

# **Computational Reproducibility:**

A how-to guide based on The Turing Way

Martina G. Vilas (she/her)

@martinagvilas



## who am !?

- PhD student in Neuroscience
   at Max-Planck-Institute AE
- Core contributor / Maintainer
   of The Turing Way



- 1. what is The Turing Way?
- 2. guide to computational reproducibility

# 1. what is The Turing Way?

2. guide to computational reproducibility



#### **Book:**

the-turing-way.netlify.app/

#### GitHub:

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

#### **Twitter:**

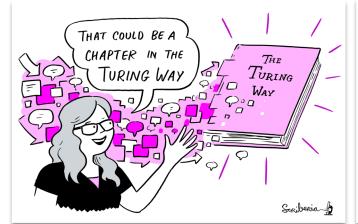
twitter.com/turingway

### Email:

theturingway@gmail.com

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### A Book



## **A Community**



## **An Open Source Project**



### A Culture of Collaboration



# The Turing Way



### **Kirstie Whitaker**

- Project Leader of The Turing Way
- Program Lead for Tools, Practices and

Systems at the Allan Turing Institute

The Alan Turing Institute

# The Turing Way

online book

moonshot goal: make reproducible research "too easy not to do"

- 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, 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.

#### 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

# 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

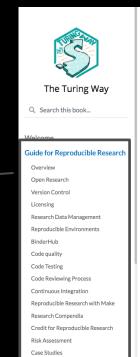
Reproducible Research with Make

Research Compendia

Credit for Reproducible Research

Risk Assessment

Case Studies







Q 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

Visit our GitHub Repository
This book is powered by Jupyter Book

### Welcome

The Turing Way is an open source community-driven guide to reproducible, ethical, inclusive and collaborative data science.

Our goal is to provide all the information that data scientists in academia, industry, government and in the third sector need at the start of their projects to ensure that they are easy to reproduce and reuse at the end.

The book started as a guide for reproducibility, covering version control, testing, and continuous integration. But technical skills are just one aspect of making data science research "open for all".

In February 2020, *The Turing Way* expanded to a series of books covering reproducible research, project design, communication, collaboration, and ethical research.



@martinagvilas, @turingway #TuringWay



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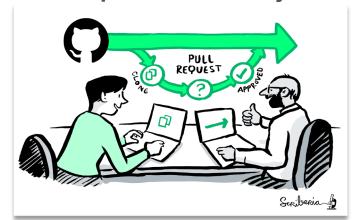
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### A Book



# An Open Source Project



### **A Community**

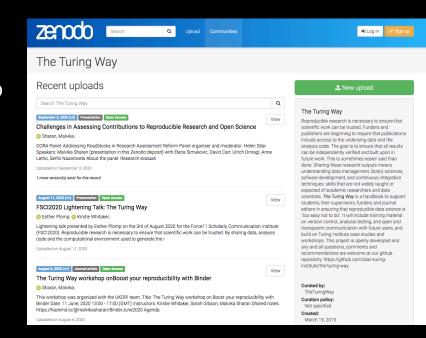


### **A Culture of Collaboration**

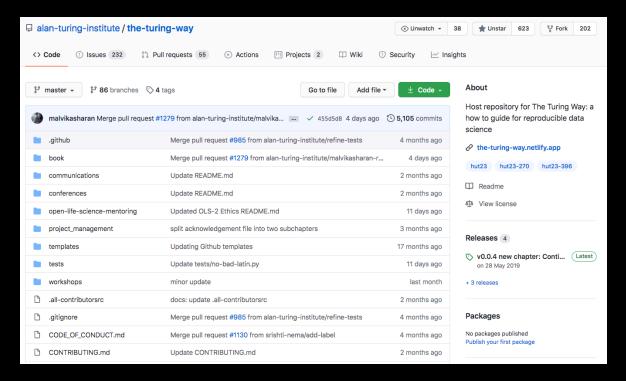


everyone can freely read, reuse,distribute, modify and help develop

the project belongs to The TuringWay community (CC-BY license)

