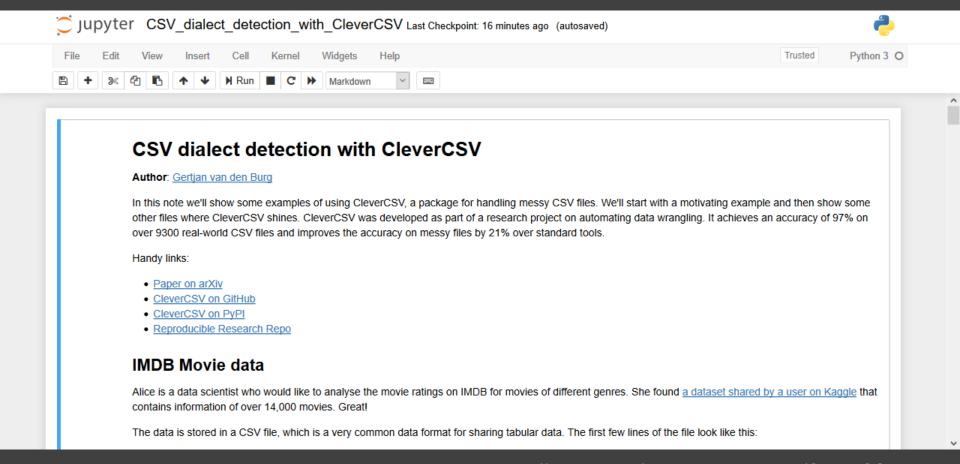
"The fun part of data science is the modelling. Being able to read in information from a csv file should not be the hardest part."

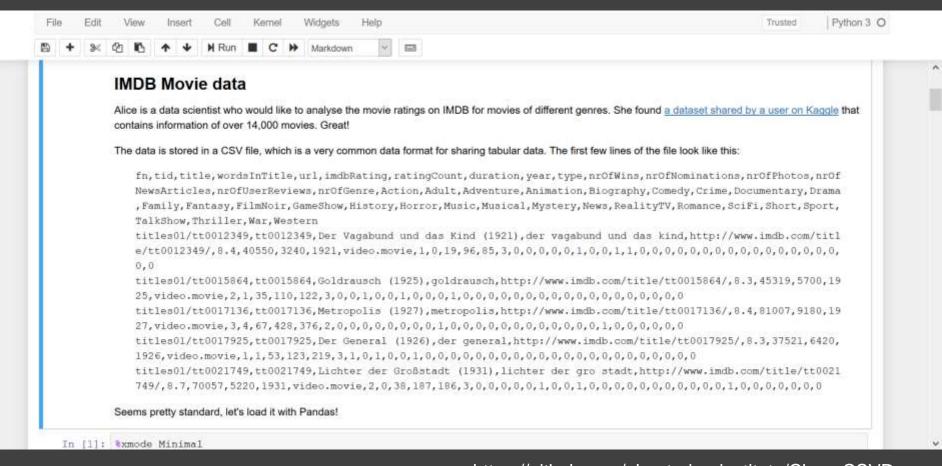


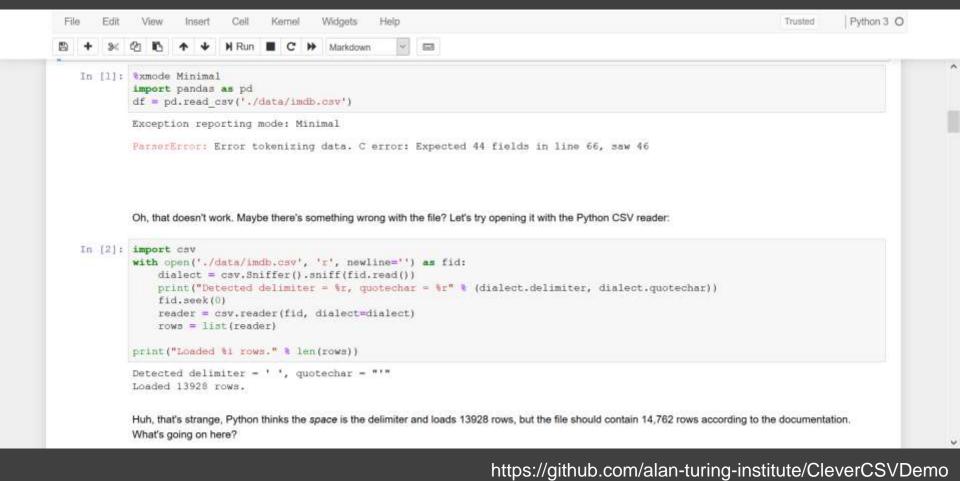
https://gertjanvandenburg.com #ORLancaster #TuringWay @kirstie\_j https://doi.org/10.5281/zenodo.3238189



