



Training in organic breeding

Module 2: Phenomics: approaches and tools for genetic resources and breeding material characterization

Unit 2.3: Guidelines and examples of good practices in data management

Authors: Yannick de Oliveira, Isabelle Goldringer





Funded by the European Union, the Swiss State Secretariat for Education, Research and Innovation (SERI) and UK Research and Innovation (UKRI).



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the European Union

Training in organic breeding organized in 5 Modules

- 1. Module 1 Plant Genetic Resources (PGRs): collection, conservation and exchange to support the increase of agrobiodiversity in farming systems
- Module 2 Phenomics: approaches and tools for genetic resources and breeding material characterisation - FEBRUARY 3rd 2025, 9:00 to 17:30 CET
- **3.** Module **3** Breeding methods fundamentals FEBRUARY 13th 2025, 9:00 to 18:00 CET
- 4. Module 4 Development and application of molecular methods in organic breeding MARCH 4th 2025, 9:00 to 18:00 CET
- 5. Module 5 Organic heterogeneous material (OHM) design and development MARCH 7th 2025, 9:00 to 18:00 CET





February 3rd 2025 - 9:00 to 17:30 CET

Unit 2.1: Main descriptors used worldwide in characterizing plant genetic resources

- 9:00-10:30 UPV (Adrian Rodríguez-Burruezo)
- 10:30-11:00 Break

Unit 2.2: Intro to ShineMas: a web tool dedicated to Seed Lots History, Phenotyping and Cultural Practices¹

- 11:00-12:30 INRAe (Yannick de Oliveira, Isabelle Goldringer)
- 12:30-14:00 Lunch Break

Unit 2.3: Guidelines and examples of good practices in data management

- 14:00-15:30 INRAe (Yannick de Oliveira, Isabelle Goldringer)
- 15:30-16:00 Break

Unit 2.4: Methods for phenotyping and selection of agronomic traits of interest in organic farming

16:00-17:30 - IPC (Pedro Mendes Moreira)

Unit 2.5: Methods for phenotyping and selection of added-value traits (e.g. taste and nutritional value)² ITAB (Solenne Jourdren)

1 - An extra practical session to use the tool with own data is scheduled for FEB 10th (9-12h)

2 - Unit 2.5 planned for the end of March 2025. Registrants will be invited for this extra training lesson

T1.4 Training in Organic Breeding

MODULE 2 – Phenomics: approaches and tools for genetic resources and breeding material characterisation

Unit 2.3: Data management

INRAE

Unit 3 – Guidelines and examples of good practices in data management

Yannick De Oliveira & Isabelle Goldringer INRAE





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Training outline

- Context of reproducibility crisis in science (10 minutes)
- Data management plan and legal constraint regarding data (15 minutes)
- What is FAIR data (10 minutes)
- Guidelines to manage data (30 minutes) :
 - Tidy data
 - Standards and metadata
 - Vocabulary
 - Licenses
 - Data warehouse
- Short quiz (10 minutes)



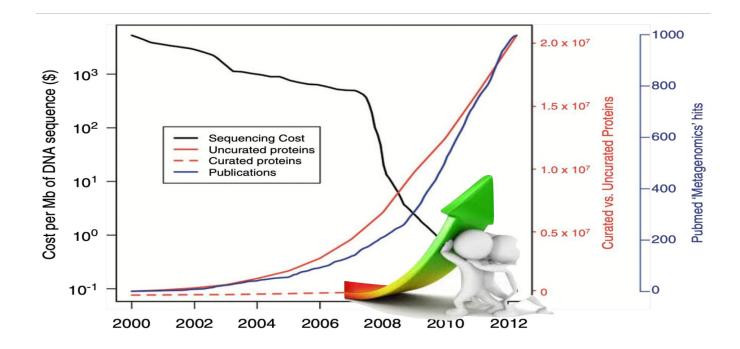


Why manage data properly ?

Context

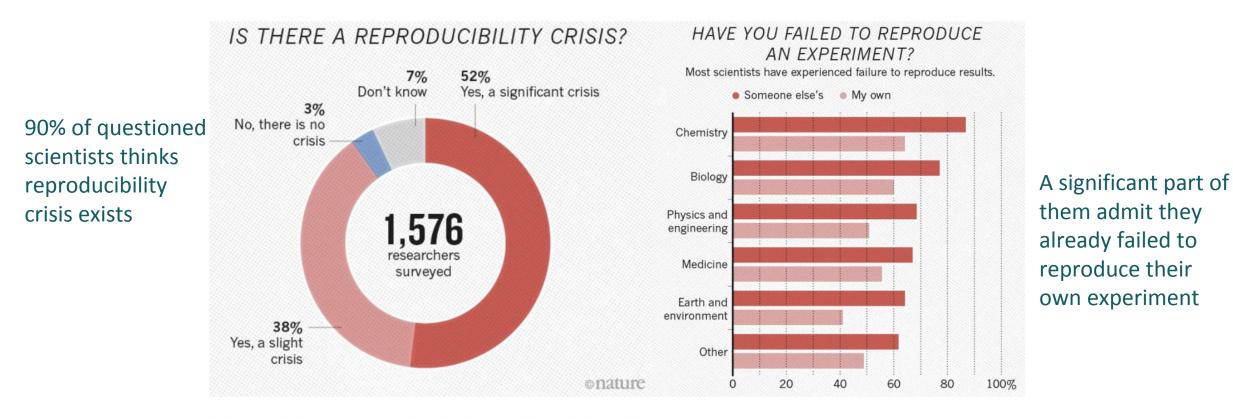
Digital transformation is changing the landscape involving a data deluge and paradigm shift that need to be to manage.

