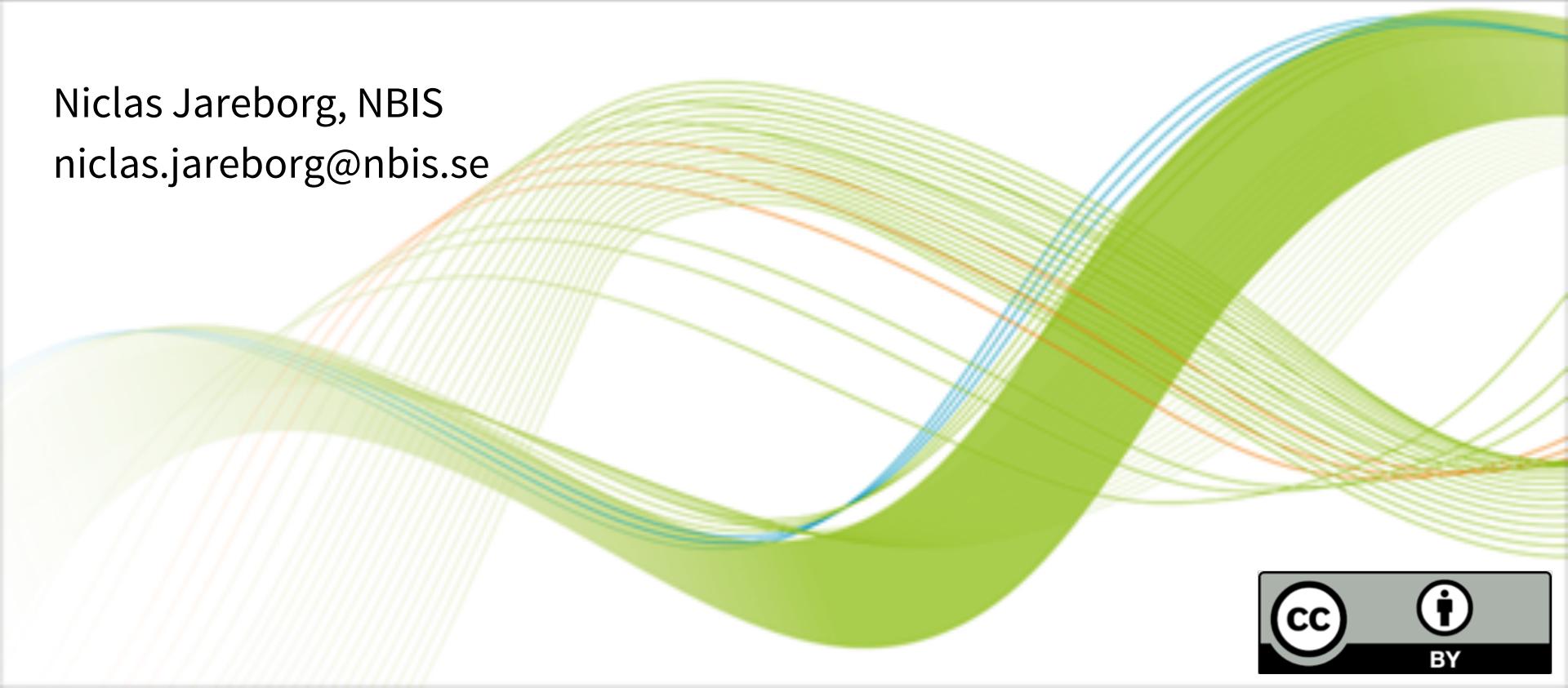
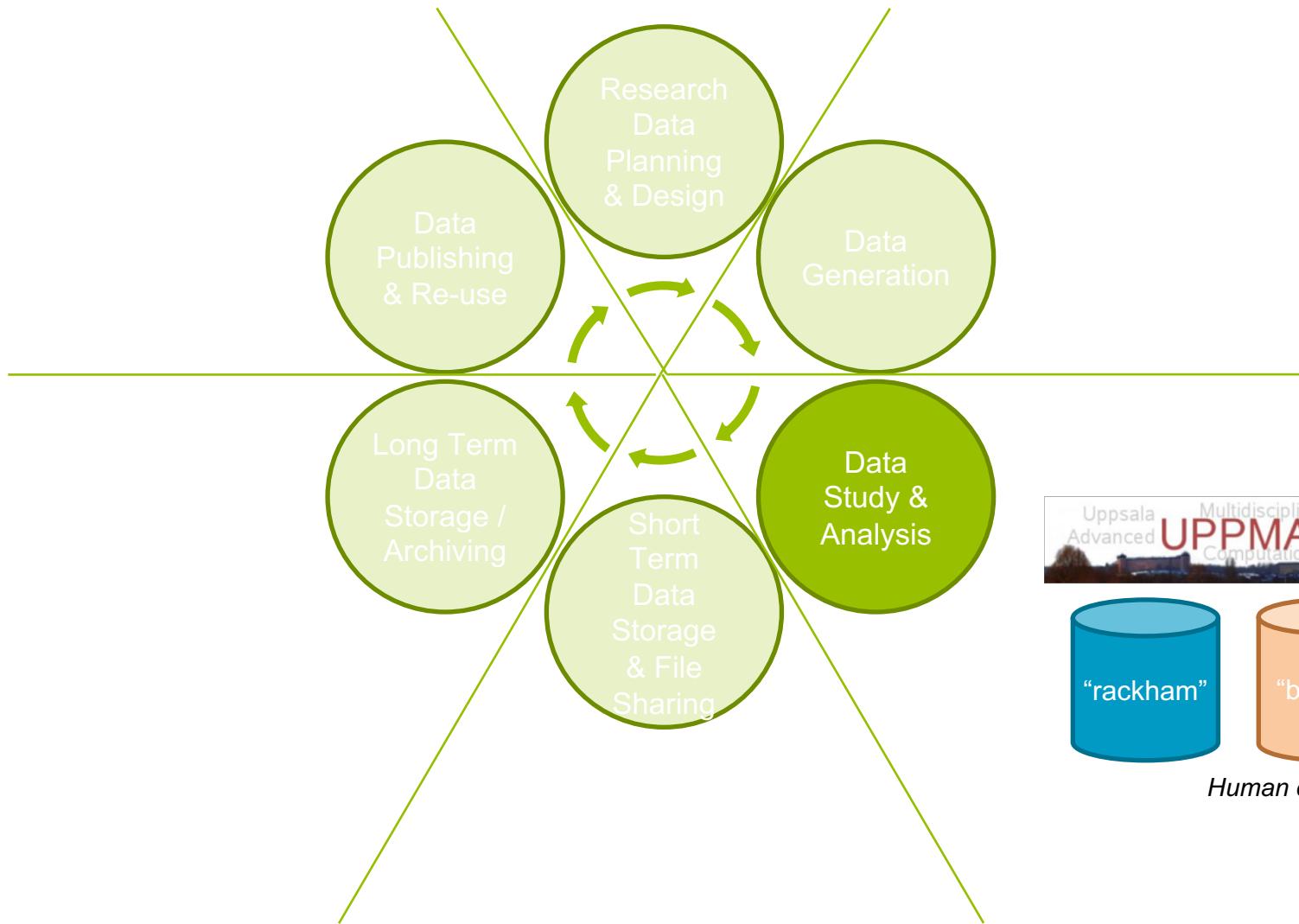

Managing your data

Niclas Jareborg, NBIS
niclas.jareborg@nbis.se



How do you know how an old result was generated?





- Guiding principle
 - “*Someone unfamiliar with your project should be able to look at your computer files and understand in detail what you did and why.*”
- Research reality
 - “*Everything you do, you will have to do over and over again*”
 - Murphy’s law

Trevor A. Branch
@TrevorABranch

Follow

My rule of thumb: every analysis you do on a dataset will have to be redone 10–15 times before publication. Plan accordingly. #Rstats



Poor organizational choices lead to significantly slower research progress

“Your primary collaborator is yourself six months from now, and your past self doesn’t answer e-mails.”



