Introduction to Data Management Practices course

NBIS DM Team

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Data Organization practices

https://nbisweden.github.io/module-organising-data-dm-practices/

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Objectives

- What to consider for maintaining data organization strategies in a project
- What to consider when settling for a file structure
- Understanding good practices for data storage, processing and documentation (**FAIR-ification**)

Credit: This image was created by Scriberia for The Turing Way community and is used under a CC-BY licence.

Welcome to Science!

Real Life scenario…

Image: SciLifeLab for Press and Media: https://www.scilifelab.se/contact/for-press-and-media

You have been recruited to the “Famous lab”!

Your research project is a continuation of previous work by PhD, Wang Fang (王芳).

You inherit a zipped folder, and a digital copy of the lab notes.

The road to success is open!

Welcome to Science!

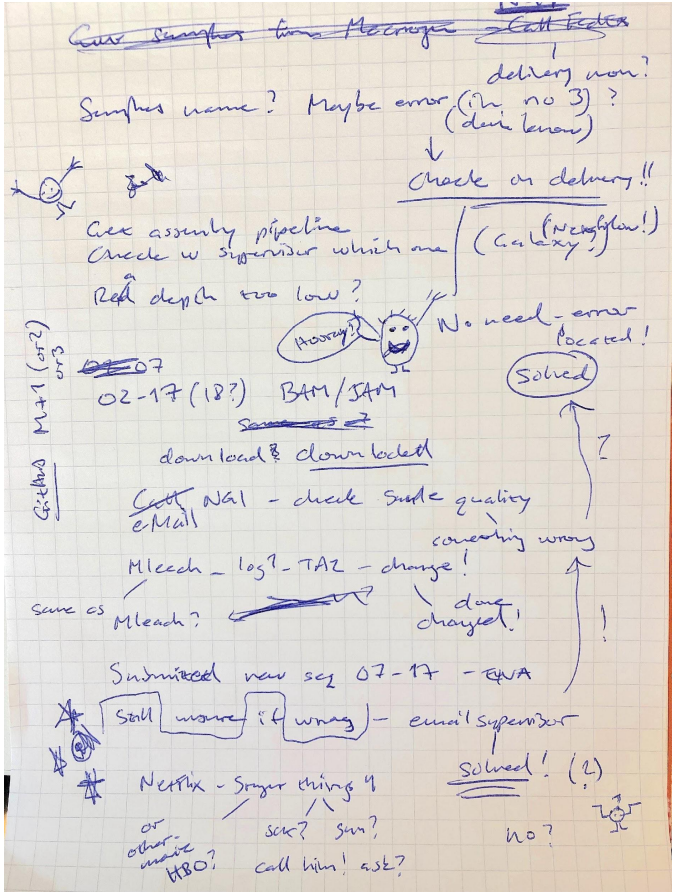
… And this is what you get…

Exercise 1

Can you list at least five major issues with the lab documentation in the image?

Exercise 2

What kind of general questions does the information raise about the work done in the lab?



Importance of good records

Why do we need to keep good quality records?

Ensures data, analysis and results to be **transparent, reproducible** and **traceable**

Prevents future issues due to **data mistakes**. In cumulative science mistakes can result in cascade effects

Reduces the risk of **data manipulation** and **research fraud**

Promotes **open science** and safeguards integrity of science itself

FAIR

Adopting good practices for data organization, makes research data more **FAIR**

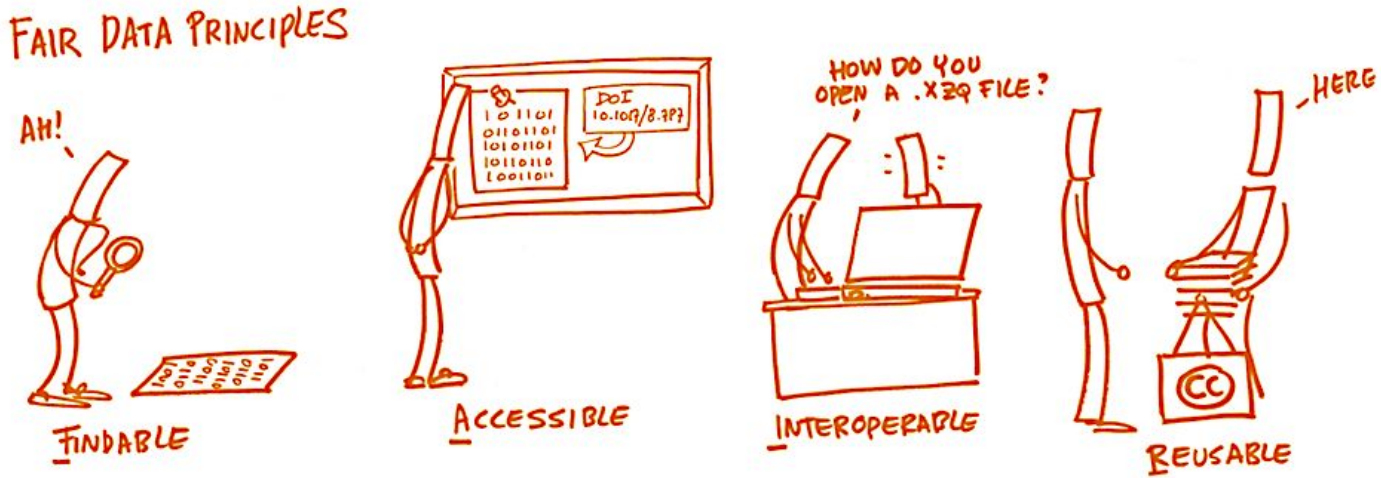
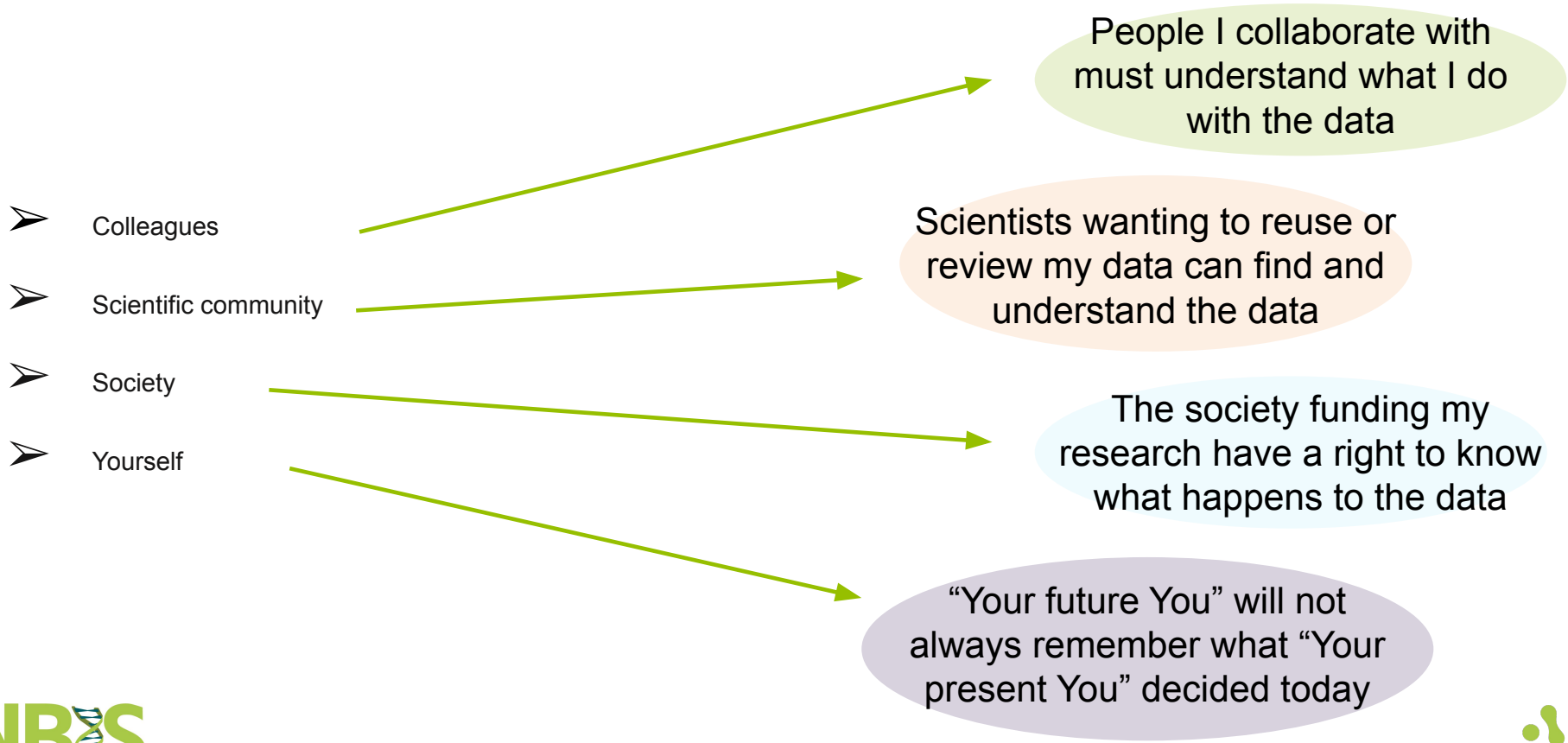