- Before: experience design > data collected > analysis
- Now: data production > organization > analysis > sharing information





Science isn't reproducible



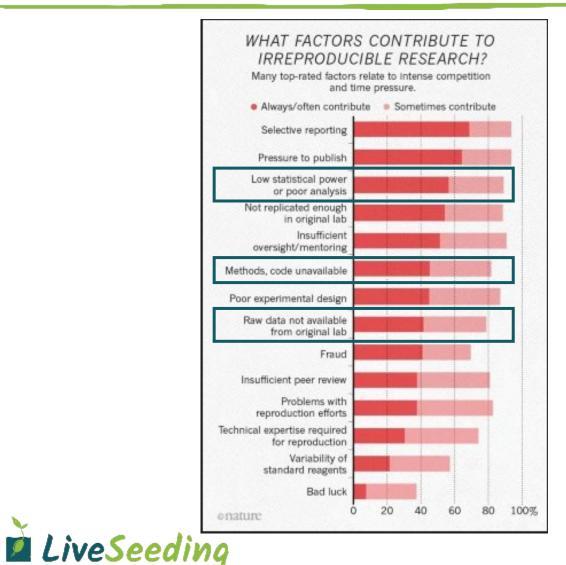
"1,500 scientists lift the lid on reproducibility". Nature. 533: 452-454 - 2016

https://doi.org/10.1038/533452a

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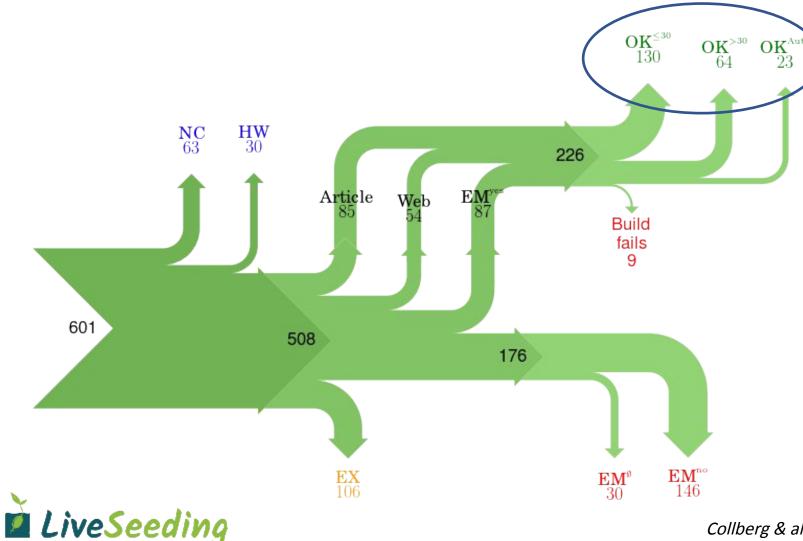
A multifactor crisis



Reasons advanced by scientists are multiple but, a significant part of them are related to data management, their analysis and the tools (source code) used to do these analyses.

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An example with source code



In this study, only 54% of source code can be build (repeatability ok).

An important part needed significant efforts for building or the help of the author.

In most cases programs can't be build because author refuse to share the code or didn't answer to email.

Collberg & al. - Repeatability in computer systems research https://doi.org/10.1145/2812803

Legal obligation

A report of the EU in 2018 estimate the annual cost of producing non-FAIR data : ~10,2bn€

European Law

- Open Data Directive (16 July 2019)
- Free movement of non-personal data in the EU (2018/1807)
- GDPR (2018)



Cost of not having FAIR research data

Cost-Benefit analysis for FAIR research data

Cost-Benefit analysis for FAIR research data - Cost of not having FAIR research data European Commission Directorate-General for Research and Innovation Directorate A — Policy Development and Coordination Unit A.2 — Open Data Policy and Science Cloud Contact Athanasios Karalopoulos E-mail Athanasios.Karalopoulos@ec.europa.eu RTD-PUBLICATIONS@ec.europa.eu European Commission B-1049 Brussels

https://data.europa.eu/doi/10.2777/02999



Focus on GDPR

Le RGPD en 5 points

- Declaration of ALL personal data processing to the institutional DPO (Data Protection Officer) and assurance of compliance
- Information for data subjects +/- consent
- Secure media and data transfers
- Individual rights (access, modification, deletion and portability)
- PIA (Privacy Impact Assessment) for sensitive data

DPO = Data Protection Officer

- Ensures the compliance of personnal data processing (information of individual, individual rights, personnal data processing register)
- He is NOT responsible







Data Management Plan

A DMP is a document that describes how the data of a research project or an entity will be managed throughout its lifecycle



DMP life cycle

Setting up the project

Section on data management Evakuate the cost of open science (data manager, storage...)