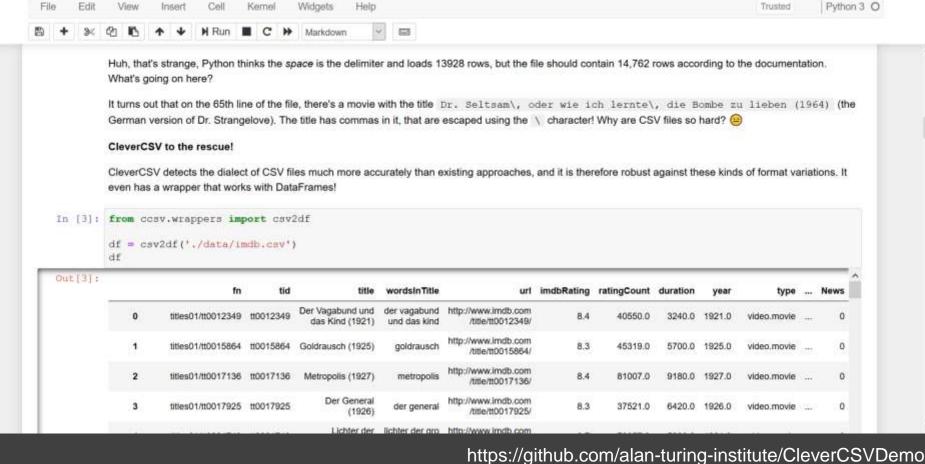
- https://github.com/ alan-turing-institute/ CleverCSVDemo
- "Wrangling Messy
   CSV Files by
   Detecting Row and
   Type Patterns"
   arXiv:1811.11242