Image: https://book.fosteropenscience.eu/

Data Recipients



Principles for good records

Protocols and lab notes should both be…

- **Detailed**
- **Up-to-date**
- **Accurate**
- **Easy to understand**

Contents in **protocols** can include

- Name, affiliation and contact information
- Originator of protocol (if not you)
- Information on ***why*** and ***how experiment*** was done
- Health and safety advice (and technical advice)
- Required software, materials and instruments
- Being self-explanatory
- Describe mistakes (for others to avoid repeating)
- Reference ethical application (if applicable)

Contents in **lab notes** can include

- Name and affiliation
- Details on ***what, when*** and ***how***
- What project the experiment is part of
- Lot and batch numbers for consumables
- Information on ***metadata**** collected
- Interpretation of outcome and outlook/plans
- Post-outcome treatment of data

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*The information needed to discover, use, and understand data

Exercise 3

Test yourself on record keeping statements

1. Analogues and digital records make information equally findable.
2. New information in digital records can be easily shared with other users.
3. Analogue records can be kept safe from any physical accidents.
4. All researchers in a shared lab should have access to the same platform for keeping records and taking notes.
5. Digital records should follow the same backup strategy as the data they describe.

Exercise 3

Test yourself on record keeping statements

1. Analogue and digital records makes information equally findable. (F)
2. New information in digital records can be easily shared with other users. (T)
3. Analogue records can be kept safe from any physical accidents. (F)
4. All researchers in a shared lab should have access to the same platform for keeping records and taking notes. (T)
5. Digital records should follow the same backup strategy as the data they describe. (T)

FAIR by README

A **README** file usually defined as the starting point of information about something

FAIRify your research by using **README files** as documentation files for:

Folder level → Explaining folder contents, naming, file history, organisation/structure etc

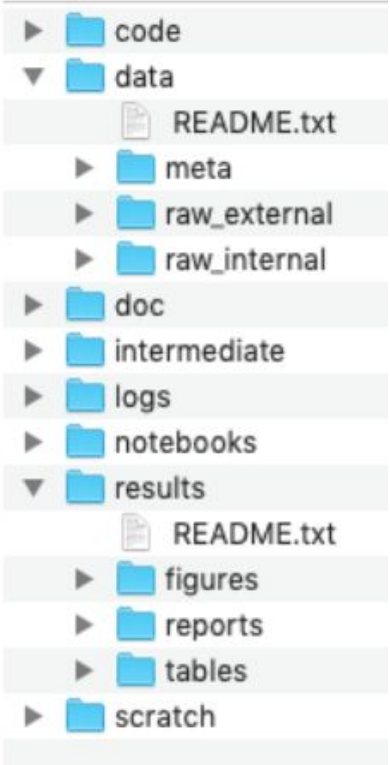
Data → Explaining file names and contents

README in Markdown (.md)