Starting the project Setting up the Data Management Plan (DMP)

During the project Data management following FAIR principle Update the DMP

End of the project Share data « as open as possible, as closed as necessary »

Submit in data warehouse in open access



DMP objectives

Implement best practices, respecting FAIR principles (Findable, Accessible, Interoperable, Reusable)

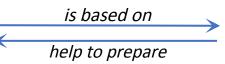
- Ensure reproducibility of experiments by describing the data and how it was obtained
- Enabling data to be understood and reused
- Avoid data loss through appropriate storage
- Establish roles and responsibilities of everyone
- Respect the law and individuals by clarifying the legal and ethical framework
- Clarify re-use rights and sharing modality



Project DMP vs Entity DMP

Project DMP

- Project funded
- Specific scope and fixed term
- Mandatory



Entity DMP

- Research laboratory,
 - plateform, breeder company etc.
- Larger scope and no fixed term
- Not mandatory



Tips : DMP tools



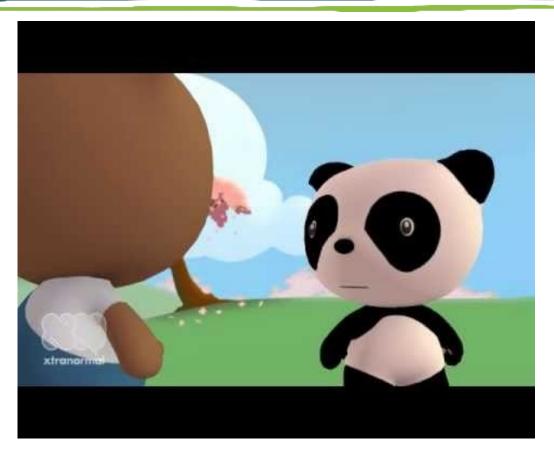
- Can include template from funders such as Horizon Europe
- Easy to use: web interface with form to fill
- -> <u>https://dmp.opidor.fr/</u>



Data stewardship wizard https://ds-wizard.org/



What is going wrong ?



https://www.youtube.com/watch?v=66oNv_DJuPc

Click on the link and share you idea on what is going wrong in this video.

https://postit.colibris-outilslibres.org/fairdataliveseeding







What is it ?

The FAIR Principles are a set of guidelines that aim to make data Findable, Accessible, Interoperable and Reusable.

- It provides guidelines for scientific data management and are relevant to all stakeholders of the digital ecosystem.
- They are aimed directly at data producers and publishers to promote maximum use of scientific data.
- They focus on the ability of machines to manage data automatically, with the minimum of human intervention.

<u>References</u>:

- Wilkinson et al. The FAIR Guiding Principles for scientific data management and stewardship. Sci Data 3, 160018 (2016). <u>https://doi.org/10.1038/sdata.2016.18</u>
- Les principes FAIR. DORANum. <u>http://doi.org/10.13143/z7s6-ed26</u> (french)



Findable

Facilitate data (and metadata) discovery for both humans and machines

- Data have a PID
- Data are described by metadata
- Thess metadata include the PID of the data they describe
- Data are submited in a data warehouse



Accessible

Enable data access and download, which may include authentication and authorization

- Data can be accessed via a standard communication protocol
- The protocol is free and open
- This protocol makes possible an access by authentication if required
- Metadata remains accessible even if data is not (disappeared or inaccessible)



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Interoperable

Enable data exploitation and integration whatever of the IT environment used

- Data are described using controlled vocabularies
- The vocabulary used is complient with FAIR principles
- Metadata are contextualized with links to other data



Reusable

Enable data to be reused for future research

- Metadata contains all information that may be useful (plurality of attributes)
- A license for reuse is assigned to the data
- The description of the data indicates its origin
- Data sharing follows scientific community standards



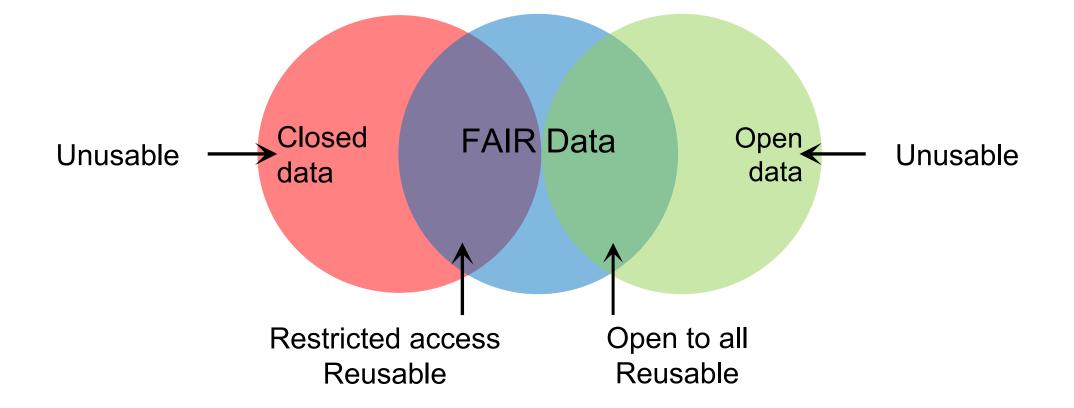
The 5 stars of FAIR data

Progress towards FAIR and Open Data requires multidisciplinary cooperation

Biologists Data linked to other datasets IT Engineer RE OF URI Data identified by a URI $\times \times \times \times$ Ontology/semantics specialists OL RE OF URI Data in a non-proprietary format $\times \times \times$ 2 OL RE OF Data uses a structured format RDF $\times \times$ 999 OL RE IT engineer Data on the web, open license CS XLS **Biogolists** W3C 66 RDF 5 OPEN DATA PDF



Accessible ≠ Open







Guidelines for data management

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Module 2 – Unit 3 Guidelines and examples of good practices in data management

Tidy data

What is it and what for?

How to move from messy to tidy data?

