BioData.pt

Ready for BioData Management?

Introduction to Research Data Management

Daniel Faria

Data, Information & Knowledge

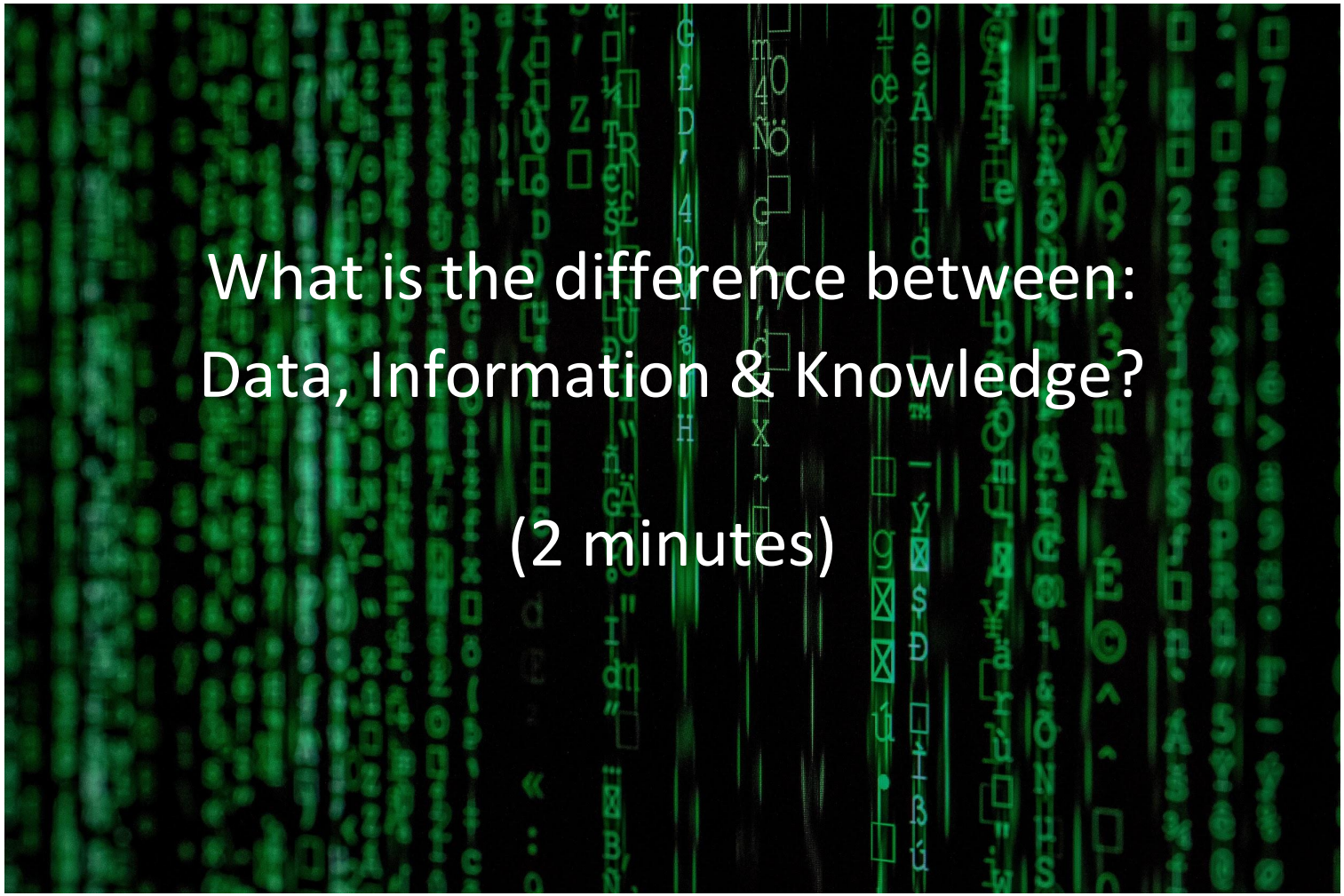
Learning Outcome 1:

Distinguish between Data, Information and Knowledge

Introduction

- The main goal of science is to discover knowledge
- This typically requires gathering / generating data
- Data, information, and knowledge are concepts that are often used interchangeably
- In this section, we will dissect their differences which bear on the dissemination of scientific outputs

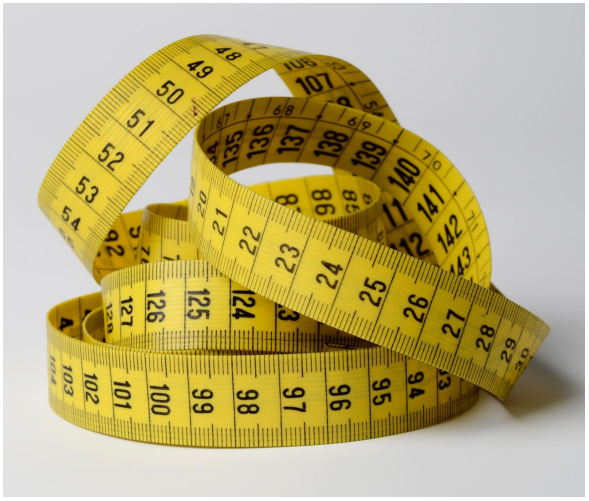
Group Discussion



By Markus Spiske temporausch.com from Pexels

Data

- Datum: an atomic fact or piece of “information”
  - Melting Point: 0℃
  - Boiling Point: 100℃
- Dataset: a collection of data that share an object or scope



By Marta Longas from Pexels

Information

- Information: data + context (metadata)
  - Substance: Water
  - Total Dissolved Solids: < 500 mg/L
  - Pressure: 1 atm

Metadata

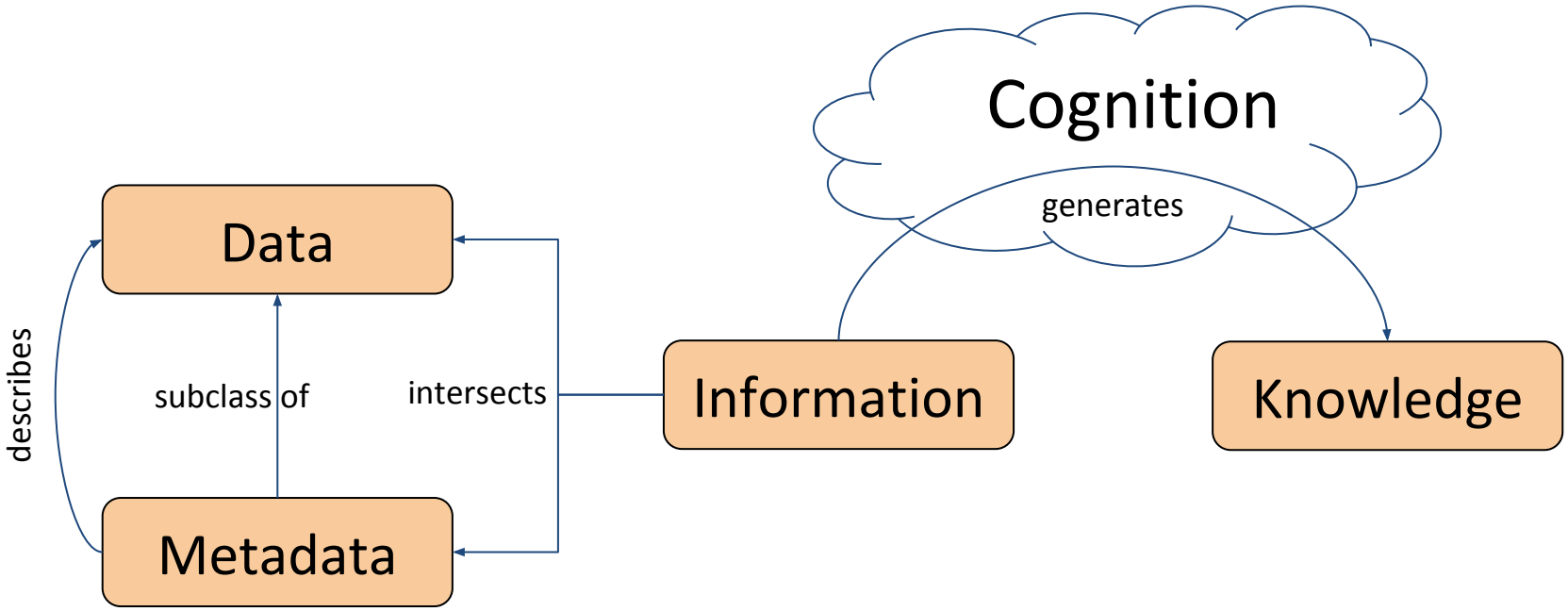
- Metadata = data about data
- Metadata = context
  - Who produced the data?
  - When was the data produced?
  - What is the data about?
  - Why was the data produced?
  - How can the data be used? (license)