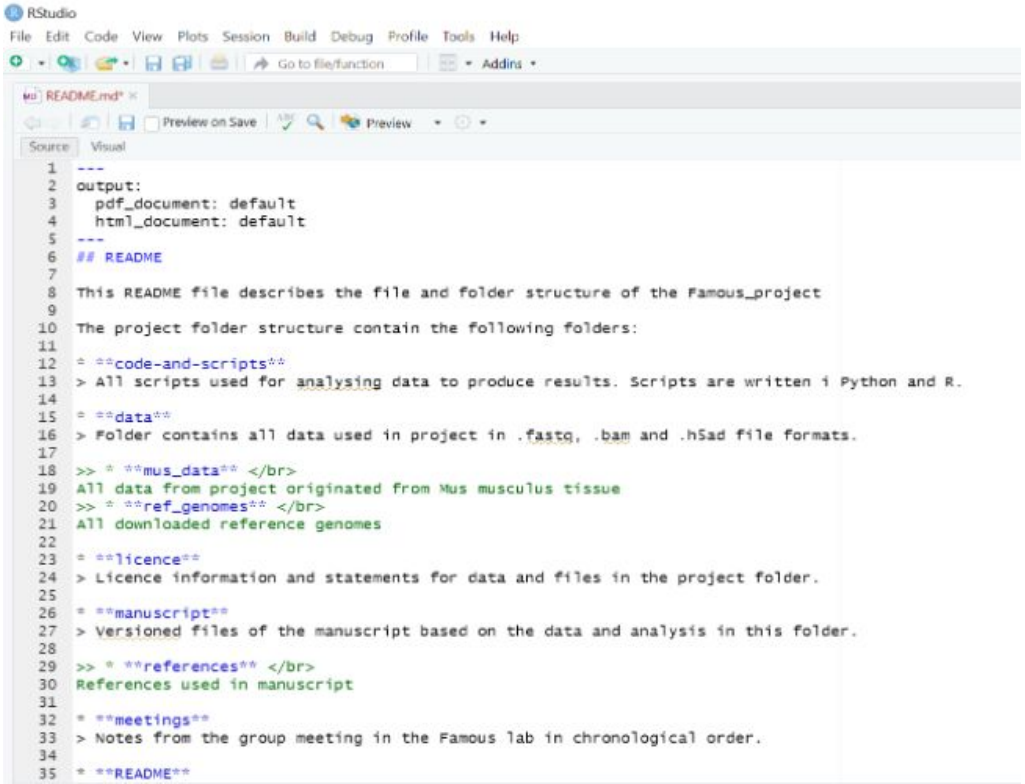
- Allows text and content formatting without interference
- Highly compatible with e.g. GitHub
- Allows inclusion of comments without having to visualize them
- Easily editable and versatile
- Does not require particular skills

README

README in Folder



README in Markdown.md



Exercise 4

Discussion

Consider an example where you would have benefited from having access to a README file when working with data.

Describe to your neighbor what you would have wanted such a file to contain.

Backup

Data and hardware failure is always a threat.

Plan early (have a backup strategy) for potential failure!

Good to know for **backup** planning purposes:

- ➔ Data sensitivity
- ➔ Ease of access
- ➔ File sizes
- ➔ Overall data volumes
- ➔ Data life cycle in project

Backup

Nearly all data, metadata and project information necessary to understand your analysis and results **require some sort of backup** strategy

Try to keep backup in **three separate copies,** on at least two different kinds of media (server, portable hard drive, cloud). Consider off-site backups

Never backup your data on **portable drives only**, and particularly not on USB sticks!

Robust backups need to be **automated**

Exercise 5

Discussion

Discuss in pairs the validity of the following statements on data backup:

1. I have my most important data backed up on my laptop. I have never experienced a hard drive failure, and my current laptop has a new state-of-the-art hard drive. Therefore, I don't need external backups.
2. All my data is stored in a cloud service.
3. My data is on a portable hard drive. There is a backup of the most important files on a shared USB stick in my research group.
4. My data is on a departmental backup administered by my University. Additionally, we have a server for all the data stored in our project.
5. We have no shared backup at all. All members in our research group are responsible for their own data.

Exercise 5

Discussion

Discuss in pairs the validity of the following statements on data backup:

1. Unsafe and not recommended. All hard drives can be subject to failure. In case of failure, all data will be lost.
2. Cloud services can be sufficient as backup, but are not fail safe. It can be sufficient in combination with a secondary backup on e.g. a shared server. For certain types of data (e.g. sensitive information), a cloud service may be outright inappropriate.
3. Not a good solution. Both portable hard drives as well as USB sticks are prone to failure.
4. A good solution in general. Data is stored independently in two separate systems. Centrally administered services are usually organised in such a way that partial failures does not affect the users.
5. Worst possible alternative. A disaster waiting to happen!

Backup

Creating a **backup strategy** in 10 steps

Find out whether **your institution** has a backup strategy

Determine **what** you want to back up

Decide **how many backups** you will need and **how frequently** to backup

Decide **where** backups will be **stored**

Determine **how much storage capacity** will be needed

Determine if there are tools you could use to **automate backup**

Determine **how long** backups **will be kept** and how they will be destroyed

Determine how **personal data** will be protected

Devise a disaster **recovery plan**

Assign **responsibilities**

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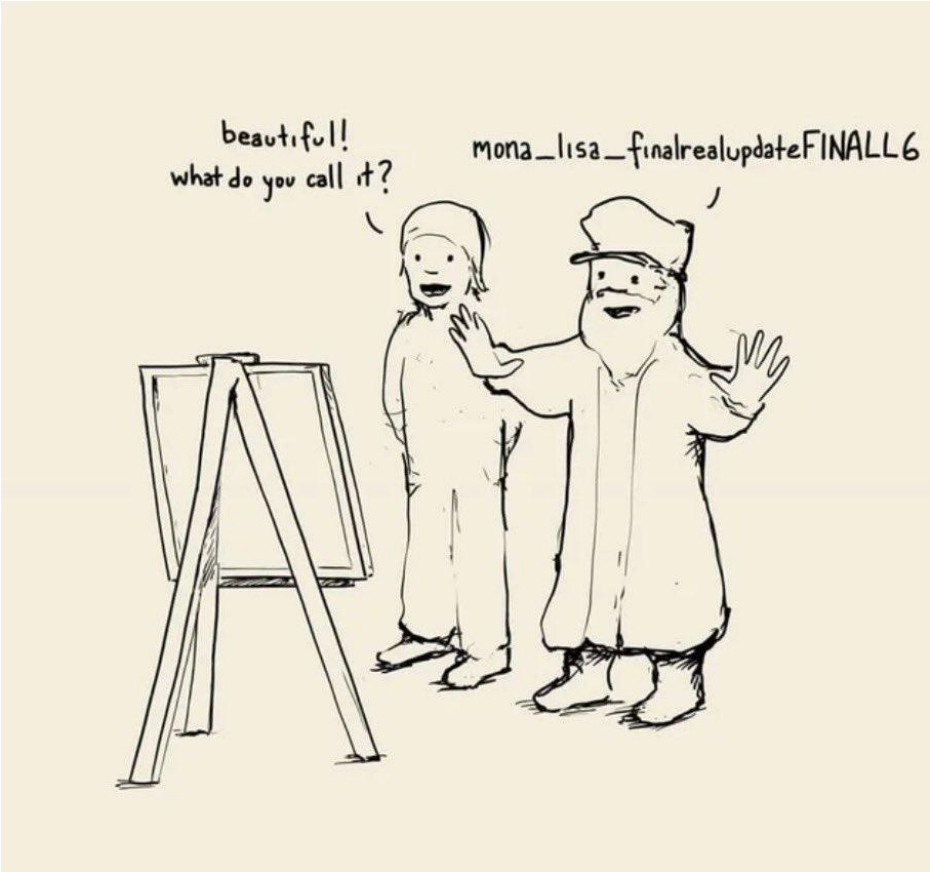
Files and Folders