Tidy data and tidy tools => everything in Whickham (2014)

(The steps further: designing a global dataset)

Additional available material



Tidy data

- 80% of data analysis is spent on the process of cleaning and preparing the data (Dasu and Johnson 2003)
- Real-world datasets = often few, if any, constraints on their organization, datasets often constructed in bizarre ways
- Data preparation is not just a first step, but must be repeated many times over the course of analysis (new problem arising, new data collected...)
- => Need to structure datasets to facilitate analysis



Tidy data

- Principles : to provide a standard way to organize data values within a dataset.
- => will make initial data cleaning easier, facilitate initial exploration and analysis of the data, and simplify the development of data analysis tools that work well together.
- Tidy datasets provide a standardized way to link the structure of a dataset (its physical layout) with its semantics (its meaning).



Data structure

•		Yield_Org	Yield_Non Org		Variety_A	Variety_B	Variety_C
•	Variety_A	-	40	Yield_Org	-	35	27
•	Variety_B	35	45	Yield_Non	40	45	30
•	Variety_C	27	30	Org			
•	Table 1			Table 2			

• Table 1 & 2 = same data but different layout



Data semantics

- Dataset = collection of values (numbers or strings)
- Every value belongs to a variable and to an observation
- A variable contains all values that measure the same underlying attribute across units
- An observation contains all values measured on the same unit across attributes



Data semantics

• Reorganizing Table 1 to make the values, variables, observations more clear

•		Yield_Org	Yield_Non Org		
•	Variety_A	-	40		
•	Variety_B	35	45		
	Variety_C	27	30		
•		Table 1			

	Yield_Org	Prot_Org
Variety_A	-	40
Variety_B	35	45
Variety_C	27	30
	Table 3	

- Table 1: mix between variables and observations
- Table 3 would be ok

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LiveSeeding

Module 2 – Unit 3 Tidy data: how to move from messy to tidy data?

Tidy data

- Each variable forms a column
- Each observation forms a row
- Each type of observational unit forms a table
- Messy data is any other arrangement of the data.

Table 4 = tidy **Table 1** => each row represents an observation, the result of one Farming practice on one Variety, and each column is a variable. Table 4



		Yield_Org		Yield_Non Org	
Table 1	Variety_A		-	40	
	Variety_B		35	45	
	Variety_C		27	30	
Varie	ties		rming actice	Yield	
Variety_A Variety_B Variety_C Variety_A Variety_B Variety_C		Organic		-	
		Organic		35	
		Organic		27	
		Non Organic		40	
		Non Organic		45	
		No	n Organic	30 - 36 -	

Tidy data

- 5 most common problems with messy datasets:
 - Column headers are values, not variable names
 - Multiple variables are stored in one column
 - Variables are stored in both rows and columns
 - Multiple types of observational units are stored in the same table
 - A single observational unit is stored in multiple tables



Table 6

Example 1: Column headers are values, not variable names

 This dataset has three variables, *Population, Flower colour* and *Frequency* => to tidy Table 5, we need to melt, or stack it = turn columns into rows

Populat ion	Flower _Blue	Flower _purple	Flower _pink	Flower _white
Pop₁	15	25	40	20
Pop₂	0	10	80	10
Pop₃	20	50	25	5
•				

Table 5



Population	Flower_ colour	Frequency
Pop ₁	Blue	15
Pop₂	Blue	0
Pop₃	Blue	20
Pop ₁	Purple	25
Pop₂	Purple	10
Pop₃	Purple	50
Pop₁	Pink	40
Pop₂	Pink	80
Pop₃	Pink	25
Pop₁	White	20
Pop₂	White	10
Pop₃	White	5 - 38

Example 2 : Column headers are values not variable names + Multiple variables stored in 1 column

This dataset has four variables, *Plant, Leaf-number, Leaf-side,* and *diseased-surface* => to tidy Table 7, we need to melt it + split a single variable *Leaf#-side* into 2 real variables *Leaf-number* and *Leaf-side*

Plant	Lf1-top	Lf1- Bottom	Lf2-top	Lf2- bottom	Lf3-top	Lf3- bottom
Plant₁	50	40	30	30	10	5
Plant₂	10	10	5	0	0	0
Plant₃	25	20	15	10	5	0



Example: Column headers are values not variable names + Multiple variables stored in 1 column

Plant	Lf1-top	Lf1- Bottom	Lf2-top	Lf2- bottom	Lf3-top	Lf3- bottom	
Plant₁	50	40	30	30	10	5	
Plant₂	10	10	5	0	0	0	
Plant₃	25	20	15	10	5	0	

LiveSeeding

Source : Wickham H (2014)

Table 8

Plant	Lf#-side	Diseased surface
Plant₁	Lf1-top	50
Plant₂	Lf1-top	10
Plant₃	Lf1-top	25
Plant₁	Lf1-Bottom	40
Plant₂	Lf1-Bottom	10
Plant₃	Lf1-Bottom	20
Plant₁	Lf2-top	30
Plant₂	Lf2-top	5
Plant₃	Lf2-top	15
Plant₁	Lf2-bottom	30
Plant₂	Lf2-bottom	0
Plant₃	Lf2-bottom	10
Plant₁	Lf3-top	10
Plant₂	Lf3-top	0
		- 40 -

Example: Column headers are values not variable names + Multiple variables stored in 1 column