By Dr. Marcus Gossler - Own work, CC BY-SA 3.0

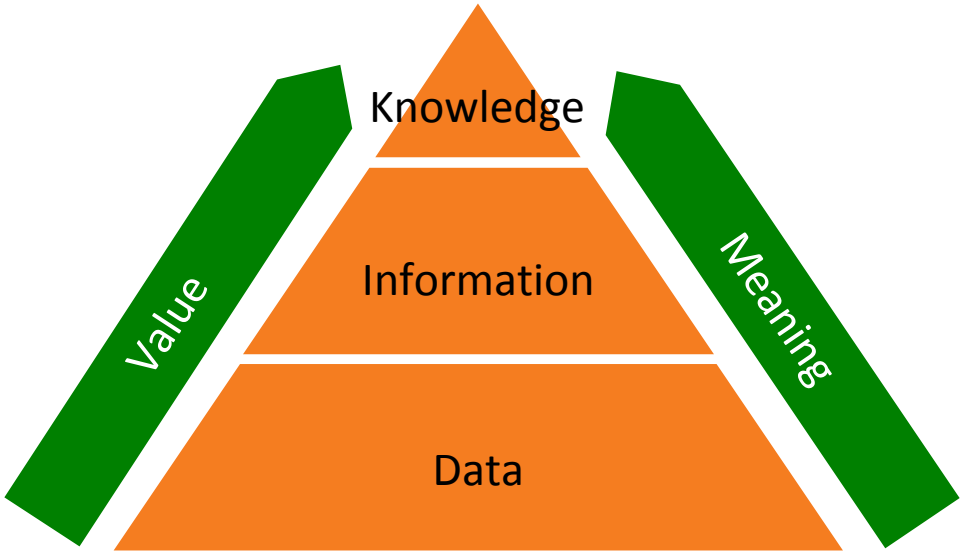
Knowledge

- Knowledge: information + (actionable) understanding
  - If I heat tap water until it starts boiling, I can cook food at 100℃
  - If I see water boiling, I shouldn't put my hand in it

Data, Information & Knowledge



Data, Information & Knowledge



The Knowledge Discovery Problem

Learning Outcome 2:

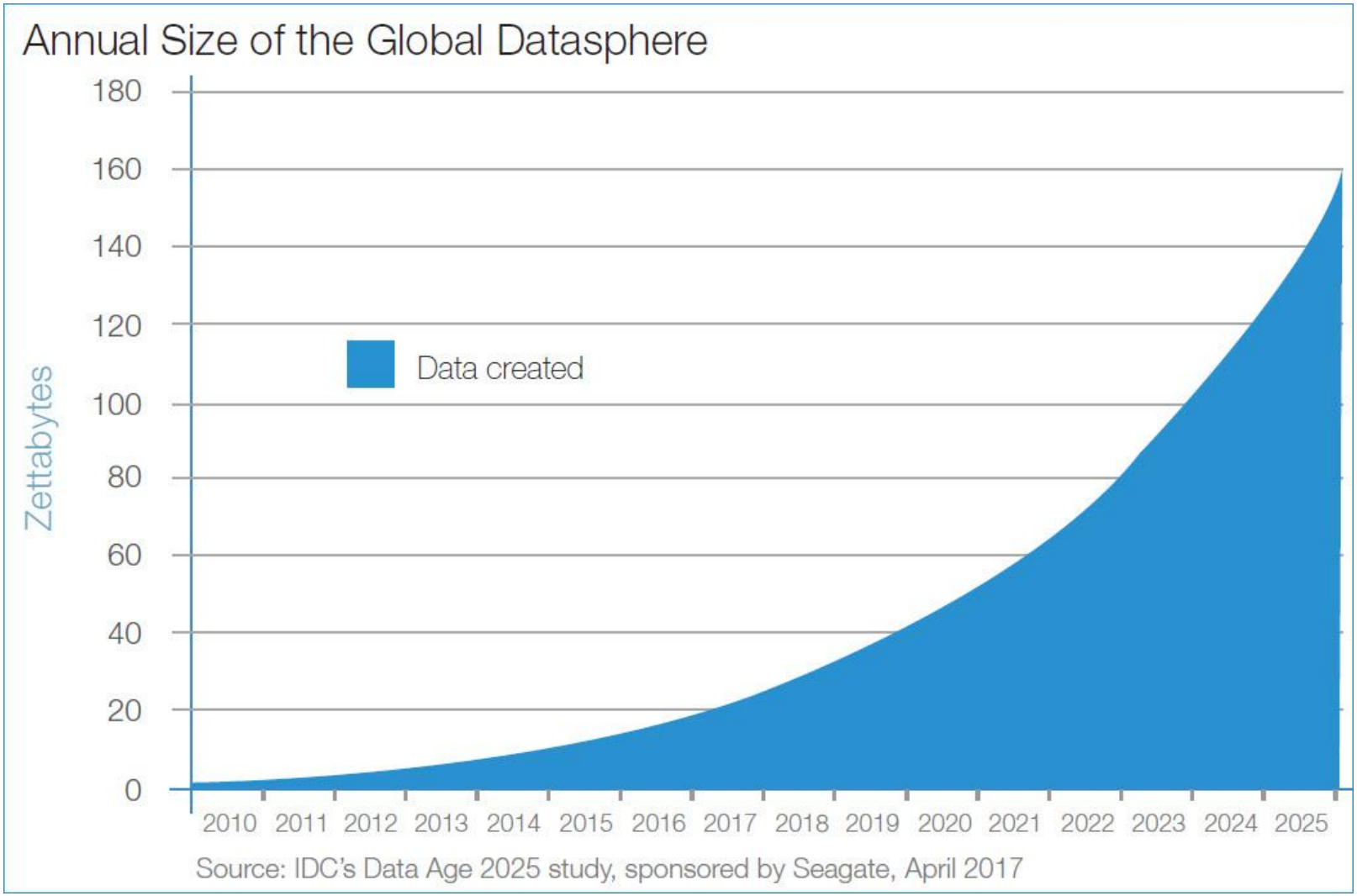
Identify the solutions to the three components

of the knowledge discovery problem

Introduction

- Scientists generate data to discover knowledge, but there is often additional value in the data (reuse)
- Scientists are assessed for sharing the knowledge, while data sharing takes on a supporting role
- To reuse research data, we often must:
  - Read paper wherein it was described
  - Extract the metadata needed for interpreting it
  - Figure out if the data is relevant, accessible and usable
- In this section, we will debate how this is not scalable and creates a bottleneck, and what can be done to address that

The Knowledge Discovery Problem



The Knowledge Discovery Problem

Findability:

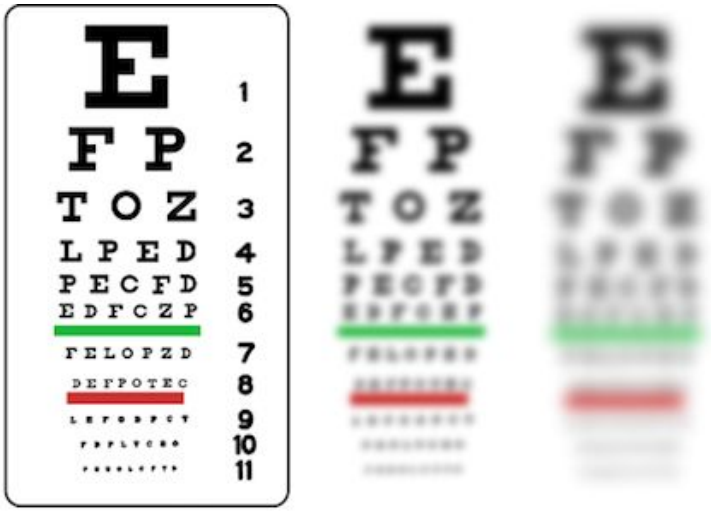
- More data ⇒ harder search
- Things can get lost amid a sea of things
- If it is not findable, it might as well not exist

By Martin Handford, retrieved from: https://exploringyourmind.com/how-does-our-brain-find-waldo/

The Knowledge Discovery Problem

Interpretability:

- More data ⇒ more costly to interpret
- We become myopic by necessity—can't afford the time to read the fine-print (e.g. full research papers)
- If we cannot interpret it readily, then it is nearly useless



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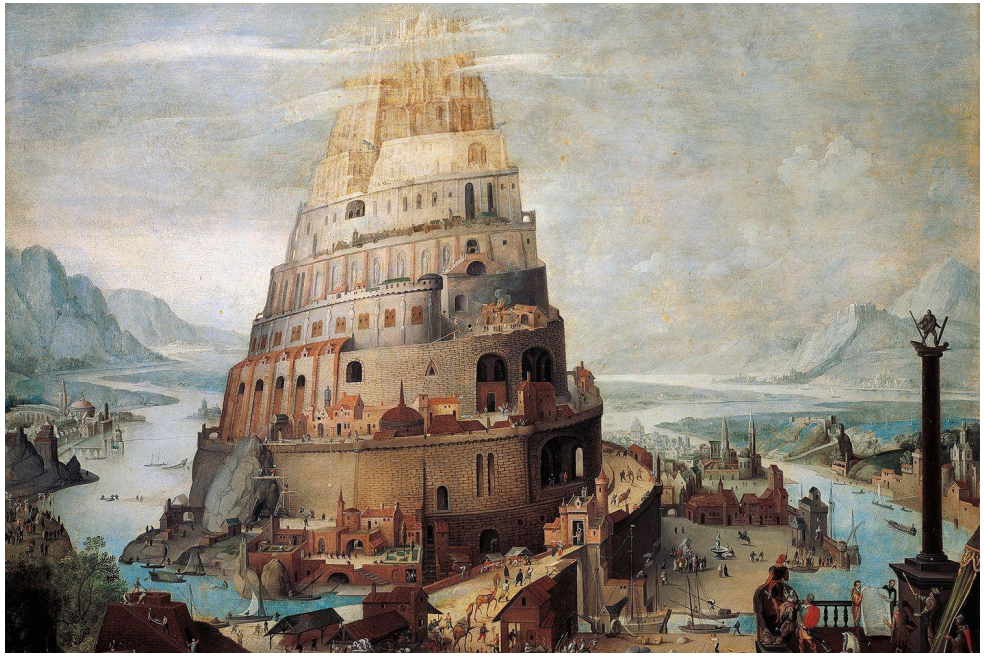
The Knowledge Discovery Problem

Interoperability:

- More data & specialization ⇒ vocabulary and viewpoint divergence
- Use of local dialects leads to sundered data and knowledge
- If we don't find common ground, we cannot integrate data from related domains



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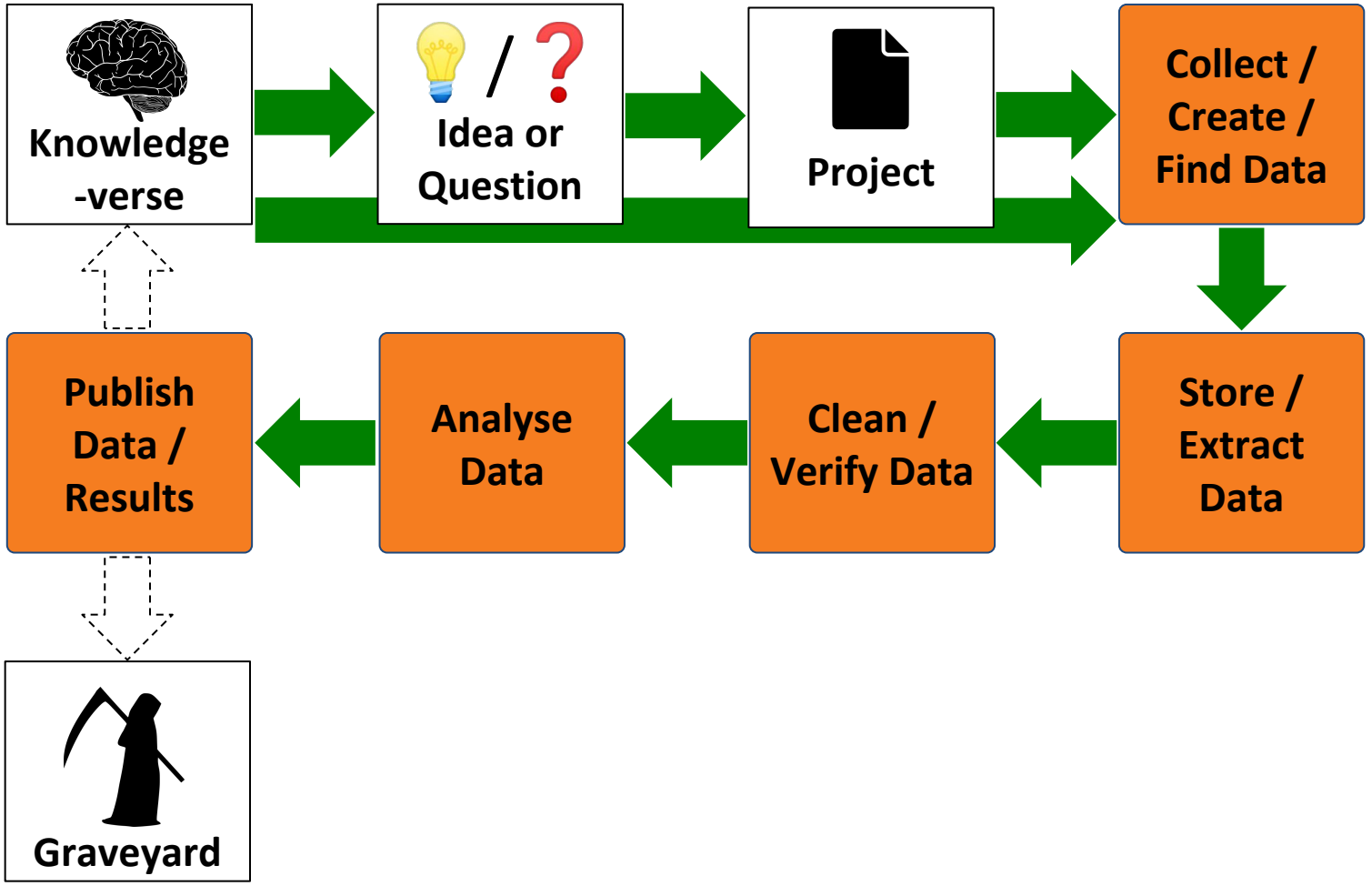
The Data Lifecycle



