

# Open science fundamentals for Bioinformatics

(and any field)

Malvika Sharan Connect @malvikasharan

15 August 2024



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link: <https://bit.ly/bon-2024-ms>, Zenodo link: <https://zenodo.org/records/13379994>

London, UK

**Co-Founded Open Life Science**

Senior Researcher - The Alan Turing Institute

**Co-lead of The Turing Way**

Lead of Community Management Team

Germany

**M.Sc, PhD, Community Building**

Worked in European Molecular Biology Laboratory,  
connected with Open Science projects

Bangalore

**Bachelor's degree  
and worked briefly**

Ranchi,  
Jharkhand

**Hometown**

**The  
Alan Turing  
Institute**



Open Life Science



Software  
Sustainability  
Institute

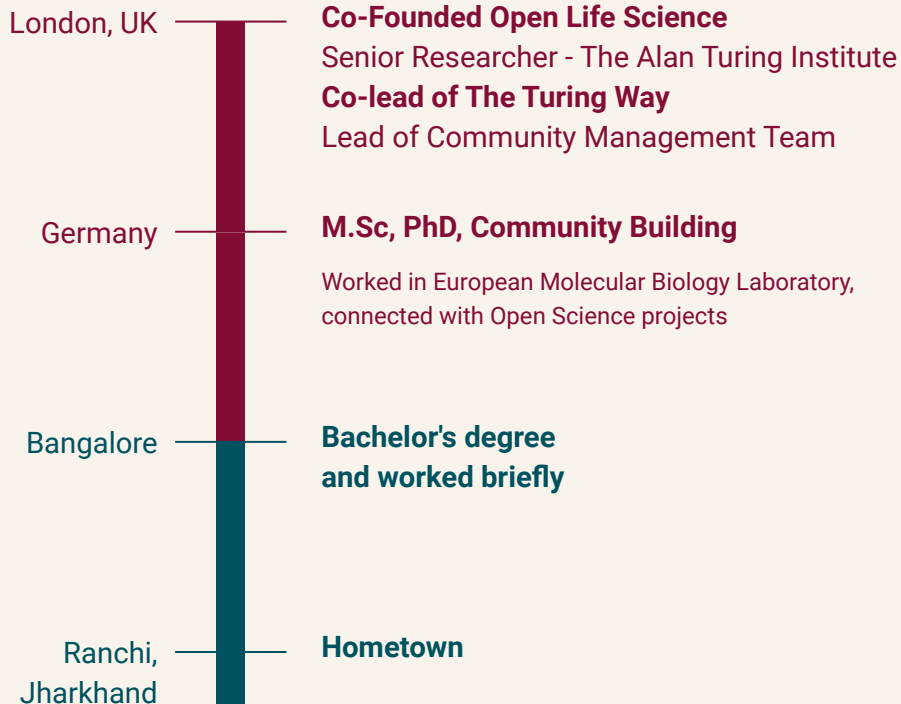




# About me



Open Source



The  
Alan Turing  
Institute



Open Life Science



Software  
Sustainability  
Institute



THE  
CARPENTRIES





# Bioinformatics heavily rely on open source and Open Data

- Sequence alignment tools: BLAST, CLUSTAL, HMMER ...
- Database: NCBI, UNIPROT, PDB, Genbank, Ensembl, KEGG ...
- Phylogenetic analysis and pattern recognition tools and databases (PHYLIP, MEME, ProViz)
- Sequence analysis by Python and R, Bioconductor, Biopython
- Omics data analysis tools and reproducible workflow (like Galaxy)



# What open Source looked like for me

- 📖 Big mystical **library books**
- 🐛 LOTS of **error messages!?**
- 🤖 Debugging sessions with my colleagues
- 😞 Late night debugging session by myself
- 🌟 Finally writing scripts that does the job
- 🔄 Repeat!

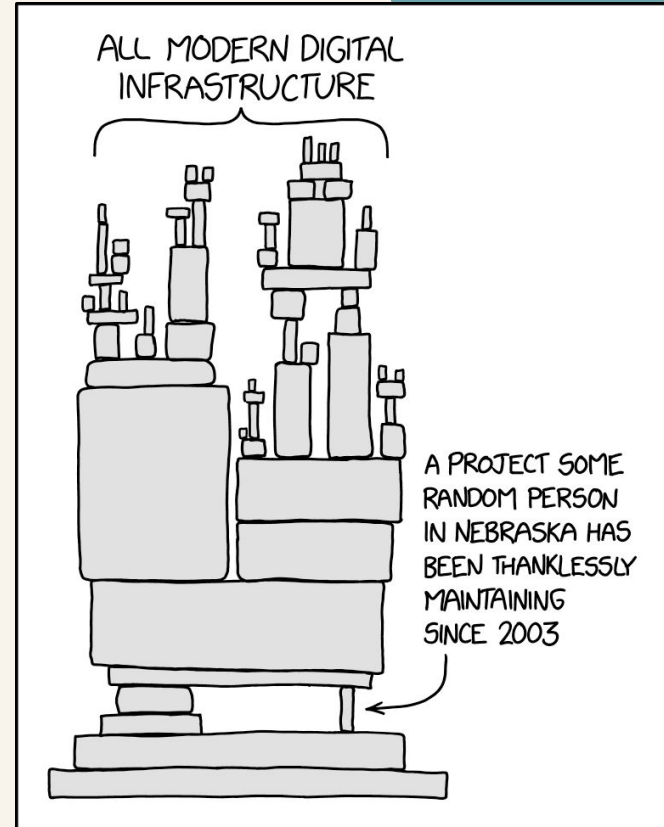


# The More you know!

We all use open source and open data even if we don't know it 'yet'!

- Most operating systems **use/rely on** open source, many apply variants of Unix (70's) and **Linux**
- **Languages:** Python, R, C, C++, Java, Scala ...
- **GitLab/GitHub** → An online platform built on the powerful '**git**' for version control
- Machine learning problems rely on open data

*If you want to learn about open, start with your daily life!*



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XKCD comics, Dependency  
<https://xkcd.com/2347>

# Good news!

- Contributed to Open Source
- Created a software, used GitHub
- Published it on PyPI
- People used it!!!! 🤖



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**Open science** is a much broader field that include Open Source and open data

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Resources that can be read, reused, modified and distributed by anyone **without any cost or access barriers.**

Improves **transparency and collaboration** with users, researchers and contributors.



*We have an obligation to consider the validity and impact our work.*

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Science including scientific errors have real world effects





# Scientific errors have real world effects

	B	C	I	J	K	L	M
2	Real GDP 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	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	=AVERAGE(L30:L44)	

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## NEWS

Home UK World Business Politics Tech Science Health Family & Education

### Magazine

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

By Ruth Alexander  
BBC News

© 20 April 2013

f t e Share

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 Debt.

Taken from Kirstie Whitaker's slides, The Turing Way, DOI: 10.5281/zenodo.7428708, <https://zenodo.org/record/10522776>

<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>



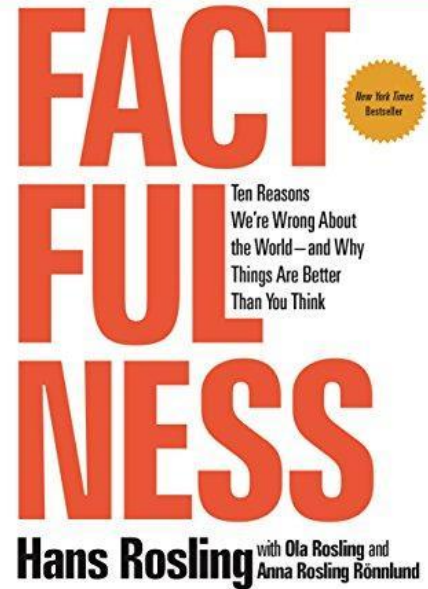
# Scientific errors have real world effects

“We will redouble our efforts to avoid such errors in the future ...” - Reinhart & Rogoff

“Our problem is that we don't know what we don't know, and even our guesses are informed by unconscious and predictable biases.” - Hans Rosling



“One of the most important books I've ever read—an indispensable guide to thinking clearly about the world.” —Bill Gates



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## Price of Popularity

Researchers in Australia publishes unreliable COVID-19 data with their preprint and misreported that an anti-parasite drug could stop the virus from replicating in cells.



*In a desperate attempt to save dying patients, doctors began justifying the drug's use against COVID-19 as the virus spread aggressively throughout Latin America.*

Reardon, S. (2021). Flawed ivermectin preprint highlights challenges of COVID drug studies. *Nature*, 596, 173–174. doi: 10.1038/d41586-021-02081-w. Mega, E. R. (2020). Latin America's embrace of unproven COVID treatment hinders drug trials. *Nature*, 586, 481–482. doi: 10.1038/d41586-020-02958-2, Slides under DOI: 10.5281/zenodo.7428708

# Public Scrutiny is Important for Accountability



## Under-reported figures

From 25 Sept to 2 Oct

**50,786**

Cases initially reported by PHE

**15,841**

Unreported cases, missed due to IT error

**8 days** of incomplete data

**1,980** cases per day, on average, were missed in that time

**48 hours** Ideal time limit for tracing contacts after positive test

Source: PHE and gov.uk [↗](#)

Kelion, B. L. (2020). Excel: Why using Microsoft's tool caused Covid-19 results to be lost. BBC News. <https://www.bbc.co.uk/news/technology-54423988>

[@turingway](#), CC-BY 4.0,  
The Turing Way, DOI: [10.5281/zenodo.7428708](https://doi.org/10.5281/zenodo.7428708)

# Lack of accountability and risks of subversion

*“We need to rely on science, but **we need to be better able to distinguish good science from bad.** We need to make science more self-correcting.”*



**Elisabeth Bik**

*Microbiologist by training,  
Scientific misconduct hunter by  
passion, professional scientific  
integrity consultant*

# Lack of accountability and risks of subversion

*“We need to rely on science, but **we need to be better able to distinguish good science from bad.** We need to make science more self-correcting.”*

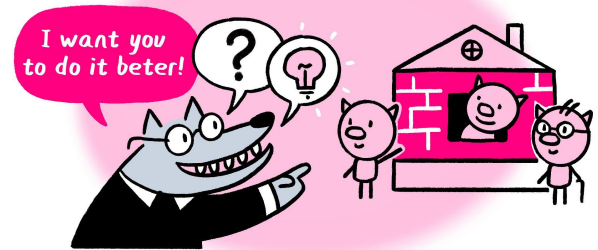
We should all learn to assess the **novelty or expected impact** of a research (output) to **validate** methodology, analysis and argumentation of a research.