data



samples.mat



data



samples.old.mat

samples.mat



data



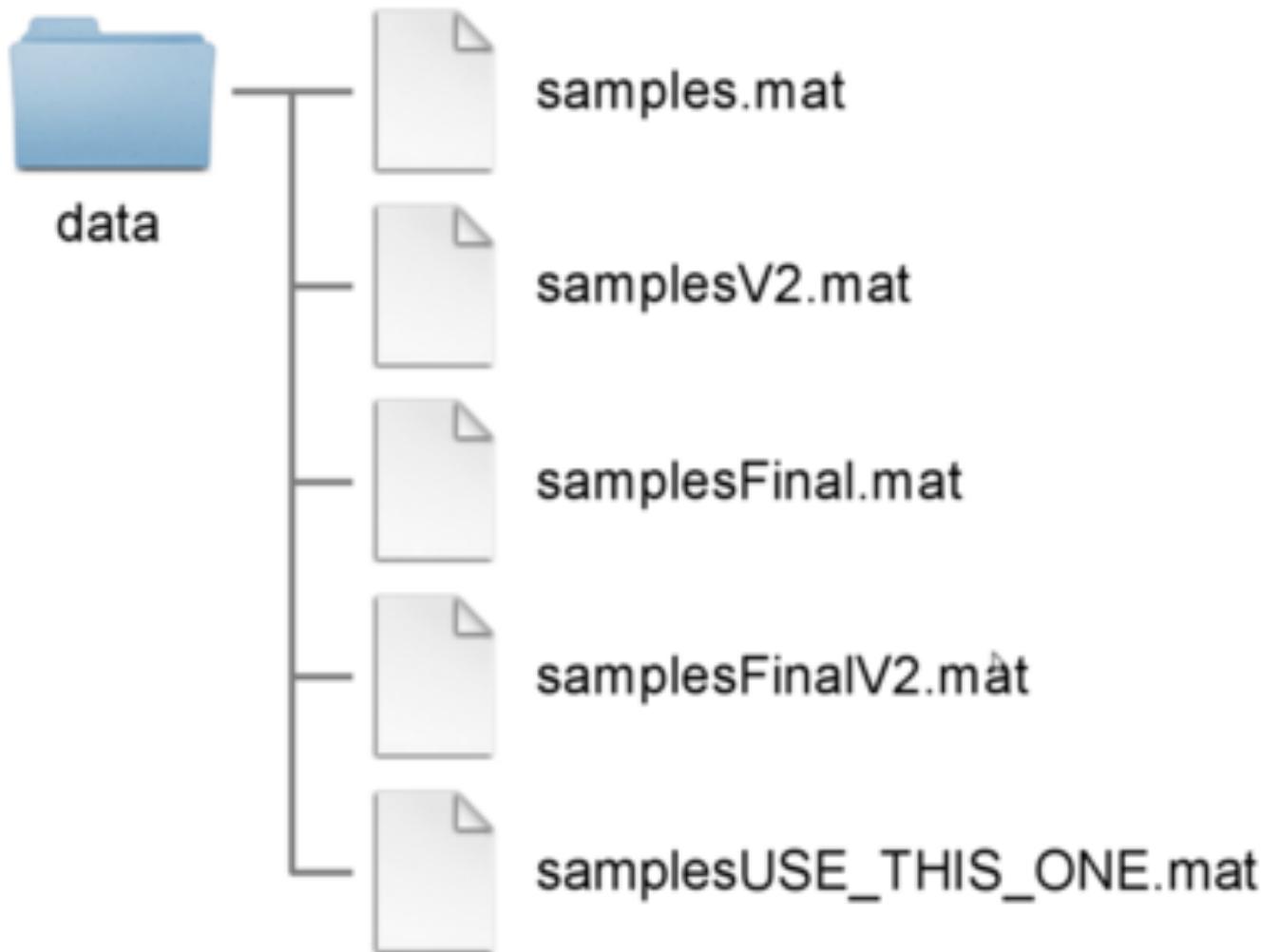
samples.old.mat

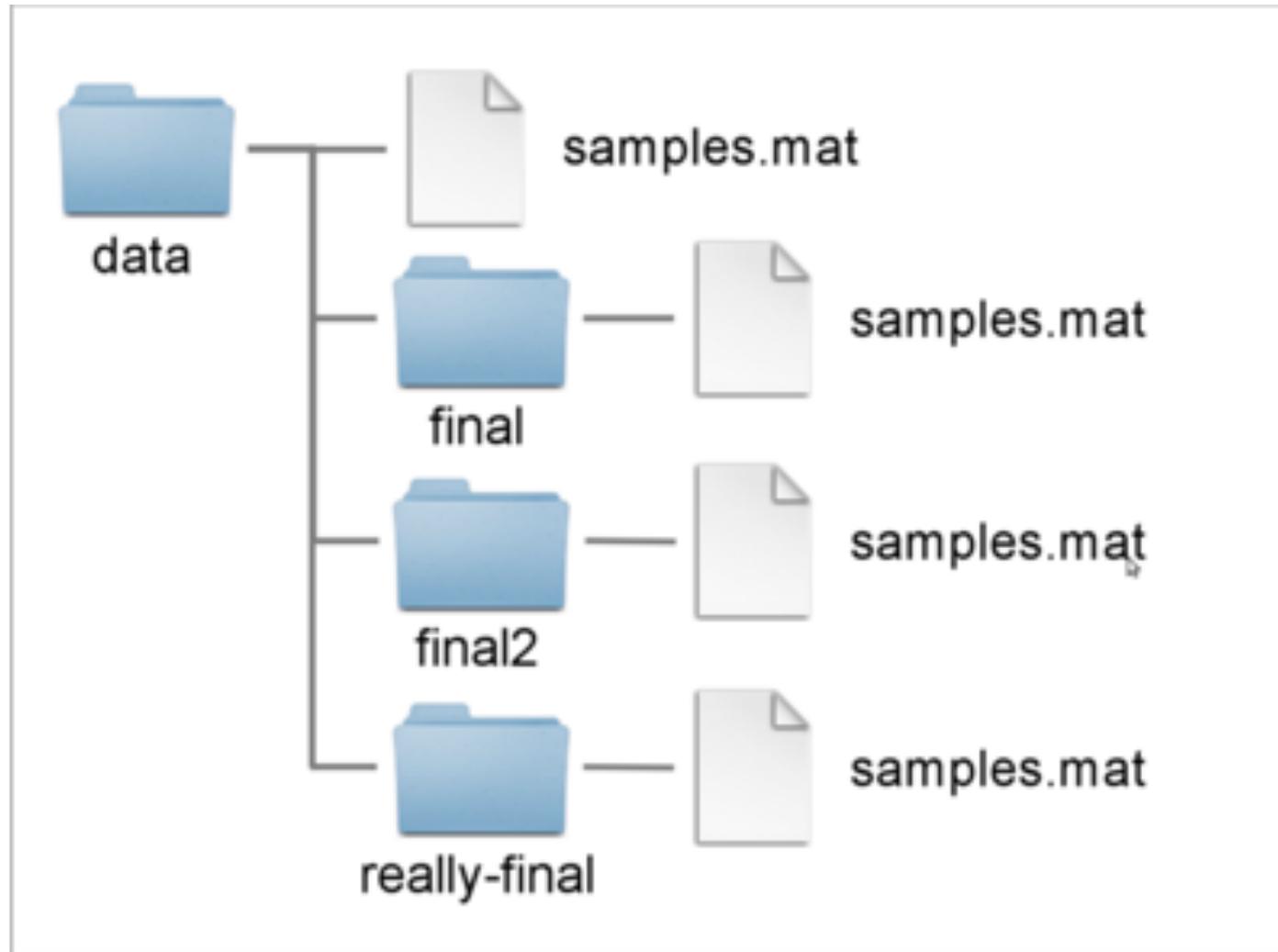


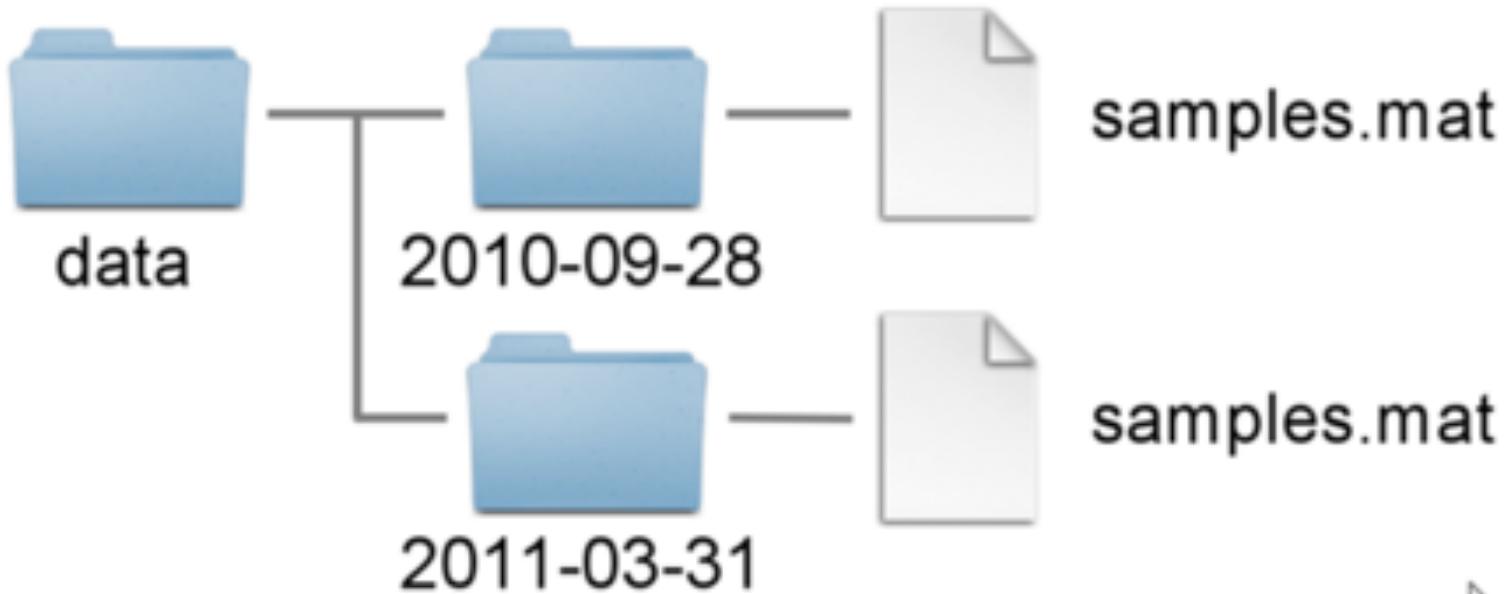
samples.old2.mat



samples.mat

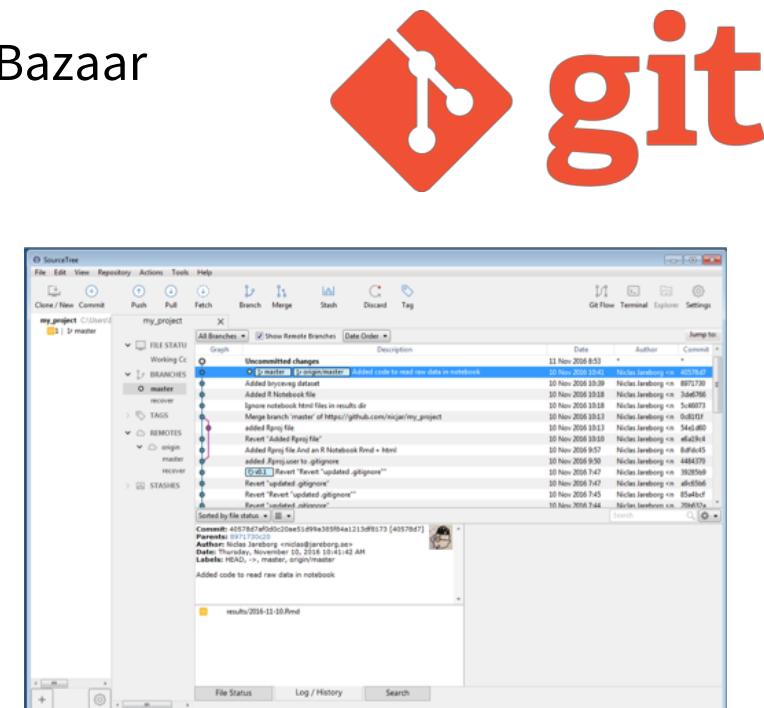






- There is a **folder for the raw data**, which do not get altered, or intermixed with data that is the result of manual or programmatic manipulation. I.e., derived data is kept separate from raw data, and **raw data are not duplicated**.
- **Code is kept separate from data.**
- Use a **version control system** (at least for code) – e.g. **git**
- There is a **scratch directory for experimentation**. Everything in the scratch directory can be deleted at any time without negative impact.
- There should be a **README in every directory**, describing the purpose of the directory and its contents.
- Use **file naming schemes** that makes it easy to find files and understand what they are (for humans and machines)
- Use **non-proprietary formats** – .csv rather than .xlsx
- Etc...

- What is it?
 - A system that keeps records of your changes
 - Allows for collaborative development
 - Allows you to know who made what changes and when
 - Allows you to revert any changes and go back to a previous state
- Several systems available
 - git, RCS, CVS, SVN, Perforce, Mercurial, Bazaar
 - git
 - Command line & GUIs
 - Remote repository hosting
 - GitHub, Bitbucket, etc



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- Use **non-proprietary formats** – .csv rather than .xlsx
- Etc...

