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Better Software, Better Data Handling

Slides DOI: 10.5281/zenodo.4282599

20 November 2020, CODATA - Webinar Series: Research Skills
(https://codata.org/initiatives/strategic-programme/codata-connect/webinar-series-research-skills/)

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The Software Sustainability Institute

The Software Sustainability Institute

Software Sustainability Institute

A national facility for cultivating world-class research through software

- "**Better Software, Better Research**"
- Software code/processes/community reaches boundaries in its development that prevent improvement, growth and adoption
- Providing the expertise and services needed to negotiate to the next stage
- Programmes, events, policy, guidance and tools to support the community developing and using research software
- **We advocate for all things Research Software**

bit.ly/BetterSoftwareTshirt

Supported by the UK Research Councils through grants EP/H043160/1, EP/N006410/1 and EP/S021779/1, with additional project funding from Jisc A collaboration between the universities of Edinburgh, Manchester, Oxford and Southampton.

Teams

Software
Helping the community to develop software that meets the needs of reliable, reproducible, and reusable research

Policy
Collecting evidence on and promoting the place of software in research & sharing with stakeholders

Outreach
Exploiting our platform to enable engagement, delivery & uptake

Training
Delivering essential software skills to researchers, partnering with institutions, doctoral schools and the community

Community
Developing Communities of Practice by supporting the right people to understand and address topical issues

Activities

Software
75+ project consultancies
200+ evaluations
4 surgeries

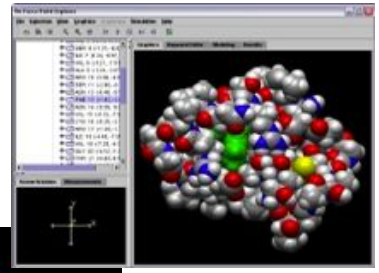
Policy
1500+ RSEs engaged
Involved in UKRI long-term strategy
On 29 national and international committees

Outreach
170+ external contributors
20k unique visitors/month
7.5k followers (Twitter)

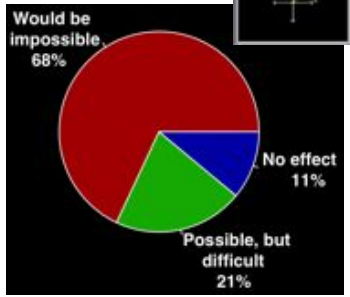
Training
300+ Carpentry workshops
7000+ learners, 250+ instructors
80+ guides

Community
140+ Fellows
35+ workshops organised

Software Sustainability Institute



The "7/10"



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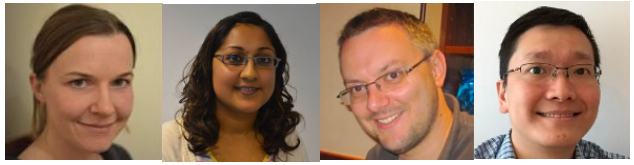

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Better Software, Better Data Handling

Today's Journey

www.software.ac.uk

- Spreadsheets
- Other options
- Resources and Training
- Data Carpentry
- Pedagogy practice and training
- Other initiatives

Photo by Zbysiu Rodak on Unsplash

Spreadsheets

Spreadsheets - data problems

- Microsoft Excel autocorrecting gene names to dates!
  - Like MARCH1 — short for "Membrane Associated Ring-CH-Type Finger 1" — Excel converts that into a date: 1-Mar
  - One study from 2016 examined genetic data shared alongside 3,597 published papers and found that roughly one-fifth had been affected by Excel errors!

www.theverge.com/2020/8/6/21355674/human-genes-rename-microsoft-excel-misreading-dates

MICROSOFT \ REPORT \ SCIENCE

Scientists rename human genes to stop Microsoft Excel from misreading them as dates

Sometimes it's easier to rewrite genetics than update Excel

By James Vincent | Aug 6, 2020, 8:44am EDT

SHARE

Illustration by Alex Castro / The Verge

Spreadsheets - format problems

www.software.ac.uk

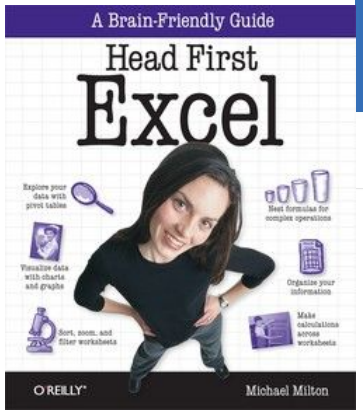
- Microsoft Excel file format caused 16,000 Covid19 cases in the UK to be lost
  - Use of XLS (65K rows) vs XLSX (1M+ rows) for integrating results
  - limit reached - rows just discarded
  - Delayed contact tracers knowing who to contact

www.bbc.co.uk/news/technology-54423988

Spreadsheets can be used properly

www.software.ac.uk

- Courses & books are available
- But the the **majority** of people **do not use best practices** in spreadsheets, probably because it **so easy not to**!
- Spreadsheets can be done in so many different ways!