Elisabeth Bik

*Microbiologist by training,  
Scientific misconduct hunter by  
passion, professional scientific  
integrity consultant*

PEER REVIEW



Serbia

---

# Avoid Errors Before the Harm Occurs

1. Mistaken research design or analysis processes
  - **Lack of reproducible and collaborative research design**
2. Lack of diverse tools, methods and expertise to draw from
  - **Lack of openness or community-developed tools**
3. Inappropriate baseline comparison and assumption of future use
  - **Lack of technical understanding and ethical implications**

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Zenodo: DOI: 10.5281/zenodo.7428708,  
<https://zenodo.org/record/10522776>



- Storing Data: **Open Data**
- Developing source code: **Open Source**
- Designing hardware: **Open Hardware**
- Sharing methods or protocols: **Open Access publications**
- Communicating results early: **Preprints**
- Peer-based Review: **Open Peer-Reviews**
- Transferring skills by training: **Open Education and training materials**
- Collaborating with public: **Citizen Science**
- Inviting & collaborating with peers contributors, maintainers: **Community Building**
- Supporting and connecting others in your field: **Scientific Network**

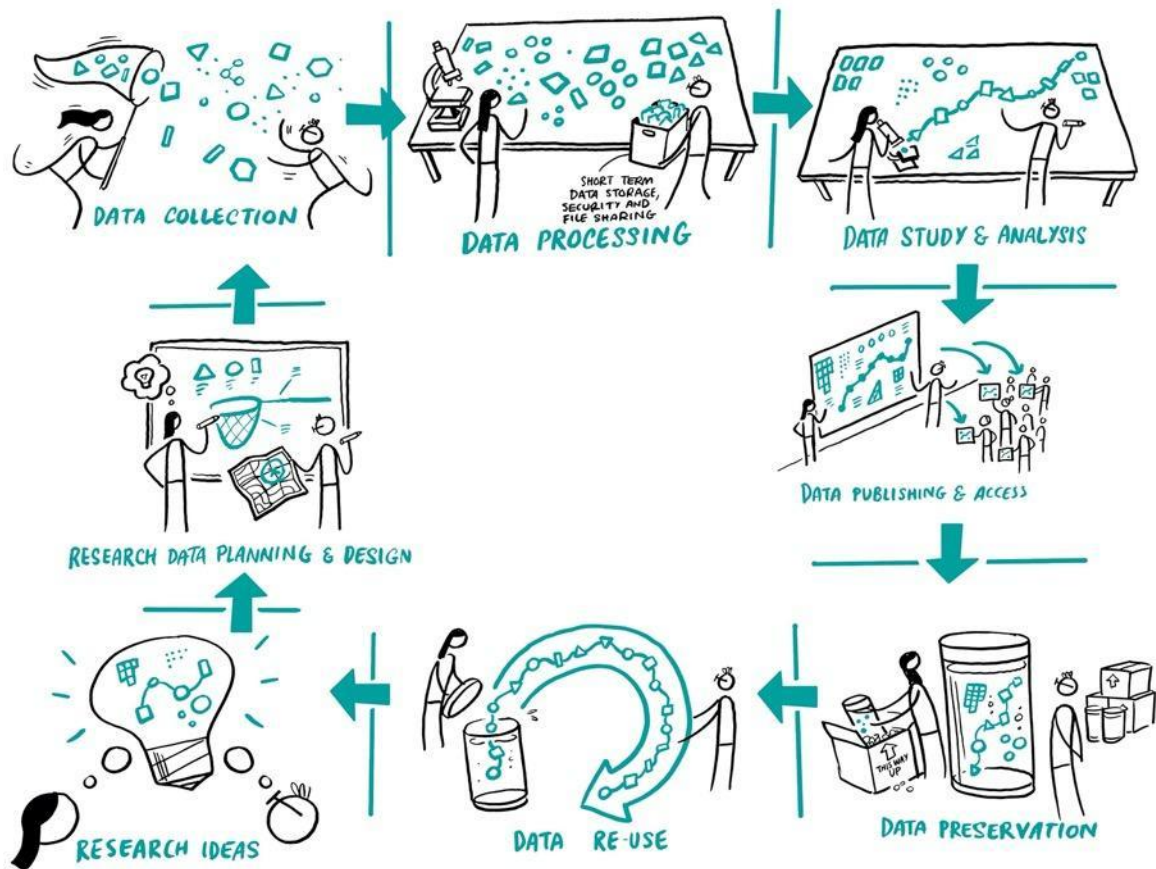


# Reproducibility

		Data	
		Same	Different
Analysis	Same	Reproducible	Replicable
	Different	Robust	Generalisable

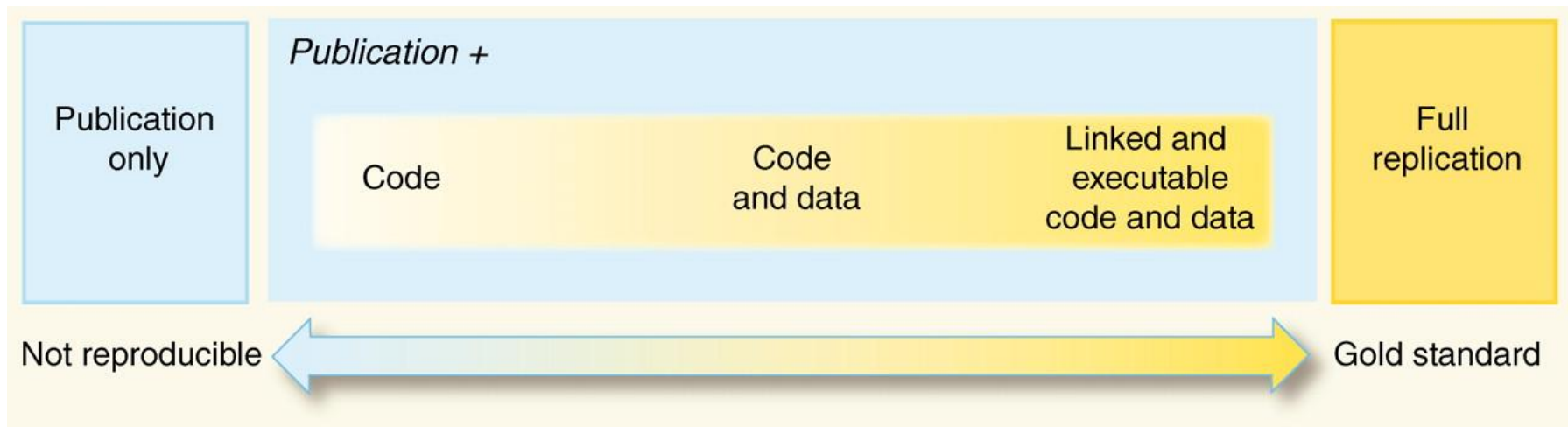


# Considering Open and Reproducibility in Research



Scriberia

# We need research environment and guidelines too!

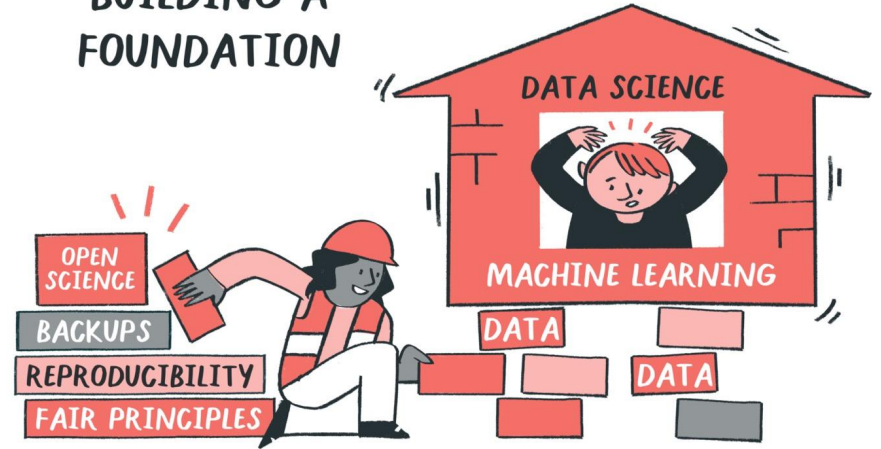


*“An article about computational science in a scientific publication is not the scholarship itself, it is **merely advertising of the scholarship**. The actual scholarship is the **complete software development environment** and the complete set of instructions which generated the figures.” - Buckheit and Donoho (paraphrasing John Claerbout, 1995)*

