The Alan Turing Institute

The Turing Way:

Open Source and reproducibility in data science

Malvika Sharan

Pronouns: she/her







- PhD in Bioinformatics
- Open Access & Open Source research publications
- Computational and Open Science skill training (2015-)
- Community Building in Open Science (2016-)
- The Turing Way (2019-)



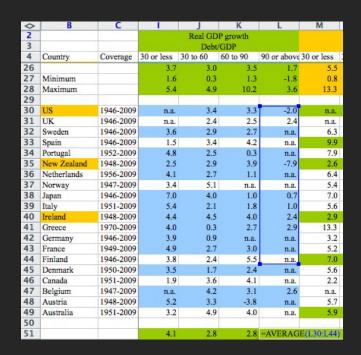






- 1. About The Turing Way
- 2. Guide to computational reproducibility
- 3. Open Source to enhance reproducibility

Academic errors have real world effects





Academic errors have real world effects

\langle	В	С		J	K	L	M
2				Real GD	P 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)

"...paper often used to make the case for austerity cuts contains major errors."

"... only included 15 of the 20 countries (of average GDP growth in countries with high public debt)."

"We will redouble our efforts to avoid such errors in the future ..."

Applying best practices in our research requires intention, resources, time and collaboration, which can be overwhelming.



Blog post: https://www.software.ac.uk/blog/2020-12-17-ten-arguments-against-open-science-you-can-win

		Data							
		Same	Different						
Analysis	Same	Reproducible	Replicable						
Ana	Different	Robust	Generalisable						

Barriers to Reproducibility & Open Research

- Reward system
- Novel findings
- Publication cost
- Training and skill transfer
- Leadership
- Institutions (often)
- Lack of trust



Added advantages

















An **Open Source** project that involves and supports its **diverse community** to make data science **reproducible**, **ethical**, **collaborative and inclusive** for you.

The Alan Turing Institute

The national institute for data science and artificial intelligence



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

Tools, Practices and Systems

- Trustworthy systems
- Transparent reporting
- Inclusive interoperable design
- Ethical integrity
- Respectful co-creation
- Leadership in open research



@malvikasharan, @turingway, CC-BY 4.0,

The Turing Way, DOI: 10.5281/zenodo.4818126



Book:

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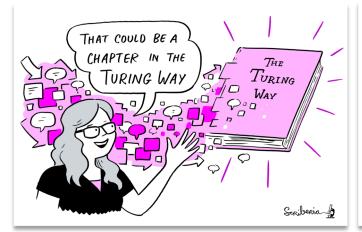
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A Book



A Community



An Open Source Project



A Culture of Collaboration



The Turing Way Book on Reproducibility



Kirstie Whitaker

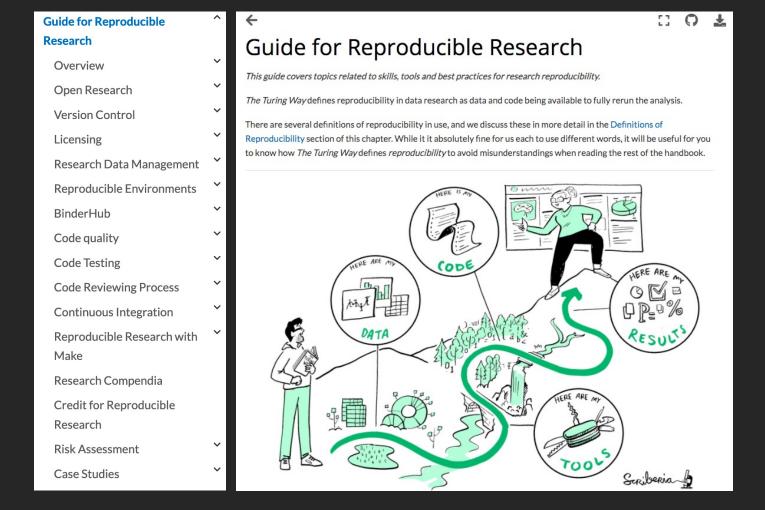
Lead of Tools, Practices & Systems Programme