Better options

Better tools & languages

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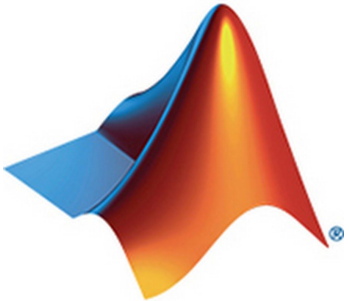
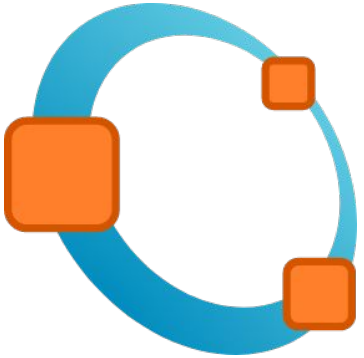
- A Scripted approach
  - Reproducible
  - Easier to compare versions
  - A more consistent version for sharing

The R Project for Statistical Computing

Python



Mathworks Matlab



GNU Octave

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Resources and Training

So you want to learn

Places to look: (that you can fit in with your day job!)

- Courses by local University IT department for ECR's
- Research Community based learning initiatives
- Self directed Learning

Out of scope for this talk:

- Fully fledged courses (that take up 30-100% of your time for more than a month) ← day job?

Research led training communities

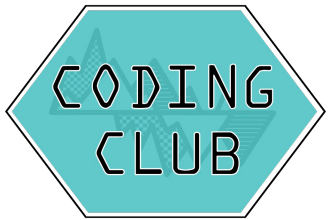
www.software.ac.uk

- The Carpentries
  - Software
  - Data
  - Library
- Code Refinery
- Our Code Club

THE CARPENTRIES

carpentries.org

coderefinery.org



ourcodingclub.github.io

Online course review sites

- Online review sites
  - Course talk
  - Class Central
  - Recommends and Rankings help choose
- MOOCs & more
  - Coursera
  - EdX
  - Future Learn etc

coursetalk
www.coursetalk.com

CLASS CENTRAL
www.classcentral.com

Coursera
edX
FutureLearn

Udacity
Swayam
Miríadax
France Université Numerique Courses

Autodidactic

- Autodidactic
  - self taught - usually complex topics e.g. calculus or a language.
  - 15%? 70%?
- The need for training & community
  - Get feedback
  - Clear blockages in your understanding
  - Builds confidence
  - Help form Learning communities

Experiences with efficient methodologies for teaching computer programming to geoscientists

Christian T. Jacobs, Gerard J. Gorman, Huw E. Rees, Lorraine Craig

Affiliation for authors #1, #2 and #4: Department of Earth Science and Engineering, South Kensington Campus, Imperial College London, London, SW7 2AZ

Affiliation for author #3: Educational Development Unit, South Kensington Campus, Imperial College London, London, SW7 2AZ

Corresponding author email address: c.jacobs10@imperial.ac.uk

Short title: Efficient methodologies for teaching programming to geoscientists

Paper type: Curriculum & Instruction (Instructional Approaches)

Keywords: computer programming, undergraduate, teaching methodology, feedback

Manuscript accepted for publication in the Journal of Geoscience Education on 9 June 2016