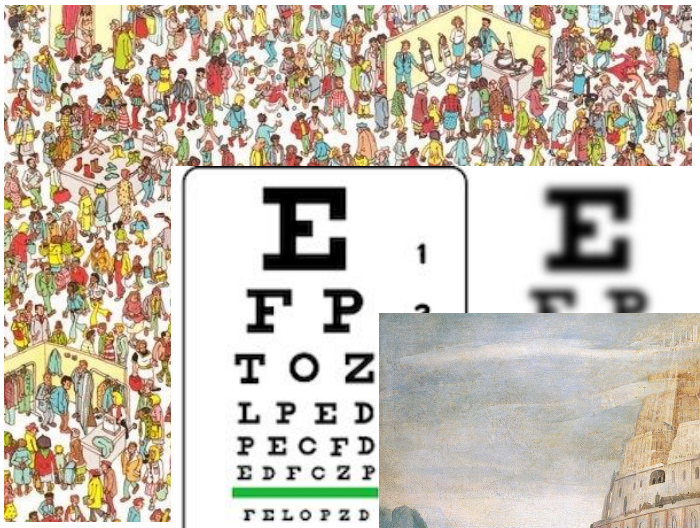
The Knowledge Discovery Problem

Wrap-Up:

- Publishing data only in scientific papers is not enough
  - Papers are not efficient vehicles for knowledge transfer!!!
- If we want our data to effectively contribute to the knowledge-verse:
  - We must publish it in a form that is:
    - Findable
    - Interpretable
    - Interoperable

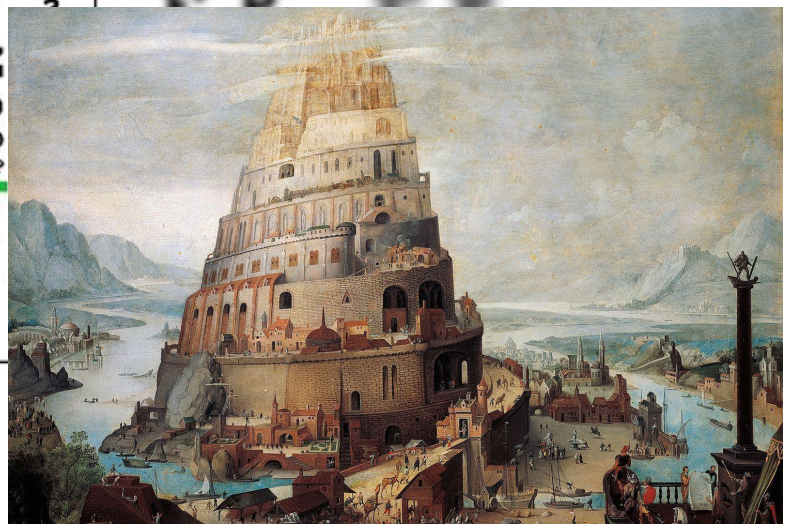
Group Discussion

How to make data:



Findable?

Interpretable?



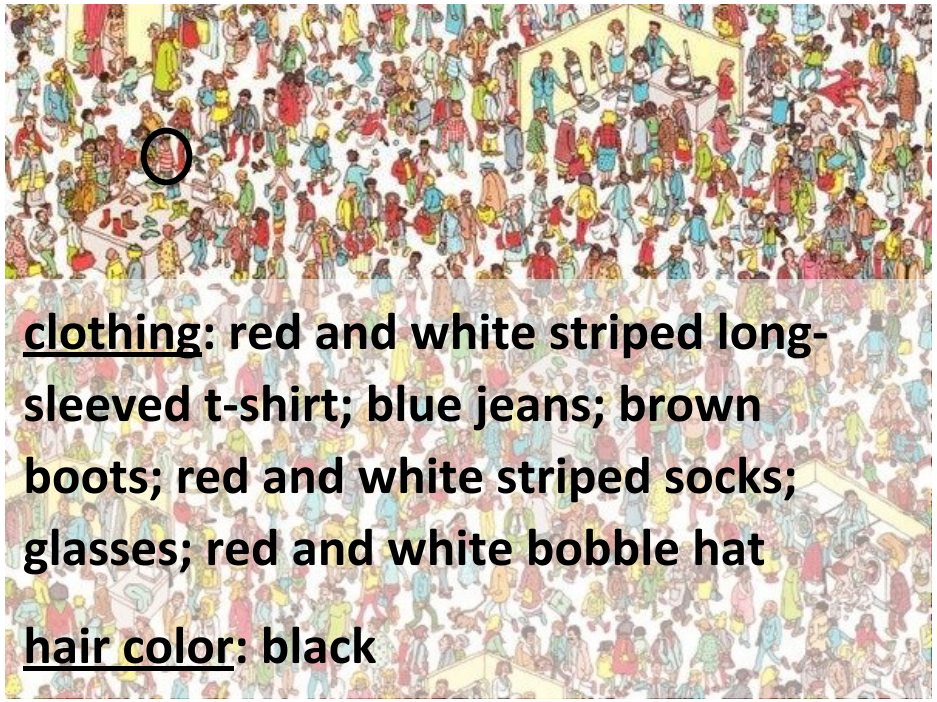
Interoperable?

(5 minutes)

The Knowledge Discovery Solution

Findability:

- Describe data with precise metadata useful for searching
- Use a common (structured) controlled vocabulary for metadata fields and values
- Put data in a repository that:
  - Uses persistent unique identifiers
  - Indexes metadata and allows searches

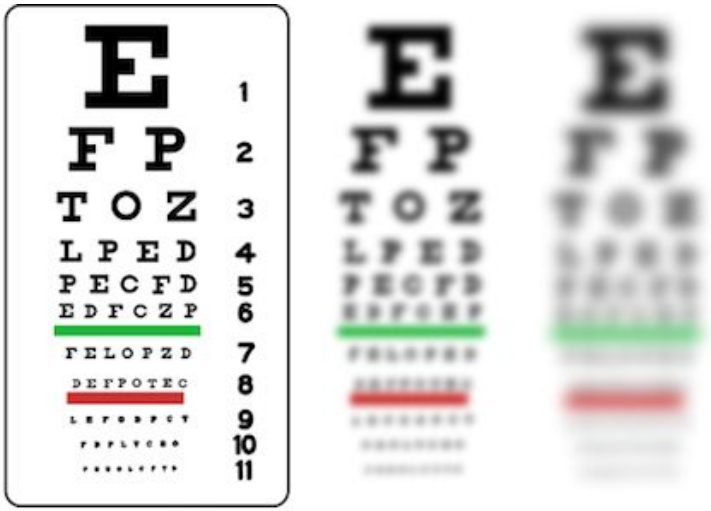


By Martin Handford, retrieved from: https://exploringyourmind.com/how-does-our-brain-find-waldo/

The Knowledge Discovery Solution

Interpretability:

- Describe data with sufficient metadata for interpreting it and understanding the experimental context—each dataset should be fully self-contained
- Use a common (structured) controlled vocabulary for metadata fields and values