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

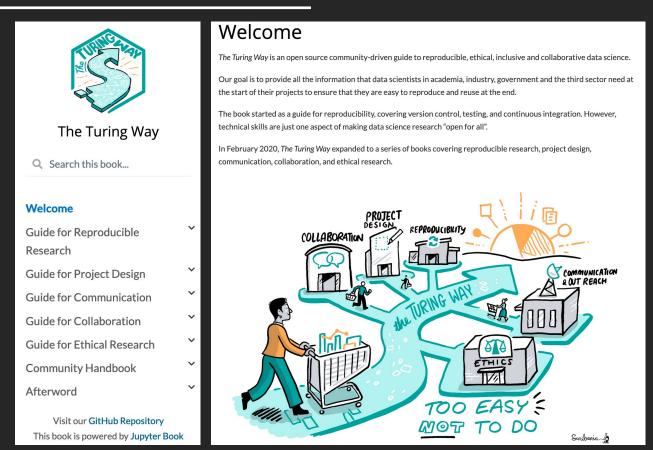
Our goal is to provide all the information that researchers need at the start of their projects to ensure that they are easy to reproduce at the end.

This also means making sure PhD students, postdocs, Pls, 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.





Moonshot Goal: Reproducibility "too easy not to do"





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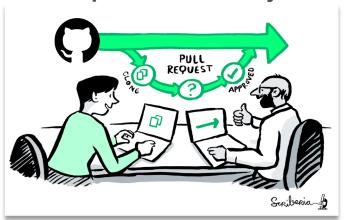
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A Book



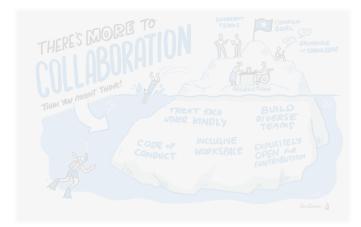
An Open Source Project



A Community



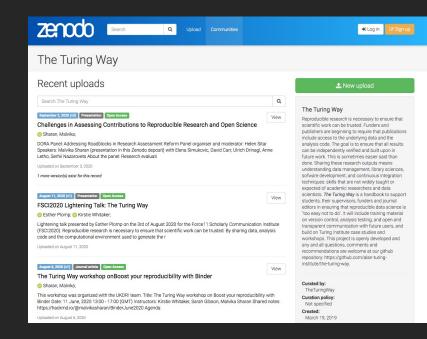
A Culture of Collaboration



An open source project

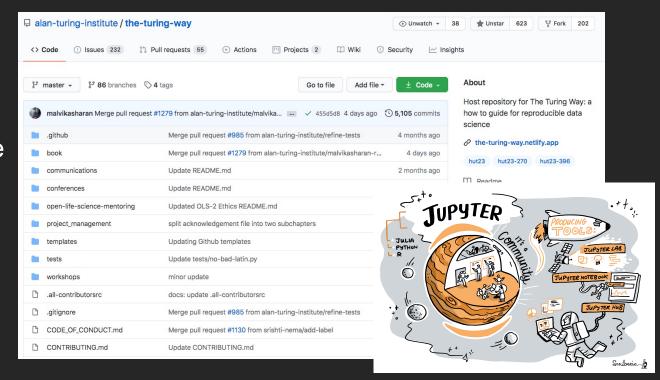
everyone can freely read, reuse,distribute, modify and help develop

the project belongs to *The Turing Way* community (CC-BY license)



An open source project

Hosted on GitHub,
builds on and uses
different Open Source
tools: Git, Netlify,
Binder, Jupyer Book,
communication tools



github .github	Remove prettier configuration	かいけんとこ
book	minor update	\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\
communications	Fix typos	
conferences	Add KW formatting pedantry	
project_management	Update online-collaboration-cafe.md	
templates	Updating Github templates	
tests tests	Add "et cetera" as a deprecated Latinism	
workshops	Remove mis-pasted text	
all-contributorsrc	Merge pull request #991 from alan-turing-institute/all-contrib	outors/a 5 days ago
igitignore	ignore pptx in workshop folder	9 months ago
: travis.yml	add html-proof file again	last month
CODE_OF_CONDUCT.md	her -> their	6 months ago
CONTRIBUTING.md	Update CONTRIBUTING.md	2 months ago
GOVERNANCE.md	Read through months later	5 months ago
LICENSE.md	Fix typo in licence	2 months ago
README.md	Merge pull request #991 from alan-turing-institute/all-contrib	outors/a 5 days ago
book_skeleton.md	Update book_skeleton.md	13 months ago
contributors.md	Add myself to contributors.md	11 months ago
tips_and_tricks_survey.md	Update tips_and_tricks_survey.md	14 months ago
ways_of_working.md	Adjust team contact section	5 months ago

Scriberia 🖢

An open source community framework

decentralized development process that encourages open collaboration and peer production.