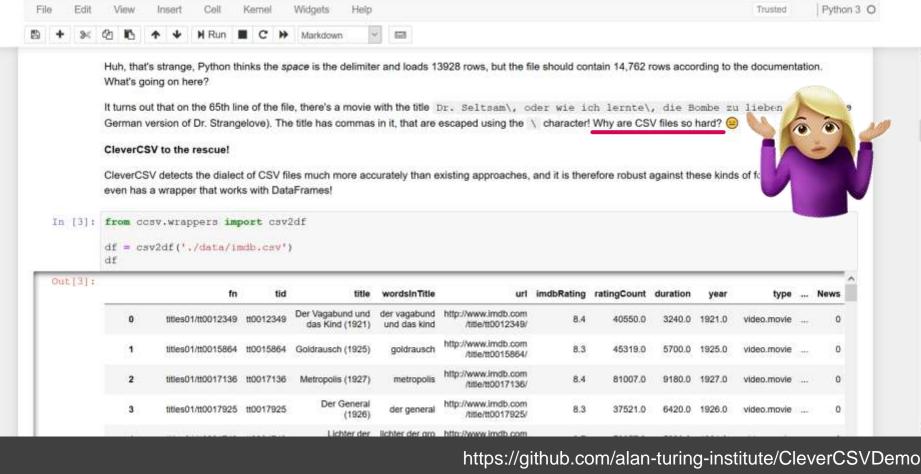


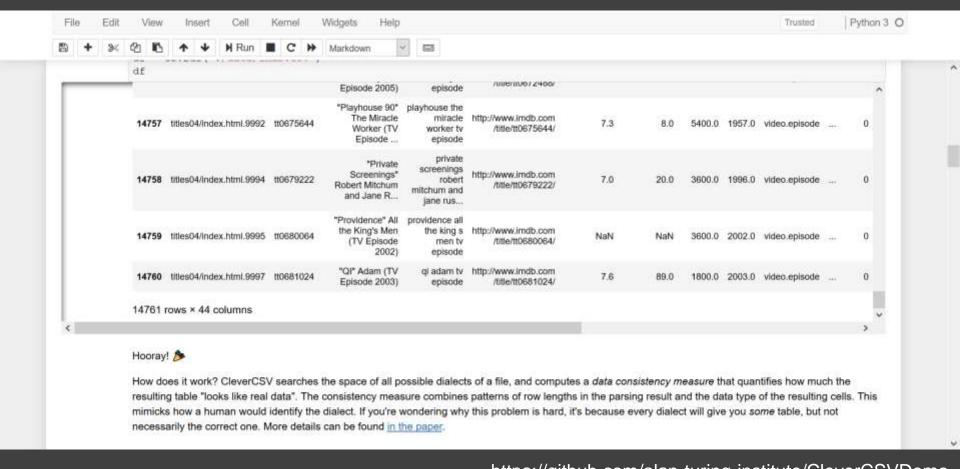
#ORLancaster #TuringWay @kirstie\_j



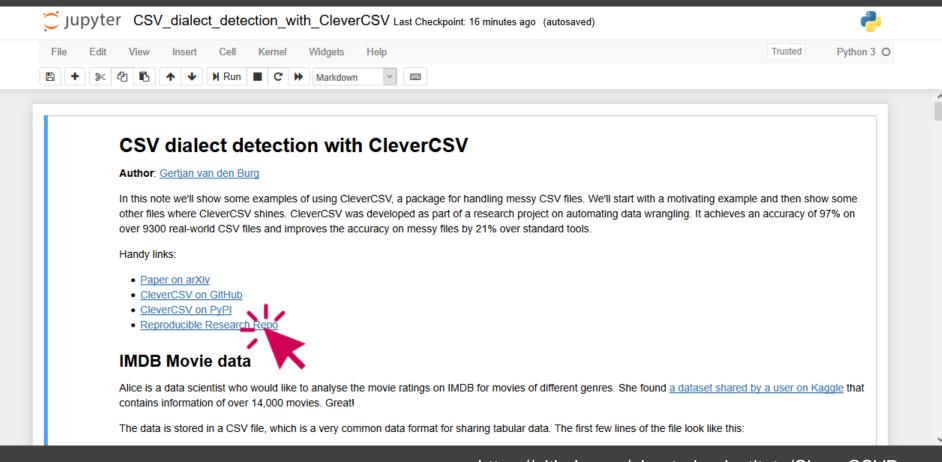
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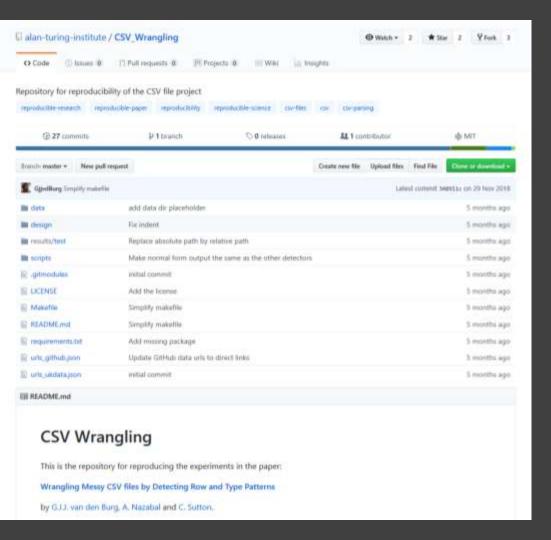




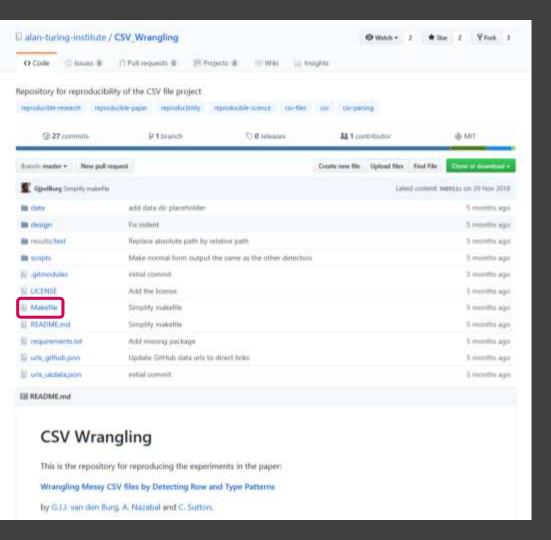
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### The Turing Way

- 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.

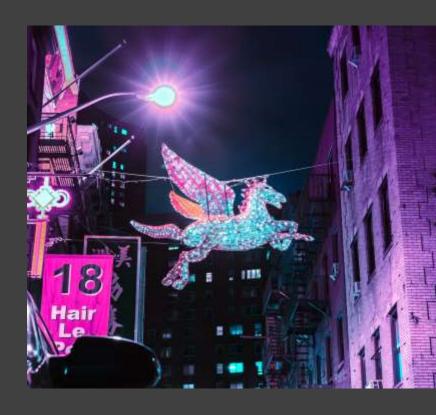
#### Learn Make by Example

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
- Generate new content
- Inspire