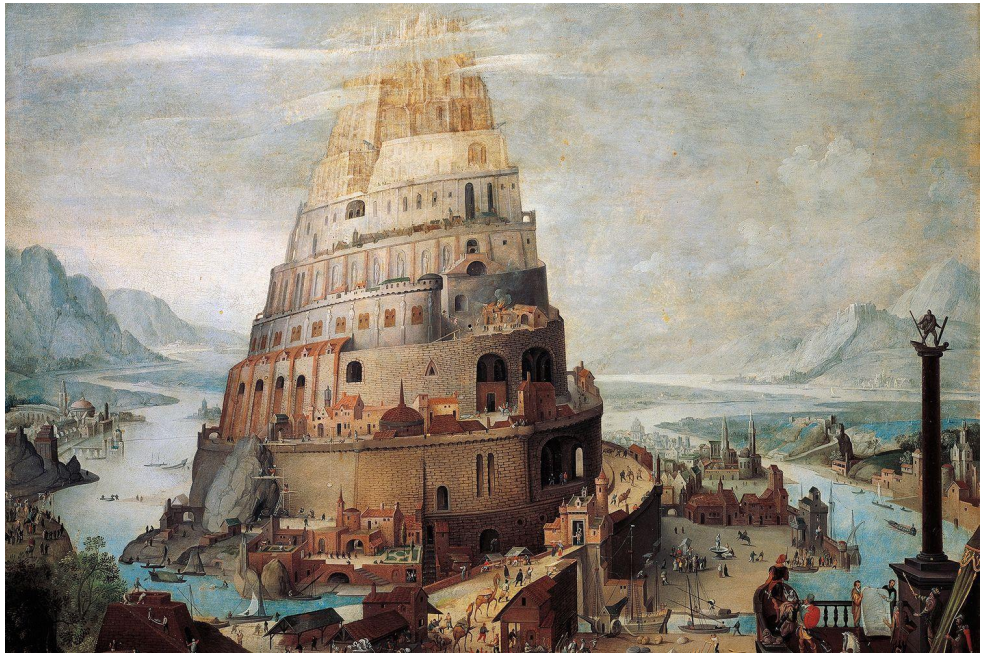


By Daniel P. B. Smith, CC BY-SA 3.0
https://en.wikipedia.org/wiki/File:Snellen-myopia.png

The Knowledge Discovery Solution

Interoperability:

- Use a common (structured) controlled vocabulary for metadata fields and values
- Include cross-references to external data objects whenever suitable (e.g. NCBI taxon id)



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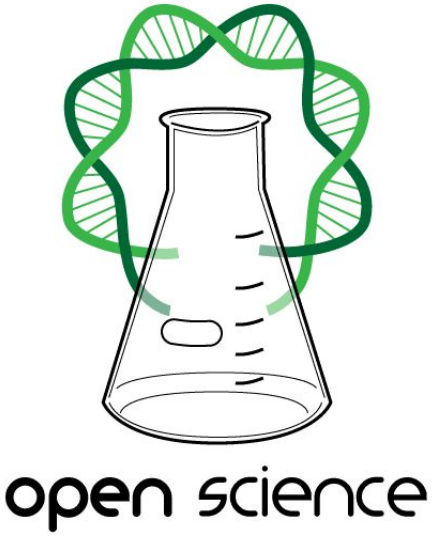

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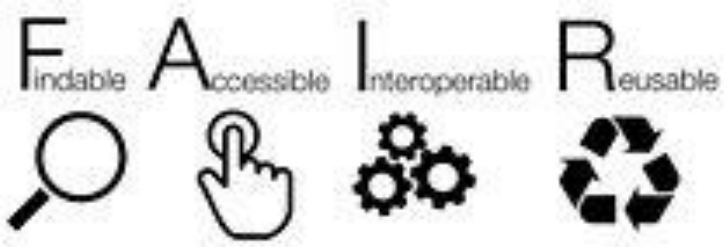

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Open Science & FAIR Principles

Learning Outcome 3:

Recognize the demands of science funders
and debate their pros and cons

Introduction

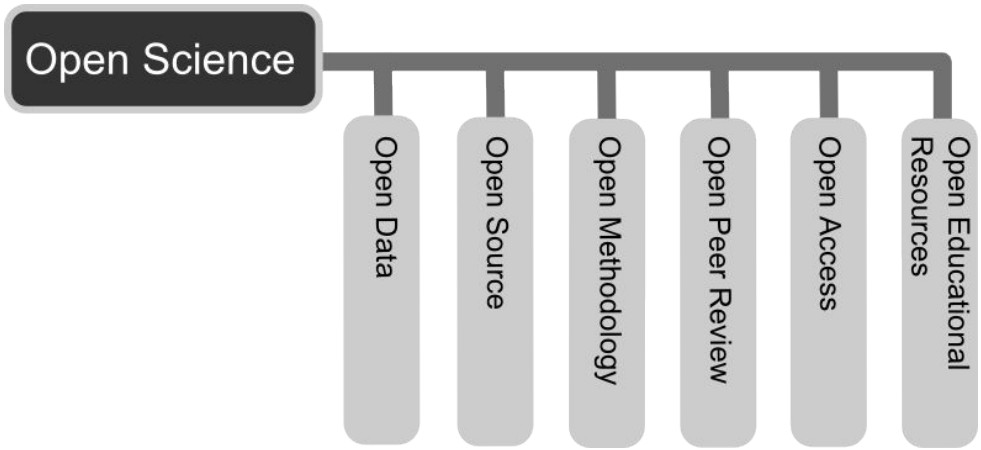
- The need to improve scientific dissemination has been recognized by research communities and publishers
- Leading to initiatives such as Open Science and the FAIR principles
- Funders recognized and are endorsing these initiatives (H2020 projects now require FAIR compliance)
- In this section, we will analyse these initiatives and the demands of funders and illustrate why complying with them is ultimately to the advantage of all

TO DO OPEN SCIENCE AND PUBLISH FAIR DATA!

What is Open Science?

Goals:

- Scientific research and its dissemination accessible to all levels of society
  - publications
  - data
  - physical samples
  - software
  - ...



- Transparent and accessible knowledge shared and developed through collaborative networks

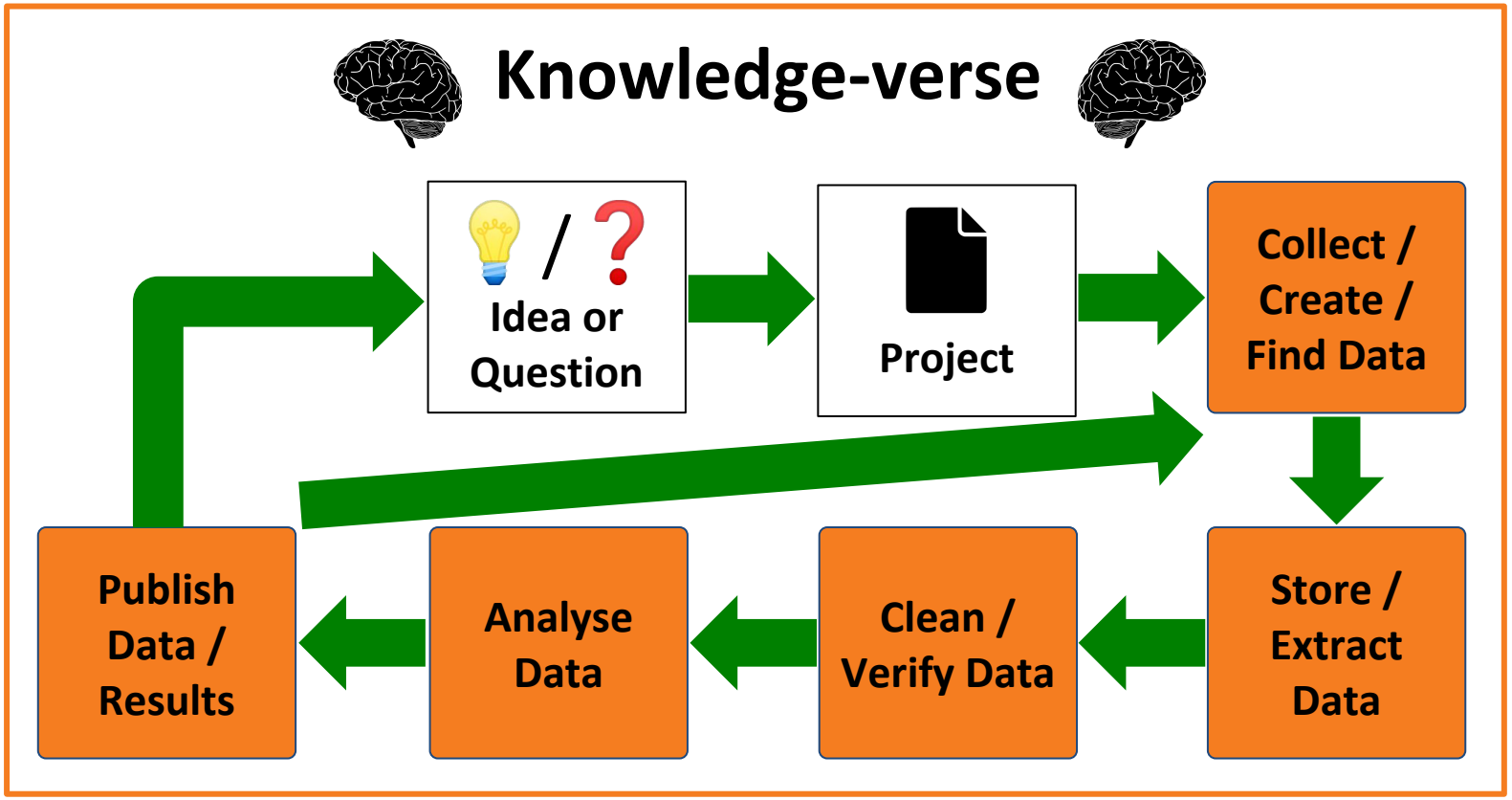
What is Open Science?