The Turing Way



Resources



Shared
Vision &
goals for
the project



- Public repo
- open source infrastructure
- collaborative development
- processes & platforms





Community building:

- transparent communication
- community handbook
- shared ownership
- value exchange
- meaningful incentive structure

Measurable outcome

Quality Assurance Sustainability

Support system

Community culture

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A Culture of Collaboration



Pathways for Collaboration



Develop & share



Review and update



Maintain & improve



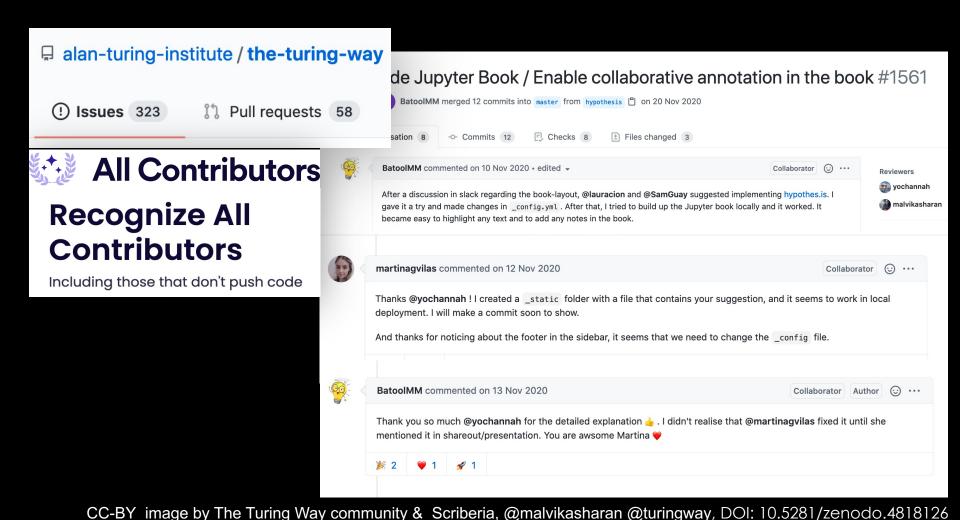
Make it global



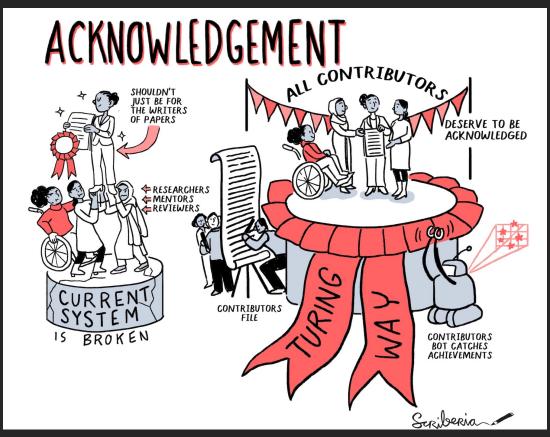
Share resources



Share best practices



Recognise All Contributions



Batool Almarzouq

- Role: Book Dash November 2020 Attendee
- ORCID: 0000-0002-3905-2751
- Short bio:

I'm the founder of R-Ladies in Saudi Arabia (Dammam). I initially majored in pharmacology but quickly developed an interest in biochemistry, structural biology, and bioinformatics. I enjoy applying deep learning to answer biological questions.

Personal highlights:

I am currently co-developing a chapter on "CI services". I have helped upgrade the Jupyter Book Infrastructure and add hypothes.is to enable collaborative annotation of *The Turing Way* chapters. I have also translated the README.me chapter in Arabic. Personal quote: "I find it hard to express my personal thoughts and feelings in words. This was such an amazing experience. It helped me to develop my technical skills. Thank you so much to everyone I met in this Book Dash event :heart:"

Supporting Development



Important

Please note that these requirements are not exhaustive or definitive, and neither are their classifications rigid. Moreover, no items are inherently more important than the other.