# Open Science and reproducibility are foundational

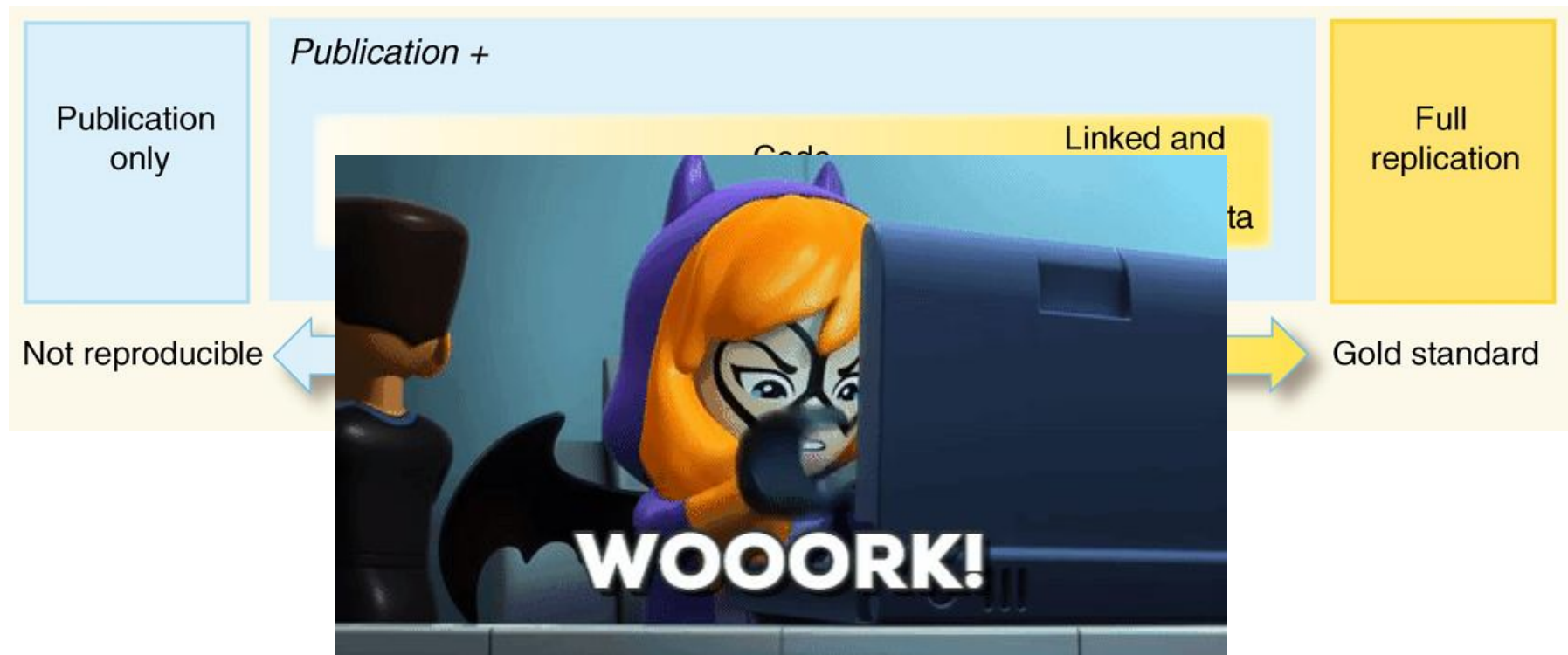


BUILDING A  
FOUNDATION



*NOTE: Not all data can or should be published.*

# We need research environment and guidelines too!



The **OLS** (formerly Open Life Science) is an open science training & capacity building organisation.



*openlifesci.org*

We create training, mentoring and learning resources with practical opportunities to apply open science, reproducibility and community approaches.



The Alan Turing Institute



*OLS-9 starting in September*





**Science can advance only when we share our  
work with others**



**... but, researchers are often skeptical about sharing their work due to their fear of getting scooped, being criticised ...**



**Together, we explore the  
important concepts and  
practices in Open Science and  
apply them in our work  
- one step at a time.**



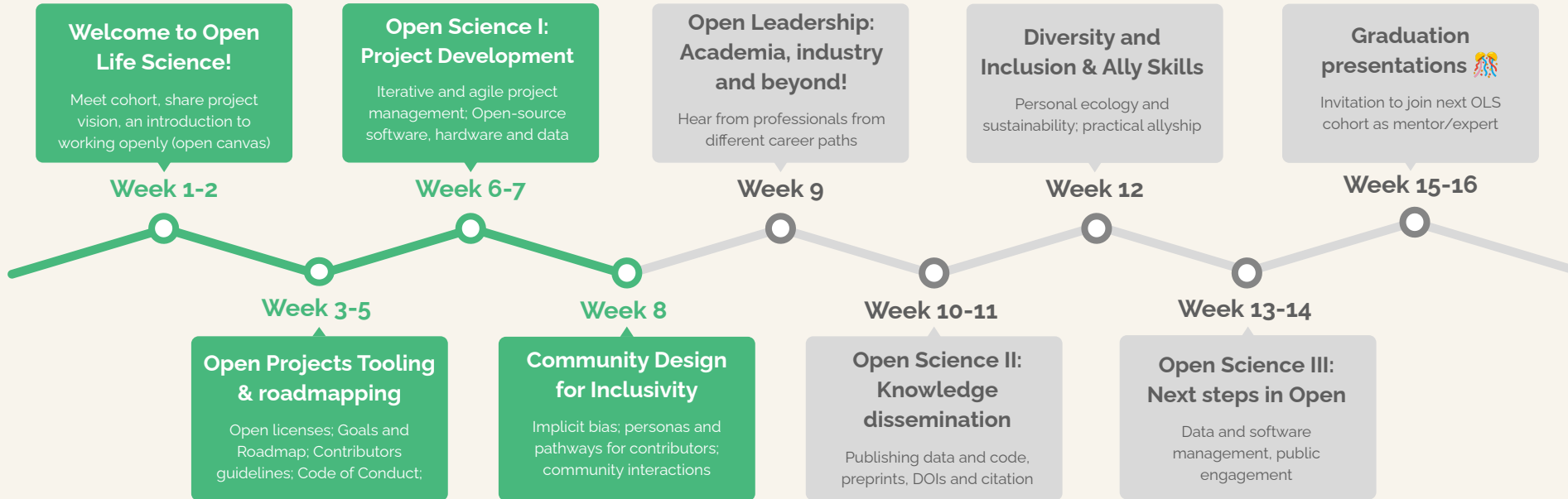
@openlifesci



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Image on Unsplash by [@joannakosinska](#)





# OLS - Program structure

16-week long mentorship and cohort-based training

Cohort-based training

**1 on 1 mentoring**

Hands on practice



# OLS's Impact in Numbers (since 2020)

8  
Cohorts

500+  
Participants

200+  
Mentors &  
Speakers

70+  
Countries

A worldwide community



## Organizational Pillars



### Open Science Training

Online mentoring and training programs for individuals and teams worldwide to learn about and adopt open research practices.



### Research on Open

Evidence base and interventions for widening participation in research.



### Open Incubator

The greenhouse: Hands-on support to empower the next generation of open leaders in research.



6-week open science training



~4 hours / week



Group projects or solo



1:1 mentorship

### Topics:

Ethos of Open

Open Data

Open Software

Open Results

Tools & Resources



<https://we-are-ols.org>



@yoyehudi



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[bit.ly/2023-ebi-repro](https://bit.ly/2023-ebi-repro)

# OLS Leadership



**Yo Yehudi**  
*Executive Director*



**Malvika Sharan**  
*Director of Partnership*



**Bérénice Batut**  
*Director of Technology*



**Patricia Herterich**  
*Chief of Staff*

## OLS Staff, Contractors and Resident Fellows



**Tajuddeen Gwadabe**

*Program Manager: Catalyst*



**Irene Ramos**

*Project Coordinator: Nebula*



**Deborah Udoh**

*Junior Web Developer*



**Bethan Illey**

*Finance Manager*



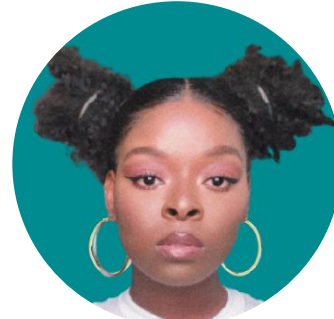
**Rowland Mosbergen**

*Resident Fellow: Practical  
Diversity and Inclusion*



**Seun Olufemi**

*Junior Resident Fellow:  
OLS-g DRI-EDIA*



**Jilaga Nneoma**

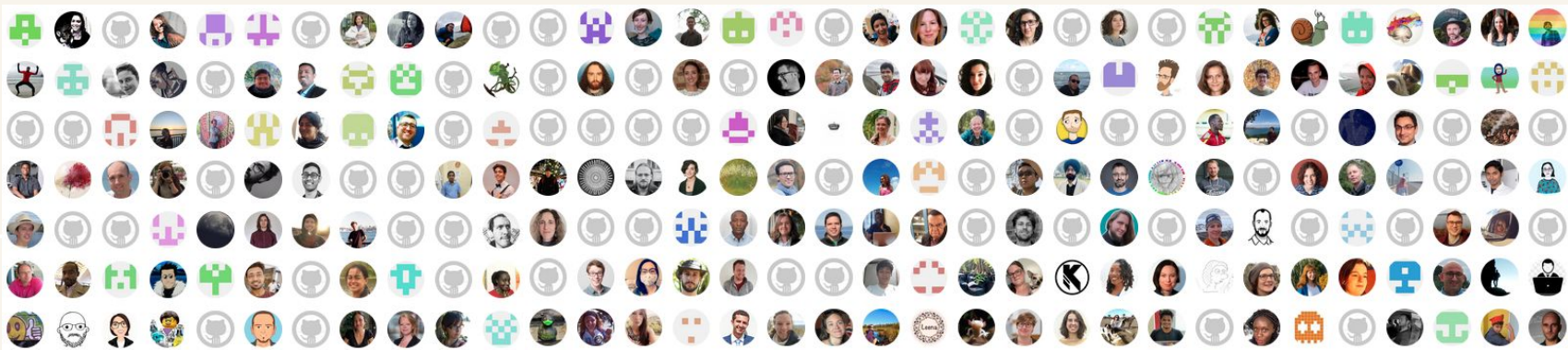
*Web Designer*



**Camille Gonzalez**

*Executive Assistant*





## Who we are:

500+ mentors, mentees,  
facilitators, and expert speakers

[Testimonials](#)

Applying open and reproducible practice require intention, resources, time, support and collaboration, which can be overwhelming.

We need open communities where we can learn with others.



**SPRINGER NATURE**

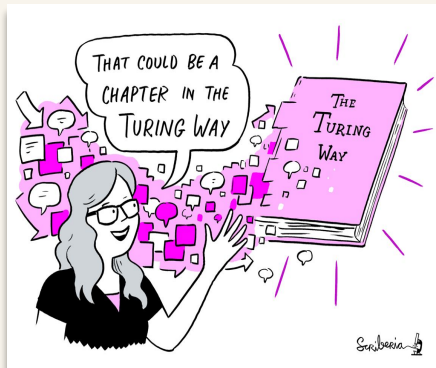


# The Turing Way



A community-led handbook to best practices in Data Science.