•	Plant	Lf#-side	Diseased surface
	Plant₁	Lf1-top	50
	Plant₂	Lf1-top	10
	Plant₃	Lf1-top	25
	Plant₁	Lf1-Bottom	40
	Plant₂	Lf1-Bottom	10
	Plant₃	Lf1-Bottom	20
	Plant₁	Lf2-top	30
	Plant₂	Lf2-top	5
Table 8	Plant₃	Lf2-top	15
	Plant₁	Lf2-bottom	30
	Plant₂	Lf2-bottom	0
Source : Wickham H	Plant₃	Lf2-bottom	10
⁽²⁰¹⁴⁾ LiveSeedi	Plant₁	Lf3-top	10
	Plant₂	Lf3-top	0

	Plant	Leaf-nb	Leaf-side	Diseased surface
	Plant₁	Lf1	top	50
	Plant₂	Lf1	top	10
	Plant₃	Lf1	top	25
	Plant₁	Lf1	bottom	40
	Plant₂	Lf1	bottom	10
	Plant₃	Lf1	bottom	20
	Plant₁	Lf12	top	30
	Plant₂	Lf12	top	5
	Plant₃	Lf12	top	15
	Plant₁	Lf12	bottom	30
-	Plant₂	Lf12	bottom	0
Table 9	Plant₃	Lf12	bottom	10
	Plant₁	Lf3	top	10
	Plant₂	Lf3	top	0
				- 41 -

Tidy data

- 5 most common problems with messy datasets:
 - Column headers are values, not variable names
 - Multiple variables are stored in one column
 - Variables are stored in both rows and columns
 - Multiple types of observational units are stored in the same table
 - A single observational unit is stored in multiple tables

=> See Wickham H (2014)



Tidy data

One way of organizing variables is by their role in the analysis:

- Fixed variables describe the experimental design (known in advance)
- => should come first
- Measured variables are what we measure in the study
- => should follow (related variables contiguous)



Tidy tools

Take tidy datasets as input and return tidy datasets as output => the output of one tool can be used as the input to another

Everything you need to know about tidy data and tidy tools is here:

- Wickham H (2014). Tidy Data. Journal of Statistical Software 59. https://doi.org/10.18637/jss.v059.i10.
- Article, codes and examples: https://www.jstatsoft.org/article/view/v059i10



Module 2 – Unit 3 The steps further: designing a global dataset

Mahmoud, R et al. A workflow for processing global datasets: application to intercropping. Peer Community Journal, Volume 4 (2024), article no. E24.

LiveSeeding

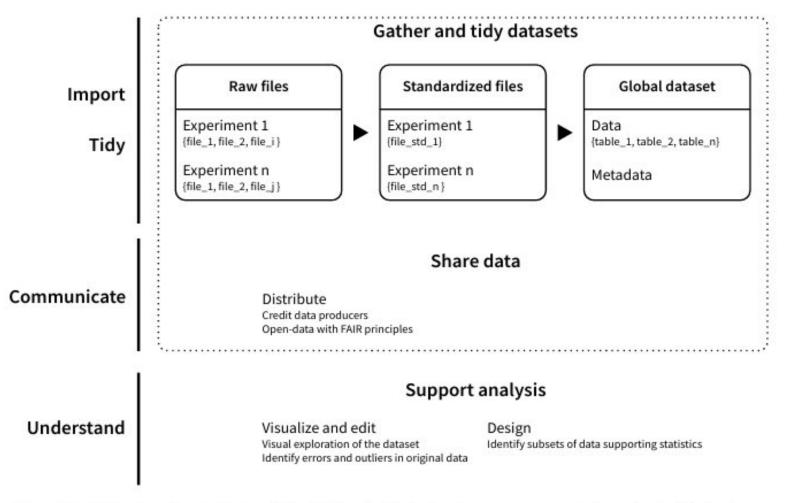


Figure 1 - Main steps for designing global datasets. The left column corresponds to a classical data science workflow. We adapted these steps for global dataset design specificities, to illustrate the importance of data gathering, tidying, and sharing (dotted frame). While some actions supporting subsequent data analysis are generic (visualization, editing), most depend on the chosen analysis strategy.

Controlled vocabulary



Why controlled vocabularies ?

A controlled vocabulary makes possible to describe concepts used by a community in the same way.

It can be a thesaurus, a glossary, an ontology etc.

A typical (and simple) example of non-controlled vocabulary, a same trait written in different ways : *plant_height, plant height, plants_height* etc.