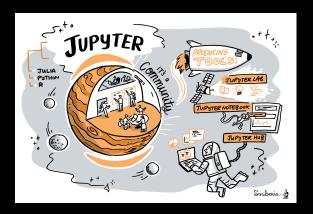


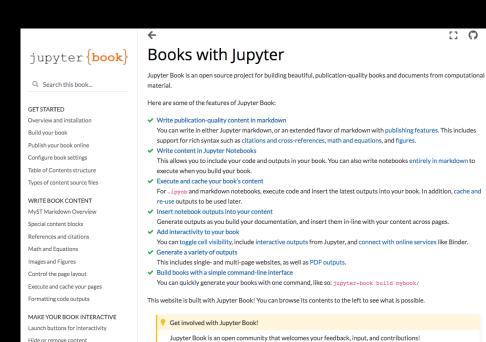
content hosted on GitHub



Interactive data visualizations
Commenting and Annotation

built with other Open Source tools





to provide feedback and new ideas, and to help others.

Get started

of Jupyter Book

Acknowledgements

A Small Example Project
Under the hood - the components

Contribute to Jupyter Book

Jupyter CON

Module 1: Welcome to the tutorial
Creating a Jupyter Book with

The Turing Way

by Malvika Sharan @malvikasharan





module 6:

Jupyter Book CI/CD

by Sarah Gibson



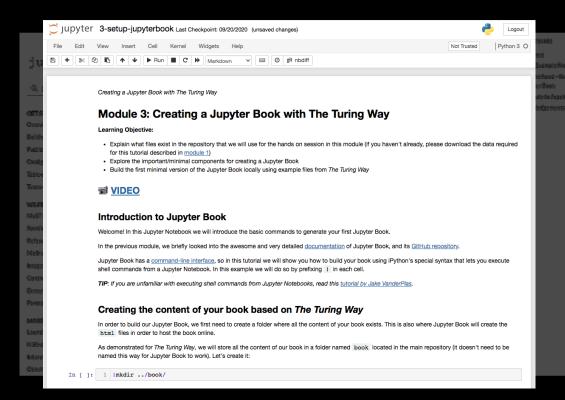


module 3:

Jupyter Book set-up

by Martina Vilas @martinagvilas





https://github.com/martinagvilas/tutorial-jupyterbook-with-turing-way/ @martinagvilas, @turingway #TuringWay



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## **An Open Source Project**

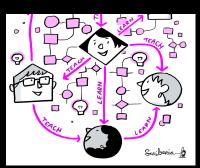


### **A Culture of Collaboration**

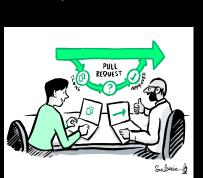


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book	minor update	\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\
communications	Fix typos	
conferences	Add KW formatting pedantry	
project_management	Update online-collaboration-cafe.md	
templates	Updating Github templates	
tests tests	Add "et cetera" as a deprecated Latinism	
workshops	Remove mis-pasted text	Seriberia S
all-contributorsrc	Merge pull request #991 from alan-turing-institute/all-contribu	
gitignore	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-contribu	itors/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

# **Contribution Pathways**



- Read/share resources



- Review pull requests



- Fix bugs/typos/errors



- Help translate



- Engage informally

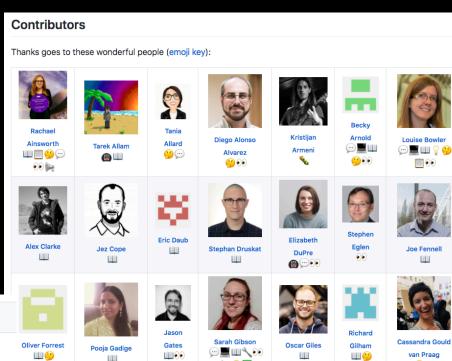


- Improve our culture

# acknowledgment

everyone gets
acknowledgement for their
work







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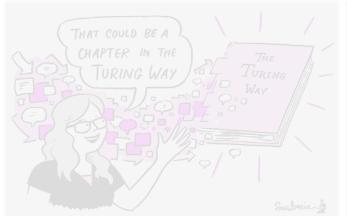
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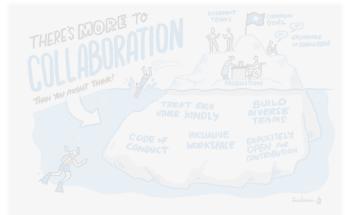
## **An Open Source Project**