Why is file organisation important for data management?



https://twitter.com/nathanwpyle/status/1108902487203958784

What level of data organisation will work for me and my project/ team?

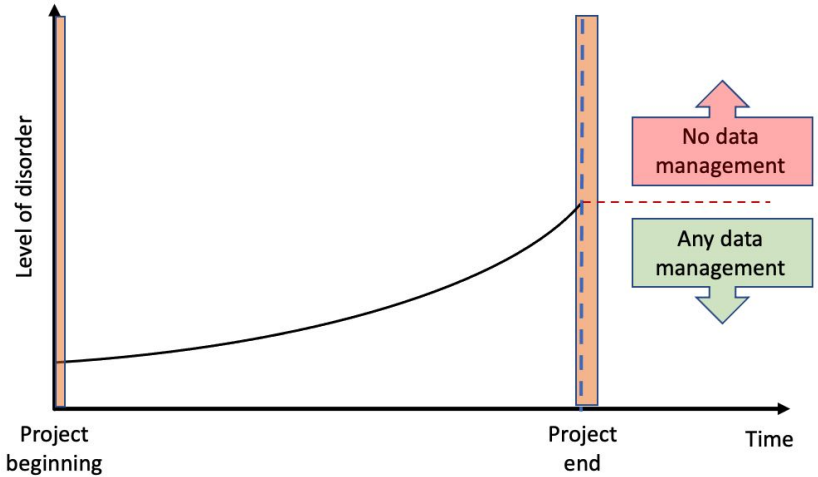
File organisation

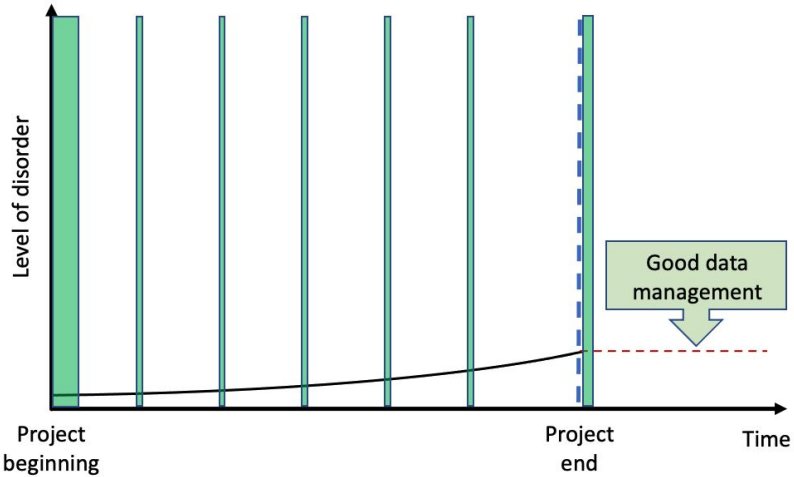
Benefits of systematically organising research and data files in your project :

- Easier to **locate** a file
- Find **similar files** together
- Easy to **identify** which files you want to **back up**
- **Moving files** becomes much easier
- Increases **productivity**
- Helps you to keep and **maintain a record** of the project
- Projects can **easily** be **understood** by others (including your future self)
- Keep **organised** in the long-run

File organisation

- ➔ Files will become ***unorganised*** over time (particularly downloads and/or desktop folders)
- ➔ Files can multiply across folders and versions, decreasing **findability**
- ➔ Organising will ***reduce clutter*** and maintenance requirements over time





File and Folder naming

Names for files and folders should be *consistent* and *meaningful* to yourself and collaborators

Example: LD_phyA_off_t04_2020-08-12_norm.xlsx

Based on the name, the file could contain information about:

LD	Long day sampling, of the
phyA	Phytochrome A genotype, in a
off	Medium without sucrose, at
t04	Time point 4
2020-08-12	Sampled on Aug 12th, 2020, with
norm	Normalised data

File and Folder naming

Names for files and folders should be *consistent* and *meaningful* to yourself and collaborators

Example: LD_phyA_off_t04_2020-08-12_norm.xlsx

Based on the name, the file could contain information about:

LD Long day sampling, of the

Not obvious from the letters and words alone. Explanation is required - README.md

2020-08-12 Sampled on Aug 12th, 2020, with

norm Normalised data

Exercise 6

Group discussion

The following example contain files from an imaginary project

- ***phyA/phyB*** - genotypes
- ***sXX*** - sample number
- ***LD/SD*** - light conditions (Long Day, Short Day)
- ***on/off*** - different growth media (on sucrose, off sucrose)
- ***date format*** - sample date
- ***tXX*** - sample time point
- ***raw***, ***norm*** - raw or normalised data

```
2020-07-14_s12_phyB_on_SD_t04.raw.xlsx
2020-07-14_s1_phyA_on_LD_t05.raw.xlsx
2020-07-14_s2_phyB_on_SD_t11.raw.xlsx
2020-08-12_s03_phyA_on_LD_t03.raw.xlsx
2020-08-12_s12_phyB_on_LD_t01.raw.xlsx
2020-08-13_s01_phyB_on_SD_t02.raw.xlsx
2020-7-12_s2_phyB_on_SD_t01.raw.xlsx
AUG-13_phyB_on_LD_s1_t11.raw.xlsx
JUL-31_phyB_on_LD_s1_t03.raw.xlsx
LD_phyA_off_t04_2020-08-12.norm.xlsx
LD_phyA_on_t04_2020-07-14.norm.xlsx
LD_phyB_off_t04_2020-08-12.norm.xlsx
LD_phyB_on_t04_2020-07-14.norm.xlsx
SD_phyB_off_t04_2020-08-13.norm.xlsx
SD_phyB_on_t04_2020-07-12.norm.xlsx
SD_phya_off_t04_2020-08-13.norm.xlsx
SD_phya_ons_t04_2020-07-12.norm.xlsx
ld_phyA_ons_t04_2020-08-12.norm.xlsx
```

Exercise 6

1. Should dates be put first, and if not, why?
2. What is the difference between using leading 0 (zero) and not?
3. Is there a difference between using upper and lower case letters?
4. What is the difference between using two letters for *on* compared to three letters *ons*?
5. What are the effects if we, as in the above example, mix naming conventions?

