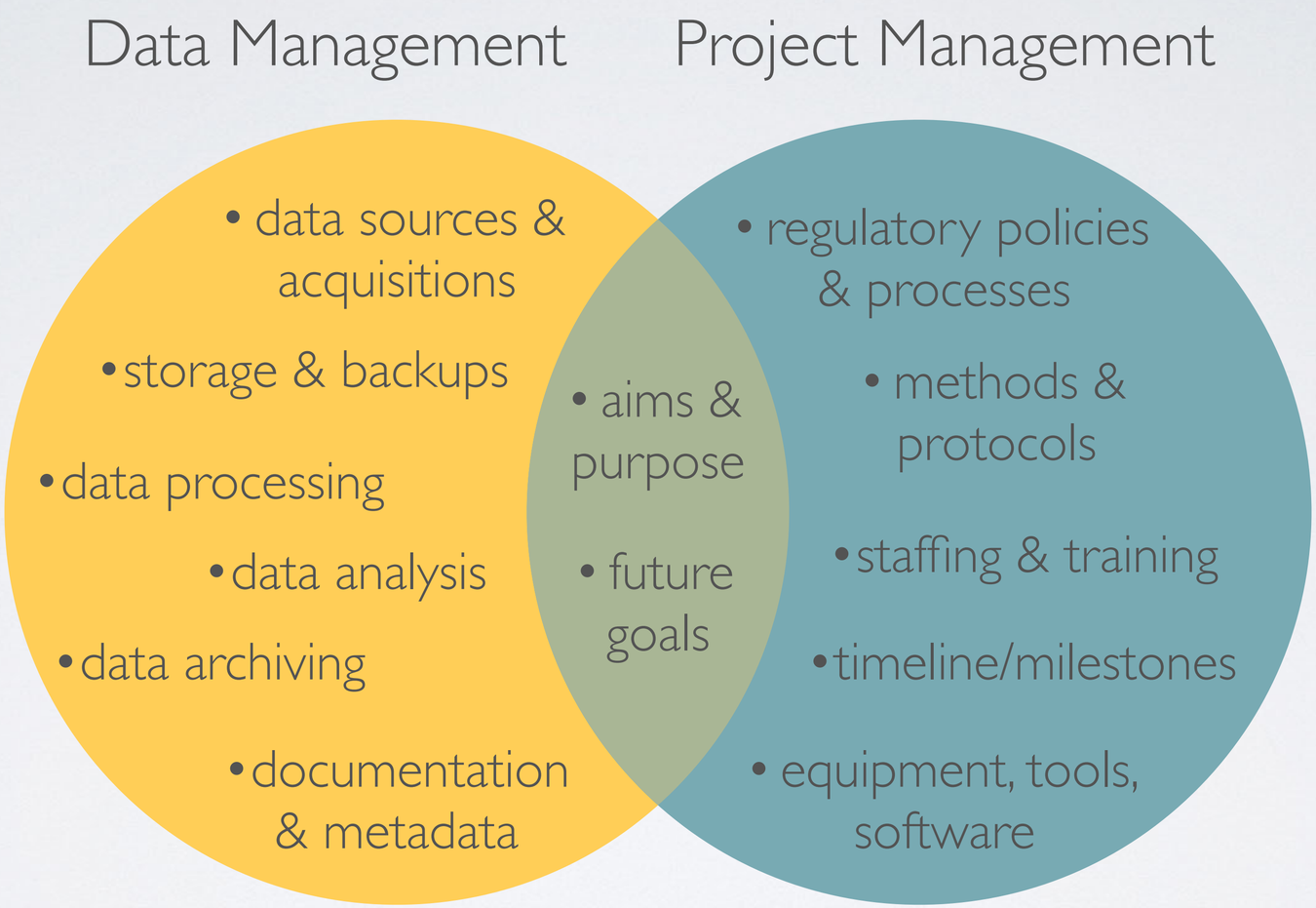
Good Enough Practices for Data Management

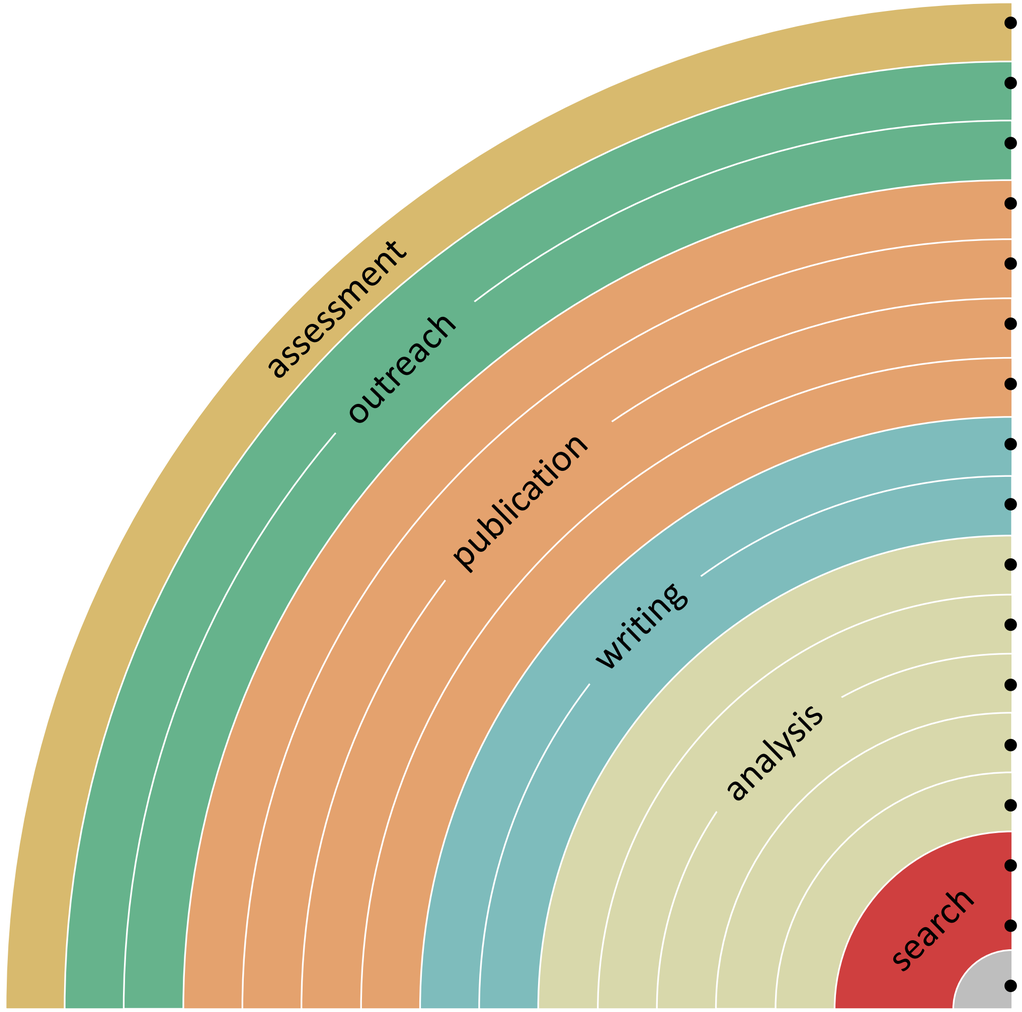
Alaina Pearce

Project vs Data Management



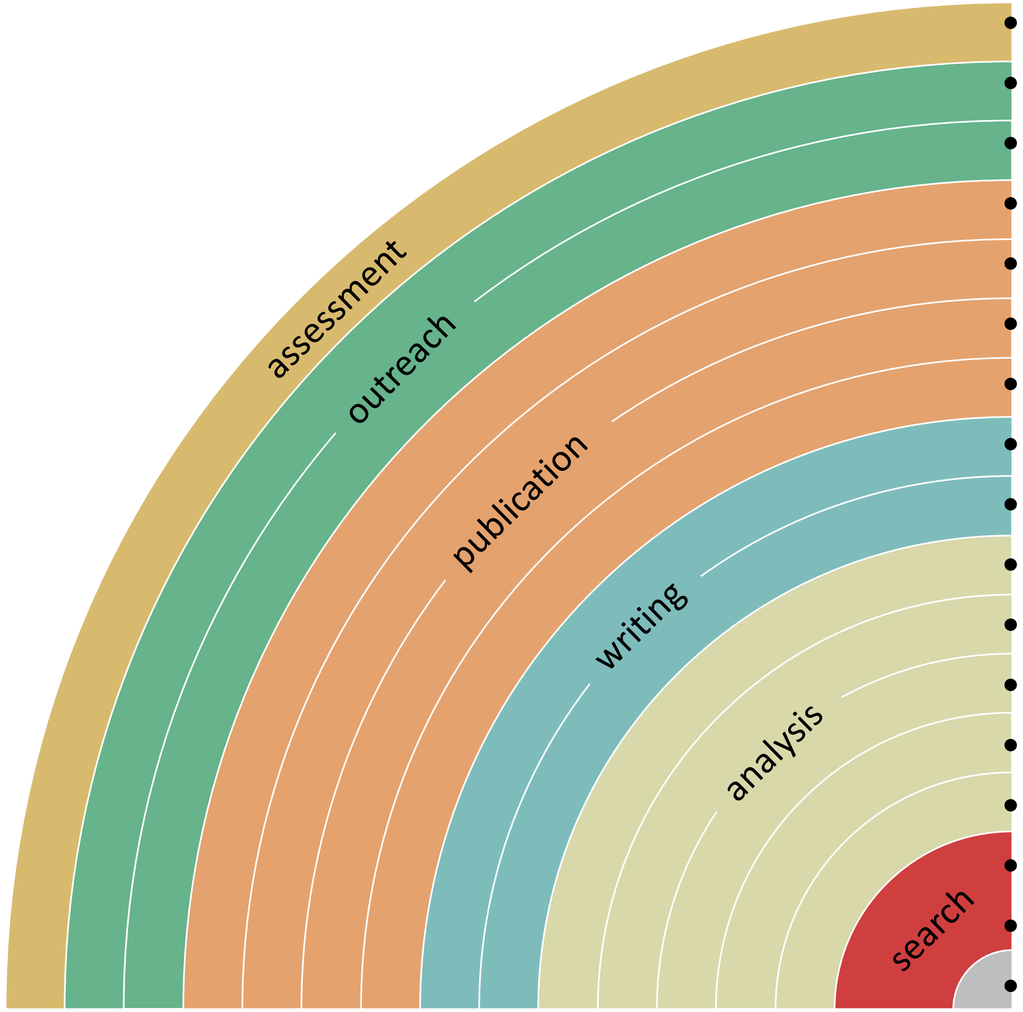
Goal: extract meaningful insight and information