- Three principles
 1. Machine readable
 2. Human readable
 3. Plays well with default ordering

NO

myabstract.docx

Joe's Filenames Use Spaces and Punctuation.xlsx

figure 1.png

fig 2.png

JW7d^(2sl@deletethisandyourcareerisoverWx2*.txt

YES

2014-06-08_abstract-for-sla.docx

joes-filenames-are-getting-better.xlsx

fig01_scatterplot-talk-length-vs-interest.png

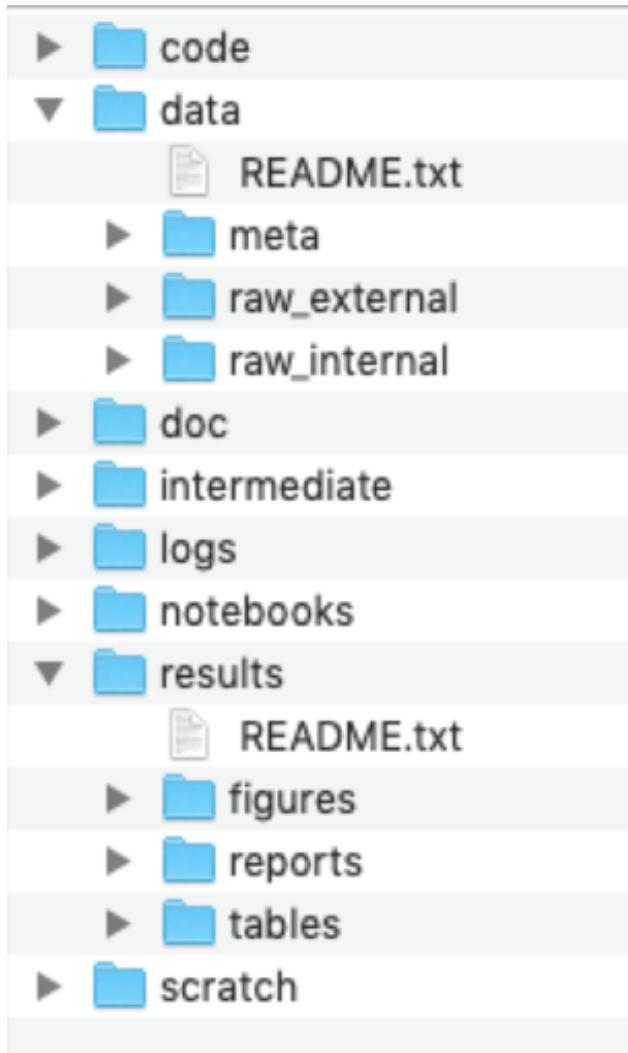
fig02_histogram-talk-attendance.png

1986-01-28_raw-data-from-challenger-o-rings.txt

- There is a **folder for the raw data**, which do not get altered, or intermixed with data that is the result of manual or programmatic manipulation. I.e., derived data is kept separate from raw data, and **raw data are not duplicated**.
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- Use **non-proprietary formats** – .csv rather than .xlsx
- Etc...

- A text-based format is more future-safe, than a proprietary binary format by a commercial vendor
- **Markdown** is a nice way of getting nice output from text.
 - Simple & readable formating
 - Can be converted to lots of different outputs
 - HTML, pdf, MS Word, slides etc
- *Never, never, never use **Excel** for scientific **analysis!***
 - Script your analysis – bash, python, R, ...





all code needed to go from input files to final results

raw and primary data, essentially all input files, **never** edit!

documentation for the study

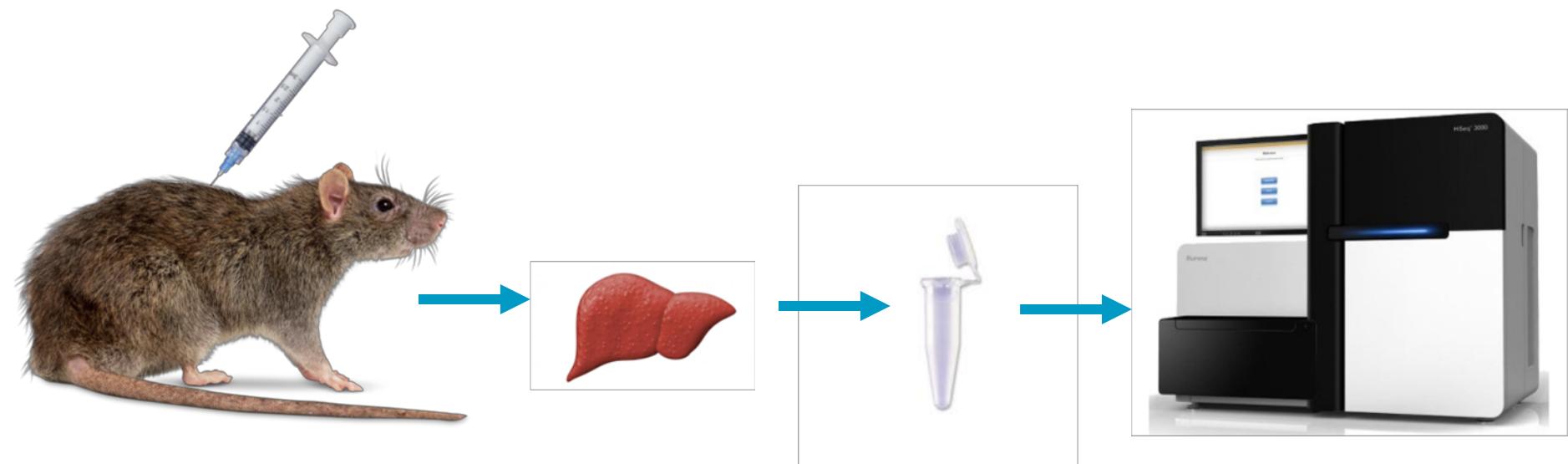
output files from different analysis steps, *can be deleted*

logs from the different analysis steps

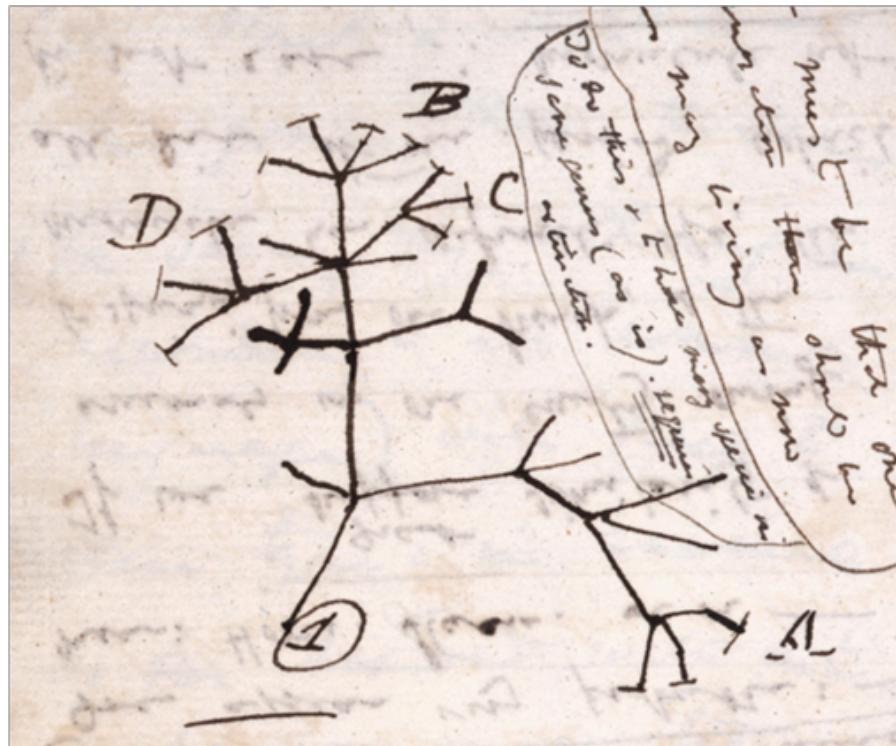
output from workflows and analyses

temporary files that can be safely *deleted or lost*

- Need context → document **metadata**
 - From what was the data generated?
 - How do the samples differ?
 - What where the experimental conditions?
 - Etc



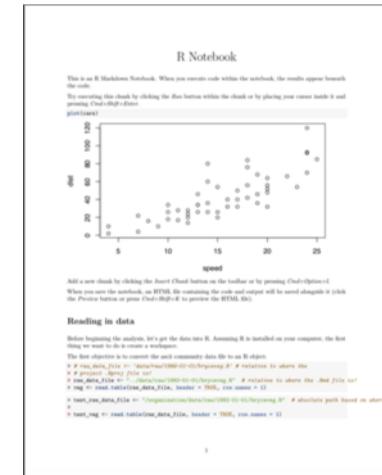
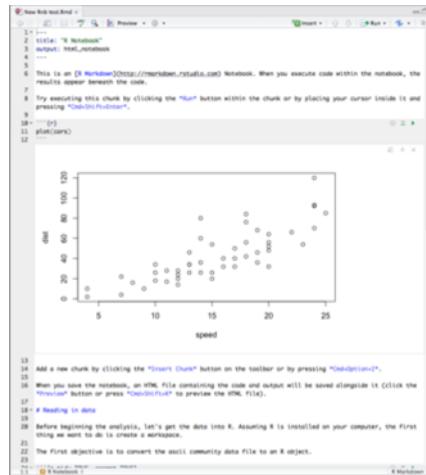
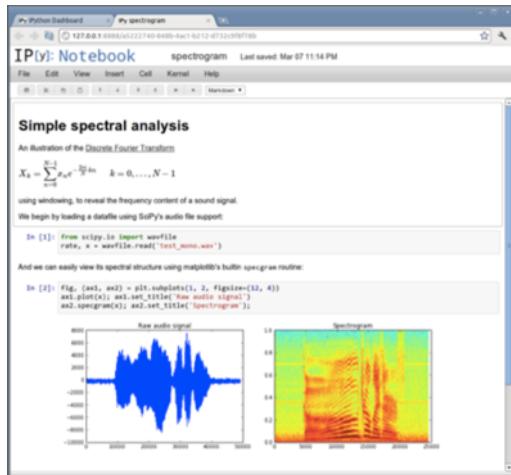
- Why?
 - You have to understand what you have done
 - **Others should be able to reproduce what you have done**