Layers:

- **Open Access**: research outputs distributed online, free of cost or access barriers
- **Open Research**: data, result and methodology clearly documented and freely available online
- **Open-Notebook Science**: primary record of a research project publicly available online as it is recorded—no insider information

What Is Open Science?

Everything documented & freely available!



What are the FAIR Data Principles?

A set of four principles detailed in fifteen guidelines, that establish what Open Research should aim for.

Findability – (Meta)data should be easy to find for both humans and computers

Accessibility – (Meta)data should have a defined access protocol with authentication and authorization rules

Interoperability – (Meta)data should be integratable with other similar datasets and interpretable by applications or workflows for analysis, storage, and processing

Reusability – (Meta)data should be well described so that it can be interpreted and reused

The FAIR Data Principles

II

The Knowledge Discovery Solution

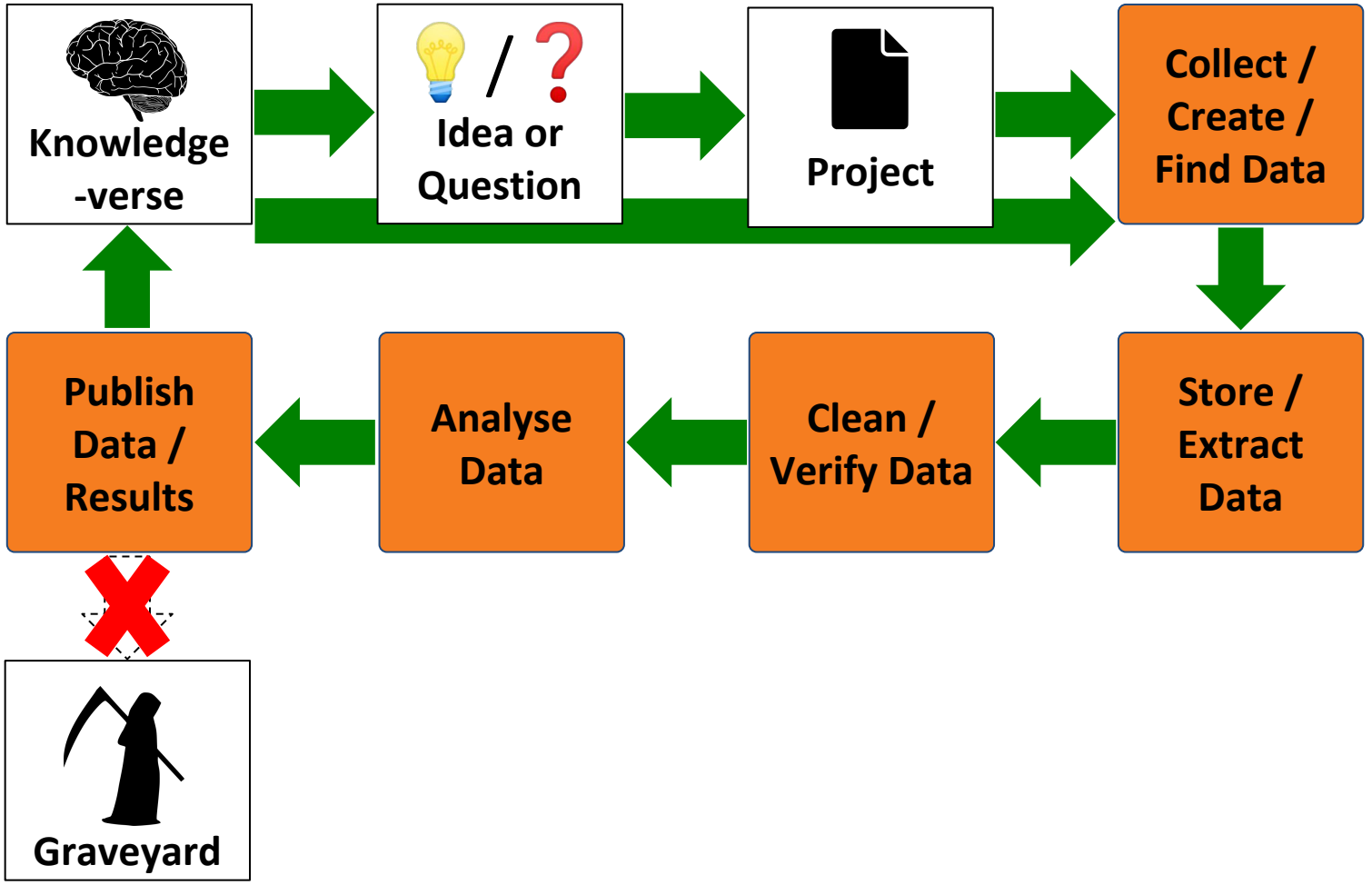
Wait, that was FII, Not FAIR...

- Reusability is the end-goal, not the problem—it is contingent on Interpretability and Interoperability.

- Accessibility concerns data repositories, not really researchers, and it is already well addressed. As long as you publish your data in a well-established repository and define an authorization policy (when applicable, such as for sensitive data) you are well off.

What Are The FAIR Data Principles?

Goal: Enable Data & Knowledge Discovery



Group Discussion

FAIR & Open Science—Pros & Cons

Pros:

- Facilitates knowledge discovery
- Promotes reproducibility / impedes fake science
- Enables networking
- Helps demystify science for the general public

Cons:

- Care with sensitive data and with knowledge that has dangerous misuse potential
- Harder to make money off of your research
- Harder to stay ahead of your competitors

FAQ

- **Can I receive credit for publishing data?**
  - This is not yet well established, but we are amidst a shift towards crediting data publishers as much as paper publishers.
- **Can't someone publish a paper ahead of me if I release my data?**
  - If someone can write a paper using your data ahead of you that supersedes yours, shame on you. If it does happen, you at least get credit for the use of your data, and will likely still be allowed to publish your paper as the original author of the data.
- **What if someone uses my data without giving me credit?**
  - The same can happen with paper publication. Reviewers and editors are expected to police this. Authors that do so can be red flagged.

