Research data management CRC 1073 / CRC 1633 / FOR 5522 / RTG 2455 13.06.2024



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Timo Henne henne@sub.uni-goettingen.de



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CRC 1073 ATOMIC SCALE CONTROL OF ENERGY CONVERSION



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Outline

- Introduction to Research Data Management
- Storing Data
- Organization of Data
- Metadata
- Data Sharing
- Publishing research software
- Further Infos





Introduction to Research Data Management





What is 'data'?





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Digital Curation Centre

What are 'data'?

"A reinterpretable representation of information in a formalized manner suitable for communication, interpretation, or processing."

Data are <u>representations</u> of observations, objects, or other entities used as <u>evidence</u> of phenomena for the purposes of research or scholarship.



(Christine Borgmann 2014)







What are research data?

Any representation of information you use in your research:

Forms: Statistics, interviews, simulations, measurement data from experiments, observational data from instruments, text with semantic annotations, 3D scans, model drawings, scripts,...

Types: Video, audio, images, spreadsheets, emails, paper documents, binary data, software, text files, lab notebooks, ...





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Types of research data

Туре	Characteristics	Example
Observations	Data is collected in real time Mostly irreplaceable	Sensor data Survey data
Experiments	Mostly created in the laboratory Reproducible but expensive	Gene sequences Chromatogram
Simulations	Generated from test models Model and metadata often more important than output	Climate models Economic models
Derived data	Derived or compiled from other data, reproducible	Text Mining 3D models
References	Collection of smaller data sets Mostly published	Gene sequence database Primary text sources
Digital copies	Digital version of an analog object, reproducible as long as the original exists	Manuscripts



Research Data – a Valuable Investment



Source: European Space Agency: Rosetta and Philae at comet. on flickr

Rosetta mission 2004-2016:

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Duration:

- >10 years preparation
- 10 years from start to data

Costs:

over € 1.000.000.000

Outcome:

- some cool photos
- lots of data
- a radically new theory on the origin of the universe?

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Research data - a resource in great demand



Data with reference to COVID-19

- medical, molecular biological, epidemiological...
- mathematical, sociological, geographical, psychological, ...

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Research cycle

Develop research question

Publish results

Plan research project

Analyze data/results

Conduct research













- Storage, Backup & Archiving
- Metadata and Documentation
- Data Quality
- File Names, Identifier and Versions
- Ethics, Rights and Licenses



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eResearch Research Data Policy of the Georg-August Universität Göttingen

- Officially issued on 28th August 2014, revised version in 2024 •
- One of the first German universities with such a policy



Research data policy of the Georg-August University Goettingen (incl. UMG) Excerpt from the Amtlichen Mitteilungen I der Georg-August-Universität Göttingen of 15.01.2024/Nr. 1, p. 1f

Preamble

The Georg August University Goettingen is committed to diligently preserve results of scholarship, to produce novel results through research, and to make results accessible and reusable for academia and the wider society, now and for future generations. The management, protection, preservation and sustainable provision of research data must therefore be carried out in accordance with recognized standards, meet the FAIR data principles and fulfill legal and ethical obligations. The University acknowledges that the implementation of this guideline will depend on the settings and requirements of each subject area.

Guideline:

1. The University commits itself to the FAIR data principles and promotes and supports open access to research data

- 2. Research data are analogue and digital objects which are collected, observed, simulated, derived, generated or analysed for the purpose of information retrieval in the course of research
- 3. Management of research data includes their planning, collection, processing, documentation and preservation. It ensures the ac to, and the reuse, reproducibility, and quality assurance of all research data underpinning research results.
- 4. Research data management is generally the responsibility of the person leading a project and the researcher who is acting in an individual capacity. A particular responsibility is the adherence to the DFG code of conduct "Guidelines for Safeguarding Good Research Practice" as well as standards in their subject area.
- 5. Research projects with research data require a data management plan that includes but is not restricted to the topics of access right to research data and necessary precautions for handling them
- 6. The University provides support and advice for research data management in the preparatory stages of research projects, du conduct and after their completion, and provides appropriate training
- 7. The University implements and maintains essential services for research data infrastructure that ensures adequate storage, technical availability and a citable publication of digital research data. Specific requirements have to be aligned among all stakeholders and may involve additional function
- 8. Storage and archiving of digital research data is carried out within the technological and informational infrastructure of the University or in acknowledged external or internal subject repositories, with specific consideration of the services of the National Research Data Infrastructure, NFOL
- 9. The University and its researchers adhere in their research data management to given conditions of ethics, data protection, intellects, property, privacy and disclosure. This leaves regulations untouched that relate to an assessment of research data according to the German employee invention act and specific contractual agreements.
- 10. If exploitation or publication rights of data were transferred to third parties, it should be a precondition that research data remain openly and freely available for research purposet