Abstract

Computer programming was once thought of as a skill required only by professional software developers. But today, given the ubiquitous nature of computation and data science it is quickly becoming necessary for all scientists and engineers to have at least a basic knowledge of how to program. Teaching how to program, particularly to those students with little or no computing background, is well-known to be a difficult task. However, there is also a wealth of evidence-based teaching practices for teaching programming skills which can be applied to greatly improve learning outcomes and the student experience. Adopting these practices naturally gives rise to greater learning efficiency - this is critical if programming is to be integrated into an already busy geoscience curriculum. This paper considers an undergraduate computer programming course, run during the last 5 years in the Department of Earth Science and Engineering at Imperial College London. The teaching methodologies that were used each year are discussed alongside the challenges that were encountered, and how the methodologies affected student performance. Anonymised

https://arxiv.org/abs/1505.05425 -

The Carpentries approach

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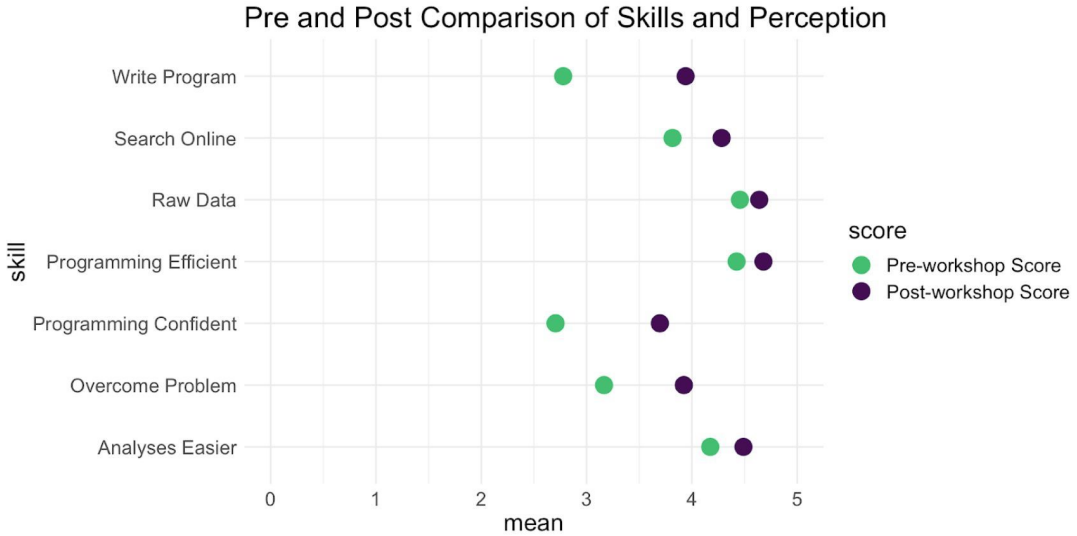
- Instruction
- Material for reference
- Learn by doing
- Helpers to clear up understanding

Evidence of Carpentries' Impact on Learners

- 66.2% of respondents use programming languages and/or the command line to automate repetitive tasks.
- 49.3% of respondents have improved their data management and project organisation.
- 46.1% of respondents use version control to manage code.

How Tools Have Helped Research/Work	*n*	%
They are improving my overall efficiency.	254	59.5
They are improving my ability to analyse data.	228	53.4
They are improving my ability to manage data.	214	50.1
I am not using the tools I learned.	65	15.2
The tools I learned have not helped me with my work.	30	7.0



carpentries.org/blog/2018/07/evidence-impact

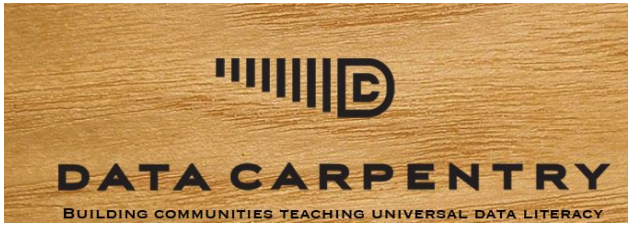
Data Carpentry

Data Carpentry (DC)

www.software.ac.uk

- Different Curriculums
  - Mature - ‘2’ days
    - Ecology, Genomics, Social Sciences, Geospatial
  - In development - ‘2’ days’
    - Image processing, Economics, Astronomy, Digital Humanities and more
  - Semester long
    - Biology

datacarpentry.org/lessons



All About Data Literacy!

A typical DC workshop

Lesson	Site	Repository	Reference	Instructor Notes	Maintainer(s)
Ecology Workshop Overview					Karen Cranston, Aleksandra Pawlik, Tracy Teal, Ethan White, Fabrice Rwasimitana
Data Organization in Spreadsheets for Ecologists					Christie Bahlai, Peter R. Hoyt, Tracy Teal
Data Cleaning with OpenRefine for Ecologists					Cam Macdonell, Deborah Paul, Phillip Doehle, Rachel Lombardi
Data Management with SQL for Ecologists					Donal Heidenblad, Timothée Poisot, Rémi Rampin, Christina Koch, Katy Felkner
Data Analysis and Visualization in R for Ecologists					Ana Costa Conrado, Auriel Fournier, François Michonneau, Brian Seok
Data Analysis and Visualization in Python for Ecologists					Tania Allard, Maxim Belkin