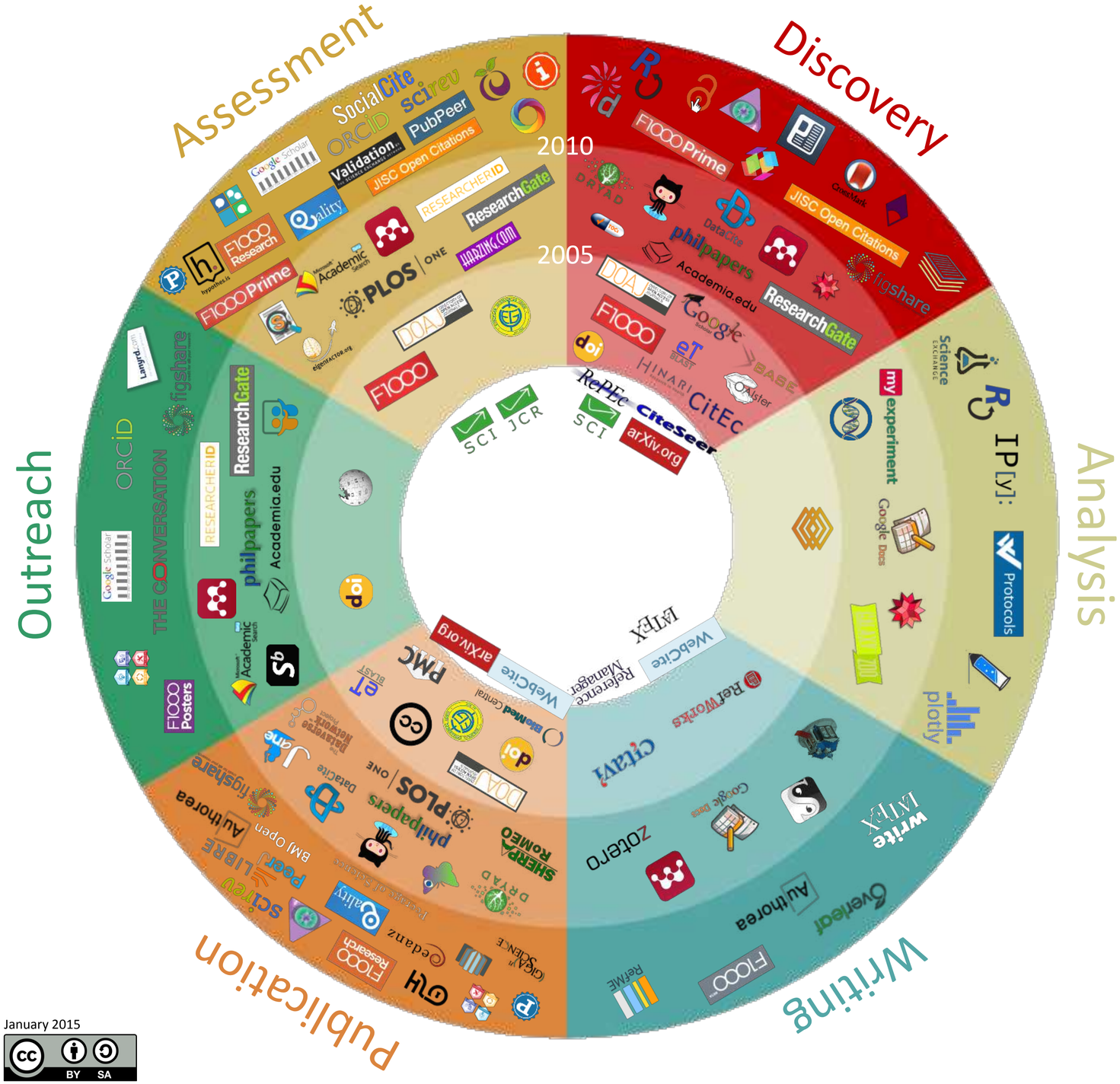
Goal: meet project goals within set timelines



- adding alternative evaluation, e.g. with altmetrics
- communicating through social media, e.g. Twitter
- sharing posters & presentations, e.g. at FigShare
- using open licenses, e.g. CC0 or CC-BY
- publishing open access, ‘green’ or ‘gold’
- using open peer review, e.g. at journals or PubPeer
- sharing preprints, e.g. at OSF, arXiv or bioRxiv
- using actionable formats, e.g. with Jupyter or CoCalc
- open XML-drafting, e.g. at Overleaf or Authorea
- sharing protocols & workfl., e.g. at Protocols.io
- sharing notebooks, e.g. at OpenNotebookScience
- sharing code, e.g. at GitHub with GNU/MIT license
- sharing data, e.g. at Dryad, Zenodo or Dataverse
- pre-registering, e.g. at OSF or AsPredicted
- commenting openly, e.g. with Hypothes.is
- using shared reference libraries, e.g. with Zotero
- sharing (grant) proposals, e.g. at RIO

DOI: 10.5281/zenodo.1147025





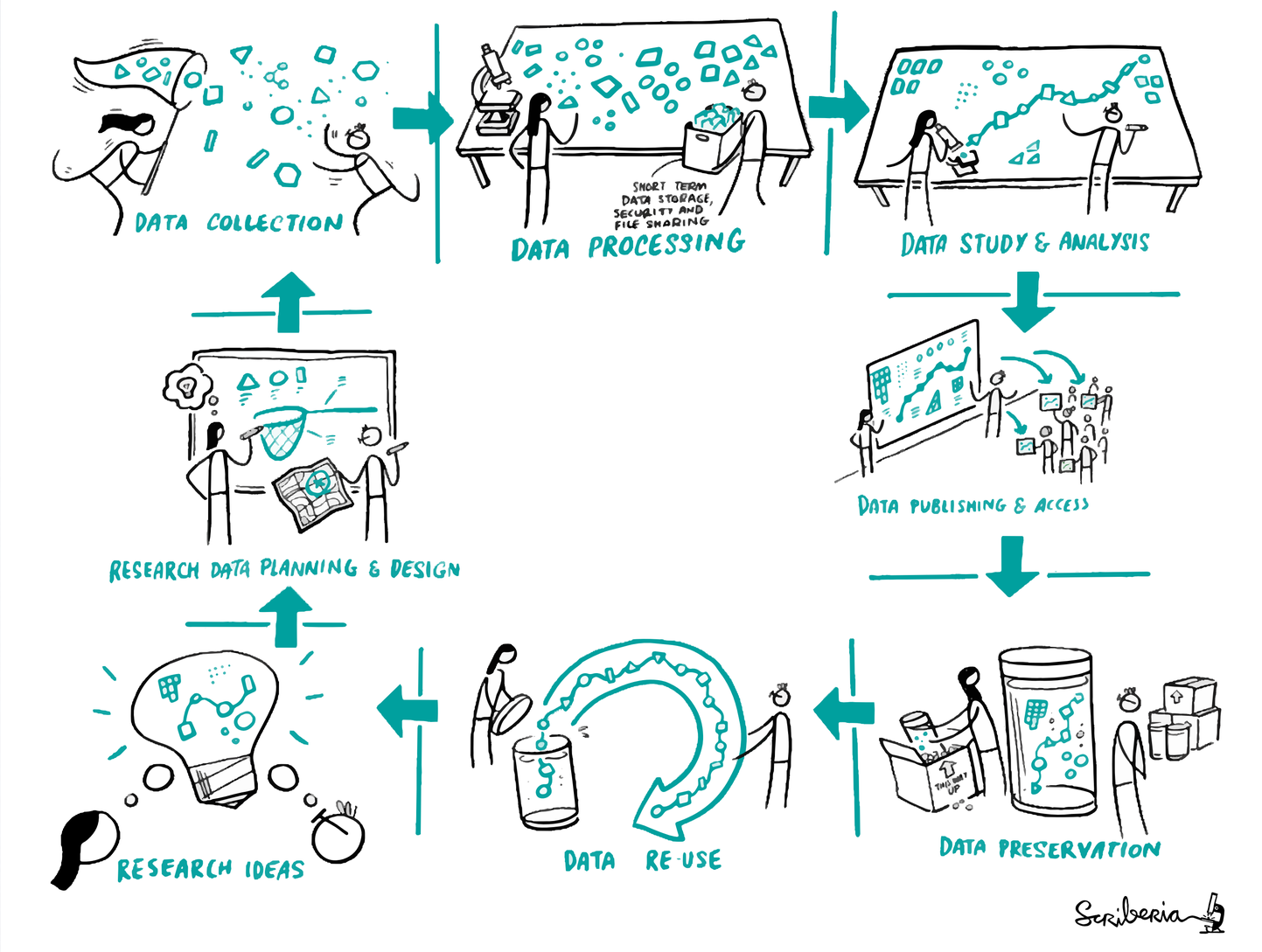
	Discovery	Analysis	Writing	Publication	Outreach	Assessment
Traditional	WEB OF SCIENCE™	SPSS	W ENDNOTE 7	nature	RESEARCHERID	Journal Citation Reports
Modern	Google scholar	R	RefWorks	arXiv.org PLOS ONE	Institutional Repository	eigenFACTOR.org PLOS ARTICLE-LEVEL METRICS
Innovative		ZOONIVERSE	Authorea	figshare PeerJ	ResearchGate ORCID	Peerage of Science Altmetric
Experimental	sparrho d	RopenSci IP[y]: Nb	Overleaf Docear The Academic Literature Suite	the WINNOWER		PubPeer
Google	Google scholar Google books		Google Research	?	Google Scholar	Google Scholar Google scholar METRICS
NPG/Macmillan		labguru do more science	Overleaf	figshare nature	Nature Blogs	nature INDEX BETA Altmetric

With What Time???

‘Good Enough’

- (relatively) low effort
- shallow learning curve
- beneficial to current and future you
- increases ‘openness’ of research

Project Lifecycle



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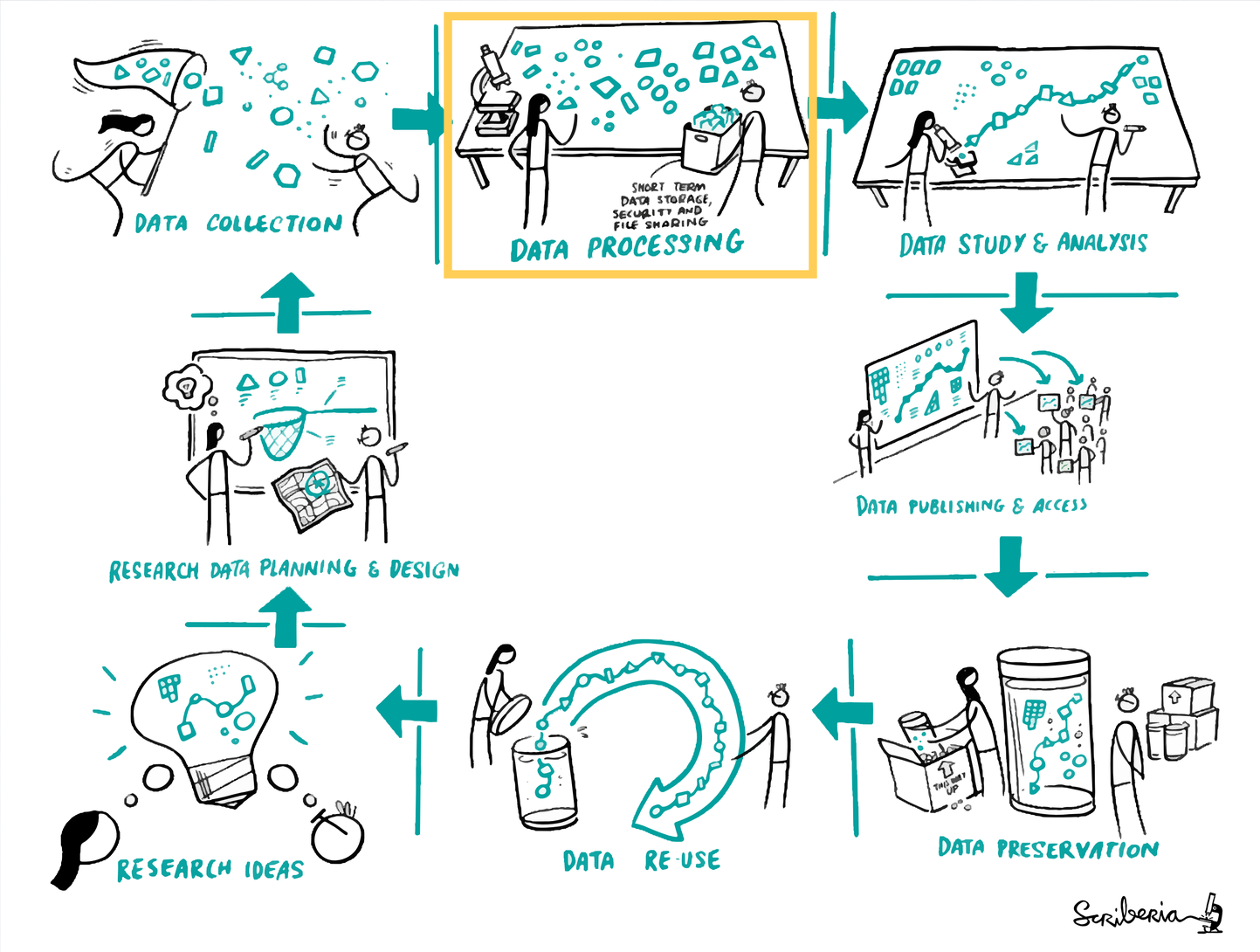