- ***phyA/phyB*** - genotypes
- ***sXX*** - sample number
- ***LD/SD*** - light conditions (Long Day, Short Day)
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2020-07-14_s12_phyB_on_SD_t04.raw.xlsx
2020-07-14_s1_phyA_on_LD_t05.raw.xlsx
2020-07-14_s2_phyB_on_SD_t11.raw.xlsx
2020-08-12_s03_phyA_on_LD_t03.raw.xlsx
2020-08-12_s12_phyB_on_LD_t01.raw.xlsx
2020-08-13_s01_phyB_on_SD_t02.raw.xlsx
2020-7-12_s2_phyB_on_SD_t01.raw.xlsx
AUG-13_phyB_on_LD_s1_t11.raw.xlsx
JUL-31_phyB_on_LD_s1_t03.raw.xlsx
LD_phyA_off_t04_2020-08-12.norm.xlsx
LD_phyA_on_t04_2020-07-14.norm.xlsx
LD_phyB_off_t04_2020-08-12.norm.xlsx
LD_phyB_on_t04_2020-07-14.norm.xlsx
SD_phyB_off_t04_2020-08-13.norm.xlsx
SD_phyB_on_t04_2020-07-12.norm.xlsx
SD_phya_off_t04_2020-08-13.norm.xlsx
SD_phya_ons_t04_2020-07-12.norm.xlsx
ld_phyA_ons_t04_2020-08-12.norm.xlsx
```

Exercise 6

1. Should dates be put first, and if not, why?
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```
2020-07-14_s12_phyB_on_SD_t04.raw.xlsx
2020-07-14_s1_phyA_on_LD_t05.raw.xlsx
2020-07-14_s2_phyB_on_SD_t11.raw.xlsx
2020-08-12_s03_phyA_on_LD_t03.raw.xlsx
2020-08-12_s12_phyB_on_LD_t01.raw.xlsx
2020-08-13_s01_phyB_on_SD_t02.raw.xlsx
2020-7-12_s2_phyB_on_SD_t01.raw.xlsx
AUG-13_phyB_on_LD_s1_t11.raw.xlsx
JUL-31_phyB_on_LD_s1_t03.raw.xlsx
LD_phyA_off_t04_2020-08-12.norm.xlsx
LD_phyA_on_t04_2020-07-14.norm.xlsx
LD_phyB_off_t04_2020-08-12.norm.xlsx
LD_phyB_on_t04_2020-07-14.norm.xlsx
SD_phyB_off_t04_2020-08-13.norm.xlsx
SD_phyB_on_t04_2020-07-12.norm.xlsx
SD_phya_off_t04_2020-08-13.norm.xlsx
SD_phya_ons_t04_2020-07-12.norm.xlsx
ld_phyA_ons_t04_2020-08-12.norm.xlsx
```

1.Using dates as leading information in file names makes finding data quickly harder as the more interesting information may be samples or timepoints (unless date is crucial to data)

2. Without leading zeros, sorting will make 10 and 11 appear before 2

3. Upper and lower cases may sort differently

4. Comparing files is easier if the file name lengths are uniform

5. Mixed naming conventions can make it difficult to locate particular files, and/or sort a large number of files

File naming Do's

For dates use the **YYYY-MM-DD standard** and place at the end of the file UNLESS you need to organize your files chronologically

Include **version number** (if applicable), use leading zeros (i.e.: v005 instead of v5)

Make sure the **end-letter file format extension** is present at the end of the name (e.g. .doc, .xls, .mov, .tif)

Add a **README.md** (PROJECT_STRUCTURE.md) file in your top directory which details your naming convention, directory structure and abbreviations

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File naming Dont's

Using spaces (use _ or -)

Long names

Repetition, e.g if directory name is Electron_Microscopy_Images, file ELN_MI_IMG1_S01_20200101.img then ELN_MI is redundant (applicable if the file is not going to be accessed independently of the location)

Dots, commas and special characters (e.g. ~ ! @ # $ % ^ & * ( ) ` ; < > ? , [ ] { } ‘ “)

Using language specific characters (e.g óężé)

Deep paths with long names (i.e. deeply nested folders with long names), as archiving or moving between OS may fail

File naming strategy

Two starting points for your file naming are:

A file name is a principal identifier of a file

- ➔ useful clues to the content
- ➔ status and version of a file
- ➔ help in classifying and sorting files
- ➔ facilitate searching and discovering files

File naming strategy should be consistent in time and among different people

- ➔ systematic and consistent across all files in the study
- ➔ a group of cooperating researchers should follow the same file naming strategy
- ➔ file names should be independent of the location of the file on a computer

Exercise 7

Group discussion

What are the potential benefits of agreeing on a ***File Naming Convention*** for a project?

Some benefits can be …

- Easier to **process** - Users will not have to over think the file naming process
- Easier to facilitate **access**, **retrieval** and **storage** of files
- Easier to browse through files, **saving time** and **effort**
- **Harder to lose**!
- Having logical and known naming conventions in place can also help you with **version control**.
- Check for obsolete or **duplicate** records

Principles for naming files

How to organise files and folders?

Consider **file name lengths**

Beware of operative systems limitations and full path names!