If you identify more consistency issues that need to be addressed, join the conversation here.





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A Book



An Open Source Project



A Community

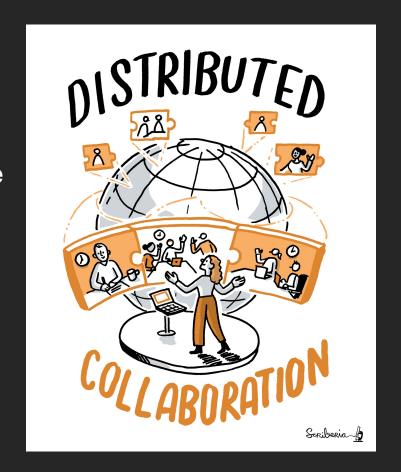


A Culture of Collaboration

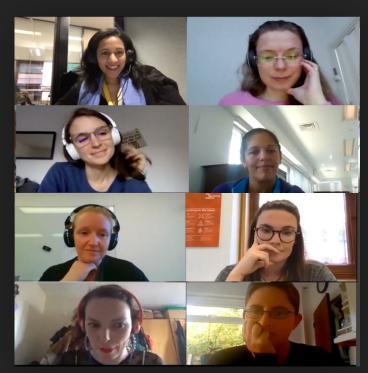


Open Community

- Interested members can join & contribute
- direction and the goals are determined collaboratively
- Governance for decentralised decisionmaking is in progress



A Community of Contributors



Collaboration Cafés & Co-working Calls



Book Dash Events



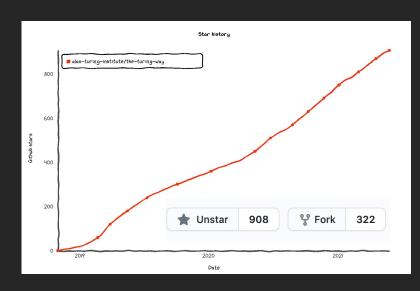
More than a Book!

The co-working hours are friendly for introverts who might be intimidated working with new people. These personal interactions are also crucial for staying motivated!

Martina G. Vilas

Project and Community Growth

- >2 years, >155 subchapters
- Community resources, guidance, templates, training
- 267 direct contributors and
 >3000 unique visits per month



https://zenodo.org/record/4323154











Adina Wagner	Aditi Shenvi	Albert Hornes Vidal	Alex Bird	Alex Chan	Alex Clarke	Alexander Morley	Charlotte Watson	Chris Holdgraf	Chris Markiewicz	Christina Hitrova	Christopher Lovell	Clare Uggins	Colin Sauze	Georgia Atkinson	Georgia Tomova	Georglana Elena	Gertjan van den Burg	Gianni Scolaro	Graham Lee	Greg Klar	Stefan Janssen	Stefan Verhoeven	Stephan Druskat	Stephen Eglen
All Seyhun Saral	Andrea Pierré	Andrew Stewart	/æn/ Andrian Nobella	Angelo Variotta	Anna Hadjitofi	Anna Krystalli	Dan Hobley	Danbee Kim	Daniel Lintott	Daniel Mietchen	Daniel Nüst	Danny Garside	David Foster	Gustavo Becelli do Nacimento	Heidi Seibold	Hieu Hoang	lan Hinder	Isil Bilgin	Ismael-KG	COMMUNICAL ITS NOT FOR DESTROOT.	Tarek Allam	Tess Gough	Thomas Sandmann	Tim Head (>)
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Kim De Ruyck	Kim De Ruyck	Kirstie Whitaker	Kristijan Armeni	Krunal Rank	Lachlan Mason	Laura Acion	Naomi Penfold	Natacha Chenevoy	Natalie Thuriby	Nathan Begbie	-		Nick Barlow	Rachael Ainsworth	Radka Jersakova	Raniere Silva	Reina Camacho Toro	Remi Gau	Reshama Shaikh	Richard Gilham	Tim Head	Tim Powell	Sansone III Tony Yang	Name of the second of the seco
Laura Carter	Lenka	Liberty Hamilton	Louise Bowler	Luca Bertinetto	Lupe CaMay	Malvika Sharan	Nico	Nicolás Alessandroni	Nomi Harris	Obi Thompson Sargoni	Oliver Clark	Oliver Forrest	Oliver Hamelijnck	Risa Ueno	Robin Long	Rohit Midha	Romero Silva	Rose Sisk	Rosie Higman	Rosti Readioff	Wieblee	Will Hulme	Wolmar Nyberg	oxpeter
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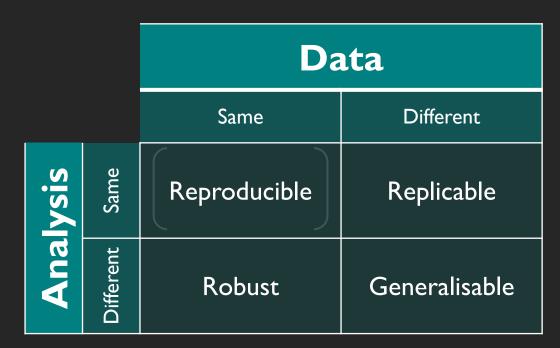
1. what is *The Turing Way*?