To Be or Not to Be Open & FAIR???

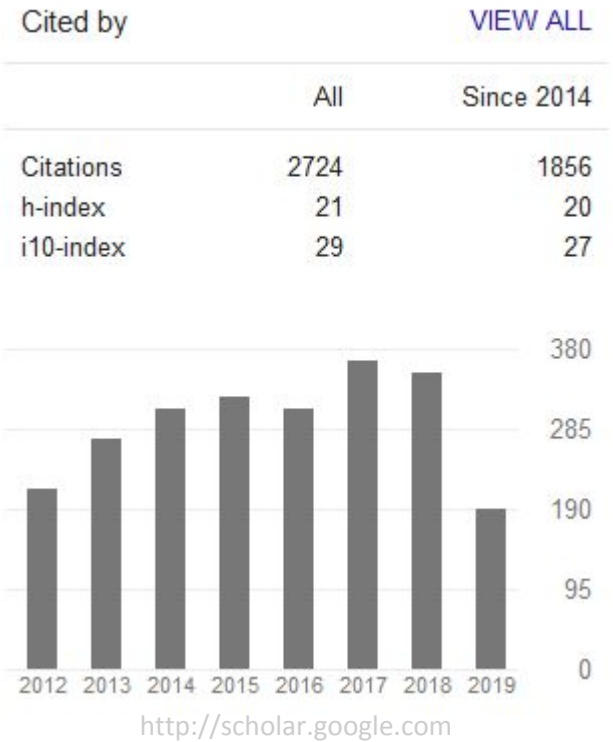
It Helps Science!

- Enables others to apply your knowledge in contexts beyond your foresight
- Enables others to reuse your data to make new research

To Be or Not to Be Open & FAIR???

It Helps You!

- It is easier to find and reuse your own data
- It is easier to write and submit a research paper
- If others apply or reuse your research, you get more citations (citing or crediting datasets is becoming common practice)

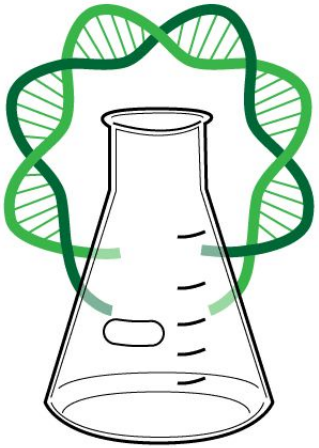


http://scholar.google.com

To Be or Not to Be Open & FAIR???

You'll Need It To Get Funded!

- Soon it will be impossible to get public funding in Europe without adherence to Open Science and FAIR
- FAIR compliance is starting to be verified
- A good track record will contribute to project approval



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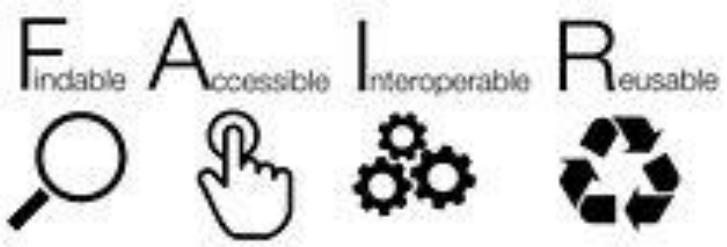


By SangyaPundir - Own work, CC BY-SA 4.0

Open Science & FAIR Principles (Again!)

Learning Outcome 4:

Comply with the demands of science funders

Introduction

- We´ve seen that adherence to Open Science and compliance with the FAIR principles are being increasingly demanded by funding agencies
- And debated the merits and demerits of compliance
- In this section, we will dissect what must be done in practice to comply with these demands

TO DO OPEN SCIENCE AND PUBLISH FAIR DATA!

How to be Open & FAIR?

Step 1 – Do Your Homework

- Is there a default public database or repository for your research domain?
  - Does it have a metadata schema?
- Are there community metadata standards?
  - Do they cover your use case?
- Are there adequate ontologies?
  - If more than one, which is best?
- Are there default data (open) file formats?

How to be Open & FAIR?

Step 1 – Do Your Homework

- Lookup the best examples of FAIR data publication in your domain and follow their practices
- Consult information hubs about existing standards, such as FAIRsharing.org
- Search for key concepts through ontology lookup services, such as BioPortal
- Consult data steward or data manager at your institution

How to be Open & FAIR?

Step 1b – Do More Homework

- If there are no standards in one or more of the previous categories, you have three alternatives:
  - Use a generic option (not valid for ontologies, and not very FAIR)
  - Use / adapt the closest option
  - Rally your community and develop / agree on a standard

How to be Open & FAIR?

Step 2 – Do Your Work-Work

- Organize, Document & Annotate:
  - Your code / scripts / workflows,
  - Your protocols
  - Your data & metadata
- According to the applicable guidelines / standards or the repository where you're depositing your data / materials
- Using domain ontologies, recommended file formats
- Cross-referencing all relevant information objects

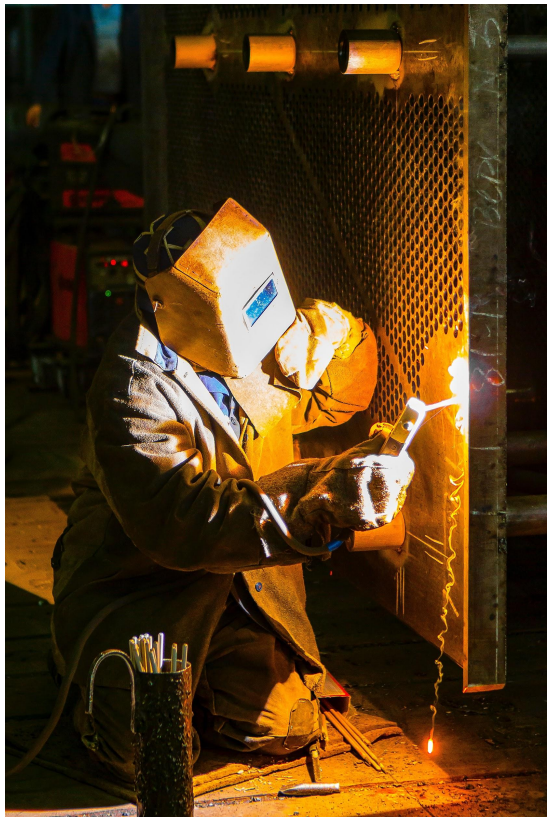


Photo by Kateryna Babaieva from Pexels

How to be Open & FAIR?

Step 3 – Deposit

- Deposit your data and materials in an appropriate public repository:
  - Code / scripts / workflows: GitHub, BitBucket
  - Protocols: Zenodo, FAIRDOMHub, Dataverse
  - Data: Domain database, one of the above
  - Metadata: Together with the data (as an accessory file, in the form of the repository)
- Under a declared usage license
- With a clear versioning policy

Photo by cottonbro from Pexels

How to be Open & FAIR?

Example – Transcriptomic Data

- Gene expression data:
  - Data repository:
    - ArrayExpress (EU) or Gene Expression Omnibus (US)
  - Metadata standard:
    - MIAME
  - Ontologies:
    - Experimental Factor Ontology
    - ...
  - Data file formats:
    - MAGE-Tab (metadata)
    - FASTQ (raw sequencing data)
    - Tabular text (read count data, differential expression data)

How to be Open & Fair?