Make names **human readable**

Name describes content of file

Make names **machine readable**

Avoid spaces, punctuations, accented characters

Explain file naming in associated info files (README.md)

File naming

Examples of a **poor** file name**:**

”Honeybee project, experiment 2 done in Helsinki, data file created on the second of December 2020”

File name - Runnew_again_2NDTRY.xls

Explanation - N/A

File naming

Examples of a **good** file name:

”Honeybee project, experiment 2 done in Helsinki, data file created on the second of December 2020”

File name - 20201202_HB_EXP2_HEL_DATA_V03.xls

Explanation - Date_ProjectAbbreviation_ExperimentNumber_
Location_TypeOfData_VersionNumber

File naming convention

Want to create your own File Naming Convention? Consider…

What **group of files** will this naming convention cover?

What **information (metadata) is important** about these files and makes each file distinct?

Do you need to **abbreviate** any of the metadata or encode it?

What is the **order** for the **metadata** in the file name?

What **characters** will you use **to separate** each piece of metadata in the file name?

Will you need to **track** different **versions** of each file?

Write down your naming convention pattern

Document this convention in a **README.md** and keep it with your files

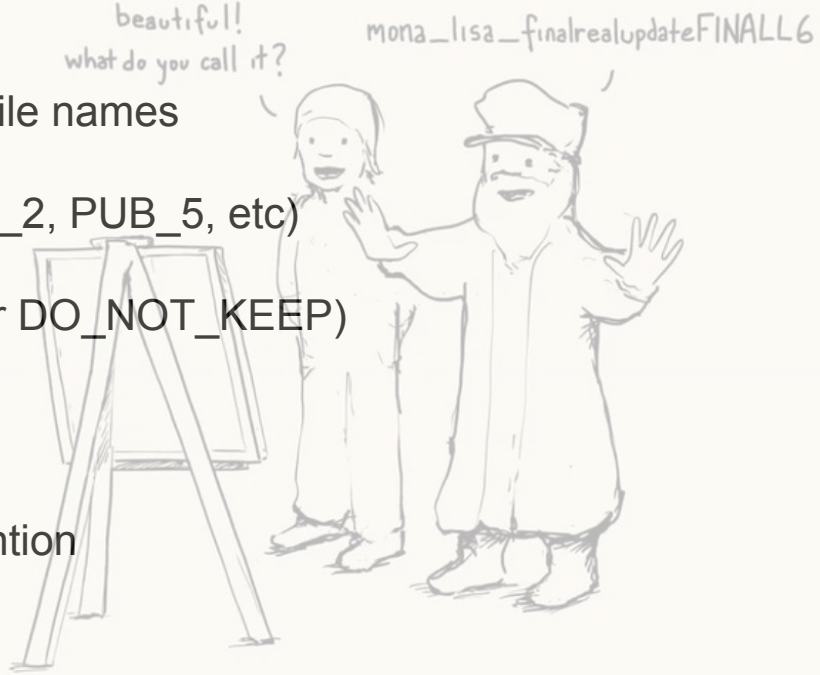
Briney, Kristin A. (2020) File Naming Convention Worksheet. [Teaching Resource]

File versioning

The simple yet powerful **Dont's** and **Do's** of file versioning:

Dont's

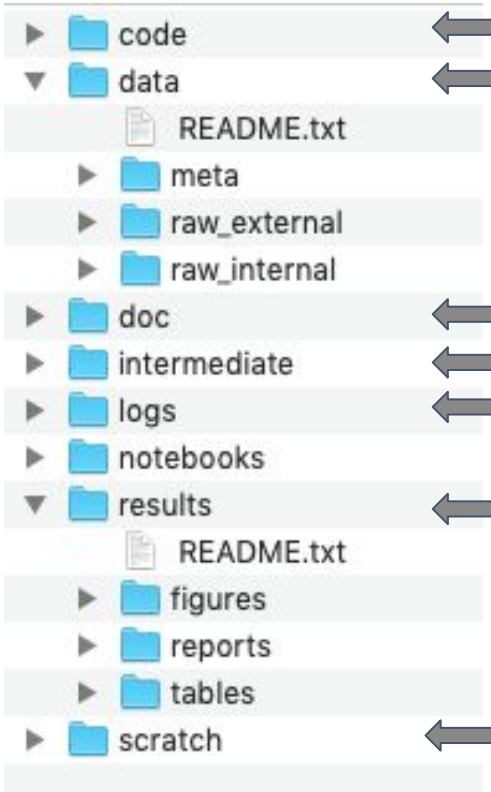
- Add suffixes like FINAL, THIS_ONE, or PUB, to file names
- Add numbers to already bad suffixes (e.g. FINAL_2, PUB_5, etc)
- Add negative information (e.g. DELETE_THIS, or DO_NOT_KEEP)



Do's

- Explicitly include versioning in file naming convention
- Use version numbers, preferably consistently

Directory structure for a sample project



- code: all code needed to go from input files to final results
- data: raw and primary data, essentially all input files, **never** edit!
- doc: documentation for the study
- intermediate: output files from different analysis steps, *can be deleted*
- logs: logs from the different analysis steps
- results: output from workflows and analyses
- scratch: temporary files that can be safely *deleted or lost*

Noble WS (2009) A Quick Guide to Organizing Computational Biology Projects. PLoS Comput Biol 5(7): e1000424.
http://journals.plos.org/ploscompbiol/article?id=info:doi/10.1371/journal.pcbi.1000424

Exercise 10

We are back in the Famous lab!

- Considering the very limited metadata we have access to, and the inherited files, what can we do in order to increase the level and quality of data organization?
- Download the zip-file containing the inherited data structure
- Consider the following:
  - File names
  - Folder structure
  - Documentation

★ Work in pairs or in smaller groups.
★ Focus on the discussion more than finishing the exercise.
★ Consider your own data and files from a third-person-view

Tabular data

Tabular data (or spreadsheet data) refers to data that is organized in **a table with rows and columns**

Tabular data is not a data *type*, but …

- a way to *organize data*

- designed for *machine readability*

Long term storage, exporting, archiving and FAIRification by converting to .CSV or .TSV

Tabular data

Good practice for structuring tabular data is to…

Think about **how** to **organize** your data both from a data entry and data analysis point of view from the beginning

Adopt good **metadata standards** and **column header formats** early in the data collection phase

Setting up **well-formatted tables** early in the research process is extremely important – before you even start entering data

Separate r**aw data** from the **analysed data** can have different layout/format

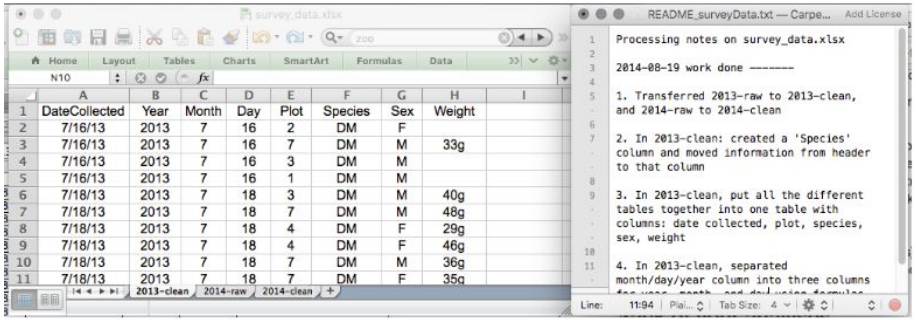
Leave the original (raw) data raw!!!