Some material is available in Spanish also - and you tend to do R or Python - ideally 2.5 days for the workshop

Using Spreadsheets in Research

- Data organisation or Data ‘wrangling’
  - The ‘sweet spot’ for spreadsheets
- Data exported for Analysis elsewhere
  - Adaptation and reproducibility is hard
  - Easy to reference wrong cells in calculations
    - Much easier to pick up this type of error using a scripting approach (e.g R, Python)
- Data presentation
  - Not optimal, use document editor for presentation
- Using Spreadsheets for “quick and dirty” analysis is OK - don’t consider it final and good data organisation helps here!

Good Data Organisation

www.software.ac.uk

- Don’t modify RAW data directly
- Take a copy and make changes to that to make a ‘clean’ data set to analyse
- Keep track of changes between RAW and ‘clean’ by keeping notes in a text file recording the steps you took to move from RAW to ‘clean’

Keep Data ‘Tidy’

- Variable in columns
- Observation in each row
- Don’t combine data into one cell
- export the data to a text-based format e.g CSV

General rules:

- columns = variables
- rows = observations
- cells = data (aka values)

“It is often said that 80% of data analysis is spent on the process of cleaning and preparing the data”

(Dasu and Johnson 2003).

Journal of Statistical Software
August 2014, Volume 59, Issue 10. http://www.jstatsoft.org/

Tidy Data

Hadley Wickham
RStudio

Abstract

A huge amount of effort is spent cleaning data to get it ready for analysis, but there has been little research on how to make data cleaning as easy and effective as possible. This paper tackles a small, but important, component of data cleaning: data tidying. Tidy datasets are easy to manipulate, model and visualize, and have a specific structure: each variable is a column, each observation is a row, and each type of observational unit is a table. This framework makes it easy to tidy messy datasets because only a small set of tools are needed to deal with a wide range of un-tidy datasets. This structure also makes it easier to develop tidy tools for data analysis, tools that both input and output tidy datasets. The advantages of a consistent data structure and matching tools are demonstrated with a case study free from mundane data manipulation chores.

Keywords: data cleaning, data tidying, relational databases, R.

www.jstatsoft.org/v59/i10

Common Formatting Problems

- Good formatting makes cleaning & analysis easier
- Multiple small tables breaks the one row per observation rule
- Keep all observation in one tab for a particular experiment
  - minimise joining
  - maintains consistency
- Zero vs null
  - and how to represent when you don’t capture values
- Formatting
  - Using formatting to represent data ← fix: new column
  - Merged cells ← fix: avoid
  - Units in cells ← fix: same unit in the column or new unit column
  - Avoid comments ← use a new column

More formatting

- Choose good column names
  - avoid spaces, make them meaningful, include units if possible, use a naming convention
- Copy and paste
  - remove formatting - use a cell as a holder of text and spaces
- Other files
  - Data files
  - Metadata files ← column name meanings, unit, exceptions, etc
  - A readme.txt to explain what each file contains and any relationships
- Date format
  - Use different columns: data, month, year or year and day of year

Better Data

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- Data validation
  - restrict the options or range
- Quality control
  - Remember to do this in a different file
  - Document your steps
- Sorting
  - Expand your sort ← maintain one row as one observation
  - Look at the start and end <- where errors tend to hide
- Conditional formatting

Guide to writing "readme" style metadata

A readme file provides information about a data file and is intended to help ensure that the data can be correctly interpreted, by yourself at a later date or by others when sharing or publishing data. Standards-based metadata is generally preferable, but where no appropriate standard exists, for internal use, writing "readme" style metadata is an appropriate strategy.

Want a template? **Download one** and adapt it for your own data!

- Best practices
- Recommended content
  - General information
  - Data and file overview
  - Sharing and access information
  - Methodological information
  - Data-specific information
- References
- Related information

data.research.cornell.edu/content/readme

Exporting data

- For analysis in other programs
  - universal, open, static format
  - Comma Separated Values - CSV or Tab Separated Values - TSV is a good choice
  - You can open them in e.g. Excel again - but remember any changes won't be saved.
  - Be careful about line endings in CSV files
    - LF (Unix) vs CR LF (Windows)

"Many people comment that this tool saves them literally months of work trying to make these edits by hand."