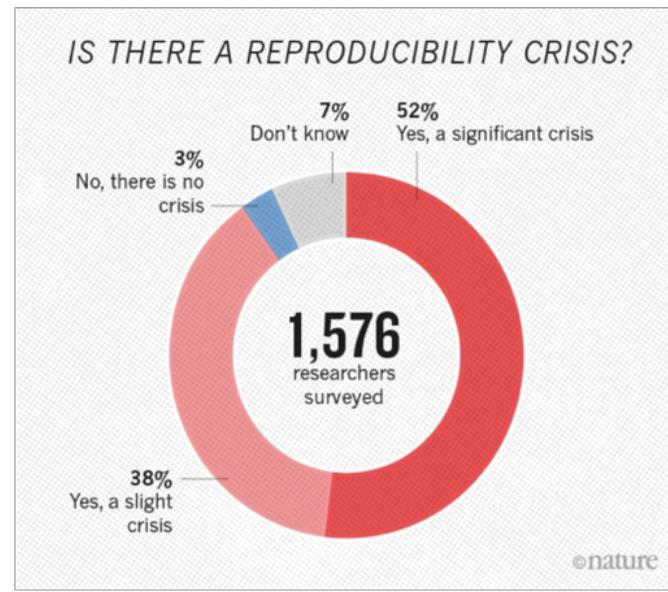
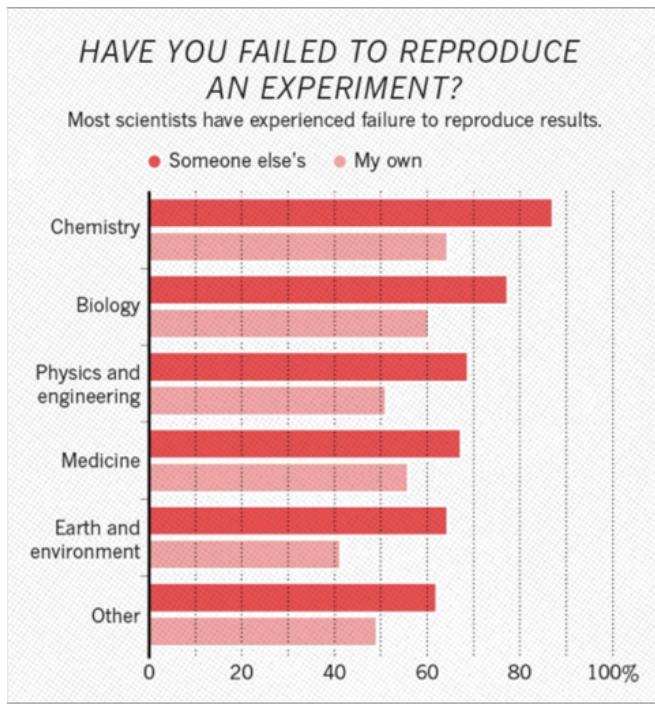
- Put in *separate* directory (e.g. *results, documentation*)
- *Dated* entries
- Entries relatively verbose
- Link to *data* and *code* (including versions)
 - Point to commands run and results generated
- Embedded images or tables showing results of analysis done
- Observations, Conclusions, and *ideas* for future work
- Also document analysis that *doesn't* work, so that it can be understood why you choose a particular way of doing the analysis in the end

Where to take down notes

- Paper Notebook
- Word processor program / Text files
- Electronic Lab Notebooks Systems
- 'Interactive' Electronic Notebooks
 - e.g. [jupyter](#), [R Notebooks](#) in RStudio
 - Plain text - work well with version control (Markdown)
 - Embed and execute code
 - Convert to other output formats
 - html, pdf, word



A reproducibility crisis



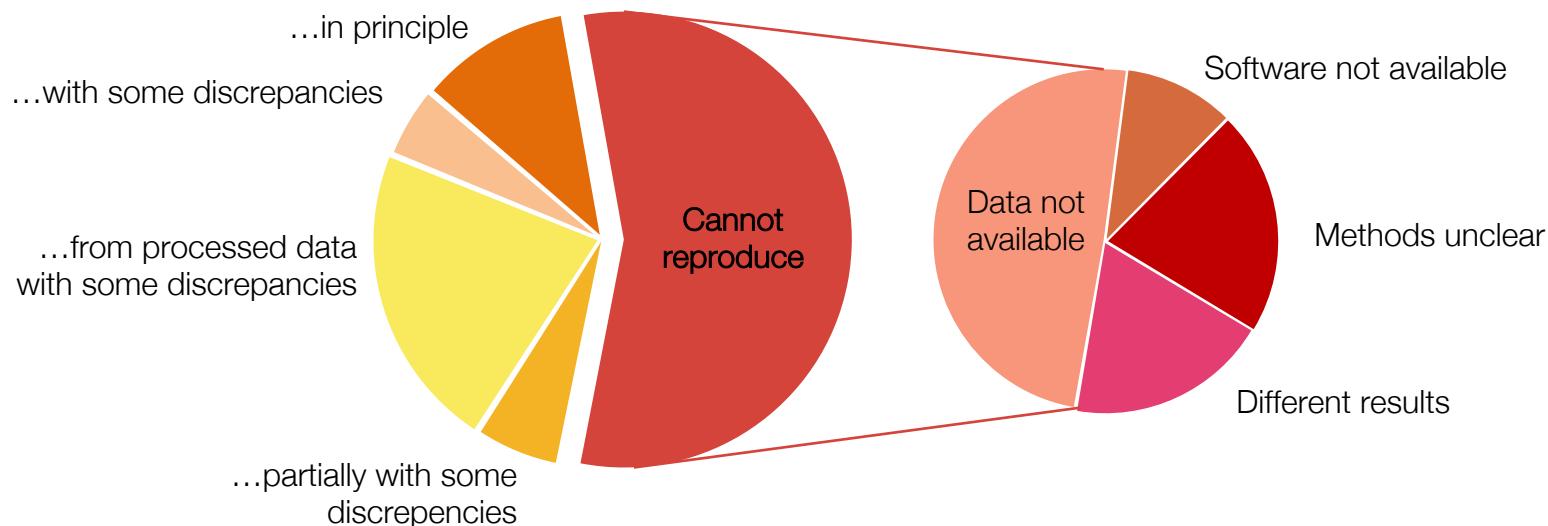
[1] "1,500 scientists lift the lid on reproducibility". Nature. 533: 452–454

[2] Begley, C. G.; Ellis, L. M. (2012). "Drug development: Raise standards for preclinical cancer research". Nature. 483 (7391): 531–533.

A reproducibility crisis

Reproduction of data analyses in 18 articles on microarray-based gene expression profiling published in *Nature Genetics* in 2005–2006:

Can reproduce...



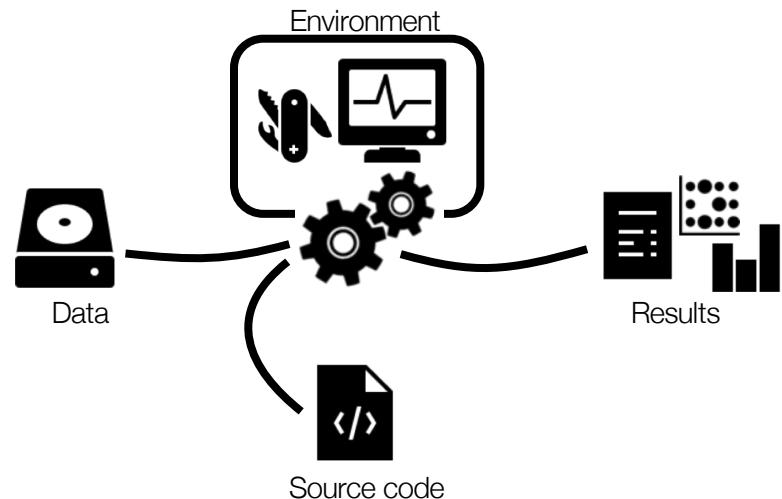
Summary of the efforts to replicate the published analyses.

Adopted from: Ioannidis et al. Repeatability of published microarray gene expression analyses.
Nature Genetics 41 (2009) doi:10.1038/ng.295

What do we mean by reproducible research?

| | | Data | |
|------|-----------|--------------|---------------|
| | | Same | Different |
| Code | Same | Reproducible | Replicable |
| | Different | Robust | Generalizable |

All parts of a bioinformatics analysis have to be reproducible:

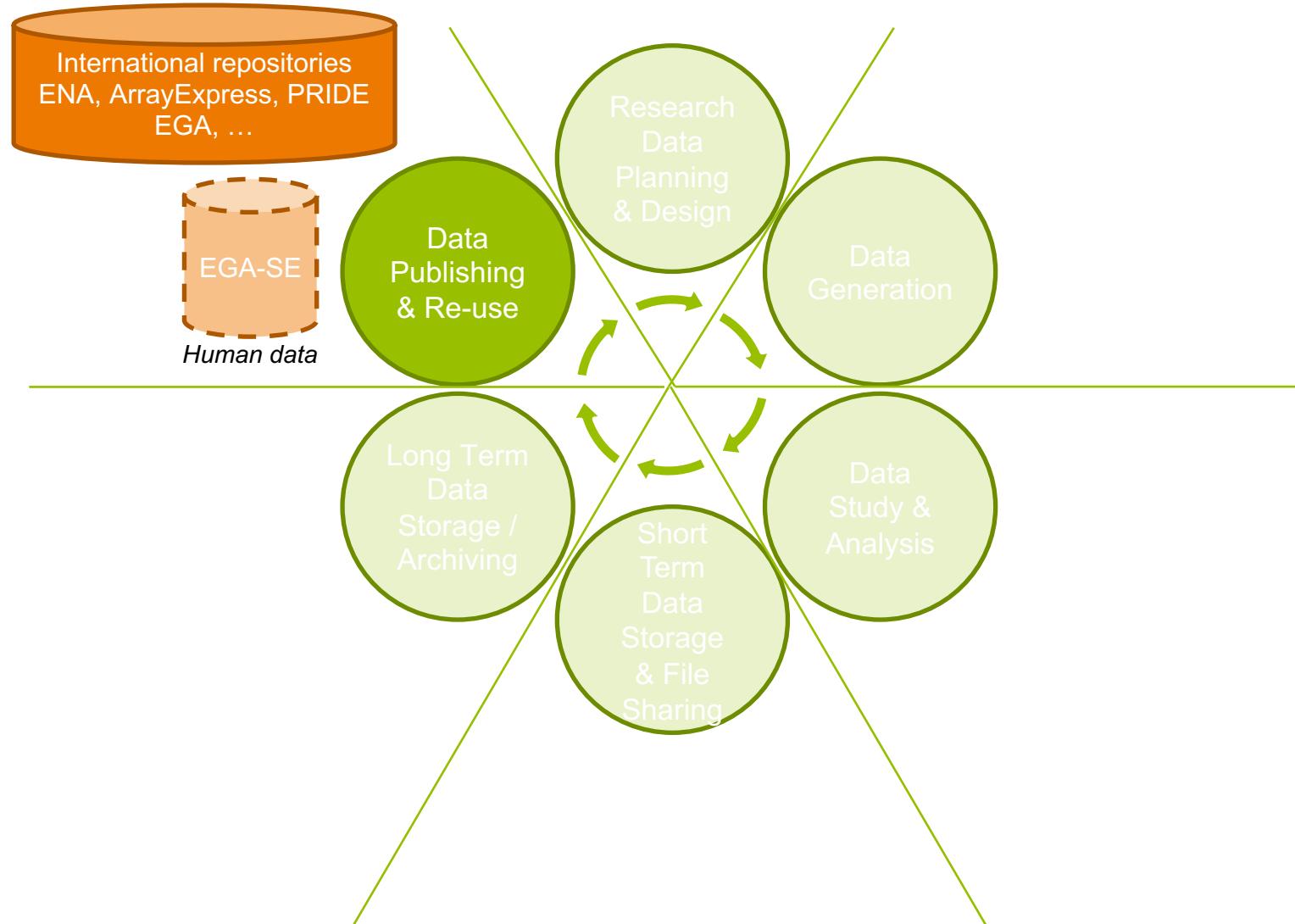


The screenshot shows the NBIS Reproducible research course website. The left sidebar includes links for Welcome, About, The course, Schedule, Travel info, Feedback, Tutorials, Introduction to the tutorials, The case study, Setup, For Mac / Linux users, For Windows users, The tutorials, Conda, Snakemake, Git, Jupyter, R Markdown, Docker, Take down, and a 'Read the Docs' link.