Data Processing Pipelines

1. Preserve Raw Data

Raw Data: data as it was originally collected

Save in data in its original form and DO NOT alter or 'improve' it

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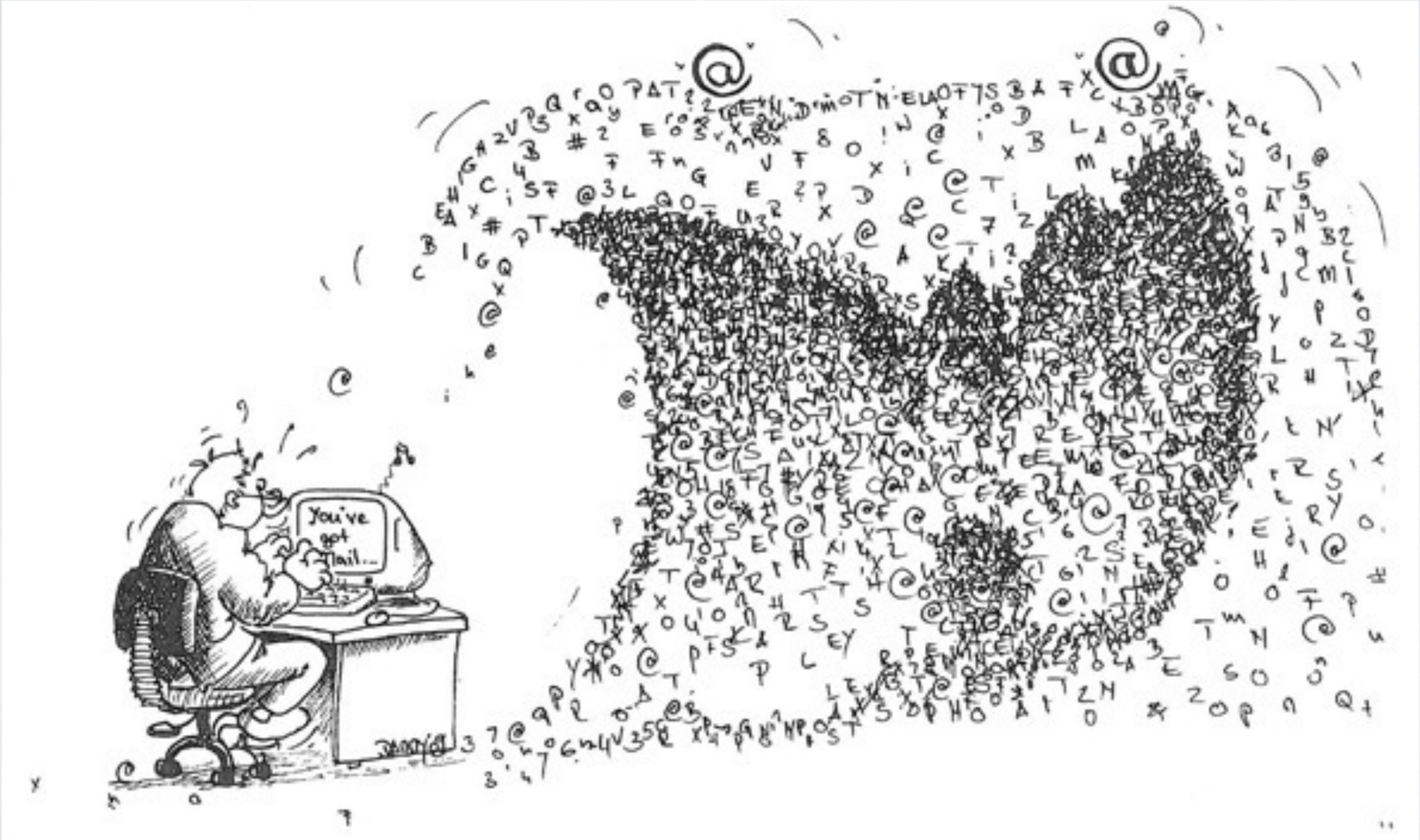
Save in data in its original form and DO NOT alter or 'improve' it

What makes this 'Open'?

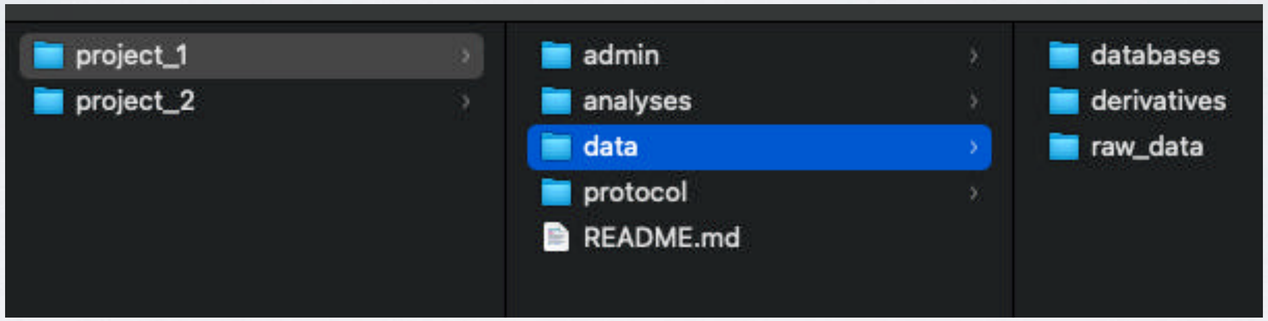
- Stable starting point
- Test reproducibility of pipeline
- Recover from mishaps
- Experiment without fear

Data Tsunami



2. Create a Central Hub

Directory Structures: organization of files into a hierarchical structure



- Create a directory for each project
- Use a consistent structure
- Separate data management from project management

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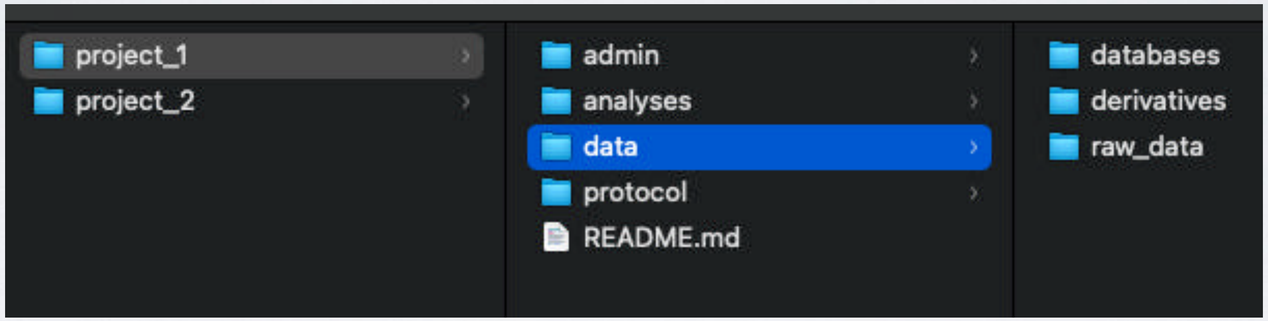


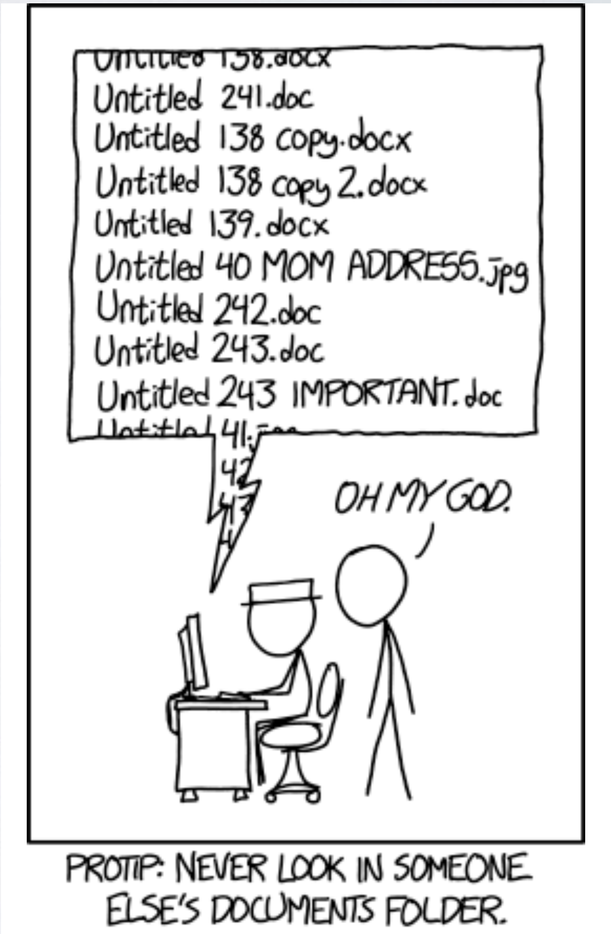
- Create a directory for each project
- Use a consistent structure
- Separate data management from project management

What makes this 'Open'?

- Easy to find data, code, protocol
- Consistent (at least within lab)
- Bigger Lift: match field standards (e.g. , BIDS, MIxS)

3. Use Meaningful Names

Leverage filenames to help you manage complex projects



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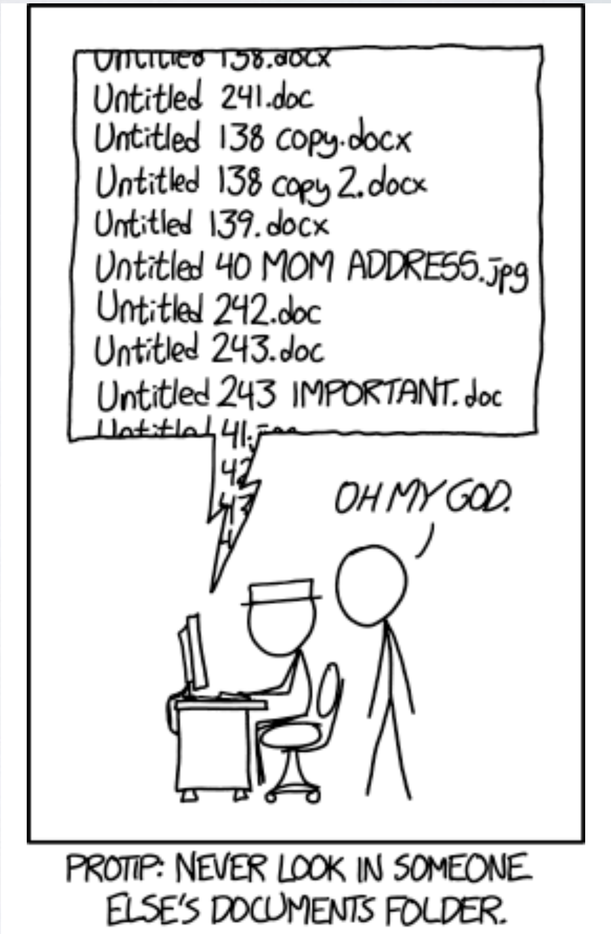
- Human Readable: names should clearly describe content in the simplest way possible (e.g., ‘code’, ‘data’)



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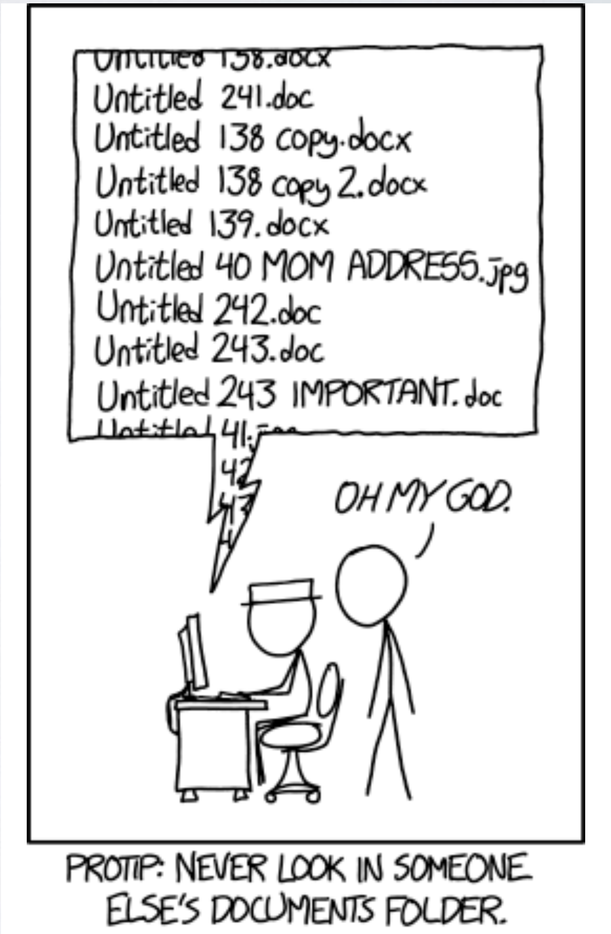
  - Use '-' or '_' in place of spaces
  - No special characters (e.g, '&', '#', '^', etc)



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- Sortable: help you find what you need in the future
  - Dates: YYYY-MM-DD
  - Pad with zeros (subject IDs, versions, etc)

```
fig_1.pdf
fig_10.pdf
fig_11.pdf
fig_12.pdf
fig_2.pdf
fig_3.pdf
fig_4.pdf
fig_5.pdf
fig_6.pdf
fig_7.pdf
fig_8.pdf
fig_9.pdf
```

→

```
fig_01.pdf
fig_02.pdf
fig_03.pdf
fig_04.pdf
fig_05.pdf
fig_06.pdf
fig_07.pdf
fig_08.pdf
fig_09.pdf
fig_10.pdf
fig_11.pdf
fig_12.pdf
```

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- Sortable: help you find what you need in the future
  - Dates: YYYY-MM-DD
  - Study IDs: Pad with zeros

What makes this 'Open'?