OpenRefine - cleaning messy data

www.software.ac.uk

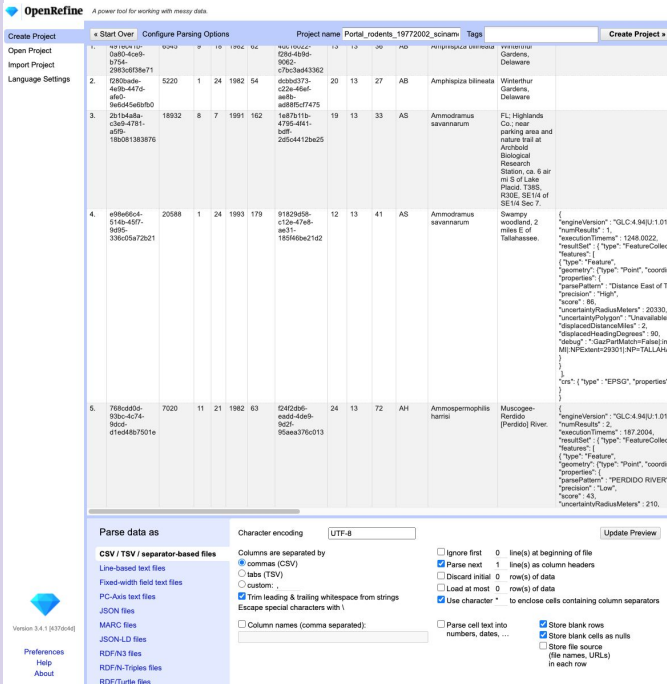
- Semi-automated cleaning that saves time
- Cleans
- Formats
- Tracks changes
- Does not overwrite raw data

Key features:

- Dataset overview
- Resolve inconsistencies
- Split data into more granular parts
- Match local data to other sets
- Enhance data from other sources
- Automation-replay steps on multiple files

openrefine.org

OpenRefine



Time for Analysis

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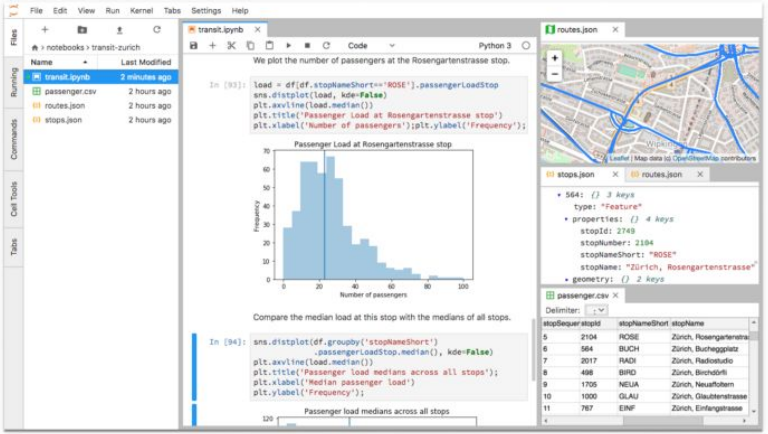
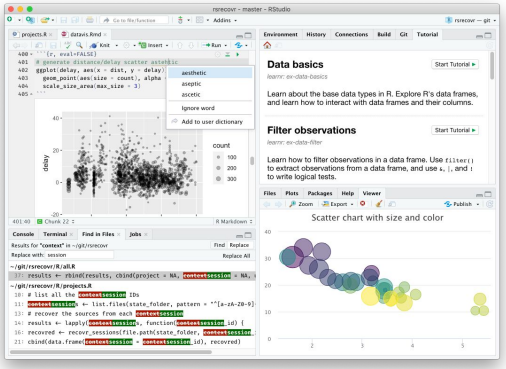
Two main DC lessons around analysis