Keeping track of your analyses

When working with spreadsheets during data clean up or analyses you **must:**

- **…create a new file or tab with your cleaned or analyzed data.**
  Do not modify the original dataset, or you will never know where you started!

- **…keep track of the steps you took in your clean up or analysis.**
  You can do this in another text file, or a good option is to create a new tab in your spreadsheet with your notes.



How to structure data tables

The cardinal rules of using spreadsheet programs for data:

- Column = Variable
- Row = Observation
- Cell = Value

Open Access training					
Date	Length (hours)	Registered	Attended	Delivered by	Canceled
16/01/17	1	26	23	JM	N
05/02/17	1	38	26	JM	N
17/02/17	1	19	25	PG	N
07/03/17	1	27	17	JM	N
29/03/17	1	32	15	PG	N
02/04/17	1	41		PG	Y
24/04/17	2	44	44	JM	N
25/05/17	1	43	37	PG	N
16/06/17	1	15	15	JM	N

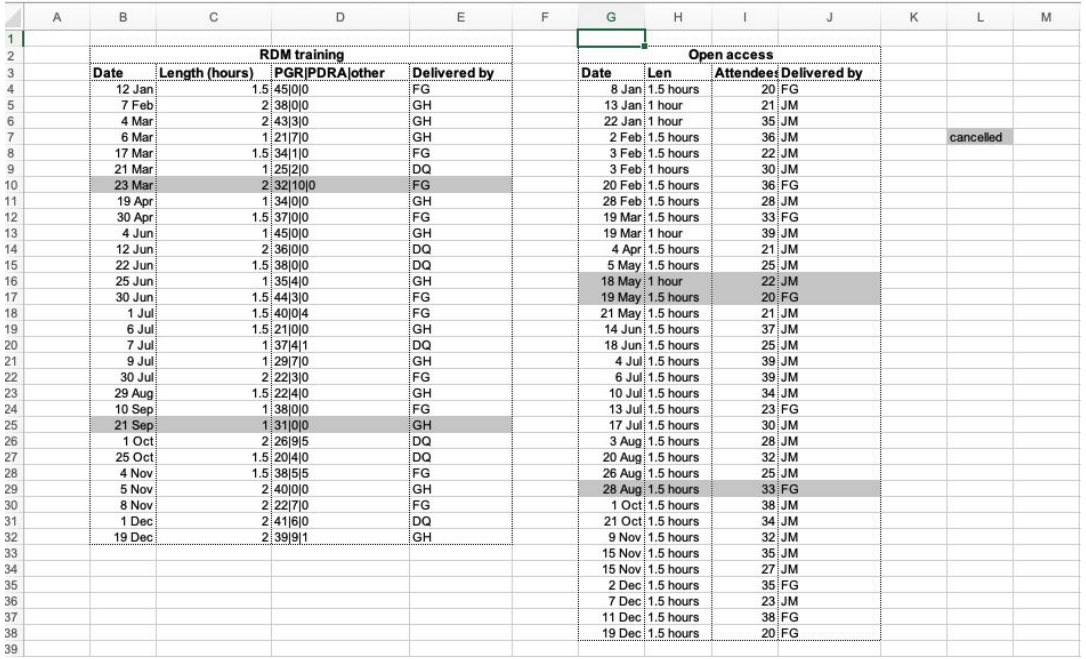
Tidy data tables

- One cell–one value
- One column–one variable
- One row–one observation

Tabular data

Do not:

- create multiple data tables within one spreadsheet tab
- combine values in cells
- merging cells
- use colors
- write comments in cells
- mix metadata and data
- use special characters
- use different date formats



	RDM training			
	Date	Length (hours)	PGR|PDRA|other	Delivered by
	12 Jan	1.5	45|0|0	FG
	7 Feb	2	38|0|0	GH
	4 Mar	2	43|3|0	GH
	6 Mar	1	21|7|0	GH
	17 Mar	1.5	34|1|0	FG
	21 Mar	1	25|2|0	DQ
	23 Mar	2	32|10|0	FG
	19 Apr	1	34|0|0	GH
	30 Apr	1.5	37|0|0	FG
	4 Jun	1	45|0|0	GH
	12 Jun	2	36|0|0	DQ
	22 Jun	1.5	38|0|0	DQ
	25 Jun	1	35|4|0	GH
	30 Jun	1.5	44|3|0	FG
	1 Jul	1.5	40|0|4	FG
	6 Jul	1.5	21|0|0	GH
	7 Jul	1	37|4|1	DQ
	9 Jul	1	29|7|0	GH
	30 Jul	2	22|3|0	FG
	29 Aug	1.5	22|4|0	GH
	10 Sep	1	38|0|0	FG
	21 Sep	1	31|0|0	GH
	1 Oct	2	26|9|5	DQ
	25 Oct	1.5	20|4|0	DQ
	4 Nov	1.5	38|5|5	FG
	5 Nov	2	40|0|0	GH
	8 Nov	2	22|7|0	FG
	1 Dec	2	41|6|0	DQ
	19 Dec	2	39|9|1	GH