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Amtliche Mittellungen der Georg-August-Universitiät Göttingen vom 15.01.2024/Nr.1 Outdated version (2014): Amtliche Mittellungen der Georg-August-Universität Göttingen vom 06.12.2016/Nr. 65



- Officially issued on 28th August 2014, revised version in 2024
- One of the first German universities with such a policy
- Topics addressed:
 - Research Data, Research Data Management and its purposes
 - Data Management Plans
 - Support, training and provision of services
 - Storage location
 - Ethical and legal standards
 - Open Access
- eResearch Alliance: support and advice on the implementation of the RDP for the Göttingen Campus













- Improve your research
 - Prevent data loss
 - Prevent unnecessary work
 - Better data quality

Good scientific practice

- Reproducibility, accountability and compliance
- "Primary data as the basis for publications shall be securely stored for ten years in a durable form in the institution of their origin." (DFG, Proposals for safeguarding good scientific practice, 1998)
- Requirement from funding agencies (e.g. EC Horizon Europe, DFG)

Data sharing with colleagues

- Research can be *very* expensive and often the only result may be data.
- Data management costs are small in comparison to data creation costs.
- Productive data sharing is simply a matter of efficiency.

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ATOMIC SCALE CONTROL





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Why Research Data Management?







Source:

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Jeffrey Brainard et al., **Rethinking retractions**, *Science* 26 Oct 2018: Vol. 362, Issue 6413, pp. 390-393 DOI: 10.1126/science.362.6413.390 GRAPHIC: J. YOU/*SCIENCE*; DATA: RETRACTION WATCH

Alison Abritis/RetractionDatabase.org

Source:

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- Improve your research
- Good scientific practice
- Data sharing with colleagues
- Data Publication
 - Required by increasing number of journals
 - Obviate retraction
 - Get credit for your data!
- Enable new kinds of research
 - Feedback loops between empirical and modeling approaches
 - Initiating research questions in completely different fields





Publications are arguments made by authors, and **data are the evidence** used to support the arguments.

(Christine Borgmann, 2014)





Levels of Data Preservation

rights, responsibilities, institutions, funding, ...

intellectual interpretability metadata on content and context

> logical re-usability readable file formats

technical stability bitstream preservation





Levels of Data Preservation



intellectual interpretability metadata on content and context

logical re-usability readable file formats

technical stability bitstream preservation



Knowledge

Information

Data

Characters





Levels of Data Preservation





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Data preservation motivation

Data Sharing and Management Snafu in 3 Short Acts by Karen Hanson, Alisa Surkis & Karen Yacobucci NYU Health Sciences Libraries August 3, 2012 (Last Update: December 12, 2012)







STORING DATA





Why do I want to store my data?

	Purpose	Solution
?	short-term storage, backup copy	institutional backupindividual backup
	long-term storage, archiving	 Data archive, institutional archive solution or individual archiving
	making data available to others	Data repository:institutional,generic orsubject-specific



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Yes, we store – what for?

	Backup	Archival	Depositing
Storage Purpose	Ability to restore data in case of data loss or error propagation	Enable validation by peers through persistent storage of data used for research results / publication	Enable verification, citation & reuse of datasets (data sharing)
Data Characteristics	Duplication of current work data & intermediate work results	Archive format (e.g. zip) containing all related & relevant data / files (ideally incl. metadata)	Format specified by repository; discipline- specific metadata standards
Process Regularity	Regularly during work phase or project runtime	Once for each relevant dataset, usually at the end of or after work phase	Once for each selected dataset, either during or after work phase
Effort	Depends – e.g.: set up once, verify regularly	Establish predefined procedure with data archive (e.g. data center)	Process documented, sometimes guided by repository





Self-Assessment: Backup

Check for yourself:

- Do you backup your research data? How?
- How often do you do it?
- Have you ever tried to recover a deleted file?
- Can you return to a previous version of a file?
- Who is responsible for Backup and Storage services at your institute?



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Why Backup?

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Laptop stolen Stop J

...relevant working material for distance

learning course... wurde mein U gerne ine Festplatte wiederhaben. A meine Dissertation, die einzige Kopie n Fernkurs den ich zurzeit absolviere wiederhaben würde. Ich war so dumr mit dem Laptop ein ganzes Jahr Art

one year's value of work disappeared

er Zukunft ie vor den Laptoptasche entwendet!

Cont

m

Finderlohn: 1.000€ in b:

s of stuff.

Jackup opies ure plans smoke



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Source: Gino on flickr



Source: steviep187 on flickr 😳 😗 🕫





Why backup?