- Python
  - General purpose language with data analysis libraries
  - Great libraries and editors - e.g. JupyterLab, Spyder, Visual Studio Code
- R
  - Built as a statistical computing language can be a bit strange to do general purpose things in
  - Great libraries and editors - R Studio

jupyter.org



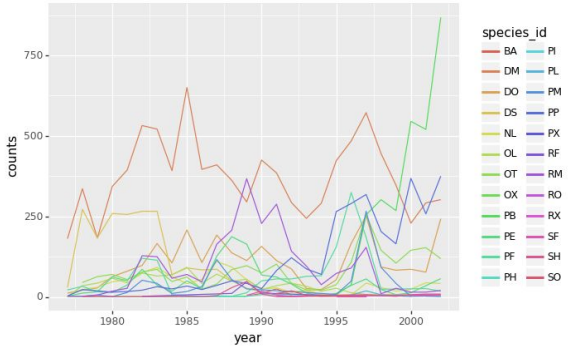
rstudio.com

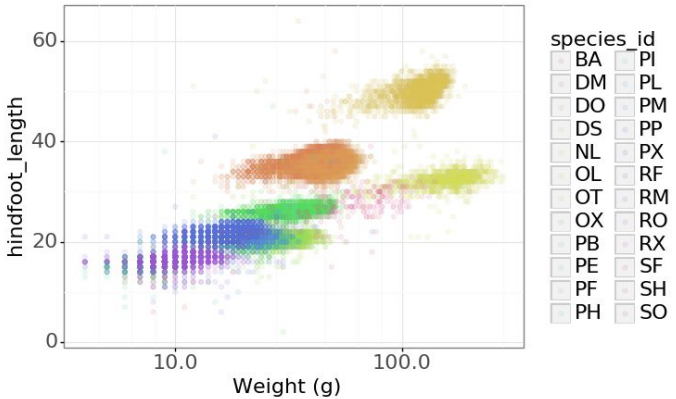


Data Analysis and Visualization in Python

www.software.ac.uk

- Python Syntax
- Jupyter notebook interface
- Importing CSV files
- pandas library to work with data frames
- Summary info from data frames
- An intro to plotting





datacarpentry.org/python-ecology-lesson/index.html

Other tools and approaches

www.software.ac.uk

- Further DC:
  - SQL ← a different approach to querying data
  - R ← similar place to Python in Analysis

Better software skills also help - more in the region of **Software Carpentry** -

- The Unix Shell ← automation
- Git ← version control
- Python / R ← more of a programming focus
- Reproducibility in R

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Pedagody practice and training

Beyond learning

THE CARPENTRIES carpentries.org

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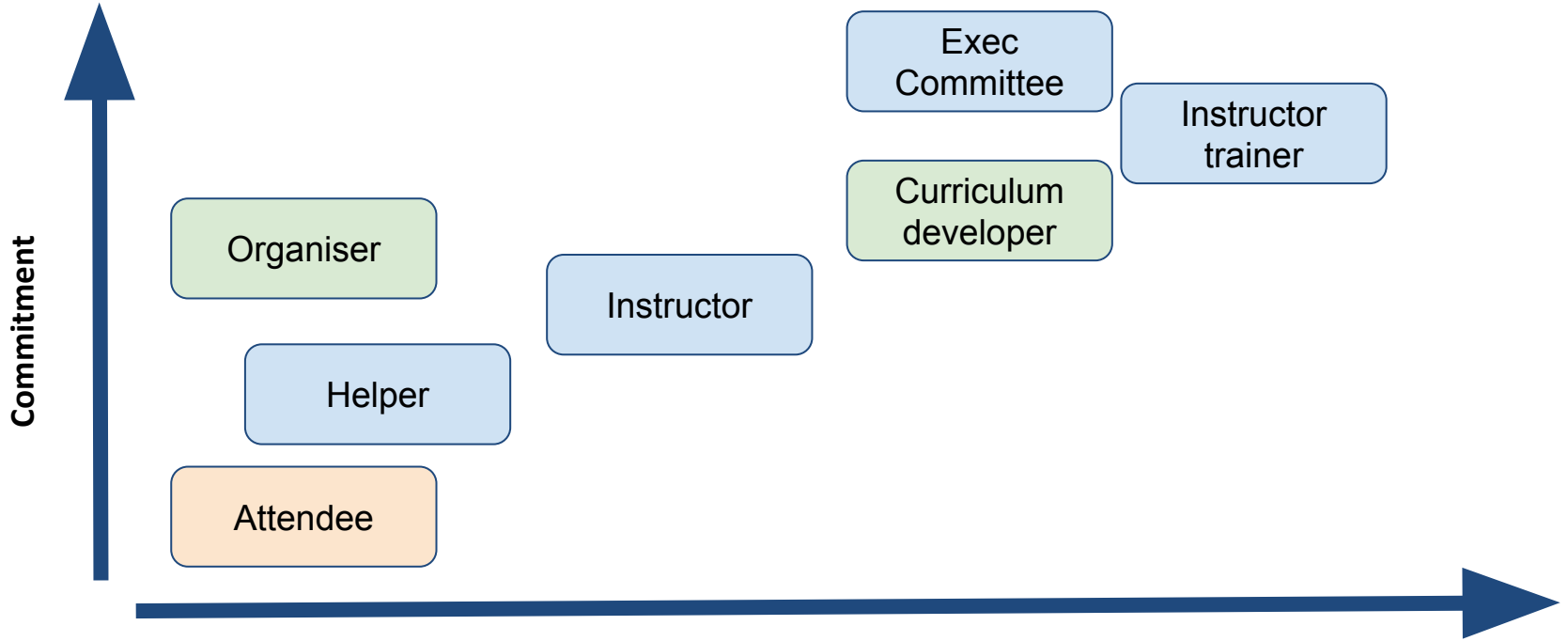