2. guide to computational reproducibility

3. Open Source to enhance reproducibility

Reproducible Research

same analysis steps on the same dataset produces same answer



https://the-turing-way.netlify.app/reproducible-research/overview/overview-definitions.html

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The Turing Way chapters on reproducibility

Guide for Reproducible Research

Overview

Open Research

Version Control

Licensing

Research Data Management

Reproducible Environments

BinderHub

Code quality

Code Testing

Code Reviewing Process

Continuous Integration

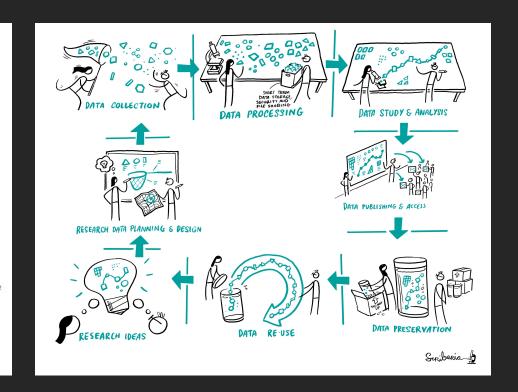
Reproducible Research with Make

Research Compendia

Credit for Reproducible Research

Risk Assessment

Case Studies



Computational Reproducibility

- → Track changes to your code/resource (version control)
- → Write clean, understandable and error free code
- → Save and share your computational environment
- → Make your code open for others to test and use

Computational Reproducibility

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Version Control

- records changes to a file or set of files over time
- provides access to any specific version

Version Control



- changes are recorded using snapshots
- distributed version control system
- Git is very complex, don't need to learn everything
- Start with the parts you need (commit, push, pull)
- Web and Desktop App GUI interface



Computational Reproducibility

- → Track changes to your code/resource (version control)
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Code Style Guide

- set of conventions on how to format code
- e.g.
 - ✓ Indentation
 - Comments
 - ✓ Imports
 - Naming

Code Style Guide: Now is better than never

- PEP 8 convention
- Enforcement tools → flake8
- Automatic formatting tools

```
!flake8 example files/bad file.py
 example_files/bad_file.py:1:80: E501 line too long (80 > 79 characters)
 example_files/bad_file.py:3:2: E225 missing whitespace around operator
# in:
j = [1,
# out:
i = [1, 2, 3]
```

https://www.python.org/dev/peps/pep-0008/

Code Review

have another programmer look over your code and assess it

Identify how you facilitate it

- → synchronous
 - lab meetings presentations
- → asynchronous
 - GitHub



Code Testing

Write tests. Any tests.

"You should not skip writing tests because you are short on time, you should write tests because you are short on time"

Code Testing

Write tests. Any tests.