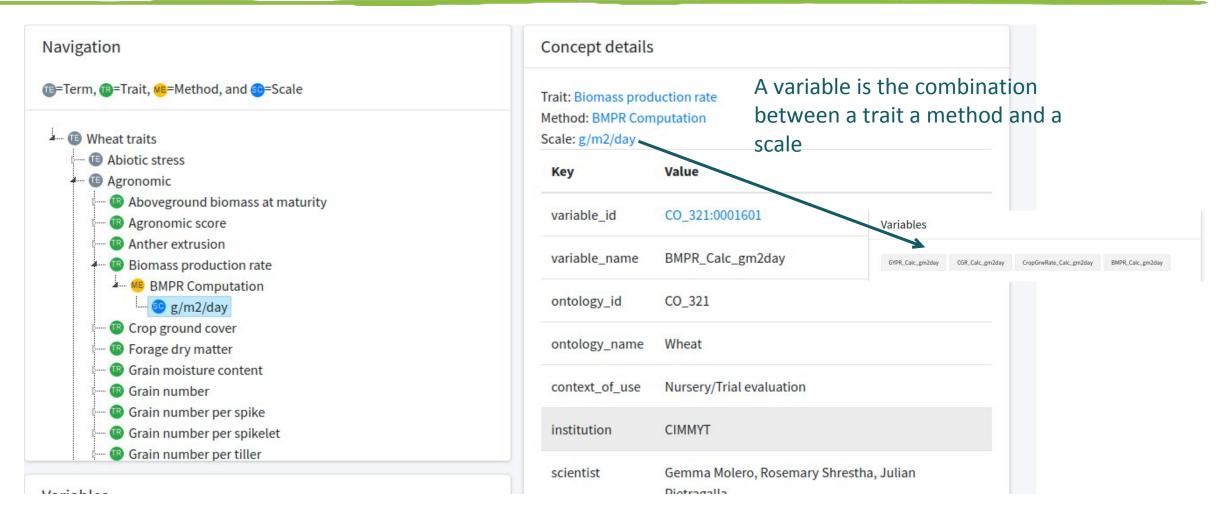
Thesaurus

Agrovoc (FAO) https://agrovoc.fao.org/browse/agrovoc/en/

Alphabetical Hierarchy design destruction of animals detection diagnosis	Groups		ternative agriculture > organic agricul ulture > farming systems > alternative (i) organic agricult	e agriculture > organic agriculture
-disinfection -dispute settlement		BROADER CONCEPT	alternative agriculture (en)	
-diving -dredging		RELATED CONCEPTS	organic certification (en)	
 economic activities agriculture agricultural practices farming systems agroforestry agroforestry systems agropastoral systems alternative agriculture biodynamic agriculture 		ENTRY TERMS	ENTRY TERMS③ organic farming (en)SCOPE NOTEAgricultural methods without use of chemical products (en)INCLUDESorganic gardening (en) organic husbandry (en)	
		INCLUDES		
		PRODUCES	organic foods (en)	
-organic agriculture permaculture -aquaculture systems -aquatic agricultural system	ems	IN OTHER LANGUAGES	 ① زراعة عضوية ① 有机农业 ① 有机耕作 	Arabic Chinese



Ontologies









What is a metadata ?

What is Metadata?

Metadata is: Data 'reporting'

- **WHO** created the data?
- **WHAT** is the content of the data?
- **WHEN** were the data created?
- **WHERE** is it geographically?
- **HOW** were the data developed?
- **WHY** were the data developed?





Why a standard ?

Why use a standard ?

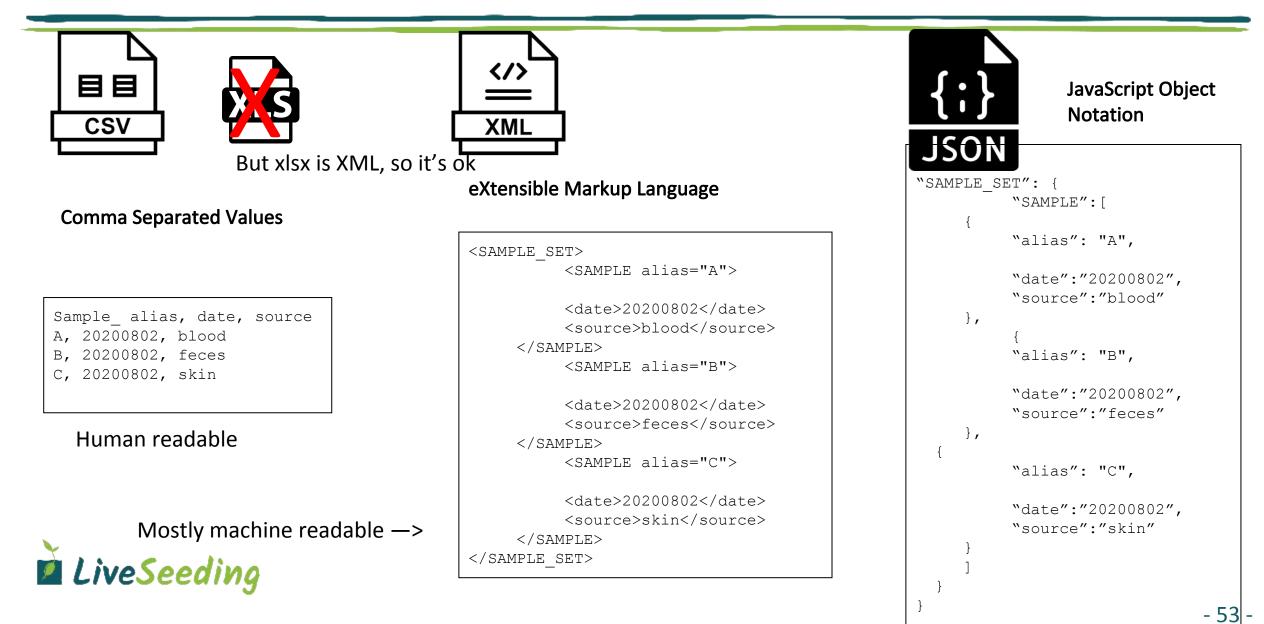
- Analyze, compare, exchange data
- Publish datasets in international data warehouse

And what about a metadata standard ?

- Describe data richly and accurately, using the same vocabulary as the rest of the scientific community
- To make your metadata interoperable and enable other systems to use them



Three text formats frequently used for metadata



Minimum Information for Plant Phenotyping Experiments (MIAPPE)

MIAPPE is a standard for phenotyping metadata Data file Investigation Study Person **Biological Material** Environment **Experimental Factor** Event **Observation Unit** Sample **Observed Variable** The object that you will describe : often a biological material at a location (plot) Variables that you will measure such as a combination between a trait x a method x a scale tidy data file : => tidy data file + MIAPPE ObservationUnit x ObservationVariables metadata file is a FAIR dataset !