- Makes data more findable
- Can be a form of metadata
- Bigger Lift: adopt field standards

4. Preserve the Journey

Version control: tracking and managing changes to documents or code

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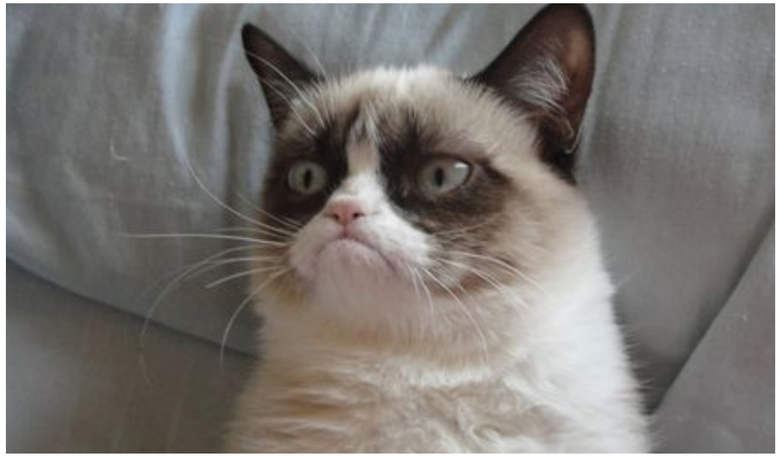

99 little bugs in the code
99 little bugs
Take one down and compile it
117 little bugs in the code...

- Manual: use file naming to document drafts (e.g., dates, version numbers)
- Software: git, GitHub, subversion
- Allows you to trace your steps

4. Preserve the Journey

Version control: tracking and managing changes to documents or code

What makes this 'Open'?

- Documents project and data history
- Can reproduce process if needed
- Bigger Lift: use a version control software (e.g., git)

- Manual: use file naming to document drafts (e.g., dates, version numbers)
- Software: git, GitHub, subversion
- Allows you to trace your steps

5. Avoid Manual Manipulations

- Manual data manipulations leave no trace
  - Hard to reproduce
  - Error prone

- Alternatives:
  - Save Syntax in SPSS
  - Include calculations in variable descriptions
  - Script data cleaning

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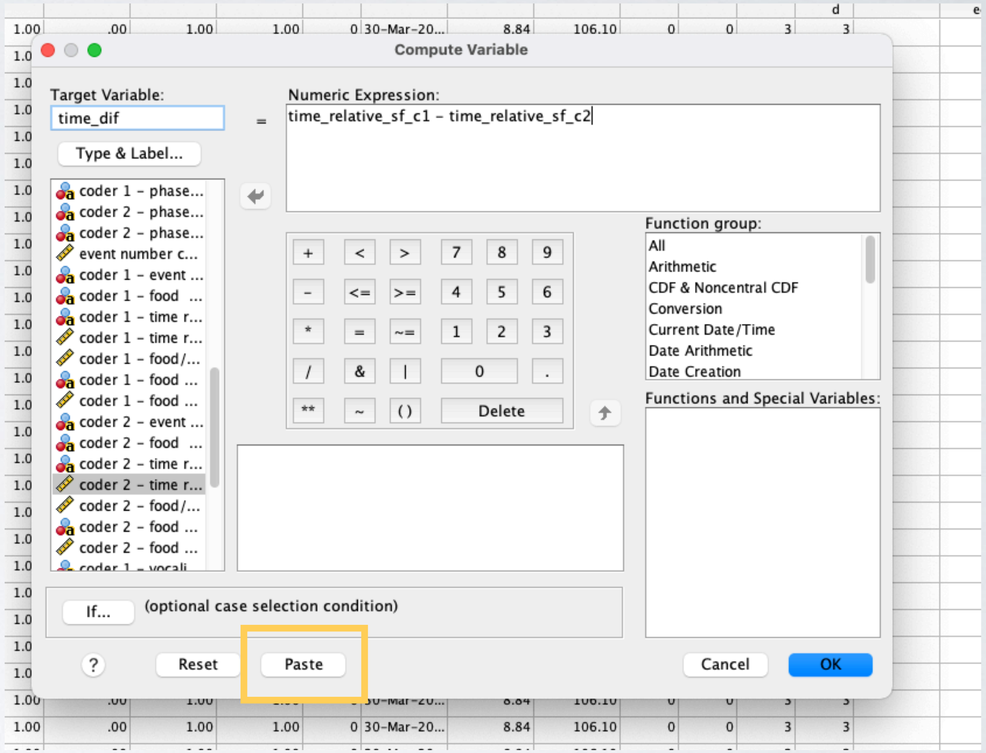

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- Alternatives:
  - Save Syntax in SPSS
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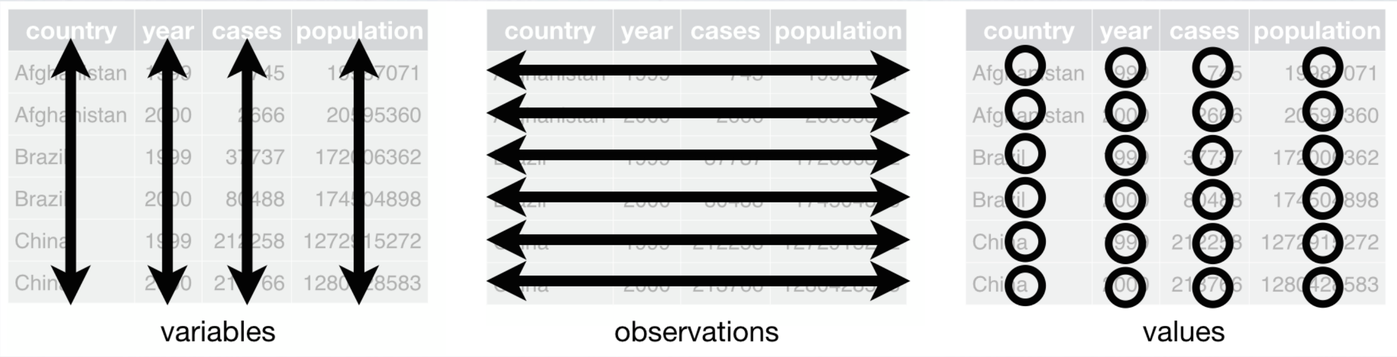
  - Script data cleaning

What makes this 'Open'?

- Data processing will be reproducible
- Can reverse to original data if needed
- Bigger Lift: move away from GUI-based analysis software to open code/syntax based programs (e.g., R, python)

6. ‘Tidy’ Your Data



- Every variable is in its own column
- Each participant/sample is in its own row
- Each value is in its own cell

6. ‘Tidy’ Your Data

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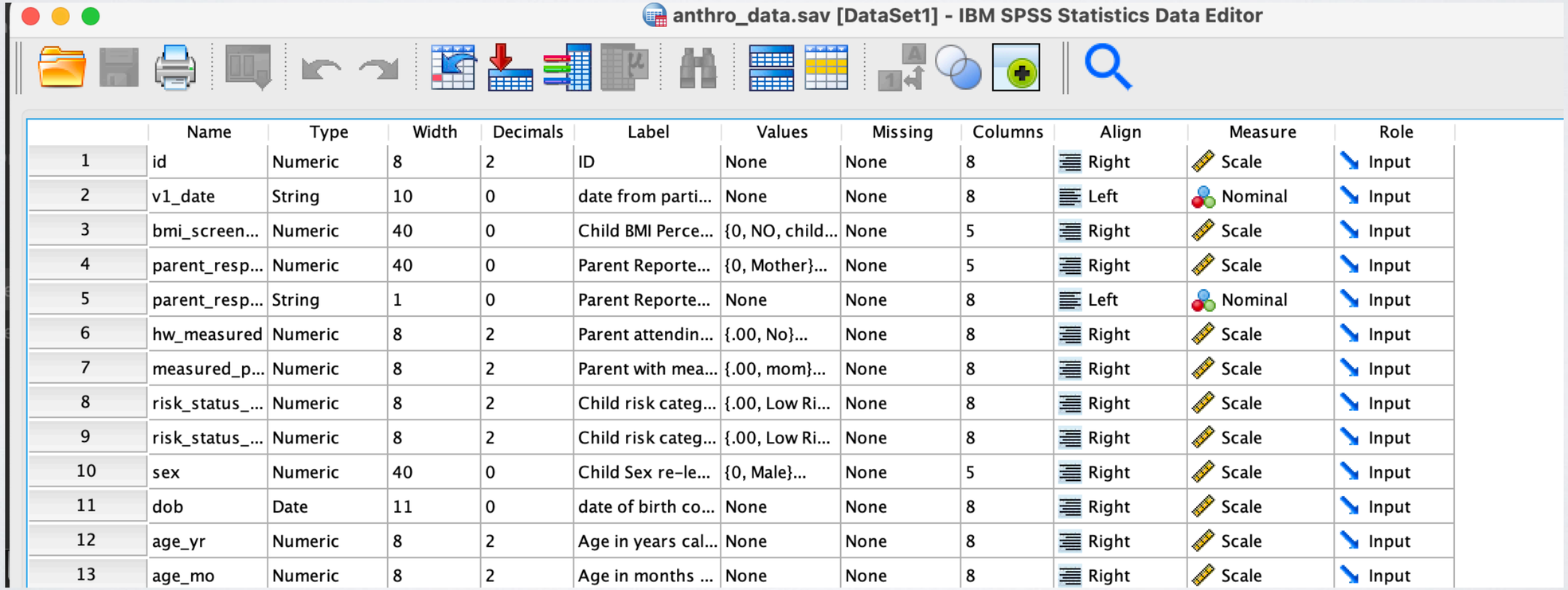

	Name	Type	Width	Decimals	Label	Values	Missing	Columns	Align	Measure	Role
1	id	Numeric	8	2	ID	None	None	8	Right	Scale	Input
2	v1_date	String	10	0	date from parti...	None	None	8	Left	Nominal	Input
3	bmi_screen...	Numeric	40	0	Child BMI Perce...	{0, NO, child...	None	5	Right	Scale	Input
4	parent_resp...	Numeric	40	0	Parent Reporte...	{0, Mother}...	None	5	Right	Scale	Input
5	parent_resp...	String	1	0	Parent Reporte...	None	None	8	Left	Nominal	Input
6	hw_measured	Numeric	8	2	Parent attendin...	{.00, No}...	None	8	Right	Scale	Input
7	measured_p...	Numeric	8	2	Parent with mea...	{.00, mom}...	None	8	Right	Scale	Input
8	risk_status_...	Numeric	8	2	Child risk categ...	{.00, Low Ri...	None	8	Right	Scale	Input
9	risk_status_...	Numeric	8	2	Child risk categ...	{.00, Low Ri...	None	8	Right	Scale	Input
10	sex	Numeric	40	0	Child Sex re-le...	{0, Male}...	None	5	Right	Scale	Input
11	dob	Date	11	0	date of birth co...	None	None	8	Right	Scale	Input
12	age_yr	Numeric	8	2	Age in years cal...	None	None	8	Right	Scale	Input
13	age_mo	Numeric	8	2	Age in months ...	None	None	8	Right	Scale	Input