We involve and support a **diverse community** to make research **reproducible, ethical, and collaborative** for everyone.



Book



Community



Global Collaboration



Culture Change

# The Turing Way: Book on Reproducibility

*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.

		Data	
		Same	Different
Analysis	Same	Reproducible	Replicable
	Different	Robust	Generalisable



## Guide for Reproducible Research

Overview

Open Research

Version Control

Licensing

Research Data Management

Reproducible Environments

BinderHub

Code quality

Code Testing

Code Reviewing Process

Reusable Code

Continuous Integration (CI)

Reproducible Research with Make

Research Compendia



**Fig. 3** The Turing Way project illustration by Scriberia. Used under a CC-BY 4.0 licence. DOI: [10.5281/zenodo.3332807](https://doi.org/10.5281/zenodo.3332807).

@malvikasharan @turingway, CC-BY 4.0, Book: <https://the-turing-way.netlify.app/welcome>,

CC-BY image by *The Turing Way* and Scriberia, Zenodo: <https://doi.org/10.5281/zenodo.3332807>. Presentation DOI: [10.5281/zenodo.7692516](https://doi.org/10.5281/zenodo.7692516)



## The Turing Way

🔍 Search this book...

Welcome

Guide for Reproducible Research

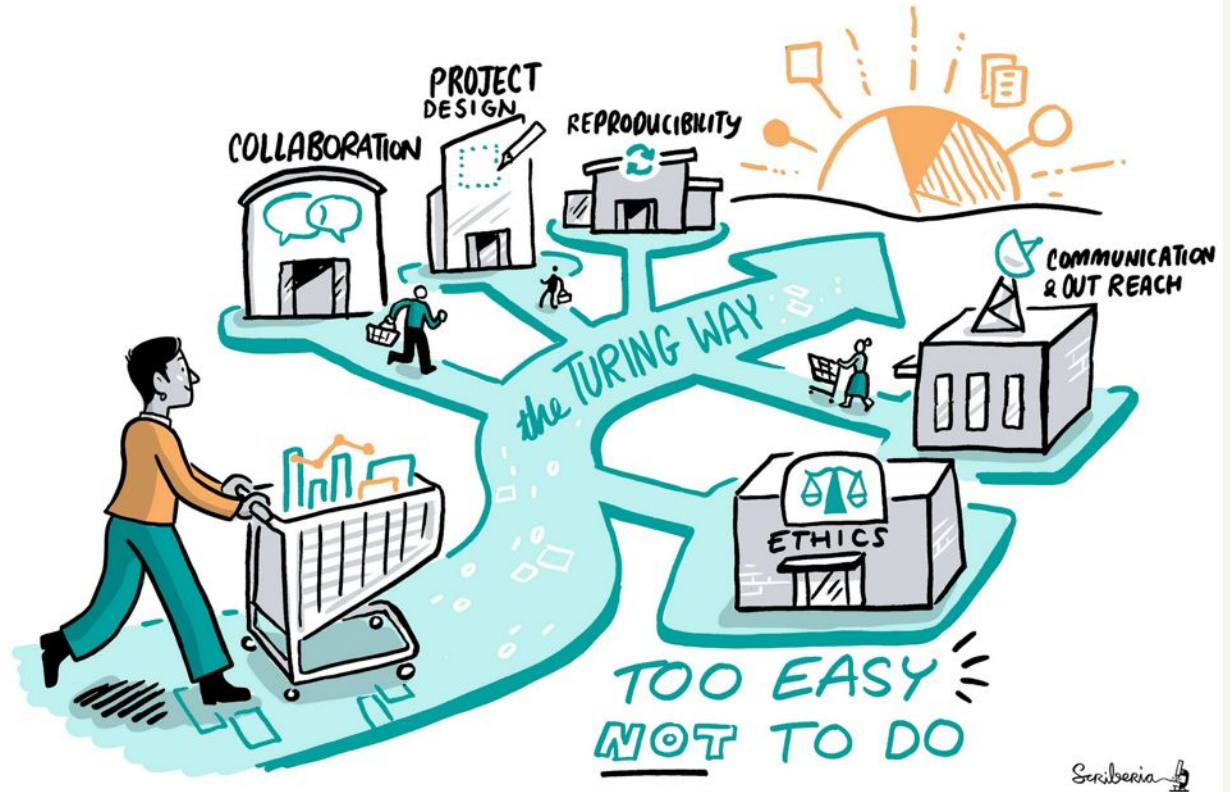
Guide for Project Design

Guide for Communication

Guide for Collaboration

Guide for Ethical Research

Community Handbook



@malvikasharan @turingway, CC-BY 4.0, Book: <https://the-turing-way.netlify.app/welcome>

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# The Turing Way Guides



Reproducibility



Project Design



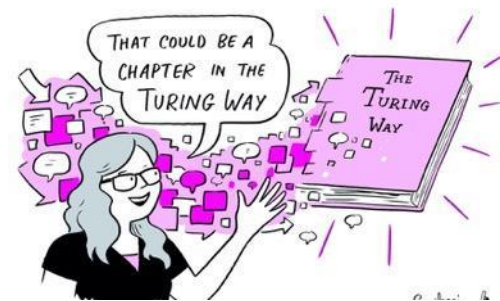
Communication



Collaboration



Ethical Research



Community Handbook

# The Turing Way: Guides on Data Science



**Kirstie Whitaker**

Director: Tools,  
Practices & Systems  
Programme (TPS)



**Malvika Sharan**



**Anne Lee Steele**

Community Manager,  
The Turing Way



**Arielle Bennett**

TPS Programme  
Manager

5 years

>350 Chapters

500+ Contributors

Numerous training  
and community  
resources.



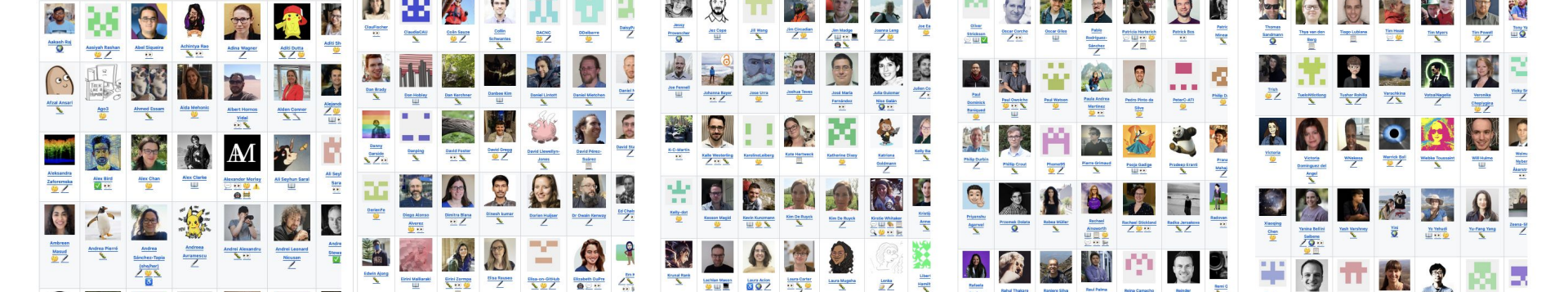
## The Turing Way

🔍 Search this book...

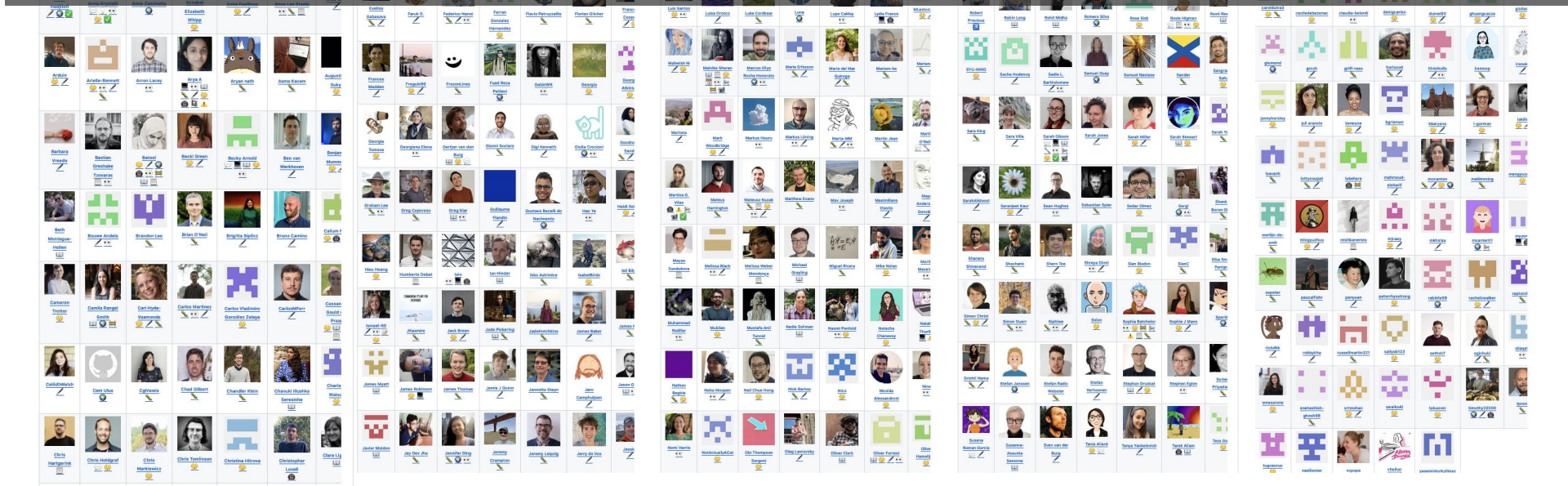
### Welcome

- Guide for Reproducible Research ▾
- Guide for Project Design ▾
- Guide for Communication ▾
- Guide for Collaboration ▾
- Guide for Ethical Research ▾
- Community Handbook ▾
- Afterword ▾





Thanks to our community of contributors & users!