Include established standard

MultiCrop Passport Descriptors (MCPD): genetic resources description

<u>https://www.miappe.org/</u> Crop Ontology: descriptions of methods, traits, measures

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Why a license

Give a framework for data sharing and reuse

- Allows users to be granted certain usage rights
- May include restrictions on use
- Strongly recommended in all cases to clearly display the related rights

Recommended Licenses

- Widely used license
- Compliant with other existing licenses (easy data aggregation)
- Taking into account the potential of the data and the restrictions applied (Etalab for distribution in France, Creative Commons for international distribution)



Creative Commons licenses

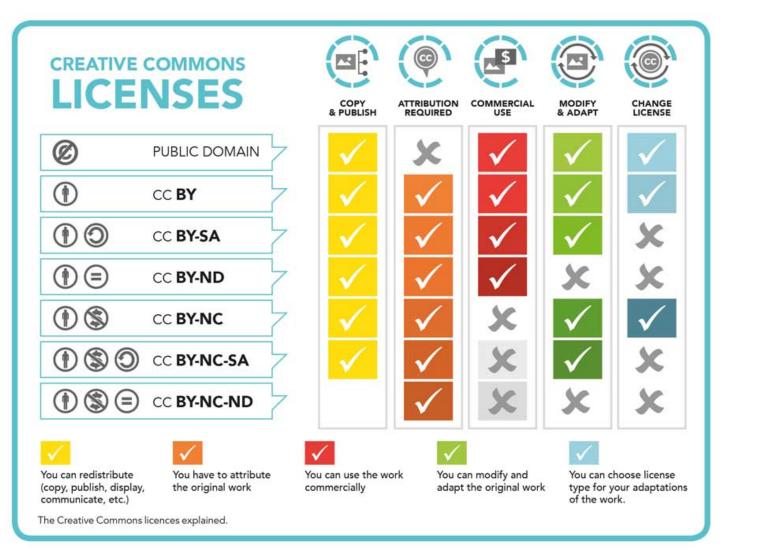
CC-0 : public domain, not cited

ND : impossible to modify/adapt data including aggregation

NC : not recommended because you prevent any commercial use, including a non-profit action such as a training that would need inscription fee

CC BY and CC BY-SA are the mostly recommended licenses





Code licenses

Permissive license means the license of the modified code can be changed. You have to be cited but the resulting code be proprietary.

Copyleft license means that the modified code must published under the same term of license.

We talk also about "viral" license.

All those licenses are good to use regarding the context.



96		BSD	l'liT	Free as in Freedom	Free as in Freedom	AGPLU Instruction Free as in Freedom
Туре	Permissive	Permissive	Permissive	Copyleft	Copyleft	Copyleft
Provides copyright protection	V TRUE					V TRUE
Can be used in commercial applications	V TRUE				V TRUE	
Provides an explicit patent license		X FALSE	X FALSE	FALSE	X FALSE	X FALSE
Can be used in proprietary (closed source) projects				FALSE	FALSE partially	FALSE for web
Popular open- source and free projects	Kubernetes Swift Firebase	Django React Flutter	Angular.js JQuery, .NET Core Laravel	Joomla Notepad++ MySQL	Qt SharpDevelop	SugarCRM Launchpad





What kind of data warehouse

Thematic data warehouses

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- Accurate dataset description and metadata
- Good quality
- Do not exists for all data types (phenotyping)
- Publication/curation of data time consuming

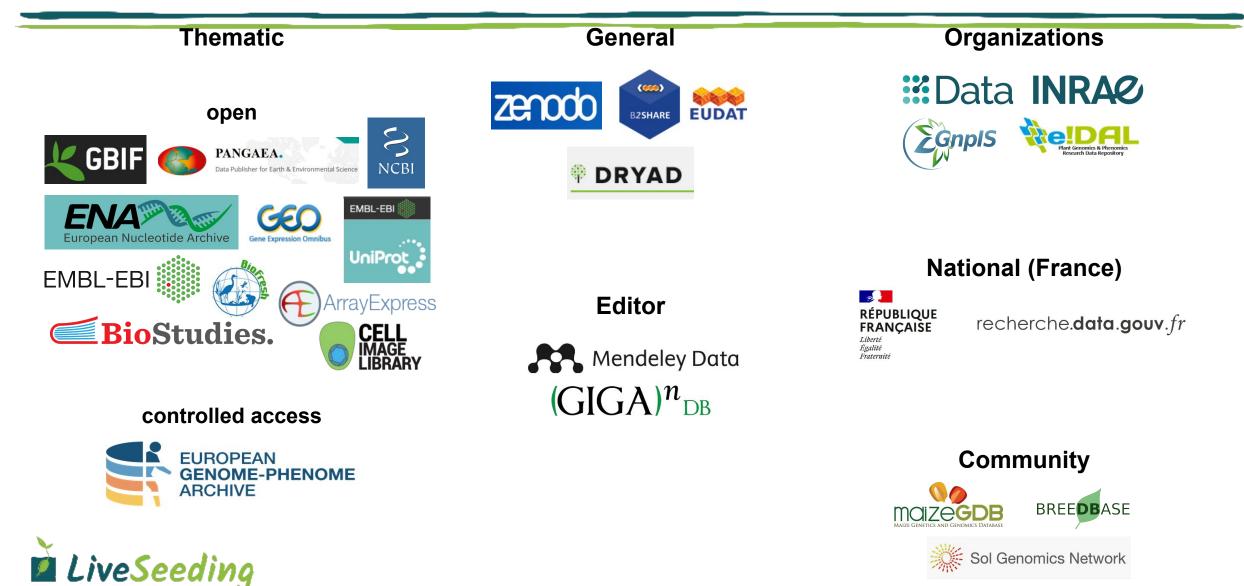
General data warehouse

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- All data types
- Minimal metadata to publish
- Fast submission
- - Poor description
 - non-standard format
 - Less FAIR