The main content area features a diagram titled 'CONDA' illustrating the interconnected nature of various tools:

- Environment management:** Set up and manage the project environment.
- Version control:** Track and backup your project history (Git).
- Workflow management:** Move from separate scripts to a connected analysis (Snakemake).
- Reports:** Connect code, output and text in fancy reports (R Markdown from R Studio).
- Notebooks:** Document your exploratory analysis (Jupyter).
- Containerization:** Make your project self-contained and distributable (Docker).

Below the diagram, four categories are listed: Do it all!, Workflow, Reproducible environment, and Interactive notebooks, each represented by a cluster of colored circles (green, red, blue, grey).



Why should you make research data available for others?

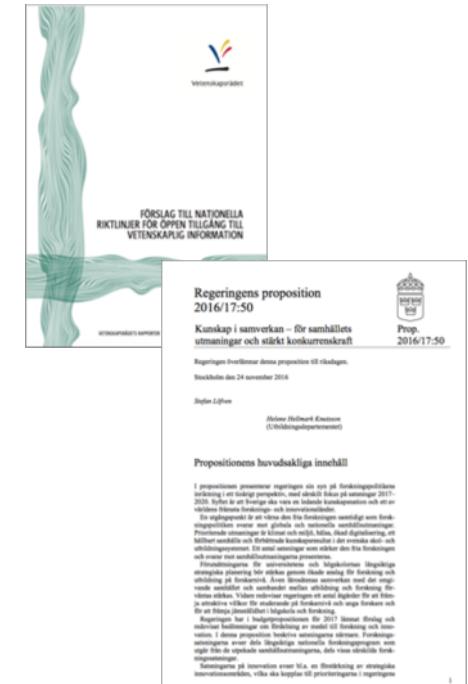
*The practice of providing **on-line access** to scientific information that is **free of charge** to the end-user and that is **re-usable**.*



- Democracy and transparency
 - Publicly funded research data should be accessible to all
 - Published results and conclusions should be possible to check by others
- Research
 - Enables others to combine data, address new questions, and develop new analytical methods
 - Reduce duplication and waste
- Innovation and utilization outside research
 - Public authorities, companies, and private persons outside research can make use of the data
- Citation
 - Citation of data will be a merit for the researcher that produced it



- Strong international movement towards Open Access (OA)
- European Commission recommended the member states to establish national guidelines for OA
 - Swedish Research Council (VR) submitted proposal to the government Jan 2015
- Research bill 2017–2020 – 28 Nov 2016
 - “*The aim of the government is that all scientific publications that are the result of publicly funded research should be openly accessible as soon as they are published. Likewise, research data underlying scientific publications should be openly accessible at the time of publication.*”
[my translation]
- 2018 – VR assigned by the government to coordinate national efforts to implement open access to research data



**What is needed for
others to be able to
re-use your data?**

- To be useful for others data should be
 - **FAIR** - Findable, Accessible, Interoperable, and Reusable
... for both Machines and Humans

Wilkinson, Mark et al. “*The FAIR Guiding Principles for scientific data management and stewardship*”. *Scientific Data* 3, Article number: 160018 (2016)
<http://dx.doi.org/10.1038/sdata.2016.18>



SCIENTIFIC DATA

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

Mark D. Wilkinson et al.*

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

Supporting discovery through good data management
Good data management is not a goal in itself, but rather is the key conduit leading to knowledge discovery and innovation, and to subsequent data and knowledge integration and reuse by the community after the data publication process. Unfortunately, the existing digital ecosystem surrounding scholarly data publication prevents us from extracting maximum benefit from our research investments (e.g., ref. 1). Partially in response to this, science funders, publishers and

Box 2 | The FAIR Guiding Principles

To be Findable:

- F1. (meta)data are assigned a globally unique and persistent identifier
- F2. data are described with rich metadata (defined by R1 below)
- F3. metadata clearly and explicitly include the identifier of the data it describes
- F4. (meta)data are registered or indexed in a searchable resource

To be Accessible:

- A1. (meta)data are retrievable by their identifier using a standardized communications protocol
- A1.1 the protocol is open, free, and universally implementable
- A1.2 the protocol allows for an authentication and authorization procedure, where necessary
- A2. metadata are accessible, even when the data are no longer available

To be Interoperable:

- I1. (meta)data use a formal, accessible, shared, and broadly applicable language for knowledge representation.
- I2. (meta)data use vocabularies that follow FAIR principles
- I3. (meta)data include qualified references to other (meta)data

To be Reusable:

- R1. meta(data) are richly described with a plurality of accurate and relevant attributes
- R1.1. (meta)data are released with a clear and accessible data usage license
- R1.2. (meta)data are associated with detailed provenance
- R1.3. (meta)data meet domain-relevant community standards

G20 HANGZHOU SUMMIT

**'We support appropriate efforts to promote open science
and facilitate appropriate access to publicly funded
research results on findable, accessible, interoperable and reusable
(FAIR)'**

HANGZHOU, CHINA 4-5 SEPTEMBER 2016



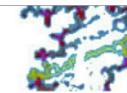
- *Research Data Publishing is a cornerstone of Open Access*
- Long-term storage
 - Data should not disappear
- Persistent identifiers
 - Possibility to refer to a dataset over long periods of time
 - Unique
 - e.g. DOIs (Digital Object Identifiers)
- Discoverability
 - Expose dataset metadata through search functionalities



- ORCID is an open, non-profit, community-driven effort to create and maintain a registry of unique researcher identifiers and a transparent method of linking research activities and outputs to these identifiers.
- <http://orcid.org>
- Persistent identifier for you as a researcher

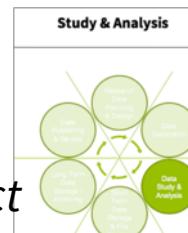
The screenshot shows the ORCID profile page for Niclas Jareborg. The top navigation bar includes links for FOR RESEARCHERS, FOR ORGANIZATIONS, ABOUT, HELP, and SIGN IN. Below the navigation, it displays 3,035,272 ORCID IDs and counting. The main profile area shows Niclas Jareborg's ORCID ID as <http://orcid.org/0000-0002-4520-044X>. It lists his education at Uppsala Universitet (Sweden) from 1989-05 to 1995-05 (Microbiology), which is a PhD, and another entry from 1985-01 to 1989-04 (Microbiology), which is a BSc. Both entries were created on 2015-04-09 and sourced from Niclas Jareborg. It also shows his employment at Stockholms Universitet (Stockholm, Sweden) from 2015-01 to present (BILS / Department of Biochemistry and Biophysics), where he is a Data Manager, created on 2015-02-23, also sourced from Niclas Jareborg. The page also lists his websites, including LinkedIn and a Personal home page.

International public repositories



- Best way to make data **FAIR**
- Domain-specific metadata standards

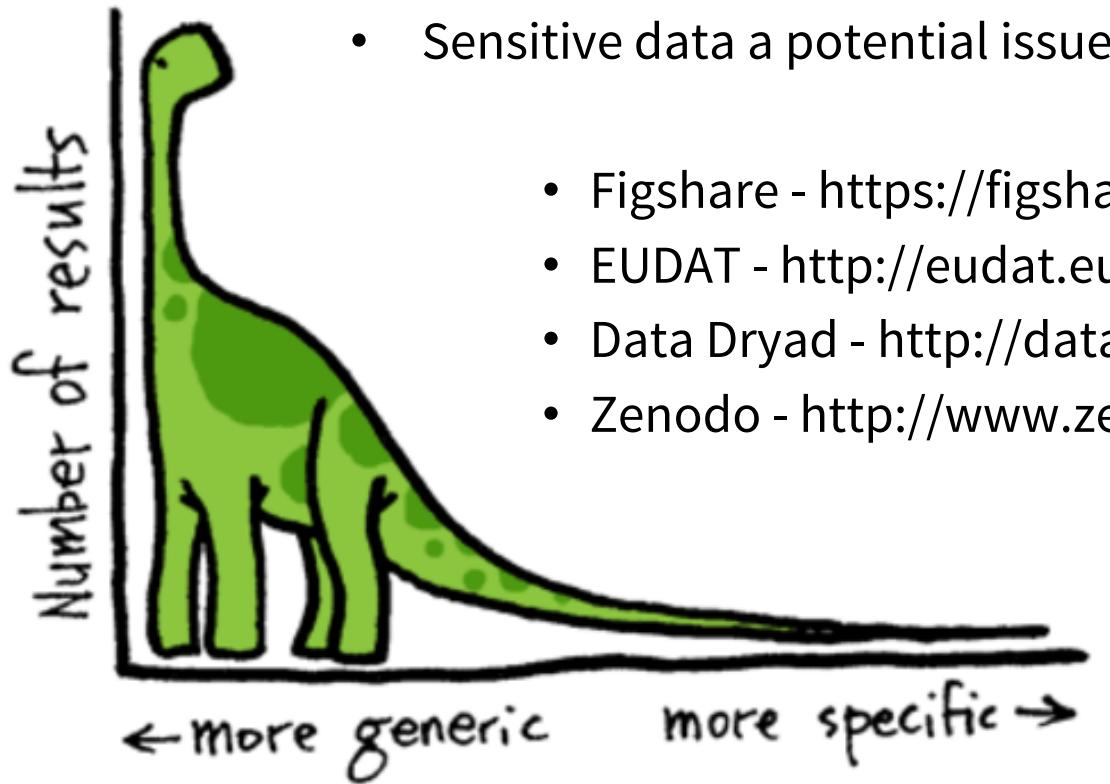
 *Strive towards uploading data to its final destination already at the beginning of a project*



| Deposition Database | Data type | International collaboration framework ¹ | Deposition Database | Data type | International collaboration framework ¹ | |
|---------------------|--|---|--|---|--|--|
| ArrayExpress | Functional genomics data. Stores data from high-throughput functional genomics experiments. | | PDBe | Biological macromolecular structures. | wwPDB | |
| BioModels | Computational models of biological processes. | | PRIDE | Mass spectrometry-based proteomics data, including peptide and protein expression information (identifications and quantification values) and the supporting mass spectra evidence. | The ProteomeXchange Consortium | |
| EGA | Personally identifiable genetic and phenotypic data resulting from biomedical research projects. | European Bioinformatics Institute and the Centre for Genomic Regulation | Pending incorporation into a Node Service Delivery Plan (see How countries join): | | | |
| ENA | Nucleotide sequence information, covering raw sequencing data, contextual data, sequence assembly information and functional and taxonomic annotation. | International Nucleotide Sequence Database Collaboration | BioSamples | BioSamples stores and supplies descriptions and metadata about biological samples used in research and development by academia and industry. | NCBI BioSamples database | |
| IntAct | IntAct provides a freely available, open source database system and analysis tools for molecular interaction data. | The International Molecular Exchange Consortium | BioStudies | Descriptions of biological studies, links to data from these studies in other databases, as well as data that do not fit in the structured archives. | | |
| MetaboLights | Metabolite structures and their reference spectra as well as their biological roles, locations and concentrations, and experimental data from metabolic experiments. | | EVA | The European Variation Archive covers genetic variation data from all species. | dbSNP and dbVAR | |
| | | | EMDB | The Electron Microscopy Data Bank is a public repository for electron microscopy density maps of macromolecular complexes and subcellular structures. | | |