## **A Community**



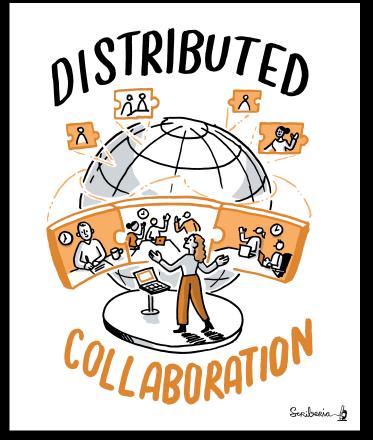
## **A Culture of Collaboration**



# open community

- anyone can join and contribute
- the direction and the goals are

determined collaboratively



# mentored contributions



Collaboration Cafés & Co-working Calls



**Book Dash Events** 

# mentored contributions



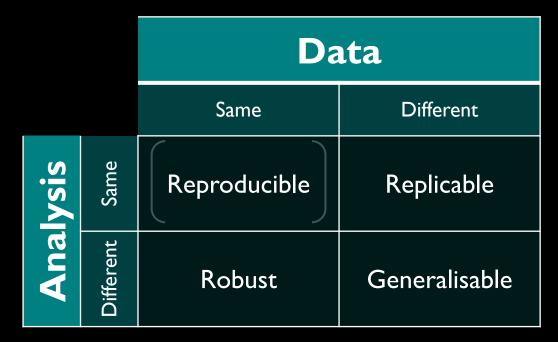
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1. what is The Turing Way?

2. guide to computational reproducibility

# reproducible research

same analysis steps on the same dataset produces same answer



# The Turing Way chapters on reproducibility

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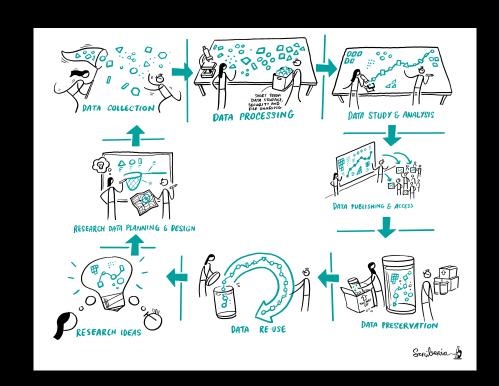
Reproducible Research with Make

Research Compendia

Credit for Reproducible Research

Risk Assessment

Case Studies



# computational reproducibility

- → Track changes to your code (version control)
- → Write clean, understandable and error free code
- → Save and share your computational environment
- → Make your code open source

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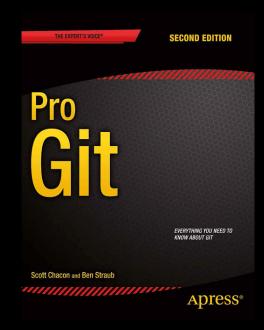
- records changes to a file or set of files over time
- provides access to any specific version



- changes are recorded using snapshots
- distributed version control system



- Web and Desktop App GUI interface
- most Open Source software hosted here



# computational reproducibility

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# code style guide

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

# code style guide

## PEP 8

e.g. imports

```
# Correct:
import os
import sys

# Wrong:
import sys, os
```

# code style guide

## PEP 8

e.g. spaces

```
# Correct:
i = i + 1
submitted += 1
x = x*2 - 1
hypot2 = x*x + y*y
c = (a+b) * (a-b)
# Wrong:
i=i+1
submitted +=1
x = x * 2 - 1
hypot2 = x * x + y * y
c = (a + b) * (a - b)
```

Style Guide Enforcement tools

Style Guide Enforcement tools → flake8

```
!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
```

Automatic formatting tools

Automatic formatting tools→ Black

### code review

have another programmer look over your code and assess it

### code review

#### types

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

### code testing

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

### code testing

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

you probably are already doing it ...

```
data = np.random.randint(0, 10, size=(4, 6))
print(data)

[[3 4 4 3 3 8]
[5 7 5 6 8 8]
[6 0 8 2 9 8]
[4 4 1 8 7 4]]
```