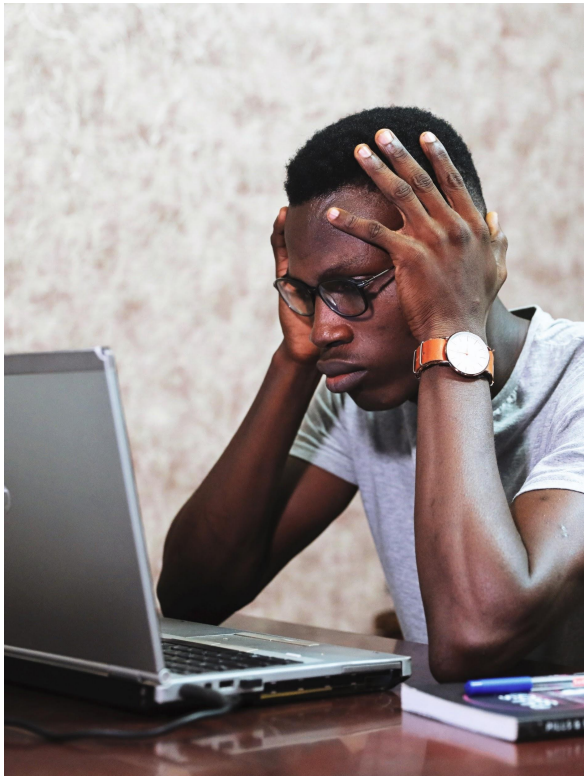
The Main Hurdles

- The Biomedical Ontology landscape is complex and hard to navigate:
  - There are often overlapping ontologies for a given domain
  - And worse, the same concepts appear in several ontologies, sometimes with the same URI!!!
  - But there are also domains with no (suitable) ontology
- Metadata standards exist only for a few domains, and not all specify a data format for publication
- Generic data repositories (e.g. FAIRDOMHub, Zenodo, Dataverse) have rigid data models that are not compatible with all domains / standards

How to be Open & FAIR?

That sounds like a lot of work!

- It is, especially if you only do it at the time of publication:
  - Have to trace all the data—risk of data loss
  - Have to recall all the details about the experiment—risk of metadata loss, compromises reproducibility
  - It is a lot of boring work to do at once—inertia and rush lead to poor job



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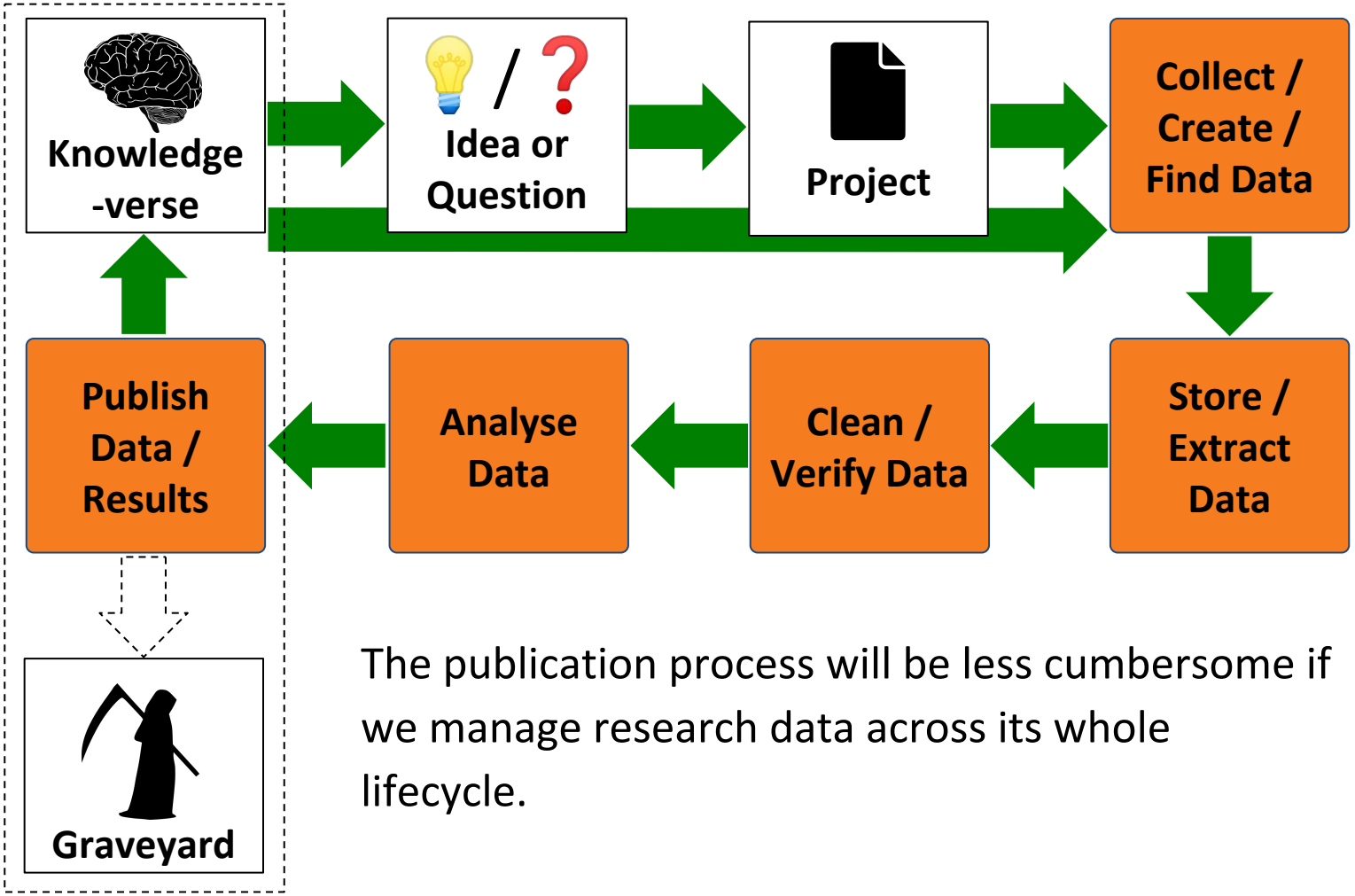
How to be Open & FAIR?



The publication process will be less cumbersome if we manage research data across its whole lifecycle.

Research Data Management

Learning Outcome 5:

Recognize the supportive role of data management in science

Introduction

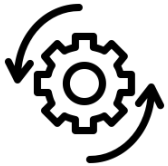
- Data management is a research domain in each own right
- Devoted to topics such as: Data Architecture, Data Modeling, Data Storage & Maintenance, Data Security, Data Integration, Metadata, Data Quality
- Researchers needn't be data management experts
- But just like driving or using a computer, basic knowledge of data management is invaluable for a life in research

Why Should I Care About Data Management?

Improve research:

By LAFS, CC BY 2.0

Effectiveness – obtain more/better results



By Youmena, CC BY 2.0

Efficiency – improve productivity and cost-efficiency

By ROZMOWA, CC BY 2.0

Security – reduce data loss / control access to data

By Nithinan Tatah, CC BY 2.0

Impact – facilitate dissemination and knowledge discovery

Data Management Commandments

- Thou shalt make a Data Management Plan for thy research project, even if it isn't funded by a grant
- Thou shalt allocate some time after each day experimenting to document everything, preferably in a digital platform (e.g. electronic lab notebook, local shared repository)
    - Thou shalt document the documentation process
    - Thou shalt use version control (e.g. git)
    - Thou shalt use controlled vocabularies (public or your own, documented)
- For every data file (or collection thereof) thou shalt create a metadata file

Data Management Resources

- Electronic lab notebooks
- Data analysis platforms
  - Galaxy
- Computing services
- Data management platforms
  - Dataverse
  - FAIRDOMHub
- Information hubs about standards
  - FAIRsharing.org
- DMP platforms
  - Data Stewardship Wizard
- Data management toolkits

Take Home Messages

Do the Best You Can!

- FAIRness is a spectrum, and FAIRer is a step forward

Reach Out For Help!

- Data stewards and data managers can provide guidance

Things Will Get Easier!

- There are people working towards more user-friendly data management solutions—they need feedback on what can be improved