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column	variable	label	value_labels	type	n_na	range
1	id	ID	NULL	double	0	c(1, 133)
2	v1_date	date from participant contacts databases ('verified_visit_da	NULL	character	0	c("2018-01-31", "2022-05-07")
3	bmi_screenout	Child BMI Percentile Screen Out	c(`YES, child is overweight, sc	double	0	c(0, 1)
4	parent_respondent	Parent Reported: Parent relationship to child re-leveled in R	c(Mother = 0, Father = 1, Oth	double	0	c(0, 1)
5	parent_respondent_o	Parent Reported: Parent specify relationship to child if other	NULL	character	0	c("", "")
6	hw_measured	Parent attending Visit 1 had measured height and weight	c(No = 0, Yes = 1)	double	0	c(1, 1)
7	measured_parent	Parent with measured BMI at Visit 1	c(mom = 0, dad = 1)	double	0	c(0, 1)
8	risk_status_mom	Child risk categor: Low risk: Mom BMI < 26, High Risk: Mom	c(`Low Risk` = 0, `High Risk` =	double	0	c(0, 1)
9	risk_status_both	Child risk category: Low Risk: Mom and Dad BMI < 25, High	c(`Low Risk` = 0, `High Risk` =	double	0	c(0, 2)
10	sex	Child Sex re-leveled in R to start with 0	c(Male = 0, Female = 1)	double	0	c(0, 1)
11	dob	date of birth converted to format yyyy-mm-dd in R	NULL	double	0	c(14333, 16391)
12	age_yr	Age in years calculated from dob and start_date	NULL	double	0	c(7, 8.99)
13	age_mo	Age in months calculated from dob and start_date	NULL	double	0	c(84, 107.9)
14	ethnicity	Parent Reported: Child ethnicity	c(`NOT Hispanic or Latino` = 0	double	0	c(0, 0)
15	race	Parent Reported: Child race -- Note: prefer not to answer (p	c(`White/Caucasian` = 0, `Am	double	0	c(0, 2)
16	income	Parent Reported: Yearly household income -- Note: prefer n	c(`Less than $20,000` = 0, `$2	double	3	c(0, 5)
17	parent_ed	Parent Reported: Parent education re-leveled in R to start w	c(`High School or GED (12 yea	double	0	c(0, 5)

6. 'Tidy' Your Data

- Use open file formats — csv, html, txt, jpeg
- Create a data dictionary
- One piece of information per cell

height
5 ft 6 in
5 ft 2 in
7 ft
5 ft 11 in

→

height_ft	height_in
5	6
5	2
7	0
5	11

6. 'Tidy' Your Data

- Use open file formats — csv, html, txt, jpeg
- Create a data dictionary
- One piece of information per cell
- Do not use highlighting/font color as data

height
5 ft 6 in
5 ft 2 in
7 ft
5 ft 11 in

→

height_ft	height_in	check_height
5	6	0
5	2	0
7	0	1
5	11	0

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What makes this 'Open'?

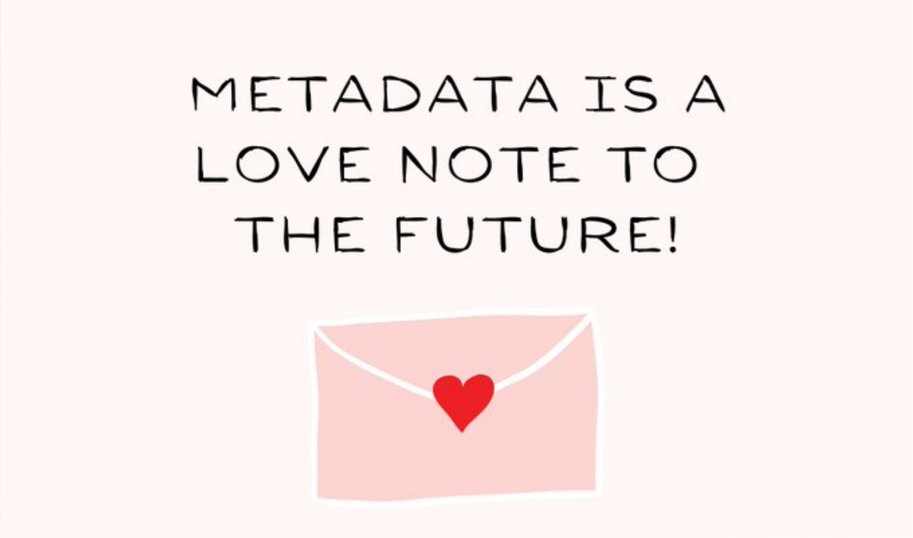
- Open formats are accessible
- All data are computer readable
- Data are documented
- Makes data re-use and sharing easier

7. Metadata Magic

Metadata: the who, what, when, where, and why of your data

What makes this 'Open'?

- Makes data more findable
- Helps others (and future you) understand the data
- Shared vocabularies help to harmonize data within a field



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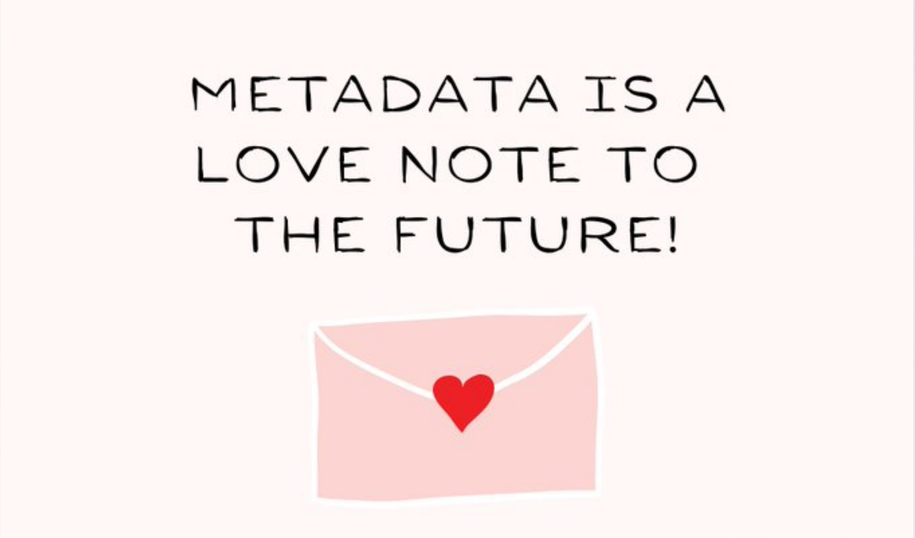
Easiest: when in doubt, document

- Data dictionaries
- Standard operating procedures manuals
- Lab notebooks
- changelog file (document versions)
- README
  - Description of folders/files
  - Can provide instructions on use of code/ data
  - License information



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- README

data/

data/raw

This folder would contain data raw data used as input for code in R/ but it will not be shared, as some datasets contain potentially identifiable information. Datasets in this folder have been copied into data/raw_deidentified with potentially identifiable information (visit 1 date, date of birth, race, ethnicity) removed.

data/raw_deidentified

This folder contains raw but de-identified datasets to use as input for code in R/. Using this data will require updating import paths in setup_data.R Files starting with dict- contain metadata for the following datasets:

- anthro_data.csv: contains anthropometric data
- demographics_data.csv: contains demographic data
- intake_data.csv: contains data from the four portion size meals
- visit6_data.csv: contains data related to the MRI visit (e.g., pre-mri fullness and anxiety; not fMRI or food-cue task data)
- FoodAndBrainR01DataP-Scansroar.csv: contains data that indicates whether each fMRI run was initiated

BIDS/code

This folder contains code to (1) process in-scanner wanting data and (2) process and analyze fMRI data

Example from Dr. Bari Fuchs

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Medium Effort: Data Manual

- Larger
- More verbose and detailed
- Can include science/rational/citations
- Like a user manual for data

7. Metadata Magic

Metadata: the who, what, when, where, and why of your data

Bigger Lift: Structured Metadata

- Often laid out in fields
- Can require use of shared vocabularies

```
"age": {
    "Description": "age of the participant",
    "Units": "years"
},
"sex": {
    "Description": "sex of the participant as reported by the participant",
    "Levels": {
        "M": "male",
        "F": "female"
    }
},
"handedness": {
    "Description": "handedness of the participant as reported by the
        participant",
    "Levels": {
        "left": "left",
        "right": "right"
    }
},
```

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- Often laid out in fields
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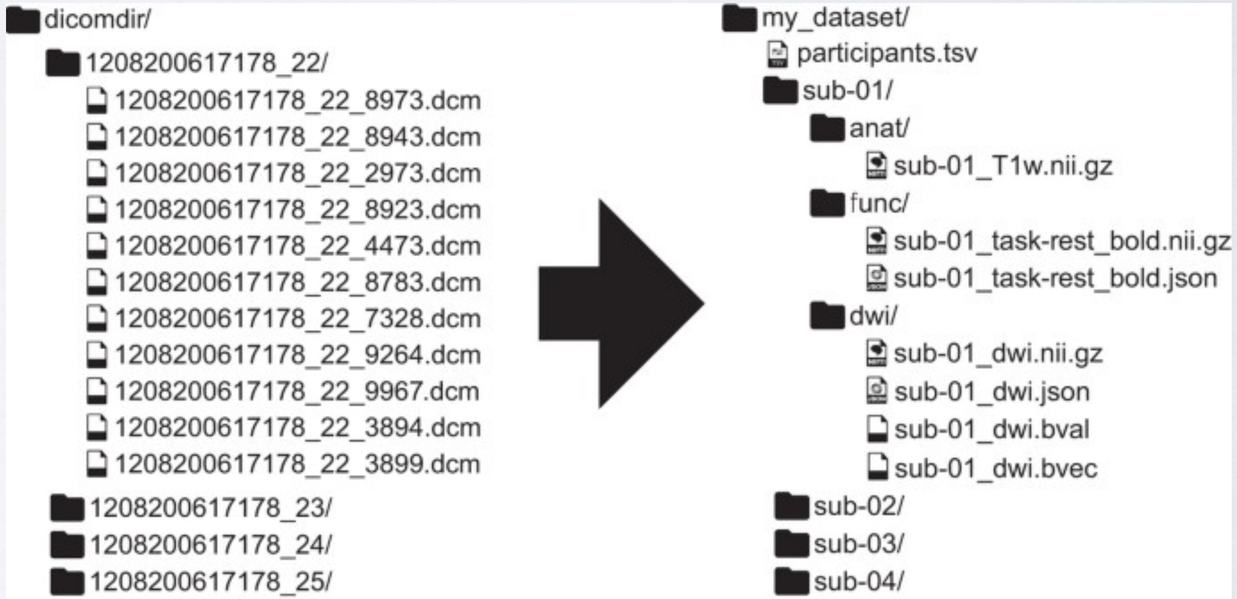
- Data standard: Often field/data type specific

Brain Imaging Data Standard (BIDS)