#### <u>assert</u>

#### <u>assert</u>

```
expected_n_rows = 3
    assert data.shape[0] == expected_n_rows, "shape mismatch"
expected_n_rows = 3
real_n_rows = data.shape[0]
assert real_n_rows == expected_n_rows, (
    f"shape mismatch, data has {real_n_rows} rows, expected {expected_n_rows} rows"
 AssertionError
                                            Traceback (most recent call last)
 <ipython-input-22-1d999f81fff0> in <module>
       2 real_n_rows = data.shape[0]
       3 assert real_n_rows == expected_n_rows, (
             f"shape mismatch, data has {real_n_rows} rows, expected {expected_n_rows} rows"
       5)
 AssertionError: shape mismatch, data has 4 rows, expected 3 rows
```

# unit testing

```
def take_fifth_power(x):
    result = x * x * x * x * x
    return result
```

```
def test_take_fifth_power():
   assert take_fifth_power(1.5) == 7.59375
```

### pytest

#### Testing framework

detailed info of assert statements

```
platform linux -- Python 3.x.y, pytest-6.x.y, py-1.x.y, pluggy-0.x.y
cachedir: $PYTHON_PREFIX/.pytest_cache
rootdir: $REGENDOC TMPDIR
collected 1 item
test_sample.py F
                                           [100%]
   test_answer _____
  def test_answer():
     assert inc(3) == 5
     assert 4 == 5
     + where 4 = inc(3)
test_sample.py:6: AssertionError
================ short test summary info ====================
FAILED test_sample.py::test_answer - assert 4 == 5
```

# pytest

#### Testing framework

- detailed info of assert statements
- auto-discovery of tests

```
setup.py
mypkg/
   __init__.py
   app.py
   view.py
tests/
   test_app.py
   test_view.py
...
```

#### Smoke test

initial checks designed to ensure very basic functionality

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initial checks designed to ensure very basic functionality

#### Integration test

individual units are combined and tested as a group

#### Smoke test

initial checks designed to ensure very basic functionality

#### Integration test

individual units are combined and tested as a group

#### etc.!

# computational reproducibility

- → Track changes to your code (version control)
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- → Save and share your computational environment
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# reproducible computational environments

#### Interaction style

		Graphical	Command line
What is	Software and versions	Binder	Conda
reproduced?	Entire system	Virtual machine	Containers

#### conda

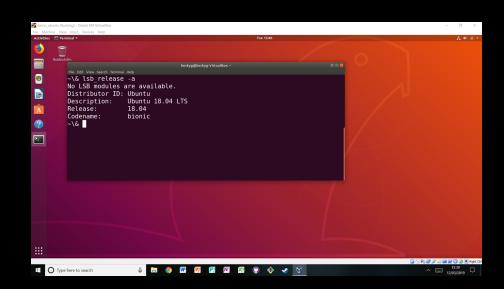


- environment management system
- package and version management system

### virtual machines

package a whole computer as an app that can be run





#### containers

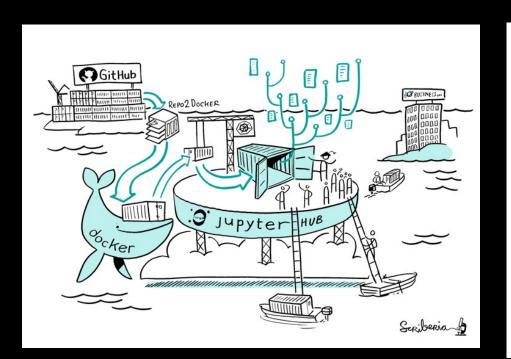


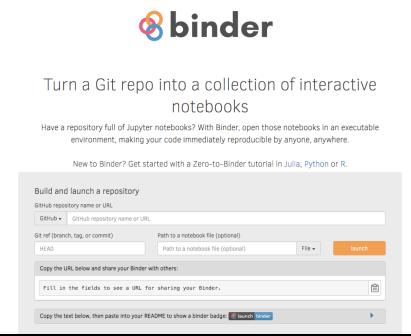
- behaves like a virtual machine
- more lightweight -> only contains the

individual components needed to operate

the project

#### **Binder**





# computational reproducibility

- → Track changes to your code (version control)
- → Write clean, understandable and error free code
- → Save and share your computational environment
- → Make your code open source