# Working with the community

- **5 years, >350 Chapters**, community resources
- **500+ contributors, 5000+ monthly users** - supported by community-based governance
- **Replication/extension** by 4 Turing & 6+ external projects (e.g. ONS, UCL, Uni Oxford, LIBER: Association of European Research Libraries)



19,098  
views

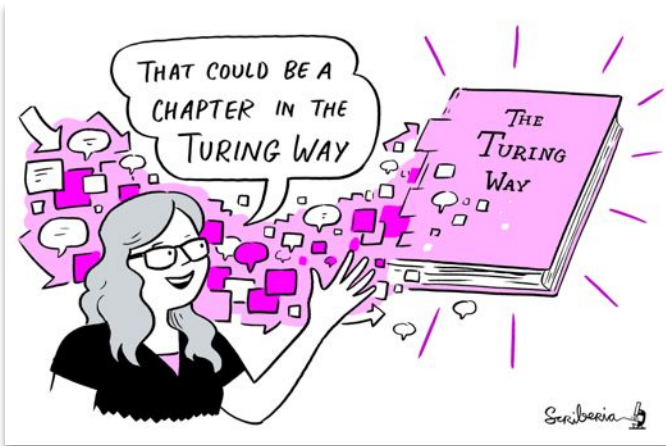
16,710  
downloads







## A Book



## A Community



## An Open Source Project



## A Culture of Collaboration



19,098

views

16,710

downloads

Start:

[the-turing-way.start.page](https://the-turing-way.start.page)

# The project belongs to the community

This is not a Turing project - although it has great support from the Institute.

This is always a work in progress - evolving with the needs in the community.

We are creating community resources together -- *it's about the way, the journey, not a set of rules.*



# Internationalisation and translation work



## The Turing Way


👤 24 followers 🔗 <https://the-turing-way.netlify.app>

**GitHub:** <https://github.com/the-turing-way>  
450+ contributors

The Turing Way > Turing Way LOG IN SIGN UP

### Turing Way

OVERVIEW README



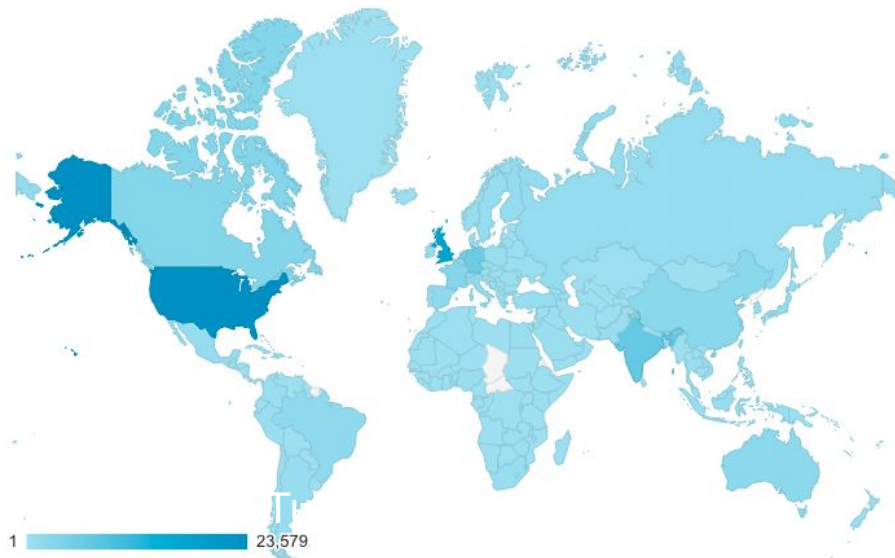
🔍 Search...

Language ↓	Progress	Words to translate
Arabic (ar)	<div style="width: 26%;"><div style="width: 1%;"></div></div> 26% - 1%	200 950
Chinese Simplified (zh-CN)	<div style="width: 15%;"><div style="width: 0%;"></div></div> 15% - 0%	228 890
French (fr)	<div style="width: 72%;"><div style="width: 0%;"></div></div> 72% - 0%	75 680
Japanese (ja)	<div style="width: 68%;"><div style="width: 0%;"></div></div> 68% - 0%	87 125
Portuguese, Brazilian (pt-BR)		
Spanish, Latin America (es-419)		
Turkish (tr)		

📄 README.md

## The Turing Way

*This README.md file is also available in Dutch (README-Dutch), French (README-French.md), German (README-German.md), Indonesian (README-Indonesian), Italian (README-Italian), Korean (README-Korean), Portuguese (README-Portuguese), and Spanish (README-Spanish) (listed alphabetically).*



# The Turing Way Community Handbook

## Community Handbook

Code of Conduct

Ways to Enter the Project

Style Guide

Maintaining Consistency

Chapter Templates and

Contribution Workflow

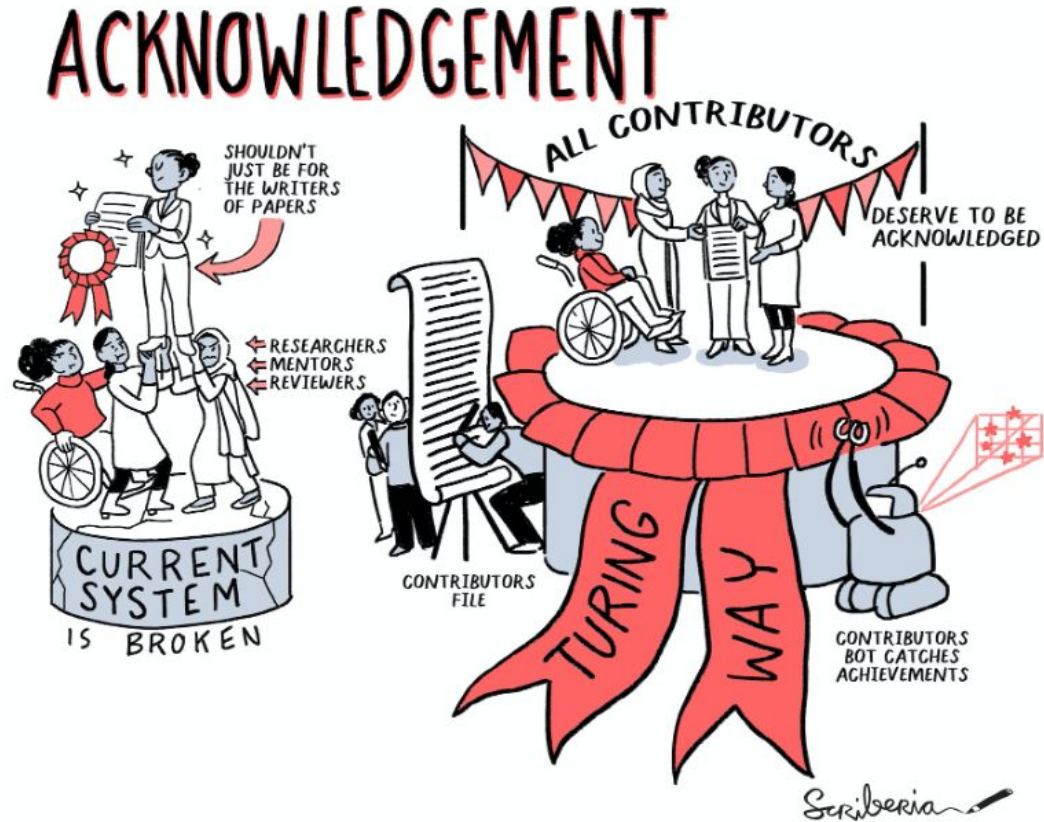
Acknowledging Contributors

Monthly Newsletters

Book Dash Events

Community Coworking Calls

Template Collection



Online book: <https://the-turing-way.netlify.app/community-handbook>, @malvikasharan @turingway

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# Open Science promotes access and equity in research and education



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# Open Science promotes access and equity in research and education

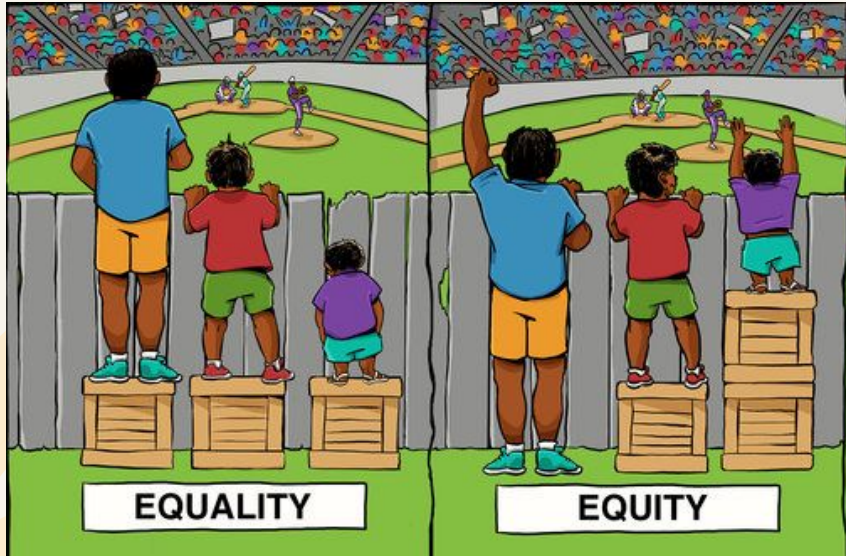


Image Credit: A collaboration between Center for Story-based Strategy & Interaction Institute for Social Change. With links to <https://www.storybasedstrategy.org/the4thbox> and <http://interactioninstitute.org/>