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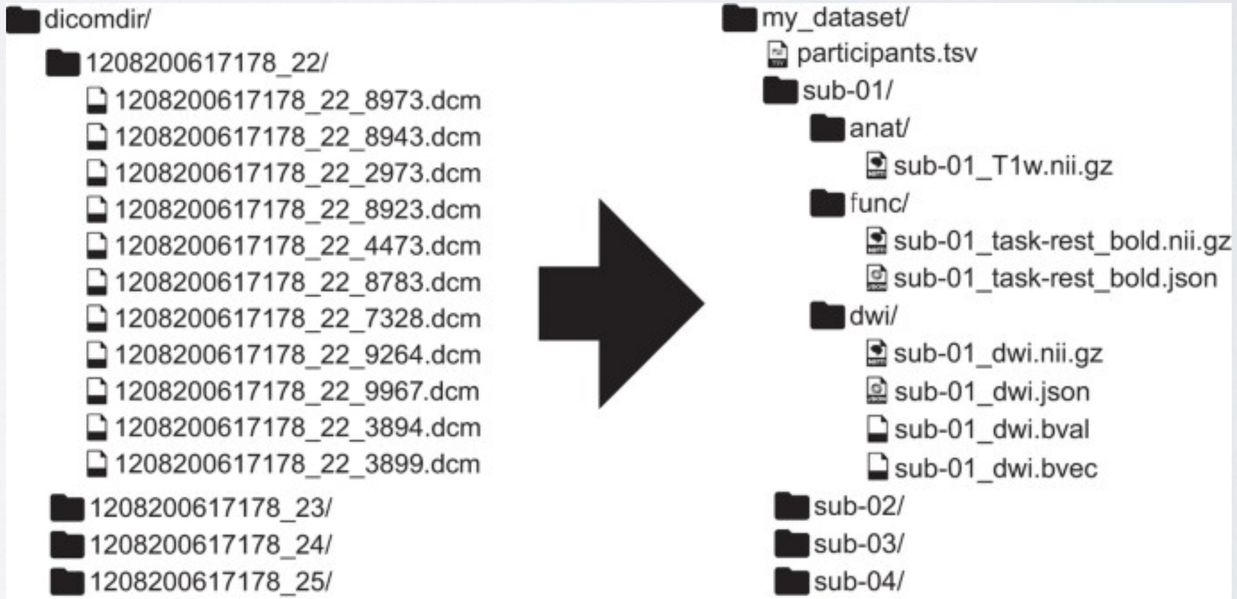
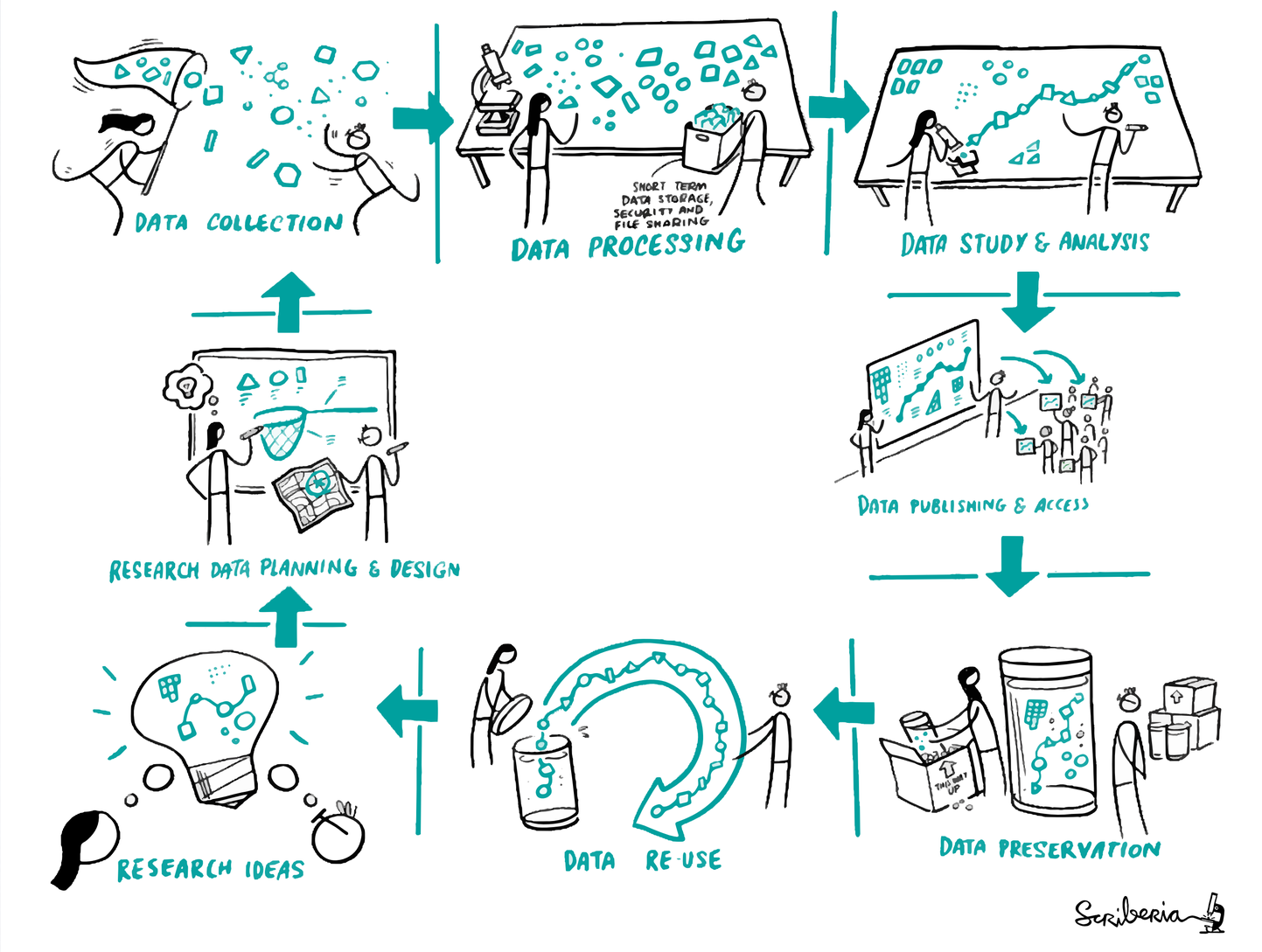


‘Good Enough’ Practices

1. Preserve Raw Data
2. Create a Central Hub
3. Use Meaningful Names
4. Preserve the Journey
5. Avoid Manual Manipulations
6. ‘Tidy’ Your Data
7. Metadata Magic

Workshop - File and Directory Organization

Project Lifecycle



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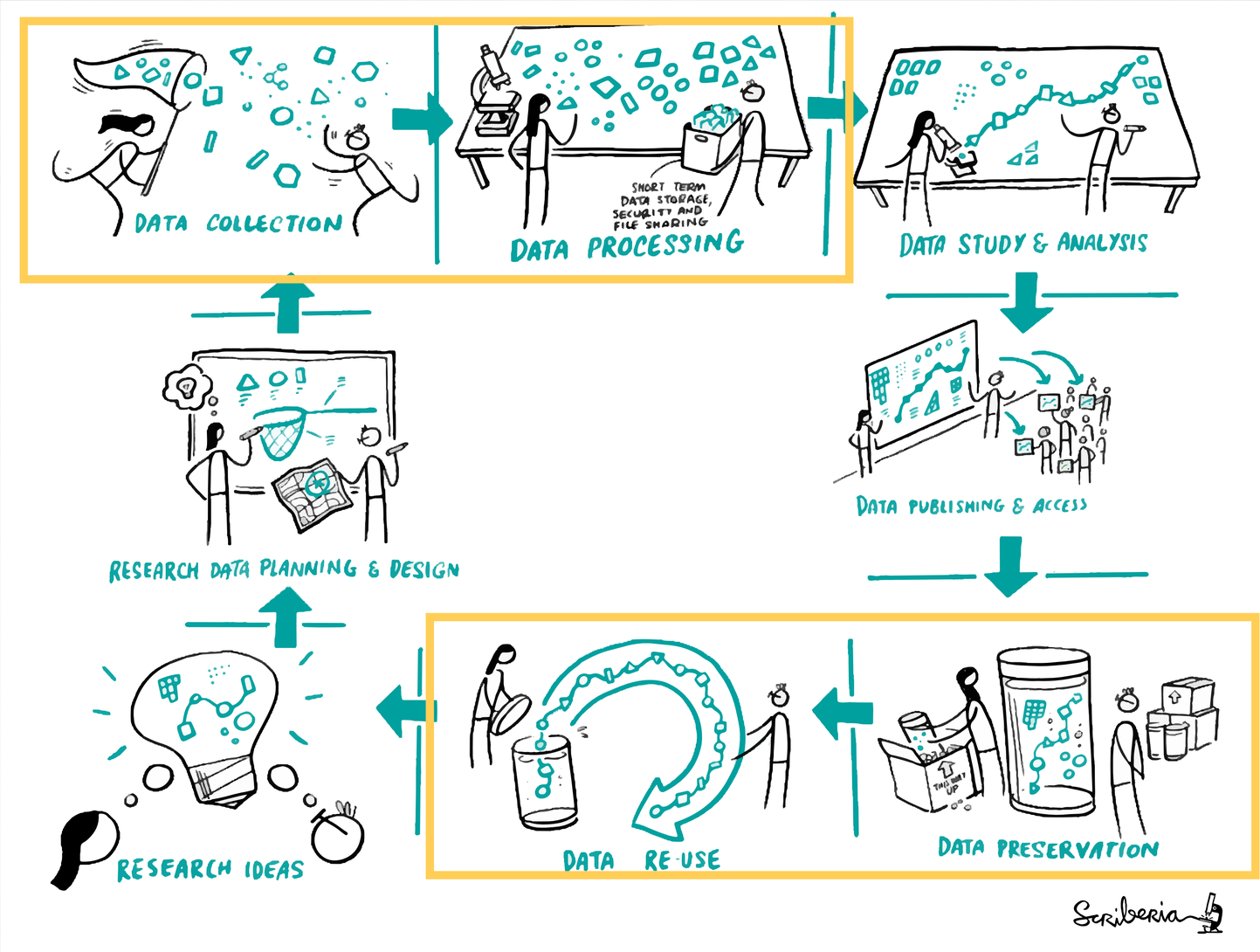

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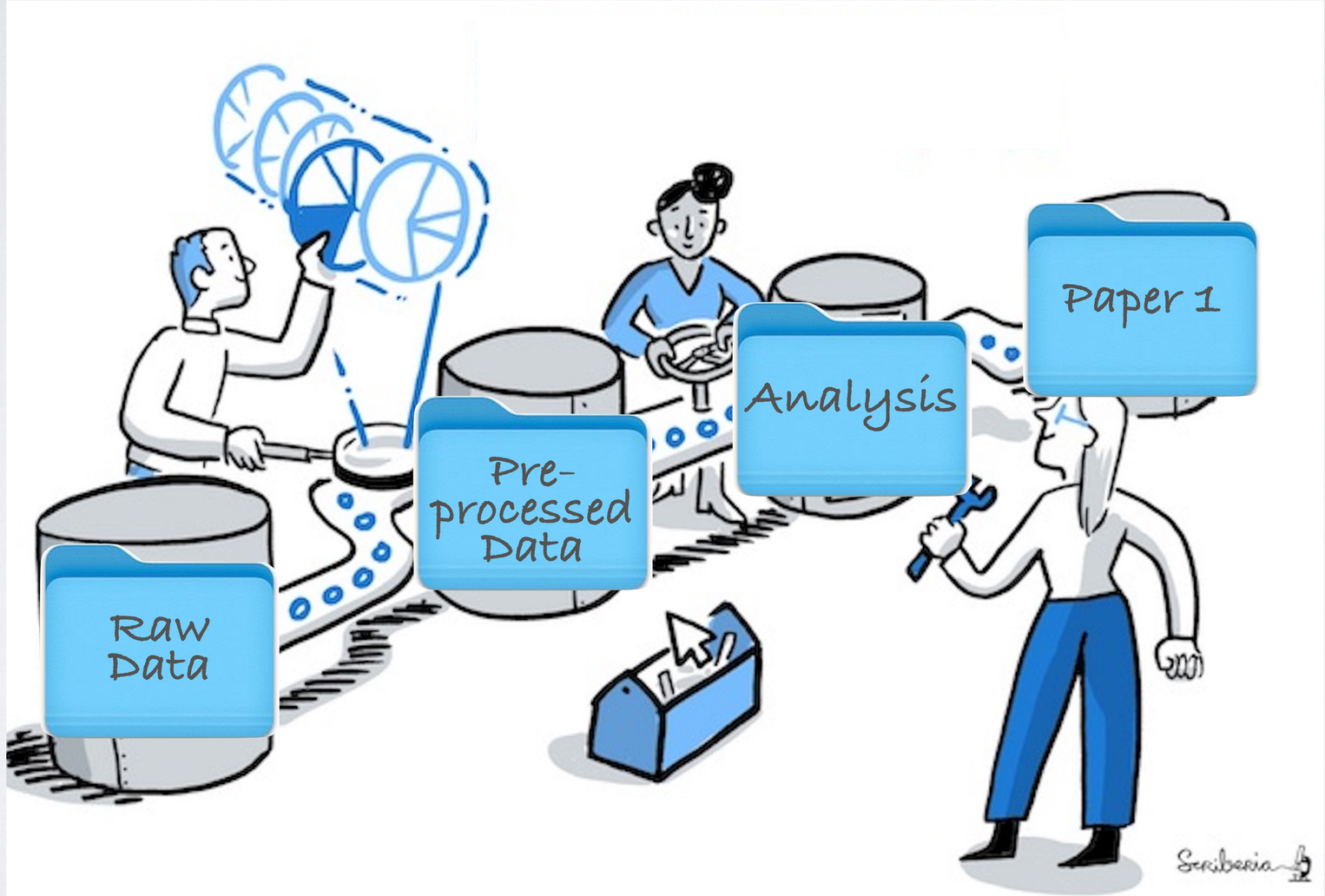