	Open access			
	Date	Len	Attendees	Delivered by
	8 Jan	1.5 hours	20	FG
	13 Jan	1 hour	21	JM
	22 Jan	1 hour	35	JM
	2 Feb	1.5 hours	36	JM
	3 Feb	1.5 hours	22	JM
	3 Feb	1 hours	30	JM
	20 Feb	1.5 hours	36	FG
	28 Feb	1.5 hours	28	JM
	19 Mar	1.5 hours	33	FG
	19 Mar	1 hour	39	JM
	4 Apr	1.5 hours	21	JM
	5 May	1.5 hours	25	JM
	18 May	1 hour	22	JM
	19 May	1.5 hours	20	FG
	21 May	1.5 hours	21	JM
	14 Jun	1.5 hours	37	JM
	18 Jun	1.5 hours	25	JM
	4 Jul	1.5 hours	39	JM
	6 Jul	1.5 hours	39	JM
	10 Jul	1.5 hours	34	JM
	13 Jul	1.5 hours	23	FG
	17 Jul	1.5 hours	30	JM
	3 Aug	1.5 hours	28	JM
	20 Aug	1.5 hours	32	JM
	26 Aug	1.5 hours	25	JM
	28 Aug	1.5 hours	33	FG
	1 Oct	1.5 hours	38	JM
	21 Oct	1.5 hours	34	JM
	9 Nov	1.5 hours	32	JM
	15 Nov	1.5 hours	35	JM
	15 Nov	1.5 hours	27	JM
	2 Dec	1.5 hours	35	FG
	7 Dec	1.5 hours	23	JM
	11 Dec	1.5 hours	38	FG
	19 Dec	1.5 hours	20	FG

cancelled

Missing data

Zero vs. Missing data - How do you make explicit something that do not exist?

Table 1. Commonly used null values, limitations, compatibility with common software and a recommendation regarding whether or not it is a good option. Null values are indicated as compatible with specific software if they work consistently and correctly with that software. For example, the null value "NULL" works correctly for certain applications in R, but does not work in others, so it is not presented in the table as R compatible.

Null values	Problems	Compatibility	Recommendation
0	Indistinguishable from a true zero		Never use
Blank	Hard to distinguish values that are missing from those overlooked on entry. Hard to distinguish blanks from spaces, which behave differently.	R, Python, SQL	Best option
-999, 999	Not recognized as null by many programs without user input. Can be inadvertently entered into calculations.		Avoid
NA, na	Can also be an abbreviation (e.g., North America), can cause problems with data type (turn a numerical column into a text column). NA is more commonly recognized than na.	R	Good option
N/A	An alternate form of NA, but often not compatible with software		Avoid
NULL	Can cause problems with data type	SQL	Good option
None	Uncommon. Can cause problems with data type	Python	Avoid
No data	Uncommon. Can cause problems with data type, contains a space		Avoid
Missing	Uncommon. Can cause problems with data type		Avoid
-,+,.	Uncommon. Can cause problems with data type		Avoid

White et al, 2013, Nine simple ways to make it easier to (re)use your data. Ideas in Ecology and Evolution

Field Name

For **field names** do not include *spaces* or *special characters* of any kind.

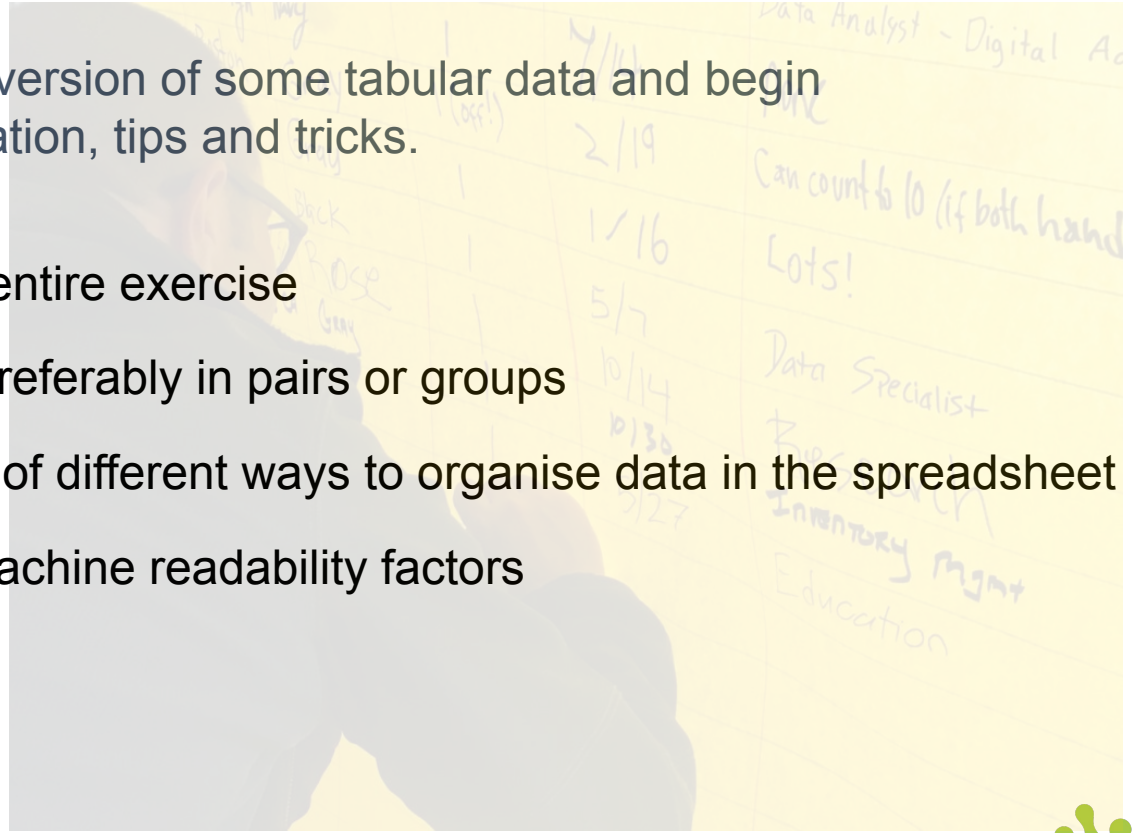
- ➔ Underscores (_) are a good alternative to spaces
- ➔ consider writing names in camelcase (LikeThis.txt) to improve readability.

Good Name	Good Alternative	Avoid
Max_temp_C	MaxTemp	Maximum Temp (°C)
Precipitation_mm	Precipitation	precmm
Mean_year_growth	MeanYearGrowth	Mean growth/year
sex	-	M/F
length	-	l
cell_type	CellType	Cell Type
Observation_01	first_observation	1st Obs

Exercise 9

We are going to take a messy version of some tabular data and begin cleaning it up using the information, tips and tricks.

- Not important to finish the entire exercise
- Work at your own speed, preferably in pairs or groups
- Discuss the pros and cons of different ways to organise data in the spreadsheet
- Consider the Human vs. Machine readability factors



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