"You should not skip writing tests because you are short on time, you should write tests because you are short on time"

Examples:

- Print (sanity check)
- Assert (assertion error)

https://the-turing-way.netlify.app/reproducible-research/testing.html

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Types of Testing

- Unit testing: individual units of a software are tested
- Pytest framework: supports complex functional testing for libraries.
- Smoke test: initial checks designed to ensure very basic functionality
- Integration test: individual units are combined and tested as a group
- ...

Computational Reproducibility

- → Track changes to your code/resource (version control)
- → Write clean, understandable and error free code
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Reproducible Computational Environments

Interaction style

What is reproduced?

Graphical Command line Software and versions **Spinder CONDA Entire** system

Computational Reproducibility

- → Track changes to your code/resource (version control)
- → Write clean, understandable and error free code
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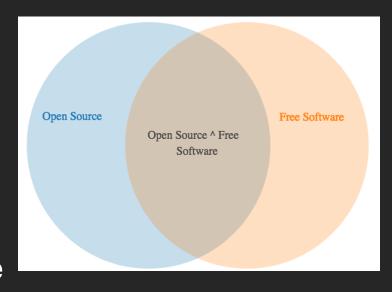
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Open Source

 Openly shared code that anybody can view, use, modify, and distribute the software for any purpose

Open Source ≠ Free

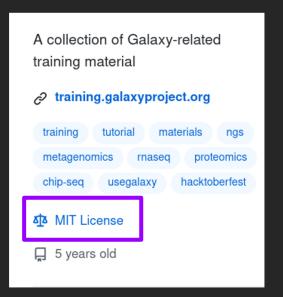
- Free software isn't always open
 - No Access to source code
 - Illegal to modify due to license
- Open source doesn't mean free
 - You can charge for your open source software!



Open Source is simply licensing your work so it can be used how YOU want.

Open Source

- Open source software has a LICENSE.
- Unless there is a licence, online code is NOT legally open for re-use.



For those who want:

Open source makes it easy for others to re-use and remix your work, and you get credit.

Why Open Source?

- code can be reviewed, re-used & integrated into other systems.
- Hacker ethic collaborate! If you benefit from Open Source, give back
- Distributed innovation: share your work, and others will share back.
 Features, bugs, ideas for improvement
- **Document for yourself**, that also helps new and existing contributors.

You are your number one collaborator!

Open Source benefits (future) you!

But what is I get scooped?

- If someone steals it, it will be more obvious to reviewers ("Hey isn't this the same code?")
- If your collaborators are still worried publish a preprint, quick way to document that you were first.
- Offsite copies (on remote servers) to access the latest version
 - Hard drive corruption? Hard drive stolen? Cryptolockers?

Risk of close

Reinhart, Rogoff... and Herndon: Th student who caught out the profs

By Ruth Alexander BBC News

() 20 April 2013

This week, economists have been astonished to find that a famous academic paper often used to make the case for austerity cuts contains major errors. Another surprise is that the mistakes, by two eminent Harvard professors, were spotted by a student doing his homework.

It's 4 January 2010, the Marriott Hotel in Atlanta. At the annual meeting of the American Economic Association, Professor Carmen Reinhart and the former chief economist of the International Monetary Fund, Ken Rogoff, are presenting a research paper called Growth in a Time of Deht

Researchers find bug in Python script may have affected hundreds of studies

"Willoughby-Hoye" scripts used OS call that caused incorrect measurements on Linux, Moiave

SEAN GALLAGHER - 10/15/2019, 3:17 PM

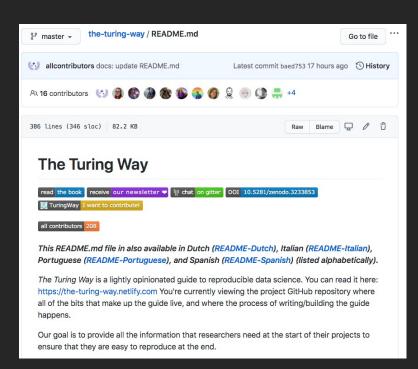


PLOS ONE PHYLOGENY/FLICKR (CC BY 2.0)