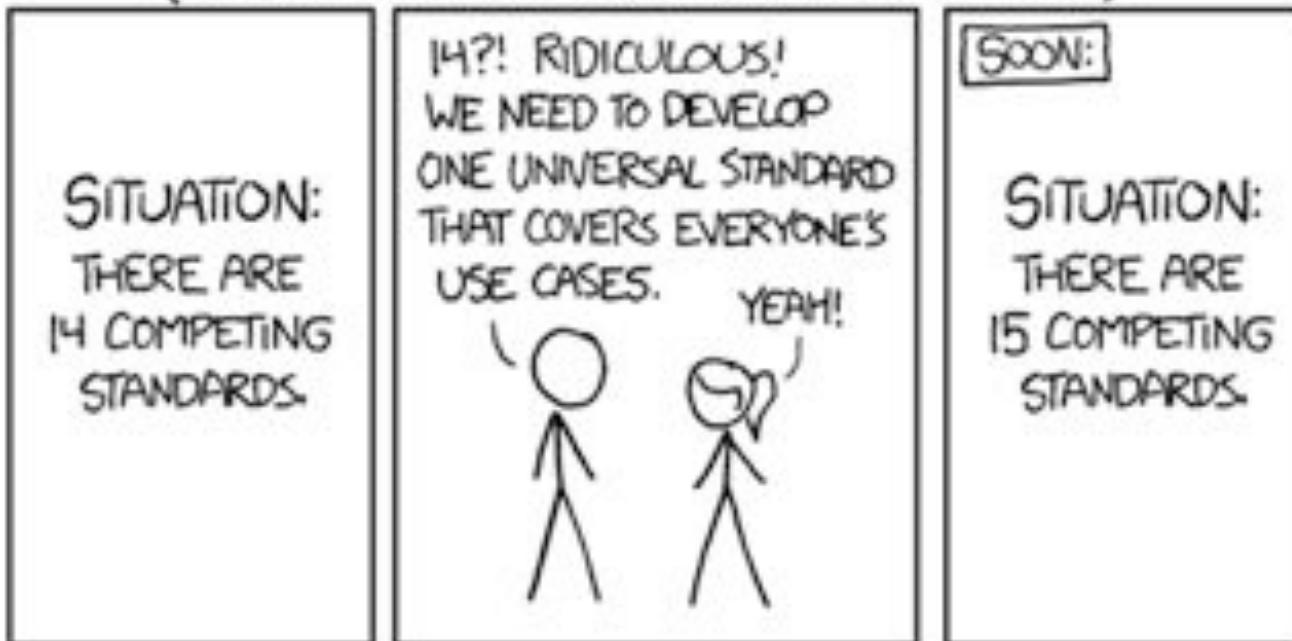
<https://www.elixir-europe.org/platforms/data/elixir-deposition-databases>

- Research data that doesn't fit in structured data repositories
- Data publication – persistent identifiers
- Metadata submission – not tailored to Life Science
 - *Affects discoverability*
 - *(Less) FAIR*
- Sensitive data a potential issue



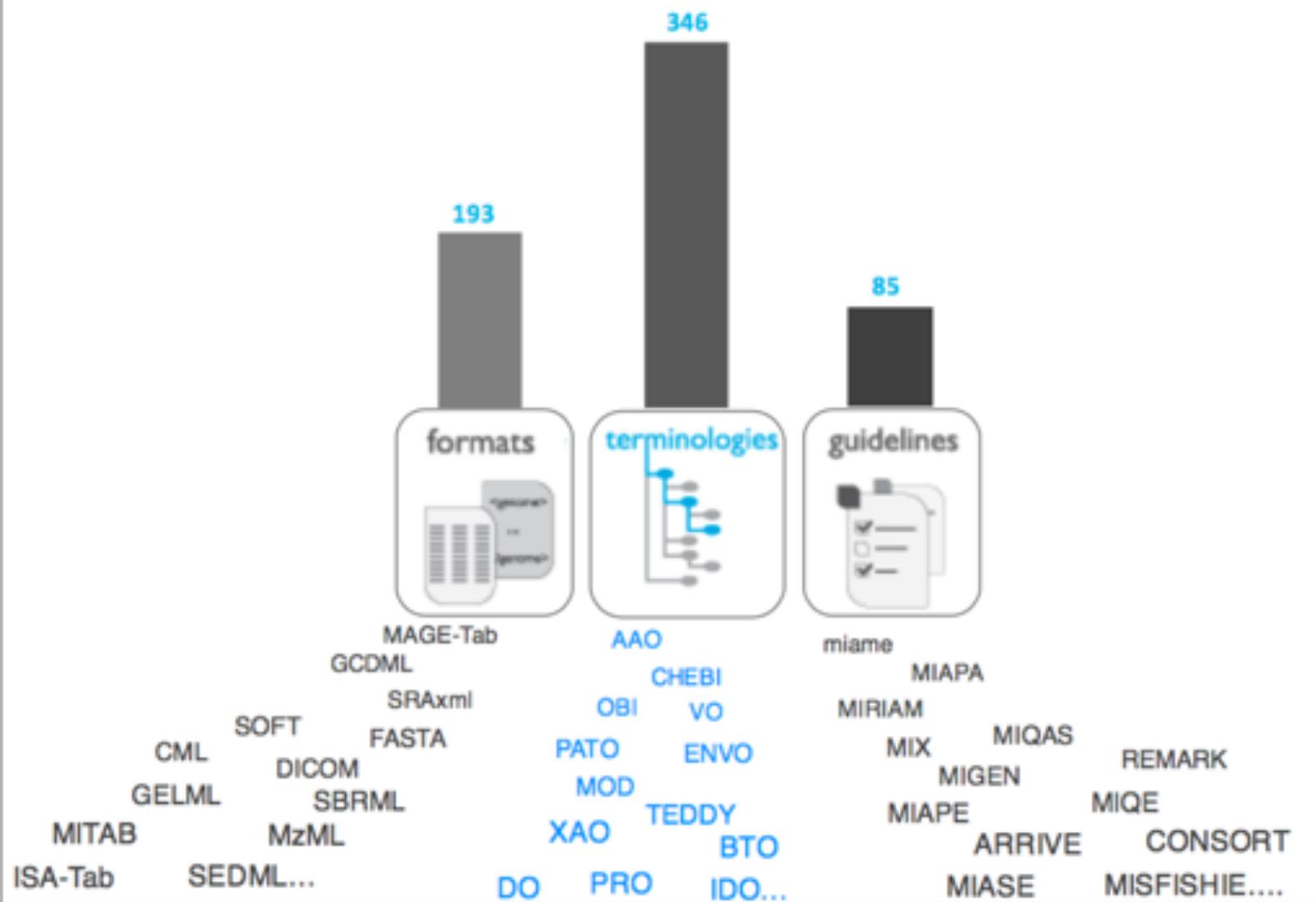
- Standards
 - Controlled vocabularies / Ontologies
 - Agreed terms for different phenomena

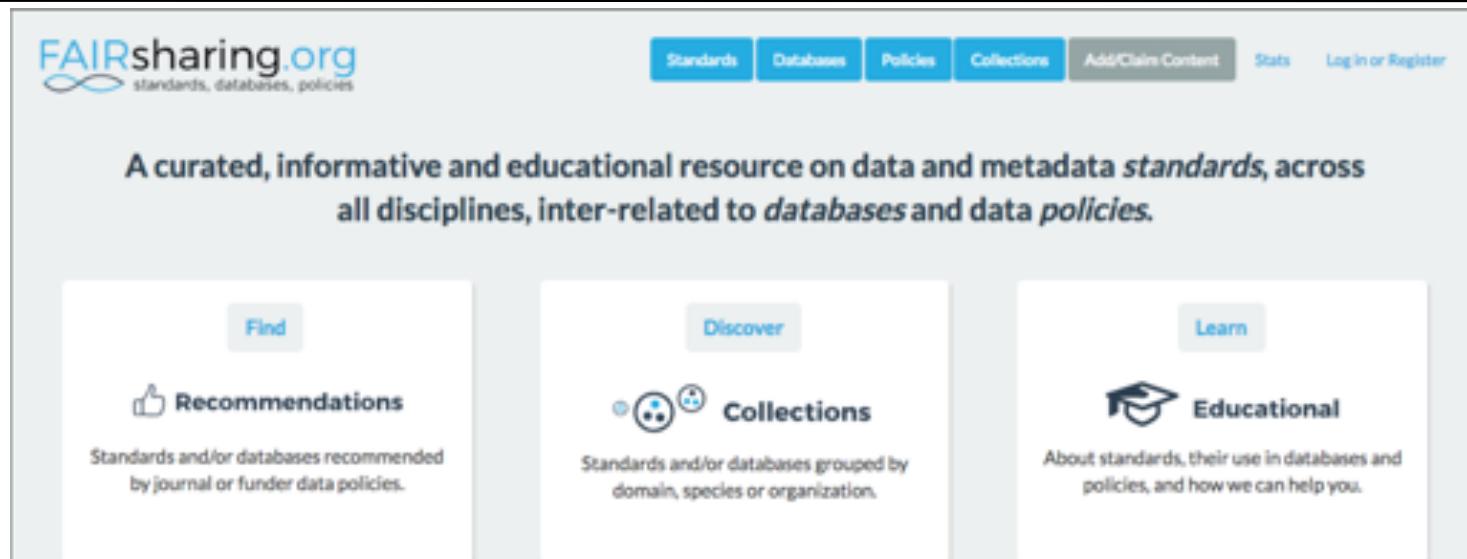
HOW STANDARDS PROLIFERATE:
(SEE: AAC CHARGERS, CHARACTER ENCODINGS, INSTANT MESSAGING, ETC.)