# Open Science promotes access and equity in research and education

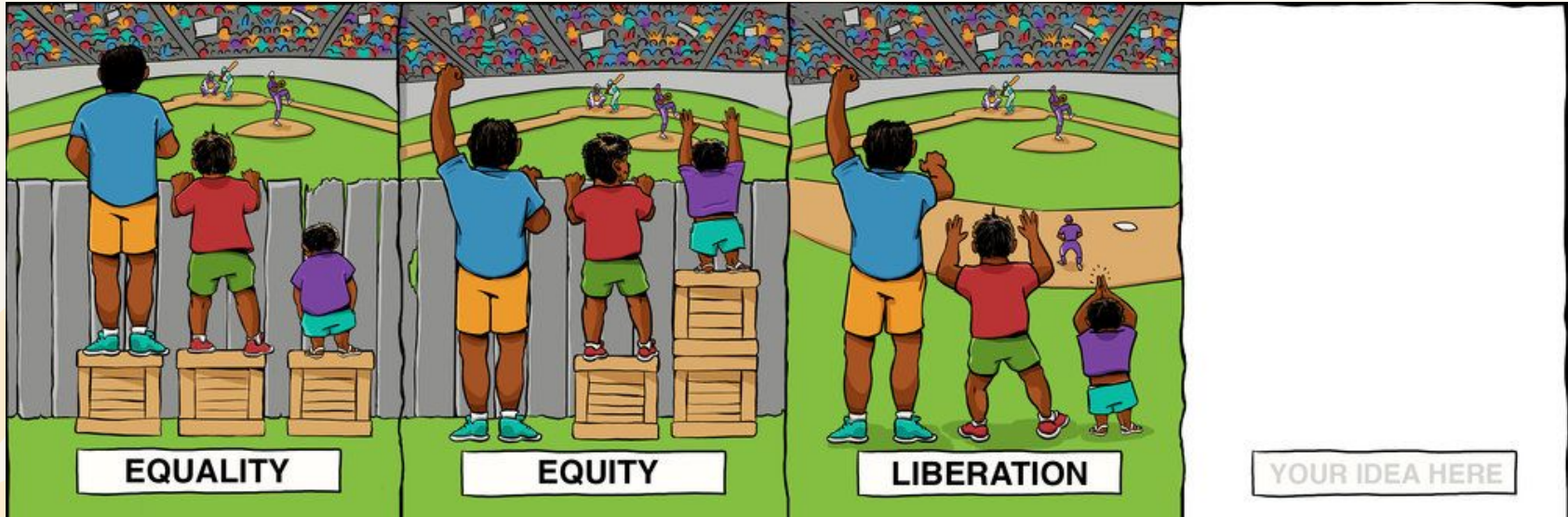
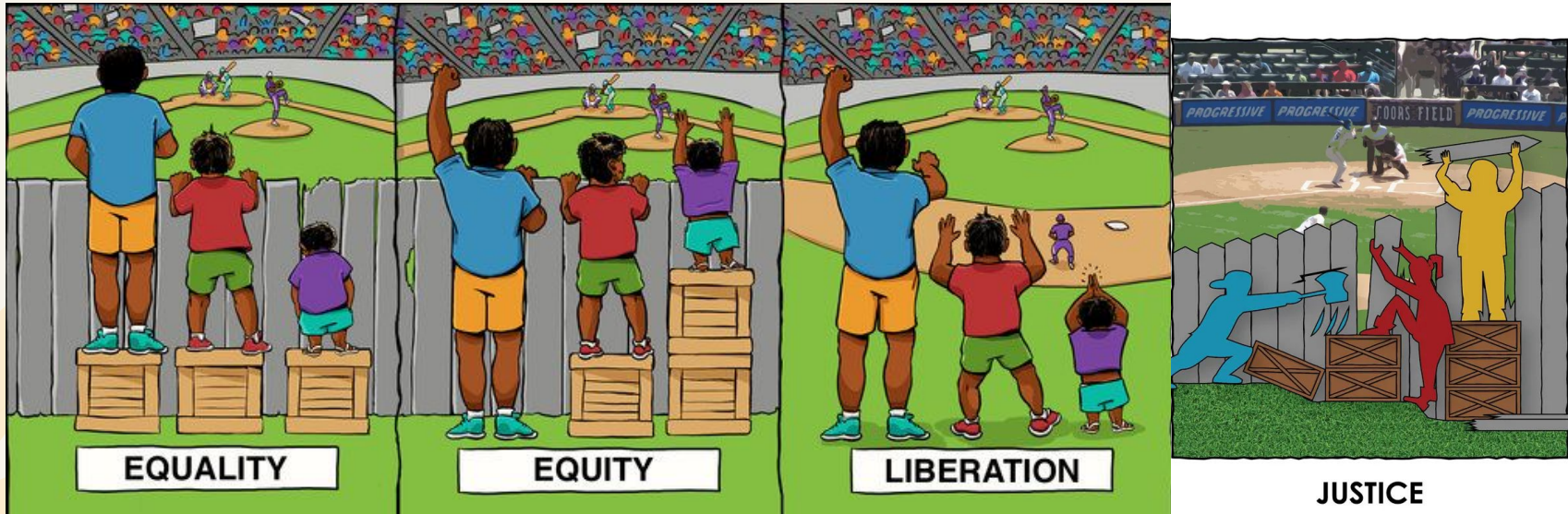


Image Credit: A collaboration between Center for Story-based Strategy & Interaction Institute for Social Change. With links to <https://www.storybasedstrategy.org/the4thbox> and <http://interactioninstitute.org/>

# Open Science promotes access and equity in research and education



Equity versus Equality (Triple Participation). (2018, September 10).

<https://ces101fall2018.wordpress.com/2018/09/10/equity-versus-equality-triple-participation>



## Equitable Open Science

Combines many forms of practices to make scientific knowledge 'open' (by design).



## Equitable Open Science

Combines many forms of practices to make scientific knowledge 'open' (by design).

**Accessible for everyone**

No price barriers, no technical barriers!





## Equitable Open Science

Combines many forms of practices to make scientific knowledge 'open' (by design).

### Accessible for everyone

No price barriers, no technical barriers!

### Inclusive for everyone

Enables everyone to participate and benefit from scientific advancements.



A top-down view of a desk with a yellow background. In the top left, a smartphone displays a social media feed. In the bottom left, a portion of a grey laptop is visible. In the center, an orange book titled 'CHANGE' by Tim Brown is the main focus. The book cover features a network diagram and the subtitle 'HOW DESIGN THINKING TRANSFORMS ORGANIZATIONS AND INSPIRES INNOVATION'. In the top right, a pair of orange-handled scissors is partially visible.

**Open by Design**

**Openness should not be a thoughtless default**






# Game time

## Open or Not Open



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- TARO loves to write **Python scripts**
- Joined a research team as a **Computer Science intern**
- **Helps** people in their research group with programming questions
- Their supervisor suggested them to **share the scripts online**
- Taro created a **public GitHub repository** and shared the scripts
- **Sent out an email** to their team members to use their repository



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# Open by Default



The repository is public and **open but**

- How can their team members **reuse** their scripts?
- Can they **help improve** the scripts?
- How **can someone credit** them if they use their work?
- Can they **share** them with others outside their lab?
- What happens if **interactions** in their repository are unpleasant?



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**The question is not "will we open this?",  
rather "how will we open this?"**



OPEN

# Open by DESIGN



1. Adds an **open source license** in their repository for reuse
2. Creates a **README file** with information on their scripts
3. Adds a **user manual** and a process for asking for help
4. Adds a **contribution guideline** for others to help improve
5. Makes it clear **how to cite/credit** their work
6. Selects a **Code of Conduct** for their repository



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**Openness is more than just putting it online!**



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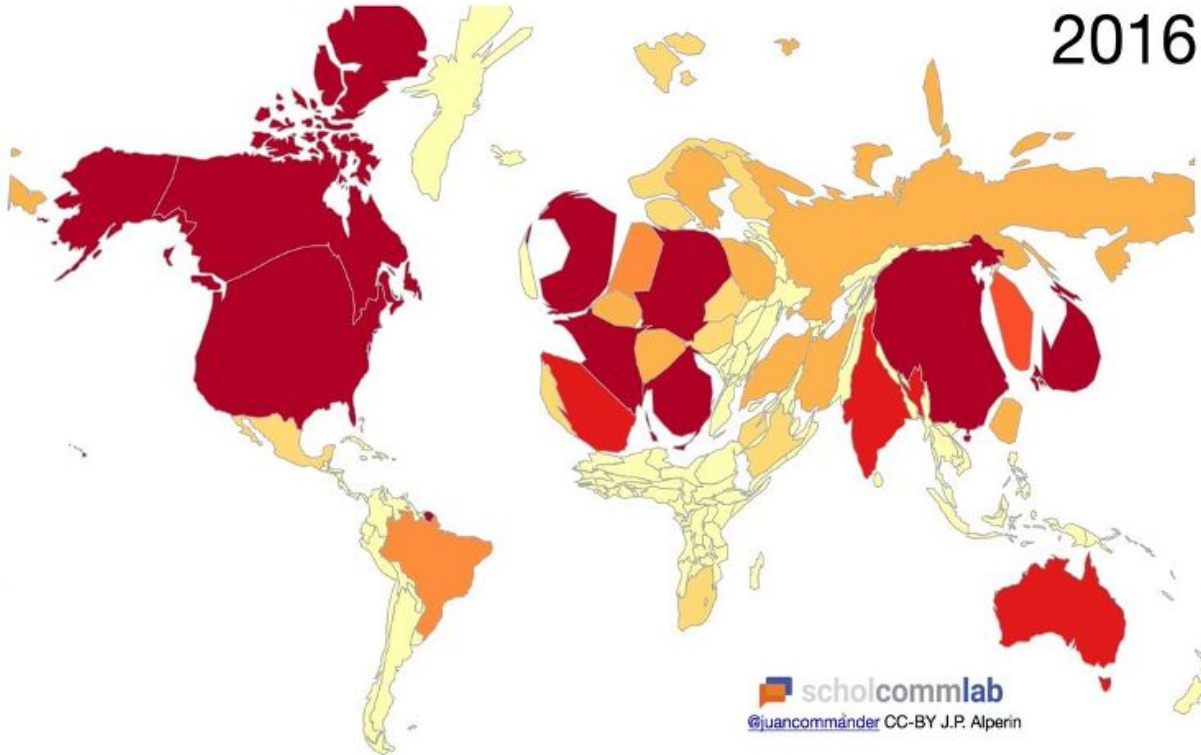