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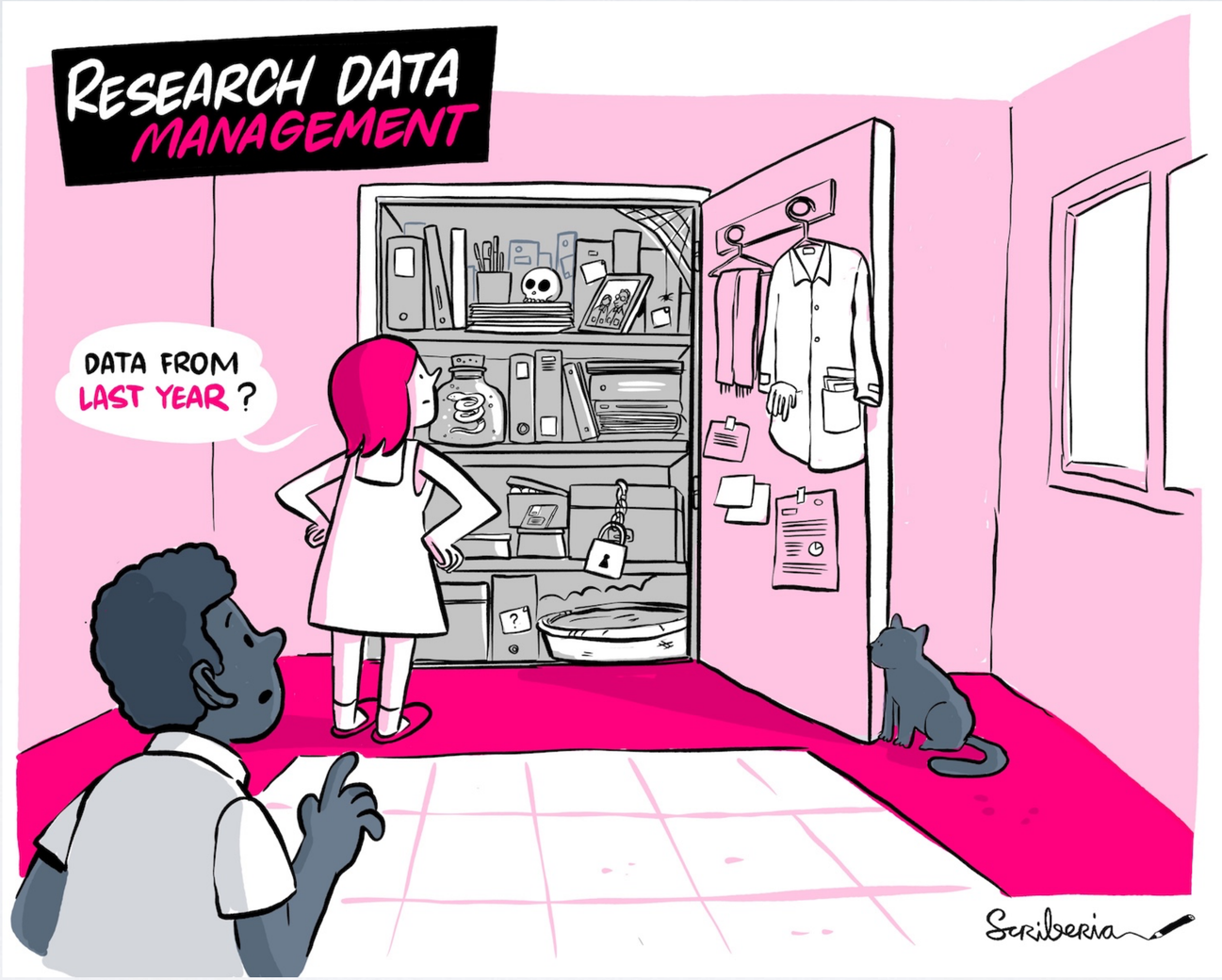

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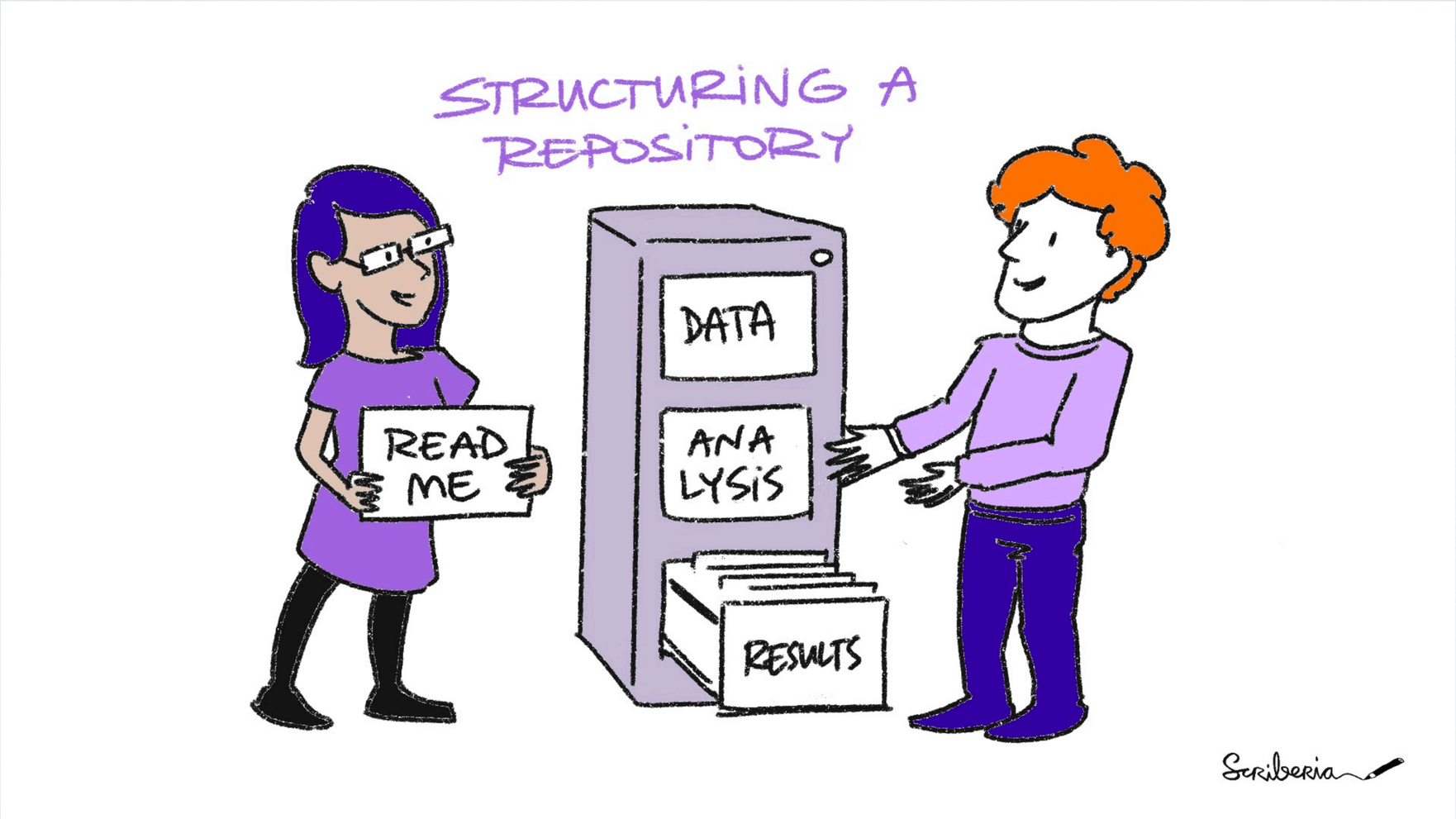
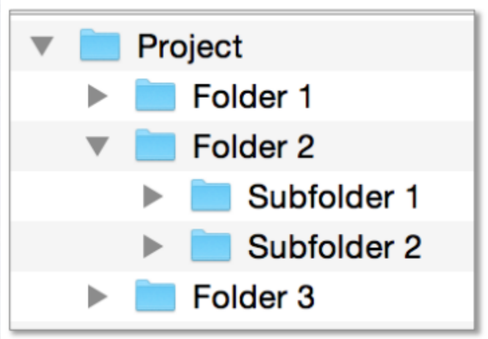
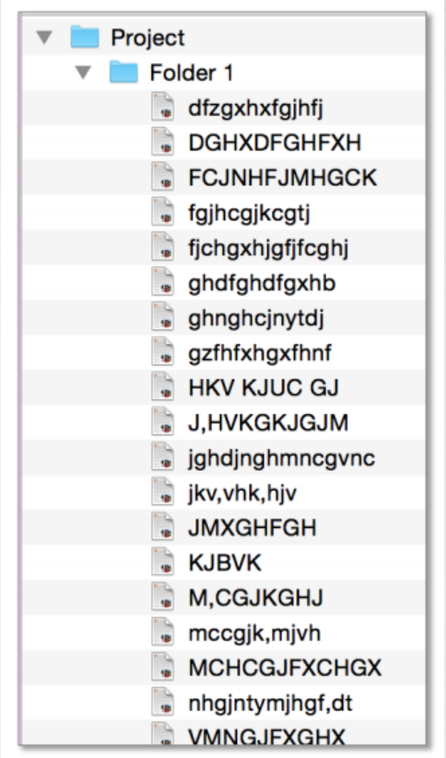


Create a Central Hub

Directory Structure - General Best Practices

- Structure logically based on project
- Keep subfolder categories narrow to limit number of files in each one
- Define abbreviations in README
- Follow file naming best practices

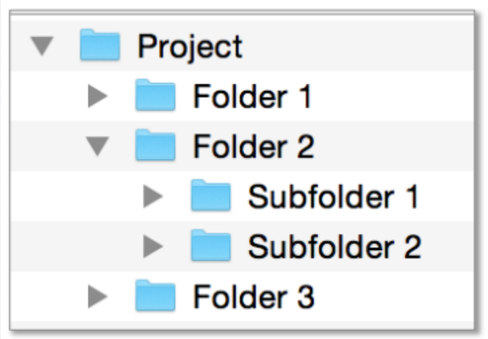


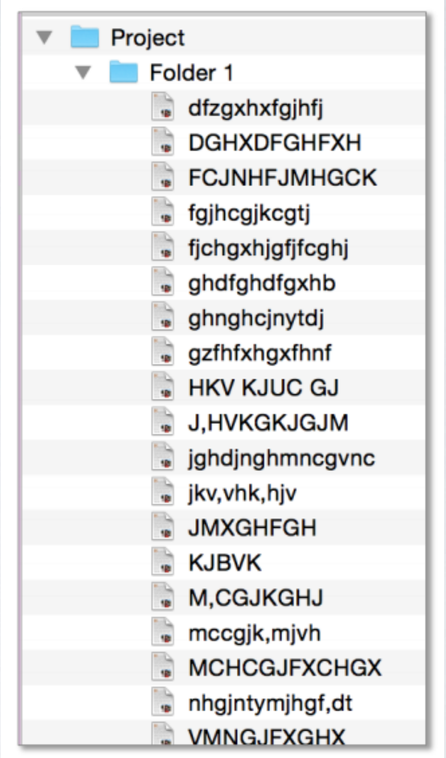


Create a Central Hub

Directory Structure - General Best Practices

- Structure logically based on project
- Keep subfolder categories narrow to limit number of files in each one
- Define abbreviations in README
- **Follow file naming best practices**





Use Meaningful Names

Goals:

- Identify file/contents in a clear way
- Have a consistent approach across projects and collaborators
- Should be meaningful but brief

Use Meaningful Names

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- Identify file/contents in a clear way
- Have a consistent approach across projects and collaborators
- Should be meaningful but brief

- Human Readable: names should clearly describe content in the simplest way possible (e.g., 'code', 'data')
- Computer Readable: ability of a computer to parse a name

Use Meaningful Names

Do **NOT** Use

- Spaces
- Periods (except for file extensions)
- Other special characters (&, *, ^, etc)

DO Use

- CamelCase
- snake_case (i.e., with underscores)
- Consistent date format - YYYYMMDD recommended
- Pad with zeros when using numbers (e.g., 001)

Example: Brain Imaging Data Structure

key1 - value1 _ key2 - value2 _ suffix .extension

- Suffixes are preceded by an underscore
- Entities are composed of key-value pairs separated by underscores
- There is a limited set of suffixes for each data type (anat, func, eeg, ...)
- For a given suffix, some entities are **required** and some others are **[optional]**.
- Keys, value and suffixes can only contain letters and/or numbers.
- Entity key-value pairs have a specific order in which they must appear in filename.
- Some entities key-value can only be used for derivative data.