Examples of data warehouses



Tips to choose your data warehouse

Consider these criterion to choose you data warehouse :

- Choose a thematic warehouse especially if it is an established one such as ENA (European Nucleotide Archive) for sequence data
- Choose a national/institutional warehouse if you have one in your country
- If you don't find a warehouse that fits this criteria find one this is : open source, general scope, provide a DOI, robustly funded.



Short test

Download the quiz : https://tinyurl.com/96dfw6wp

And send it to <u>yannick.de-oliveira@inrae.fr</u>



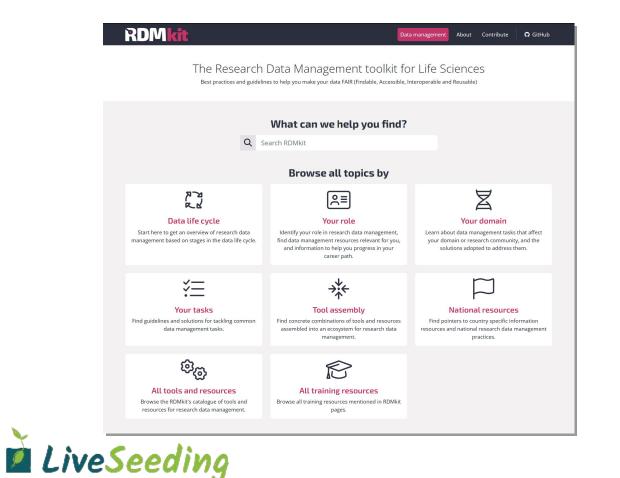
Key messages

- Be FAIR with your data :)
- Use tidy data, standard and controlled vocabularies to increase quality of your data
- Share your data with appropriate license and warehouse to make them reusable



Resources

<u>https://rdmkit.elixir-europe.org/data_life_cycle</u>



RDM	cit l	Data management About Contribute 🖓 GitHub 🔍 Search RDMkit
Data manageme	ent	Your domain
Data life cycle	~	Plant sciences 🕢 📭
Your role	~	
Your domain	^	Introduction
Bioimaging d	ata	Plant biological materials: (meta)data collection and sharing
Biomolecular simulation da		Phenotyping: (meta)data collection and publication
Epitranscripto data	ome	Genotyping: (meta)data collection and publication
Human data		Related pages More information
Intrinsically disordered proteins		Relevant tools and resources
Marine metagenomic	CS	Introduction
Microbial		Data management challenges in plant sciences
biotechnolog		The plant science domain includes studying the adaptation of plants to their environment,
Plant science	S	with applications ranging from improving crop yield or resistance to environmental conditions, to managing forest ecosystems. Data integration and reuse are facilitators for
Proteomics		understanding the play between genotype and environment to produce a phenotype, which

Resources

Controlled vocabularies :

https://agrovoc.fao.org/browse/agrovoc/en/ https://cropontology.org/

Data Management Plan :

https://dmp.opidor.fr/ https://ds-wizard.org

Metadata standard :

https://www.miappe.org/ https://fairsharing.org/

Interoperability

https://brapi.org/

Licenses

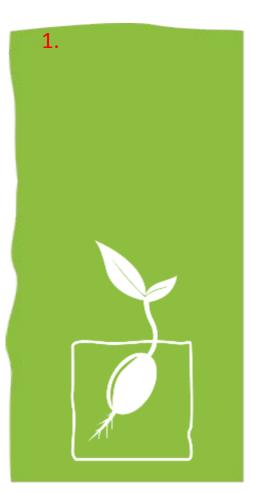
https://creativecommons.org/

Data warehouse

https://zenodo.org/ https://recherche.data.gouv.fr/fr



Module 2 – Unit 3 Additional available materials





Initial steps toward reproducible research

Karl Broman's tutorial: http://kbroman.org/steps2rr/

- 1. Everything with a script:
 - Get the data in the most-raw form, Download external data, Convert a data file, Don't handedit data files, Data cleaning should be in scripts, Analysis should be in scripts, Save your seeds for random number generation.

2. Organize your data and code:

- Encapsulate everything within one directory, Separate raw data from derived data, Separate the data from the code, Use relative paths, Choose file names carefully, Avoid using "final" in a file name (rather version number), Write ReadMe files
- 3. Automate the process
- 4. Turn scripts into reproducible reports
- 5. Turn repeated code into functions
- 6. Package functions for reuse

Module 2 – Unit 3 Additional available materials

Initial steps toward reproducible research:

- Karl Broman's tutorial: <u>http://kbroman.org/steps2rr/</u>
- Teach yourself:
 - Software Carpentry (https://software-carpentry.org/),
 - MOOC RR (https://www.fun-mooc.fr/fr/cours/recherchereproductible-principes-methodologiques-pour-unescience-transparente/ in French),
 - Forum RR (https://forum.recherche-reproductible.fr/)





LiveSeeding

Thank you !