- Teaching training and experience - help transition from postdoc to faculty
- CV worthy material

Teaching Infrastructure

www.software.ac.uk

carpentries.org/become-instructor

Apply to become an Instructor

carpentries.github.io/instructor-training

- Introduce you to evidence-based best-practices of teaching.
- Teach you how to create a positive environment for learners at your workshops.
- Provide opportunities for you to practice and build your teaching skills.
- Help you become integrated into the Carpentries community.
- Prepare you to use these teaching skills in teaching Carpentries workshops.

The Carpentries Incubator

Community Developed Lessons

carpentries.org/community-lessons

Development guidebook

cdh.carpentries.org

Template

github.com/carpentries/styles

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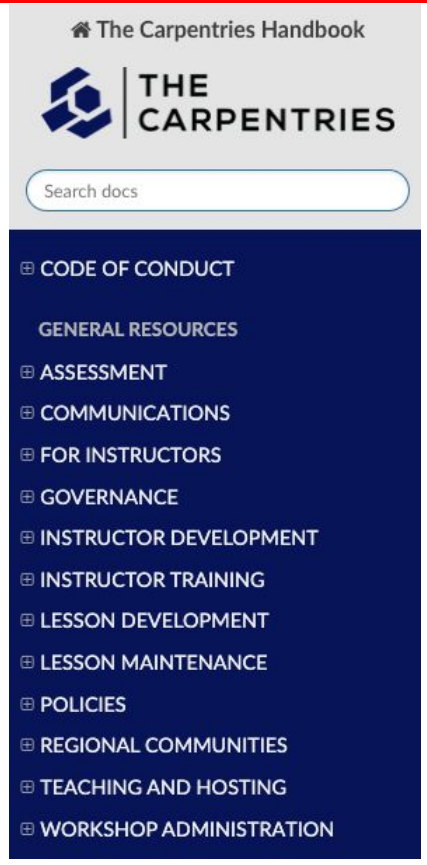
docs.carpentries.org



Teaching Community

www.software.ac.uk

Community Discussions

carpentries.org/community_discussions

1. **Pre- and Post-Workshop Discussions** These discussions are designed for those getting ready to teach or having recently taught to come discuss their workshop with the community. They occur twice per week.

2. **Themed Discussion Sessions** These discussions are centered around a particular topic ranging anywhere from teaching your first workshop to community building strategies. They occur once per month.

3. **Carpentries Conversations** These Conversations are hosted by one of our Committees or Task Forces to provide the community with the opportunity to learn about and discuss new developments and programs in our organisation. They occur once per month.

twitter.com/thecarpentries

Join **The Carpentries** on Slack.
2242 users are registered so far.

swc-slack-invite.herokuapp.com

Other initiatives

Open Science & Reproducibility

www.software.ac.uk

Open Science / Research

- Open Access
- Open Data
- Open notebook science
- Open Source
- It's about transparency and access

Benefits:

- Verification
- Reduce duplication
- Reuse
- Trustworthiness
- Quality

Rein in the four horsemen of irreproducibility

Dorothy Bishop *describes how threats to reproducibility, recognized but unaddressed for decades, might finally be brought under control.*

Problems:

- Publication Bias
- Low statistical power
- P-value hacking
- Harking (hypothesis after results are known)

www.nature.com/articles/d41586-019-01307-2

International Level

OECD BETTER POLICIES FOR BETTER LIVES

www.oecd.org/science/inno/open-science.htm

OECD Science, Technology and Industry Policy Papers No. 25

Making Open Science a Reality

OECD

doi.org/10.1787/23074957

National & Institutional

UKRN

RN UK Reproducibility Network

www.ukrn.org

- Training
- Best practice / primers
- Culture
- Researcher led
  - Local network model