# A global collaboration

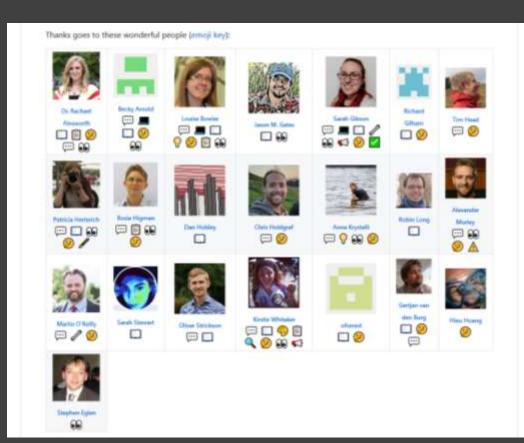


### **Patricia Herterich**

"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 #ORLancaster #TuringWay @kirstie\_j https://doi.org/10.5281/zenodo.3238189





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

https://allcontributors.org/docs/en/bot/overview https://allcontributors.org/docs/en/emoji-key

## **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**

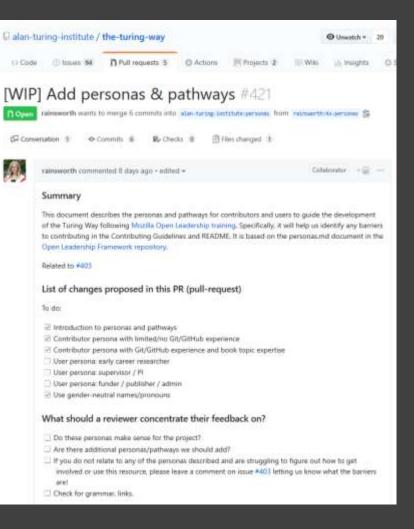
You build shared ownership and agency to make the work inviting and sustainable for all.

### 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 #ORLancaster #TuringWay @kirstie\_j https://doi.org/10.5281/zenodo.3238189



- 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 #ORLancaster #TuringWay @kirstie\_j https://doi.org/10.5281/zenodo.3238189

# The future



### **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



http://www.scriberia.co.uk #ORLancaster #TuringWay @kirstie\_j https://doi.org/10.5281/zenodo.3238189

### **Funding extension**

- Expand the scope to all of data science practices
- Full time community
   manager, contributions
   from Turing and
   beyond



https://github.com/ alan-turing-institute/the-turing-way/ blob/master/ project\_management/ tps-funding-application-20190429.md

## **Alex Morley**

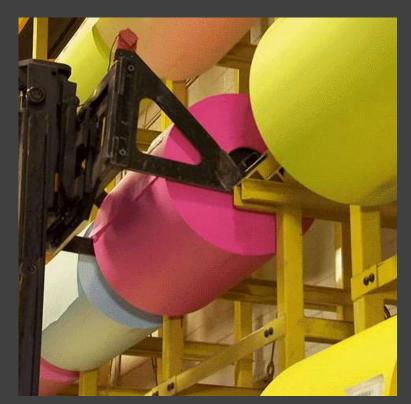
"I think the coolest part of The Turing Way is the balance it strikes between being authoritative and being an open communitydriven project."



https://alexmorley.me #ORLancaster #TuringWay @kirstie\_j https://doi.org/10.5281/zenodo.3238189

## **Carpentries & beyond**

- Workshop at CarpentryConnect
- Interactive tutorials
- JOSE papers
- Train the trainers
- Interoperability & reusability at all times



https://www.software.ac.uk/ccmcr19 #ORLancaster #TuringWay @kirstie\_j https://doi.org/10.5281/zenodo.3238189

## Sharing the responsibility for reproducibility

- Handbook, a place to capture knowledge easily
- Technology, to make it easy for senior investigators to review code
- Case studies, to show that it can be done
- Checklists, for researchers, Pls, funders and business team members
- Community, to support each other

# It takes a village

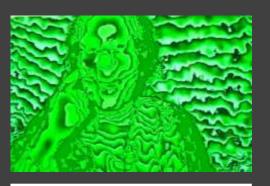




Rachael Ainsworth



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

Alan Turing Institute

The

Book: <a href="https://the-turing-way.netlify.com">https://the-turing-way.netlify.com</a>

moz://a

- Newsletter: <a href="https://tinyletter.com/TuringWay">https://tinyletter.com/TuringWay</a>
- GitHub: https://github.com/alan-turing-institute/the-turing-way
- Chat: <a href="https://gitter.im/alan-turing-institute/the-turing-way">https://gitter.im/alan-turing-institute/the-turing-way</a>
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https://doi.org/10.5281/zenodo.3238189