### open source

 anybody can view, use, modify, and distribute the software for any purpose

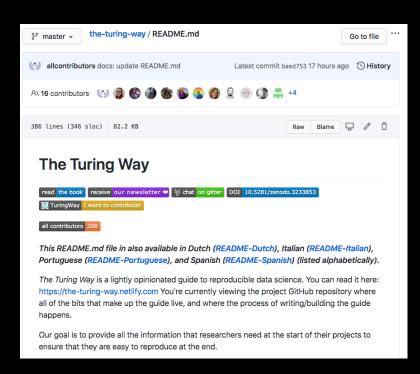
# licensing

	Copyleft		Permissive	Duamietem	
	Strong	Weak	Permissive	Proprietary	
Use for anything	Yes	Yes	Yes	Sometimes	
Private changes	Yes	Yes	Yes	Rarely	
Distribute original	Same license, with source	Same license, with source	Same license, also binary-only <sup>1</sup>	Rarely	
Distribute modified	Same license, with source	Same license, with source <sup>2</sup>	Any license, also binary-only	Rarely	
Distribute combined	Same license, with source	Any license, binary additions	Any license, also binary-only	Rarely	
<sup>1</sup> Under any license for the MIT license <sup>2</sup> Relicensing LGPL to GPL is allowed					

Free				
Copyleft		Permissive	Proprietary	
Strong	Weak	Permissive		
GPL <sup>1</sup> CDDL <sup>2</sup>	LGPL <sup>3</sup> MPL <sup>4</sup>	BSD <sup>5</sup> MIT <sup>6</sup> Apache	Research Only: No copying, No modification	

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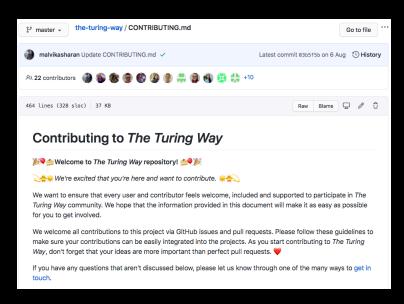
### community files



#### README.md

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

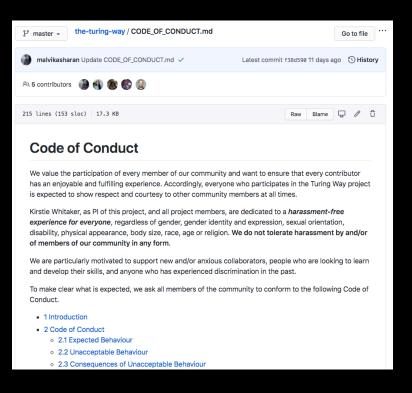
### community files



#### 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

### community files



#### CODE OF CONDUCT.md

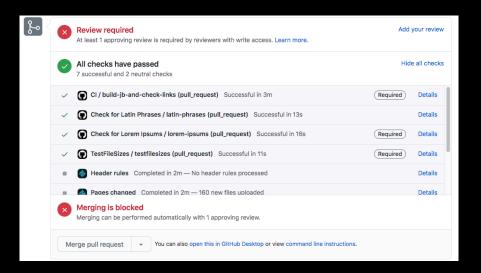
- how you expect participants to behave
- who these expectations apply to
- when they apply
- what to do if a violation occurs

### continuous integration

practice of integrating changes to a project made by individuals

into a main, shared version

frequently



# continuous integration

- Travis
- CircleCi
- GitHub Actions
- Azure

#### .yml

```
language: python
python:
- "2.6"
- "2.7"
- "3.2"
- "3.3"
```

```
os:
- linux
- osx
```

#### etc.

- documentation
- packaging
- interactivity

#### **Acknowledgements:**

- Kirstie Whitaker (@kirstie\_i), Project Lead
- Malvika Sharan (@malvikasharan), Community Manager
- 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: <a href="https://tinyurl.com/jointuringwayslack">https://tinyurl.com/jointuringwayslack</a>
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