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World scaled by number of documents with authors from each country in Web of Science

2016



References: Mewa, & Goudarzi. (2018). Mapping Academic Publishing: Locating Enclaves of Development Knowledge. Electronic Publishing, Connecting the Knowledge Commons: From Projects to Sustainable Infrastructure, Image: <https://doi.org/10.6084/m9.figshare.953177>, Quote: <https://www.force11.org/blog/open-access-inclusion-interview-juan-pablo-alperin>

World scaled by number of documents with authors from each country in Web of Science

2016

*Access is not only about being able to read but  
being able to have a voice and shape the  
directions, economic models and infrastructure.*

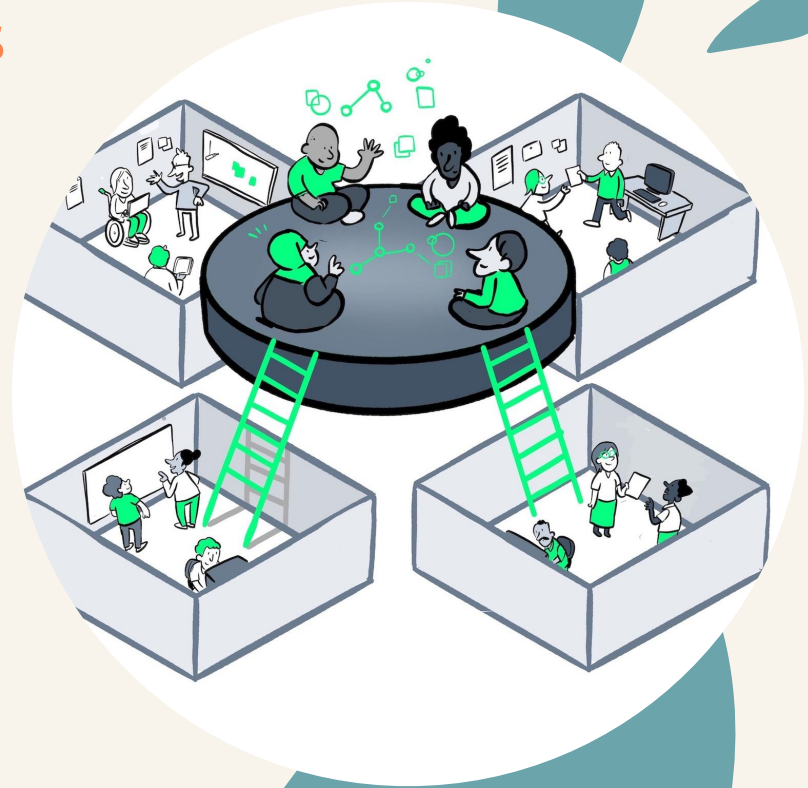
- Juan Pablo Alperin

 scholcommlab  
@juancommander CC-BY J.P. Alperin

References: Mewa, & Goudarzi. (2018). Mapping Academic Publishing: Locating Enclaves of Development Knowledge. Electronic PUBLISHING, Connecting the Knowledge Commons: From Projects to Sustainable Infrastructure, Image: <https://doi.org/10.6084/m9.figshare.953177>, Quote: <https://www.force11.org/blog/open-access-inclusion-interview-juan-pablo-alperin>

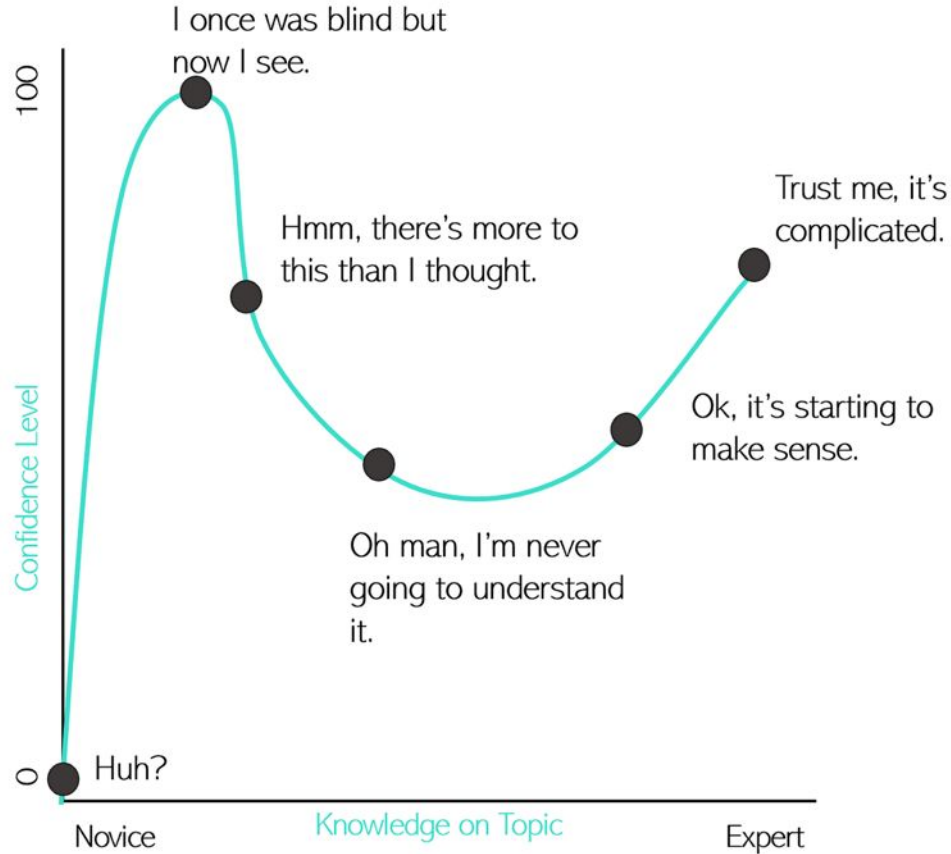
# You are participant and organiser of open science in bioinformatics

- Systems to get involved and access support and mentorship
- Opportunities for diverse representation in all spaces
- Recognition for all contributions and rewards through visible roles
- Community-led process for transparent decision-making



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# The more I know!



Haylee Somerville, The Hidden Power of Intellectual Humility - The Decision Lab. 2020.  
<https://thedecisionlab.com/insights/society/the-hidden-power-of-intelle>

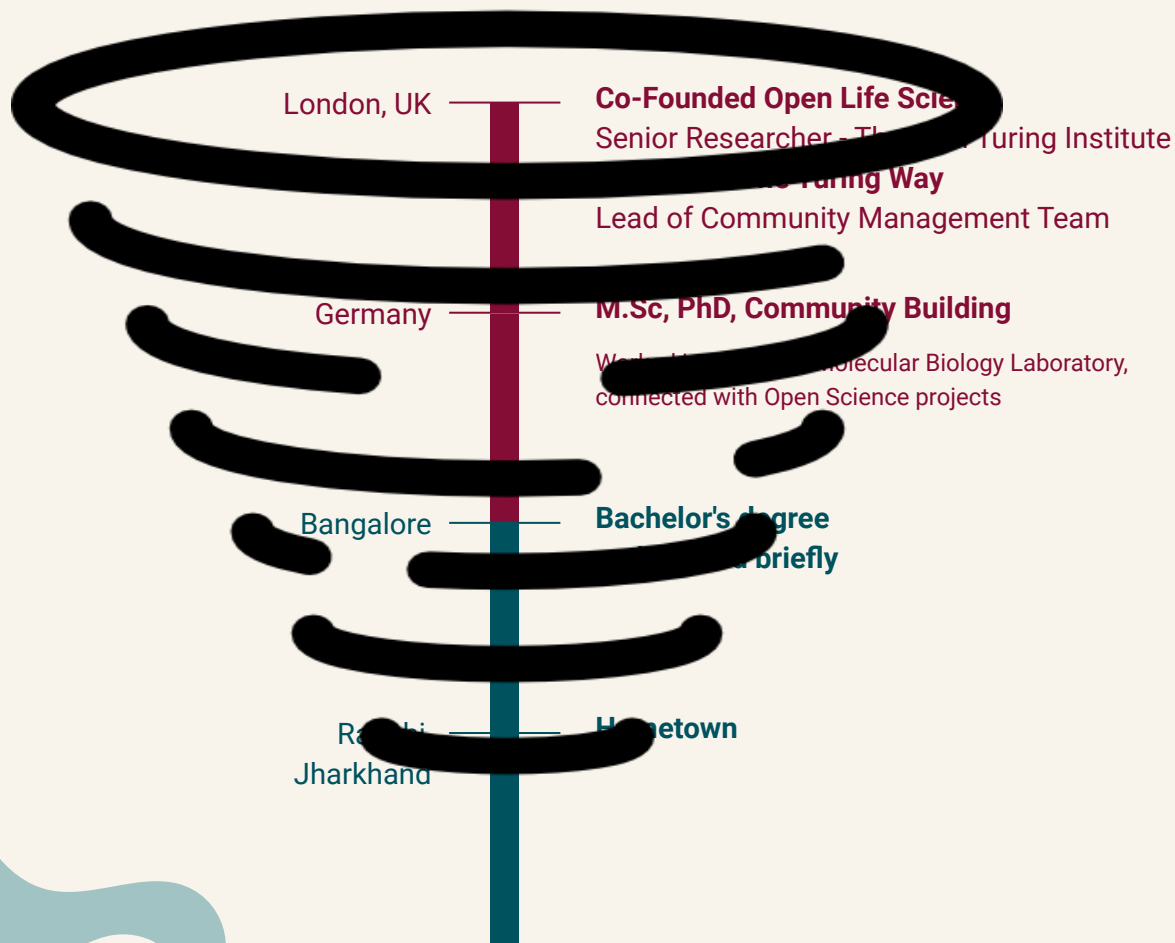
Adapted from: Squad. (2018, December 13). Dunning-Kruger Effect: Definition, Test, Examples & Quiz. Science Terms. <https://scienceterms.net/psychology/dunning-kruger-effect/>





I only know the directions I  
want to take, I don't know  
where I will end up!