| Human Phenotype Ontology | |
|--|--|
| Summary | Classes |
| Jump To: | Details Visualization Notes (0) Class Mappings (21) Edit |
| <ul style="list-style-type: none"> • All • Clinical modifier • Developmental • Disease • Homeostatic • Phenotypic abnormality • Abnormality of blood and blood-forming tissues • Abnormal bleeding • Abnormal thrombosis • Abnormality of bone marrow cell morphology • Abnormality of coagulation • Abnormality of heart • Abnormality of thrombocytes • Extramedullary hematopoeisis • Hematological neoplasm • Leukemia <ul style="list-style-type: none"> • Acute leukemia • Acute lymphoblastic leukemia • Acute myelogenous leukemia • Acute monocytic leukemia • Acute myeloid leukemia • Acute myelomonocytic leukemia • Acute promyelocytic leukemia • Bilingual acute leukaemia • Chronic leukemia • Lymphoid leukemia • Myeloma • Myeloproliferative disorder • Lymphoma • Lymphoproliferative disorder | <p>Preferred Name Acute myeloid leukemia</p> <p>Synonyms Acute myeloblastic leukemia Acute myelogenous leukemia Acute myelocytic leukemia</p> <p>Definitions A form of leukemia characterized by overproduction of an early myeloid cell.</p> <p>ID http://purl.obolibrary.org/obo/HP_0004808</p> <p>database_cross_reference MeSH:D015470 UMLS:C0023467</p> <p>definition A form of leukemia characterized by overproduction of an early myeloid cell.</p> <p>has_alternative_id HP:0004843 HP:0001914 HP:0006728 HP:0006724 HP:0005516</p> <p>has_exact_synonym Acute myeloblastic leukemia Acute myelogenous leukemia Acute myelocytic leukemia</p> <p>has_obo_namespace human_phenotype</p> <p>id HP:0004808</p> <p>label Acute myeloid leukemia</p> <p>notation HP:0004808</p> <p>prefLabel Acute myeloid leukemia</p> <p>treeView Acute leukemia</p> <p>subClassOf Acute leukemia</p> |

In the life sciences there are >600 *content standards*





FAIRsharing.org standards, databases, policies

Standards Databases Policies Collections Add/Claim Content Stats Log in or Register

A curated, informative and educational resource on data and metadata *standards*, across all disciplines, inter-related to *databases* and *data policies*.

Find

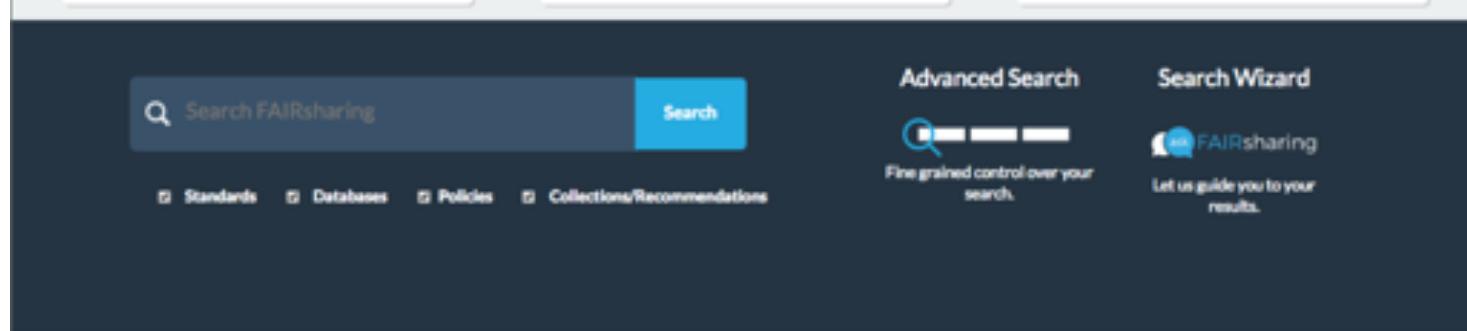
 **Recommendations**
Standards and/or databases recommended by journal or funder data policies.

Discover

 **Collections**
Standards and/or databases grouped by domain, species or organization.

Learn

 **Educational**
About standards, their use in databases and policies, and how we can help you.



Search FAIRsharing Search

Advanced Search Search Wizard

FAIRsharing

Standards Databases Policies Collections/Recommendations

Fine grained control over your search.

Let us guide you to your results.



699 Standards

View all

| Terminology | Artifact | 343 |
|---------------------|----------|-----|
| Model/Format | | 239 |
| Reporting Guideline | | 117 |

974 Databases

View all

| Life Science | 733 |
|--------------------|-----|
| Biomedical Science | 181 |
| General Purpose | 10 |

97 Policies

View all

| Funder | Journal | Society |
|--------|---------|---------|
| 22 | 68 | 3 |

**Can you share all types
of data publicly?**

**If not, what would be the
reasons?**

Personal data



- GDPR – General Data Protection Regulation (*Dataskyddsförordningen*) + others
- Act concerning the Ethical Review of Research Involving Humans (*Lag om etikprövning av forskning som avser människor*)



- All kinds of information that is directly or indirectly referable to a natural person who is alive constitute personal data
- To process personal data:
 - *All processing of personal data must fulfil the **fundamental principles** defined in the Regulation, among them are:*
 - Decide a **purpose** and stick to it
 - Identify the **legal basis** for data processing before it starts
- *Have you defined the **purpose** and **legal basis** for handling personal data in your project?*

- Special categories (*Sensitive data*)
 - ... **racial or ethnic origin**, [...] **genetic data**, [...], data concerning **health** ... Art. 9 (1)
 - Processing is **prohibited** unless...
 - **explicit consent** is given Art. 9 (2)a
 - processing is necessary for **scientific research** in accordance with Article 89(1) based on Union or *Member State law* which shall be proportionate to the aim pursued, respect the essence of the right to data protection and provide for suitable and specific measures to safeguard the fundamental rights and the interests of the data subject. Art. 9 (2)j
 - Member State specific conditions and *limitations possible* for processing of health & genetic data Art. 9 (4)
 - **Sweden**
 - Consent?
 - Public interest → Ethical review necessary (often includes consent)

- **A Data Protection Officer (*dataskyddssombud*)**
 - The natural person that is responsible for ensuring that the organization/company adheres to the GDPR
 - Educate
 - Audit
 - Contact point between organization and Data Protection Agency

GU

<https://medarbetarportalen.gu.se/projekt-process/aktuella-projekt/dataskyddsforordning>

KI

<https://ki.se/medarbetare/gdpr-pa-karolinska-institutet>

KTH

<https://intra.kth.se/anstallning/anstallningsvillkor/att-vara-statligt-an/behandling-av-person/dataskyddsforordningen-gdpr-1.800623>

LiU

<https://insidan.liu.se/dataskyddsforordningen/anmalan-av-personuppgiftsbehandling?l=sv>

LU

<https://personuppgifter.blogg.lu.se>

SU

<https://www.su.se/medarbetare/organisation-styrning/juridik/personuppgifter/dataskyddsforordningen>

UmU

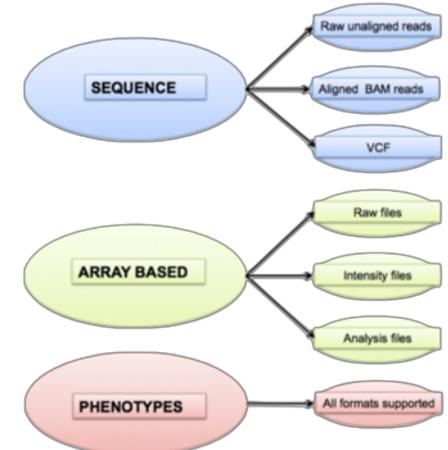
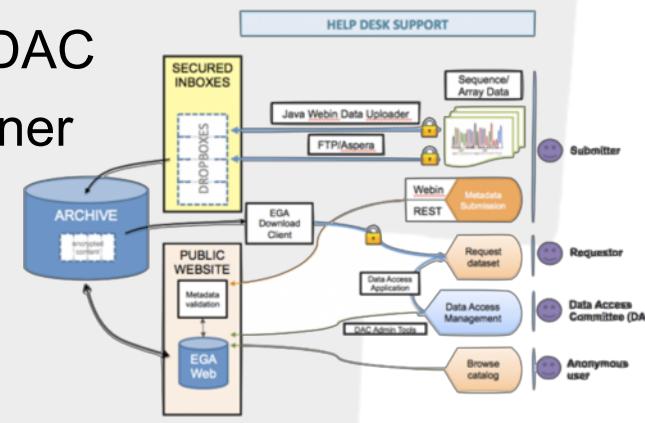
<https://www.aurora.umu.se/regler-och-riktlinjer/juridik/personuppgifter/>