One in five genetics papers contains errors thanks to Microsoft Excel

A Few Steps to Make Your Work Open Source

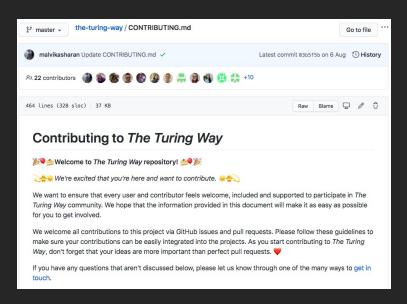
Community Files



README.md

- project name and main features
- installation instructions
- how to run associated tests
- list of authors/contributors
- contact information
- links to related material

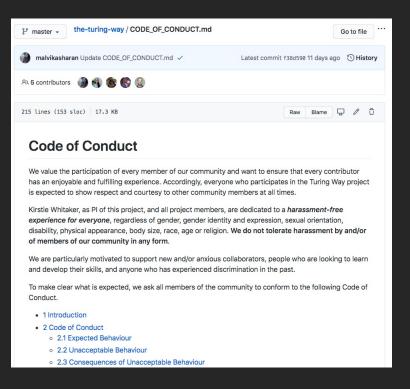
Contribution Guideline



CONTRIBUTING.md

- how to file a bug report
- how to suggest a new feature
- how to contribute changes
- roadmap or vision for the project
- how contributors should (or should not) get in touch with you

Code of Conduct



CODE_OF_CONDUCT.md

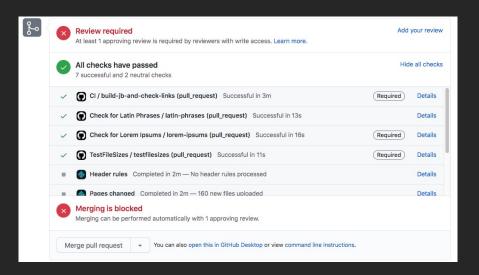
- how you expect participants to behave
- who these expectations apply to
- when they apply
- what to do if a violation occurs

Continuous Integration

practice of integrating changes to a project made by individuals into a

main, shared version

frequently





"Make research resources available online without price barriers and without most permission barriers."

- Suber et. al., 2012

Toward a UNESCO Recommendation on Open Science: Canadian Commission for UNESCO By Ella Chan, Dick Bourgeois-Doyle, Michael Donaldson, and Eleanor Haine-BennettOttawa, Canada, April 2020



Open Science involves many concepts.

Take possible steps to make your work open.

Ask for feedback and help whenever you can.

Practice reproducibility with open science



Laurent Gatto

Open science, reproducible research, data champion, computational biology, proteomics, more omics, emacs, a lot of R, quite a bit of running, and parenting.

Becoming a better scientist with open and reproducible research (2)

25 minute read

This is an modified version of the Becoming a better scientist with open and reproducible research talk that I gave at TU Delft in May 2019. This version was modified and prepared for the Virtual Bioinformatics Student Symposium on the 4 December 2020. The slides are available here and the recording is available on youtube.

ON THIS PAGE

The Turing Way Guides



Reproducibility



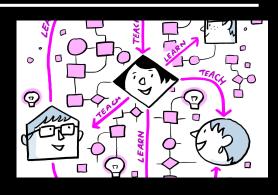
Collaboration



Project Design



Ethical Research



Communication

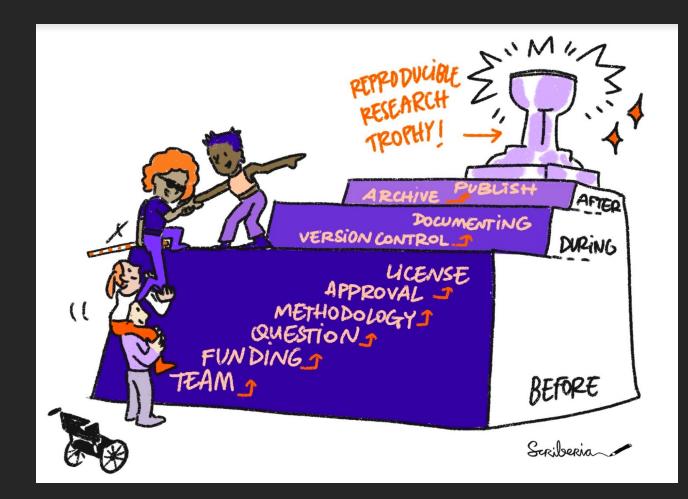


Community Handbook

Share your skills, methods, practices, case studies, while using The Turing Way as a tool.