Software Sustainability Institute

Institutional & Grassroots

started 2018, 109 institutions in 25 different countries

ReproducibiliTea

reproducibilitea.org

- Open Science Journal clubs
- Setup you own

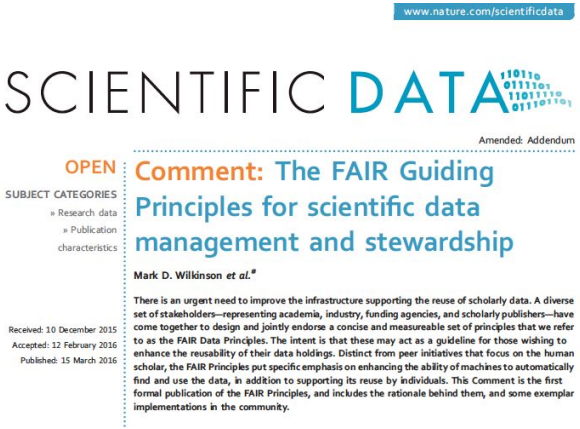
FAIR - Findable, Accessible, Interoperable, Reusable

www.software.ac.uk

FAIR (2015)

Turning FAIR into reality (2018)

FAIR 4 Research Software (2019)


www.nature.com/scientificdata

SCIENTIFIC DATA

Amended: Addendum

OPEN

SUBJECT CATEGORIES
» Research data
» Publication characteristics

Comment: The FAIR Guiding Principles for scientific data management and stewardship

Mark D. Wilkinson *et al.*

Received: 10 December 2015
Accepted: 12 February 2016
Published: 15 March 2016

There is an urgent need to improve the infrastructure supporting the reuse of scholarly data. A diverse set of stakeholders—representing academia, industry, funding agencies, and scholarly publishers—have come together to design and jointly endorse a concise and measureable set of principles that we refer to as the FAIR Data Principles. The intent is that these may act as a guideline for those wishing to enhance the reusability of their data holdings. Distinct from peer initiatives that focus on the human scholar, the FAIR Principles put specific emphasis on enhancing the ability of machines to automatically find and use the data, in addition to supporting its reuse by individuals. This Comment is the first formal publication of the FAIR Principles, and includes the rationale behind them, and some exemplar implementations in the community.

www.nature.com/articles/sdata201618

op.europa.eu/s/oriv

FAIR for Research Software (FAIR4RS) WG

www.rd-alliance.org/groups/fair-research-software-fair4rs-wg

3 subgroups:

- How do FAIR principles map to Software
- How has FAIR been applied to workflows, notebooks, training etc
- Definition of research software

Why is this important?:

- **Understanding how to make your analysis FAIR will help make it Reproducible and mindfully Open**

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In conclusion

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- Better ways to handle and analyse data
- Learn best practices
- Make your work reproducible
- Get involved in training communities for career credit
- Be aware of the wider context
- Do what you do better - make coding/scripting/ aka better software your data handling superpower!

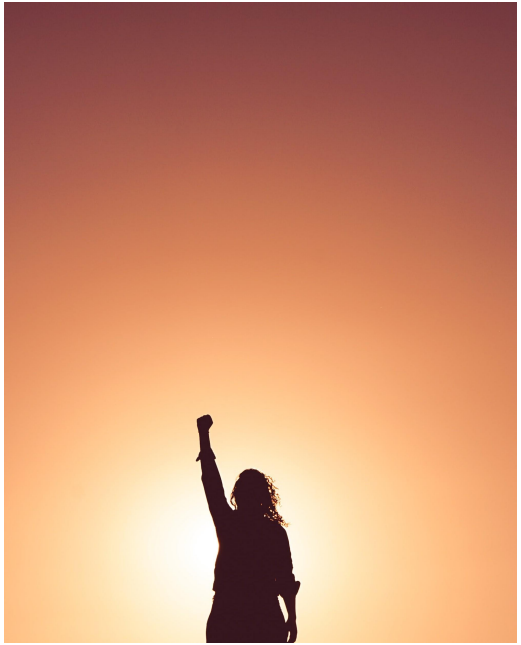

Photo by Miguel Bruna on Unsplash

Acknowledgements

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The SSI team/*alumni*:

- Agata Dybisz
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- Claire Wyatt
- Clem Hadfield
- Dave De Roure
- *Devasena Prasad*
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- *Malcolm Illingworth*
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Questions?

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