UU

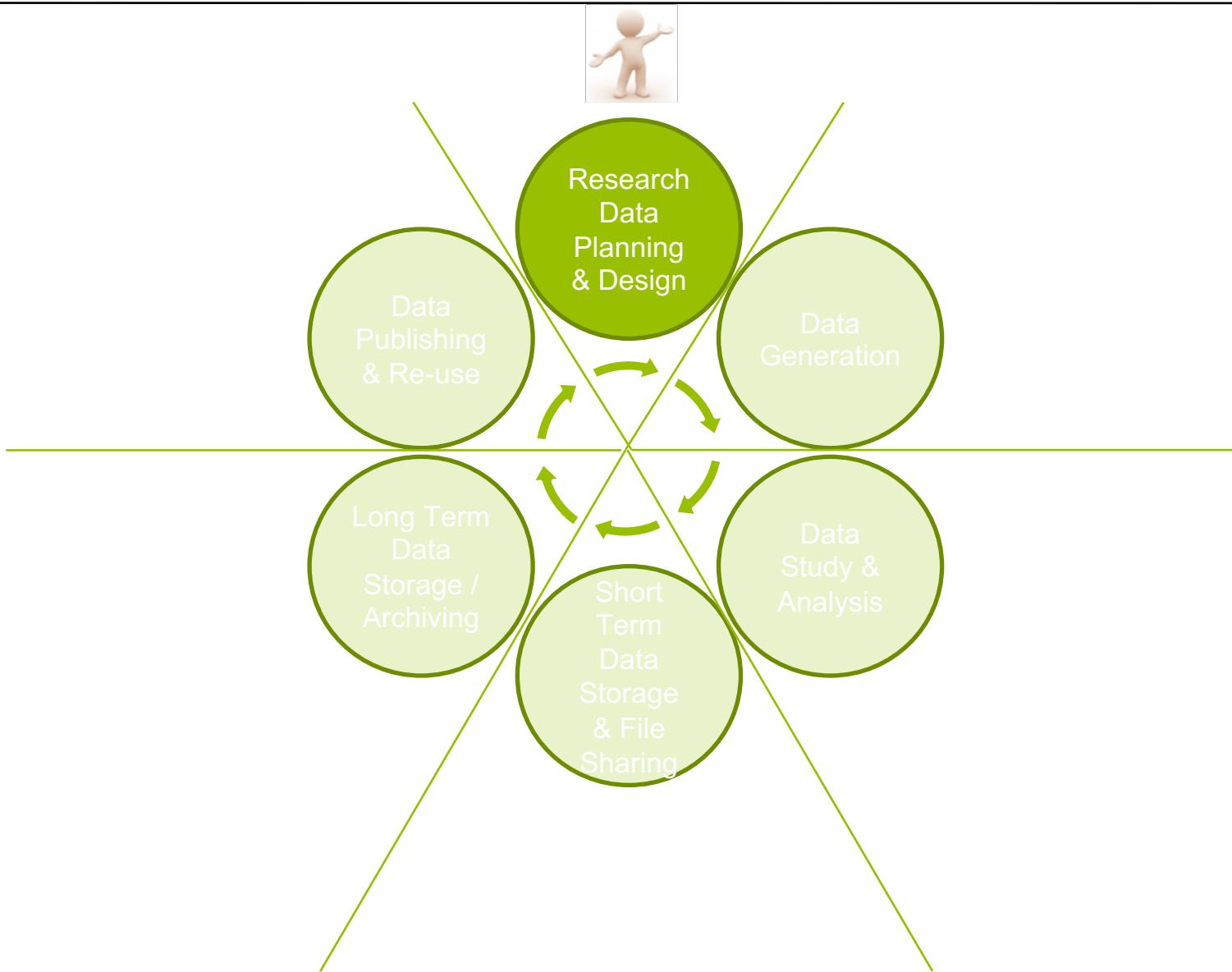
<https://mp.uu.se/web/info/stod/dataskyddsforordningen>

“As open as possible, as closed as necessary”

- **EGA – European Genome-phenome Archive**
 - Repository that promotes the distribution and sharing of **genetic and phenotypic data** consented for specific approved uses but **not fully open, public distribution**.
 - All types of sequence and genotype experiments, including case-control, population, and family studies.
- Data Access Agreement
 - Defined by the data owner
- Data Access Committee – DAC
 - Decided by the data owner



When should you start planning for how to manage your data?



Will become a standard part of the research funding application process

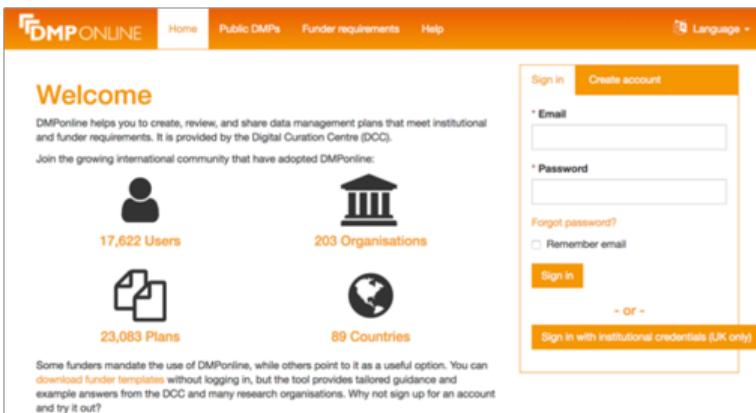
- **Data collection** - data types and volumes, analysis code
- **Data organization** - folder and file structure, and naming
- **Data documentation** - data and analysis, metadata standards
- **Data storage** - storage/backup/protection & time lines
- **Data policies** - conditions/licences for using data & legal/ethical issues
- **Data sharing** - *When and How* will *What* data (and code) be shared
- **Roles and responsibilities** - who's responsible for what & is competence available
- **Budget** - People & Hardware/Software

The screenshot shows the homepage of the **nature** journal website. At the top, there is a red header bar with the **nature** logo and the text "International Journal of science". To the right of the logo are four buttons: "Search", "E-alert", "Submit", and "Login". Below the header, there is a horizontal line followed by the word "EDITORIAL" and the date "13 MARCH 2018". The main headline reads "Everyone needs a data-management plan". A subtext below the headline says "They sound dull, but data-management plans are essential, and funders must explain why.".

- 💡 *Consider structuring metadata in the format needed by the repository already at planning stage*

DMP tools

DMPonline



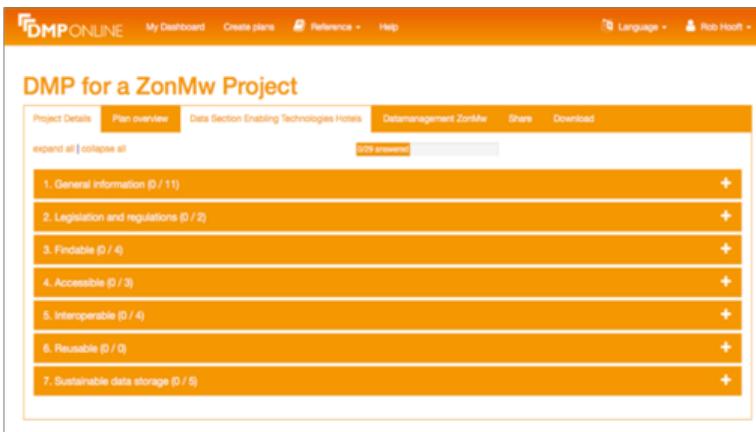
The screenshot shows the DMPonline homepage. It features a top navigation bar with links for Home, Public DMPs, Funder requirements, Help, and Language selection. Below this is a "Welcome" section with a brief introduction and statistics: 17,622 Users, 203 Organisations, and 89 Countries. To the right is a sign-in form with fields for Email and Password, and options for Remember email, Sign In, or Sign in with institutional credentials (UK only). A sidebar on the left provides links to My Dashboard, Create plans, Reference, Help, and a user profile for Rob Heath.

<https://dmponline.dcc.ac.uk/>

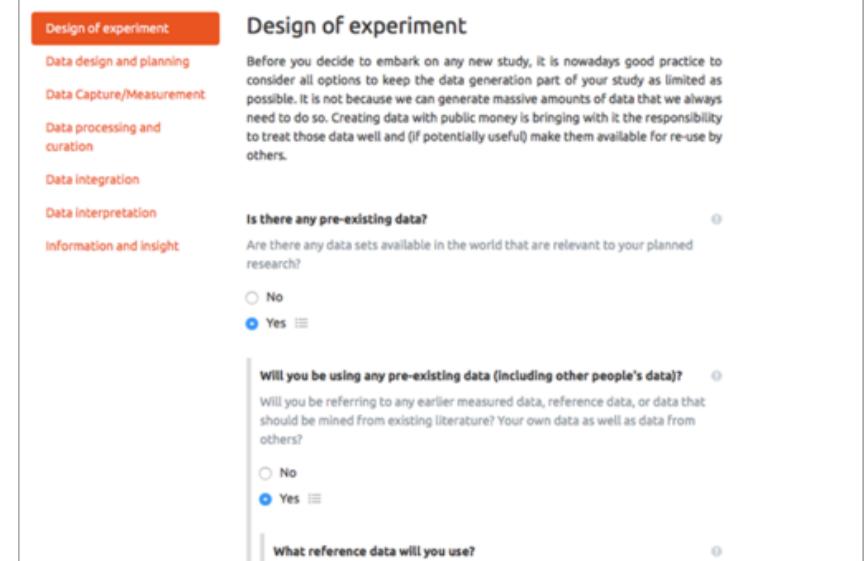
ELIXIR Data Stewardship Wizard



The screenshot shows the ELIXIR Data Stewardship Wizard homepage. It has a warm orange background with a network graph of interconnected nodes. The title "ELIXIR Data Stewardship Wizard" is at the top, followed by the subtitle "Smart Data Management Plans for FAIR Open Science". Below this is the tagline "For serious researchers and data stewards". A "Go to App" button is in the top right corner.



This screenshot shows the "Plan overview" tab of a DMPonline project titled "DMP for a ZonMw Project". The interface includes tabs for Project Details, Plan overview, Data Section Enabling Technologies Hotels, Datamanagement ZonMw, Share, and Download. The "Plan overview" tab displays a list of 7 sections with counts: 1. General information (0 / 11), 2. Legislation and regulations (0 / 2), 3. Findable (0 / 4), 4. Accessible (0 / 3), 5. Interoperable (0 / 4), 6. Reusable (0 / 0), and 7. Sustainable data storage (0 / 5). Each section has a plus sign icon to expand it.



The screenshot shows the "Design of experiment" section of the ELIXIR Data Stewardship Wizard. It starts with a heading "Design of experiment" and a list of categories: Data design and planning, Data Capture/Measurement, Data processing and curation, Data integration, Data interpretation, and Information and insight. Below this is a question "Is there any pre-existing data?" with two radio button options: "No" and "Yes". The "Yes" option is selected. Further down are questions about using pre-existing data and what reference data will be used, each with "No" and "Yes" radio button options.

<https://dsw.fairdata.solutions/>

- Project planning
 - Metadata
 - File formats
 - Licensing
 - *Data Management Plans*
- Data analysis
- Data publication and submission
 - Support submissions to public repositories
 - Metadata
 - DOIs to dataset (if needed)

- Consider doing a Data Management Plan for your project
 - How do you ensure that your research output is FAIR?
- Plan for submitting "raw data" to public repositories as early as possible
- Organize project metadata from the start
 - In ways that makes it easy to submit to public repositories
 - Use available standards
- Pick a thought-through file and folder structure organization for your computational analyses
- Strive for reproducibility
 - Data & Code
- Be aware that there are legal aspects to processing human data
- *Ask for help if you need it!*

- Research Data Management, EUDAT - <http://hdl.handle.net/11304/79db27e2-c12a-11e5-9bb4-2b0aad496318>
- Noble WS (2009) [A Quick Guide to Organizing Computational Biology Projects. PLoS Comput Biol 5\(7\): e1000424. doi:10.1371/journal.pcbi.1000424](https://doi.org/10.1371/journal.pcbi.1000424)
- Reproducible research
 - Reproducible Science Curriculum – <https://github.com/Reproducible-Science-Curriculum/rr-init>
 - Leif Väremo & Rasmus Ågren
 - https://bitbucket.org/scilifelab-lts/reproducible_research_example/src
 - https://nbis-reproducible-research.readthedocs.io/en/course_1803
- GDPR
 - Datainspektionen – <https://www.datainspektionen.se/lagar-regler/dataskyddsforordningen/>
- ... and probably others I have forgotten