# Everyone fails - learns - grows (whirlwind!)



The  
Alan Turing  
Institute



Open Life Science



Software  
Sustainability  
Institute

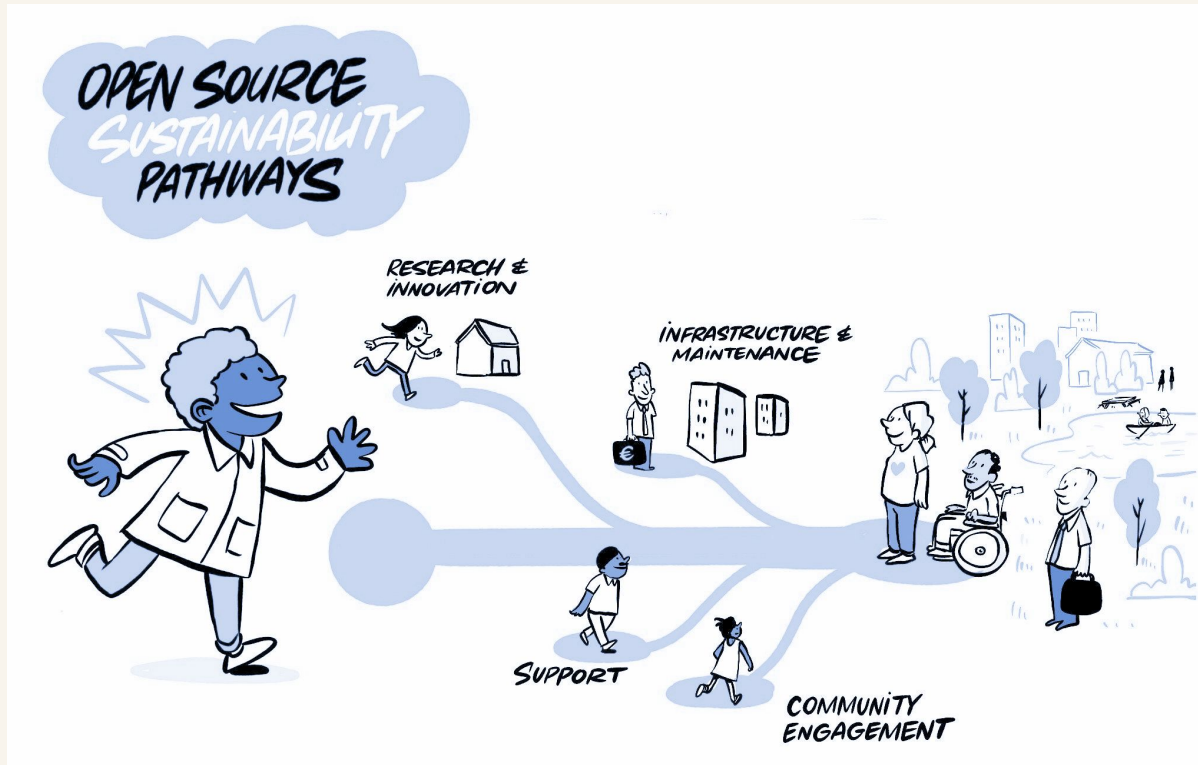


THE  
CARPENTRIES



CS&S Code for  
Science &  
Society

# Your Open Source/Science Journey

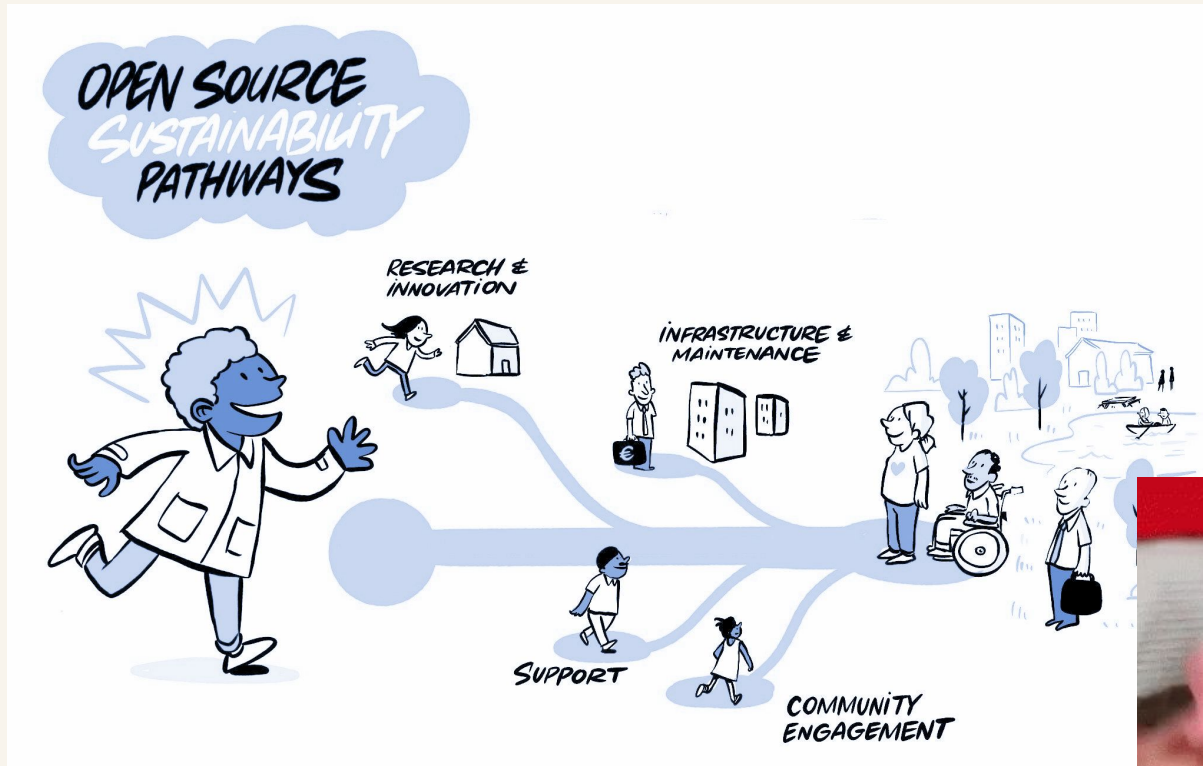


Our skills aren't fixed in place. **You can be good at lots of things.** You can do anything. – Tania Reilly

**Technical Leadership and the Glue Work.**

@malvikasharan @turingway, CC-BY 4.0, CC-BY image by *The Turing Way* and Scriberia, Presentation DOI: 10.5281/zenodo.7692516

# I can't wait to see amazing things you will do



Our skills aren't fixed in place. **You can be good at lots of things.** You can do anything. – Tania Reilly

**Technical Leadership and the Glue Work.**

@malvikasharan @turingway, CC-BY 4.0, CC-BY image by *The Turing Way* and Scriberia, Presentation DOI: 10.5281/zenodo.7692516

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## Acknowledgements & Links

### *The Turing Way*

- Kirstie Whitaker, The Turing Way core contributors and community
- Anne Lee Steele, Alexandra Araujo Alvarez, Arielle Bennett, **All** TPS members
- Book: [the-turing-way.netlify.com](https://the-turing-way.netlify.com), Twitter: [twitter.com/turingway](https://twitter.com/turingway)
- GitHub: [github.com/alan-turing-institute/the-turing-way](https://github.com/alan-turing-institute/the-turing-way), Start: [the-turing-way.start.page](https://the-turing-way.start.page)

### *OLS (Open Life Science)*

- Open Life Science community; Yo Yehudi, Bérénice Batut, Emmy Tsang
- Website: [openlifesci.org](https://openlifesci.org), Twitter: [twitter.com/openlifesci](https://twitter.com/openlifesci)
- GitHub: [github.com/open-life-science/open-life-science.github.io](https://github.com/open-life-science/open-life-science.github.io)

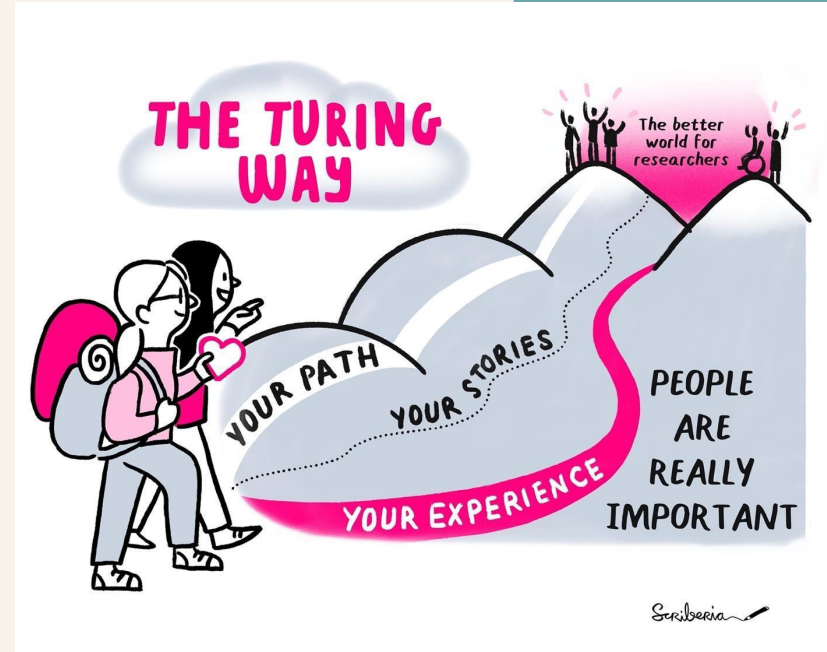
*Parts of my talk reuse materials from presentations given previously in Open Life Science and The Turing Way by the team members listed in this slide.*



## Meeting you where you are!

- i. Join the community
- ii. Learn a new skill
- iii. Share your skills
- iv. Collaborate with others
- v. Mentor others' contributions
- vi. Represent this community

*Join us, participate, learn, share!*



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5. **Instructions for use**.
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  - The **fonts and colors** used in the template.
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