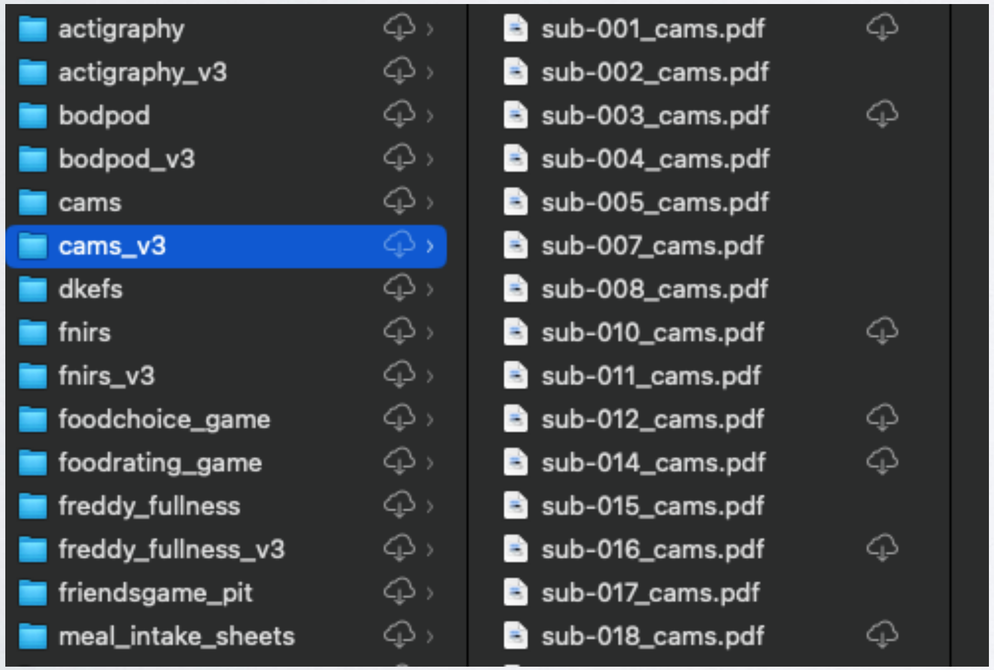
sub-035_task-flanker_events.txt
sub-035_ses-2_task-flanker_events.txt

https://bids-standard.github.io/bids-starter-kit/folders_and_files/files.html

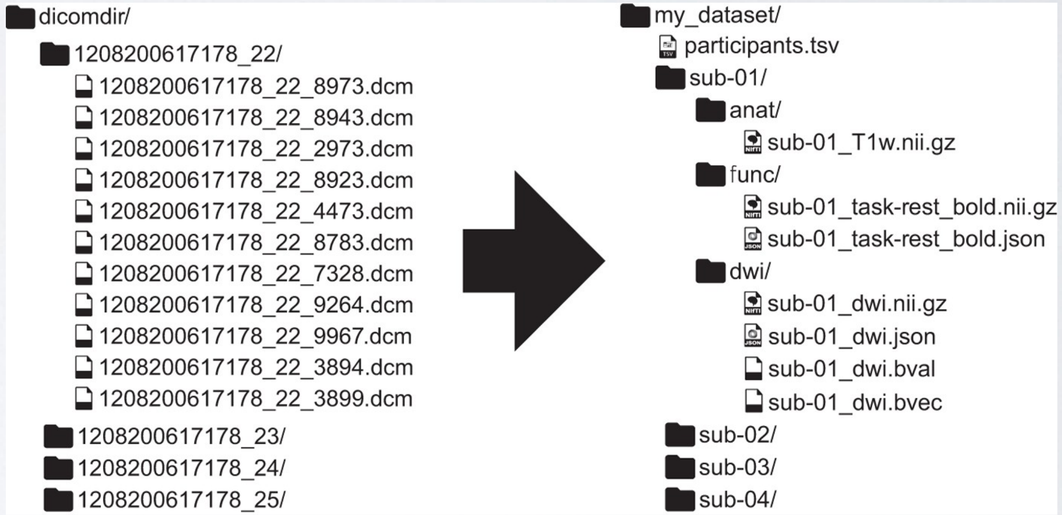
Tricky Choices

Organize by data type vs sample/participant?

raw_untouched directory



Brain Imaging Data Structure



Tricky Choices

How to handle raw data in mixed structures?

- Raw data with files for each observation/participant

AND

- Raw data exported with multiple observations in a single file

Key Considerations

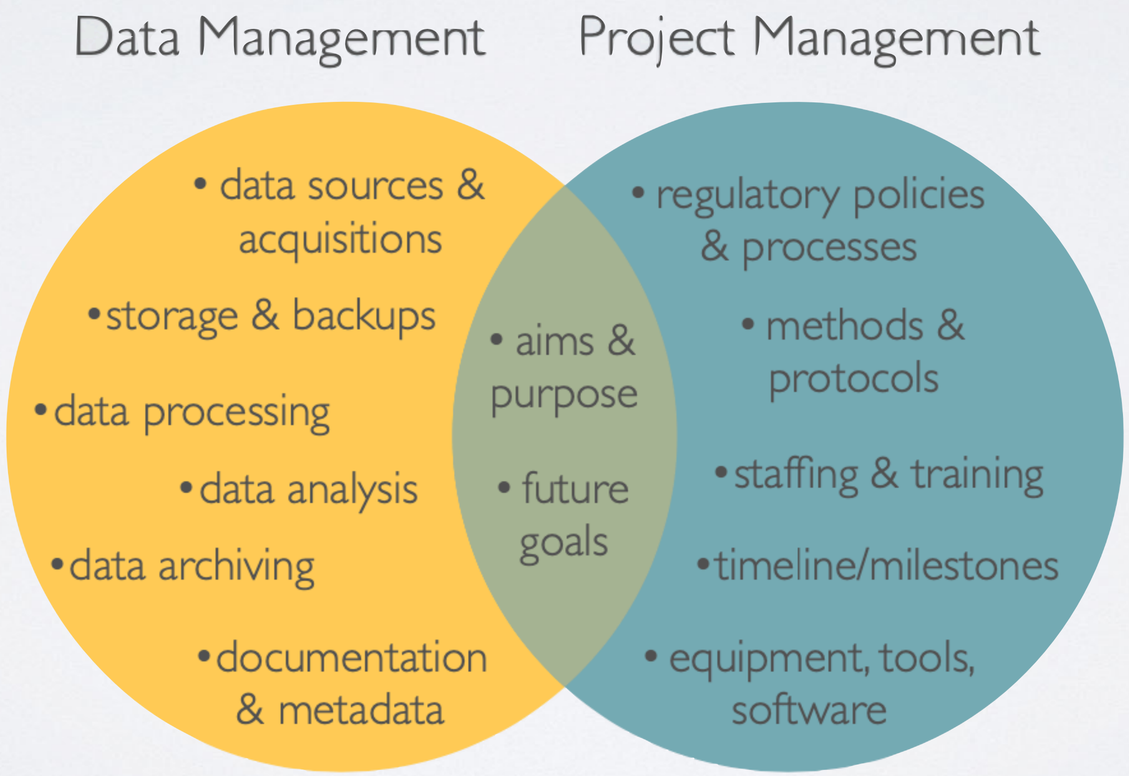
1. Preserve Raw Data

Raw Data: data as it was originally collected

Save in data in its original form and DO NOT alter or 'improve' it

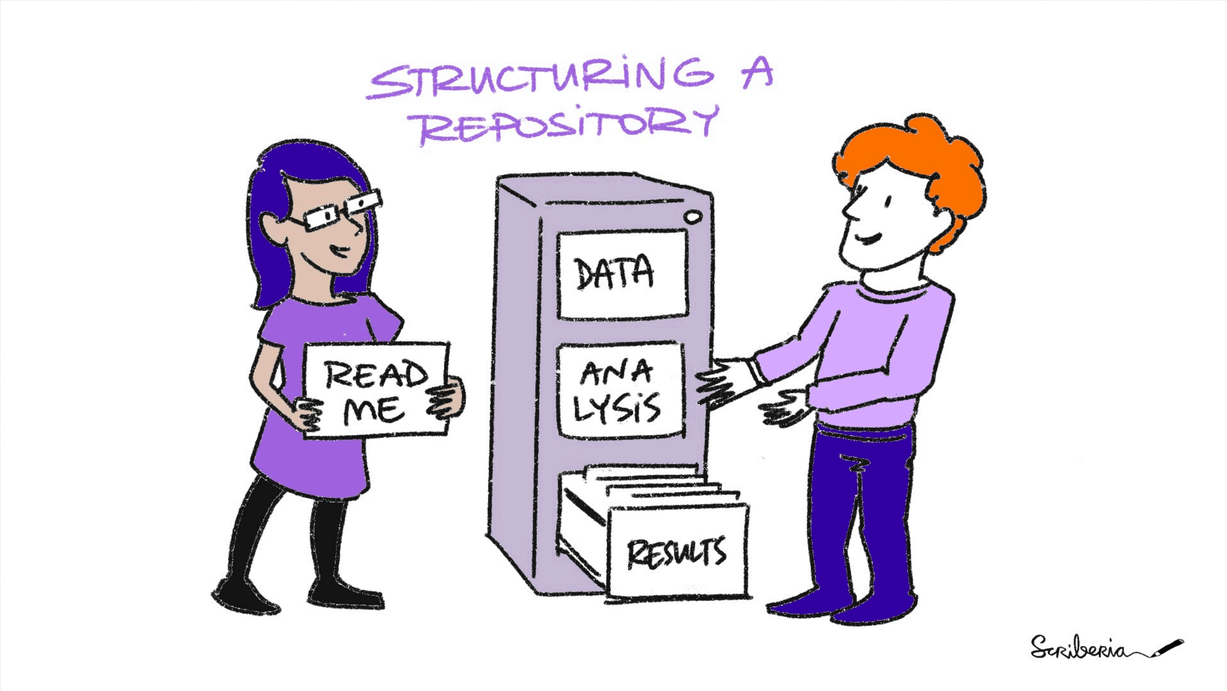
Key Considerations

1. Preserve Raw Data
2. Separate Project and Data Management



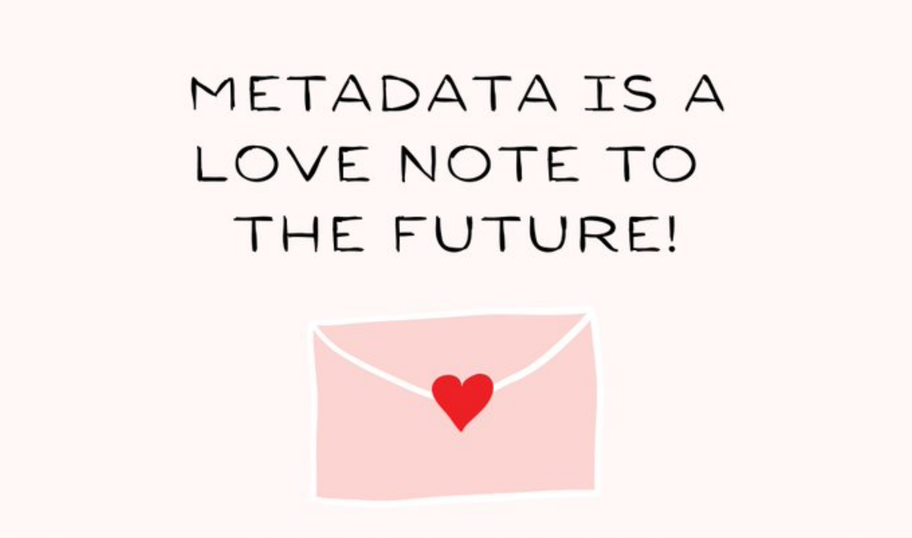
Key Considerations

1. Preserve Raw Data
2. Separate Project and Data Management
3. Skeleton Consistent Across Projects



Key Considerations

1. Preserve Raw Data
2. Separate Project and Data Management
3. Skeleton Consistent Across Projects
4. Metadata - the who, what, when, where, and why of your data



Project

Study Overview: A multidisciplinary team is conducting a laboratory based study to examine environmental, cognitive, and biological drivers of pediatric obesity.

Key Protocol/Data Elements:

- Parent-report surveys via REDCap - home food environment, feeding practices, child traits and behaviors
- In-Lab Test Meal - measure children's intake of a controlled lab meal
- Anthropometrics - height and weight, BodPod
- Reward Processing - child PIT task call the Friends Game
- Urinary Metabolites - first void urine samples processed by the Metabolmics Core

Goals (10-15 min)**:**

- Design a directory structure based on files for 10 participants
- Determine a file naming convention that will work for all files

https://bit.ly/4iLWdTk