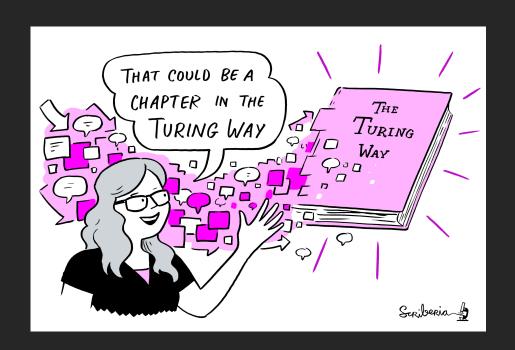


Guide your project design



Join us!

- Reading/sharing
- Editing
- Writing
- Reviewing
- Linking
- Automating
- Curating
- Translating
- Promoting



Create your own version of *The Turing Way*

Module 1: Welcome to the tutorial

Creating a Jupyter Book with The Turing Way

by Malvika Sharan



|upyter**c⊚N**

module 3:

Jupyter Book set-up

by Martina Vilas



jupyter**c**•N

module 6:

Jupyter Book CI/CD

by Sarah Gibson @sgibson91



Creating a Jupyter Book with The Turing Way

Module 6: Continuous Integration and Deployment - An Introduction

Learning Objectives:

- Explain what Continuous Integration (CI) and Continuous Deployment (CD) are and how they are useful for reproducible workflows
- Explain how we can use CI and CD when publishing a Jupyter Book
- Introduce GitHub Actions and discuss why we use it in The Turing Way
- Guide our learners setup a GitHub Action on their repository

Continuous Integration (CI)

Continuous Integration (CI) is the process of automating the integration of code changes from multiple contributors into a single software project. This process is often comprised of a range of automatic tooling to assert the new code's correctness before integration. A version control system is the crucial element of CI processes and is often supplemented with other checks such as code quality, syntax style reviews, and more.

CI for Jupyter Book

When building a Jupyter Book, we may use CI processes to achieve tasks like spellchecks, checking for broken links, code cells are bug-free and don't hang, and so on.

Continuous Deployment (CD)

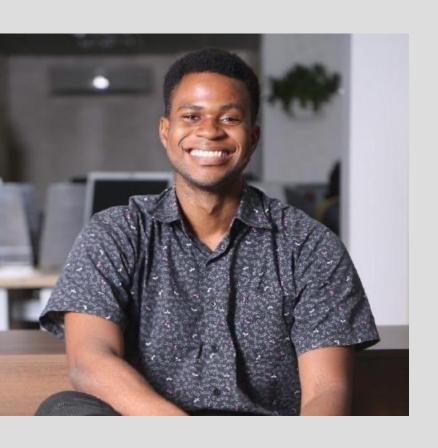
Continuous Deployment (CD) is a software release process that uses automated testing to validate if changes to a code base are correct and stable before immediate deployment to a production environment. This is beneficial as bug fixes and new features can often be in the hands of users as soon as they are pushed.

CD for Jupyter Book

A CD process for Jupyter Book might include a deployment preview so that we can automatically check what the rendered book will look like with the added content before releasing it.

https://github.com/martinagvilas/tutorial-jupyterbook-with-turing-way/

@malvikasharan, @turingway, CC-BY 4.0, The Turing Way, DOI: 10.5281/zenodo.4818126



Pay it forward!

I realised that the value I left behind in The Turing Way is not in the amount of work I did, but how I enabled other contributors.

Paul Owoicho, GSoD intern

Acknowledgements:

- Kirstie Whitaker (@kirstie j), Project Lead
- Martina G. Vilas (<u>@ martinagvilas</u>), Core Contributor
- The Turing Way community, friends & collaborators

Useful links:

- Book: <u>the-turing-way.netlify.com</u>
- Twitter: <u>twitter.com/turingway</u>
- Newsletter: <u>tinyletter.com/TuringWay</u>
- GitHub: github.com/alan-turing-institute/the-turing-way
- Slack: https://tinyurl.com/jointuringwayslack
- Artwork by Scriberia: https://doi.org/10.5281/zenodo.3332808

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