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Source: University of Southampton, Department of Electronics and Computer Science, 2005

> **Source:** reuters.com, image by Sapeurs-Pompiers du Base-Rhin, 2021:

OVHCloud data center in Strasbourg, France

Source: Frankfurt University of Applied Sciences, March 2020 © Frankfurt Fire Department







As **you** are responsible for your research methods and results, **you** are also responsible for your research data.

If you rely on others to store your data, make sure you know:

- where the data are stored
- what measures are in place for data safety and data security
- how you or someone else can access and retrieve backups
- whom to contact in case of emergency or for support





Sources of Data Loss






Sources of Data Loss

- Malware / Theft / Destruction
- Software failures
 - Program errors / bugs / software updates
 - Features

(e.g.: Dropbox overwriting on synchronization)

- Hardware failures
 - Bad design / cheap parts / defects
 - Age
 - Dropped laptops / HDDs
 - Liquids (water, coffee, coke)
 - Lightning strikes / electric pulses
- Human errors
 - Accidental deletion
 - Missing knowledge



Source: a man working at home while eating breakfast by Socialeurope via flickr: https://www.flickr.com/photos/socialeurope/4303391587



Source: Kroll Ontrack, 2007, Robin Harris, http://www.zdnet.com/blog/storage/how-data-gets-lost/167

Further reading: disasters and tales of data loss, statistics on how data gets lost





Is backing up really worth the effort?

- PhD or postdoc salary costs for employer: € 79.800 - 86.100 / year *
- Estimated costs for losing data of one year's work: usually even higher Hours
- Besides, you can lose a lot of time ... and possibly your nerves

Required investments:

- External hard drives start at € 50,-
- Backup Software is included in most modern operating systems

> When will you start? When will you be required to?

* DFG staff appropriation rates for 2024: https://www.dfg.de/de/formulare-60-12-246894



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Backup Principles

- Create multiple backups
- Expect human errors (keep older versions)
- Do not use backup drives for sharing files
- Store backups physically separate from your PC / laptop
- Check your backups regularly
- Practice the worst case and make a full recovery dry-run
- Discuss the topic with friends to learn their best-practices
- Include required software, scripts, documentation in your planning



- 3 copies
- 2 different media
- 1 remote



eResearc **Backup Strategy Recommendations**

- 1. Use an **institutional storage solution** for backing up your work and data on a daily basis (e.g. network drive, ownCloud)
- 2. Use your OS built-in backup software or an external software to regularly back up your data to external media
 - Predefine files/folders that are regularly backed up
 - Automate the process, eventually make a calendar entry
- Keep one backup copy at a remote place 3.
- **4.** Check your backups regularly (e.g. once/month) on integrity by performing by random checks
- 5. Practice doing a **full recovery dry-run** at least once
 - Possibly have a workstation set up at work for practicing



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Backup-Software

Operating system	Integrate Backup S		Comment						
Windows 7	File Recovery		Requires configuration, to not only copy local librariesCan create bootable image						
Windows 8/10	File History ("Dateiversions- verlauf")		 Saves only local libraries Can be configured by individual libraries and excluding folders Cannot create bootable image 						
Mac OS	Time Machine		 Saves everything except excluded folders Can use encryption Can be used to recover a non-booting Mac 						
Ubuntu Déjà Dup)	Uses encryption and compressionCan use cloud storage						
Operating system Free		Free other	ree other Backup Software						
Windows Pe		Personal Backup, PureSync, Paragon Backup&Recovery, Robocopy,							
Mac OS		Carbon Copy Cloner, SuperDuper,							
Ubuntu		Rsync, Timeshift							



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GWDG Storage Services

Name	Backup	Archival	Sharing	Comment
Fileservice / Active Directory	Yes	No	Possibly	Network drives, e.g. P: , possibly more Are backed up automatically
IBM Tivoli Storage Manager (TSM)	Yes	Partially	No	Offer for institutes to centrally back up servers or local workstations
CrashPlanProE	Yes	No	No	Individual Backup-Solution GWDG License: €29,- per year
ownCloud	Partially	No	Yes	Free storage: 50 GB, extendable
GRO.data	Partially	Partially	Yes	Primarily for data exchange and data storage for subsequent publication
HSM	No	Yes	No	For archiving data from finished projects
GitLab	No	Partially	Yes	Versioning; not for large data amounts

More info: <u>https://info.gwdg.de/dokuwiki/doku.php?id=en:services:storage_services:start</u> ⁴²





Organisation of Data











Organize your files so that you and others can find and access things when you need them



File Naming Conventions

To stay organized, you should define:

- A self-describing folder structure or tagging scheme
- What information should be in filenames
- How filenames should be structured
- How to group and label related files
- · How to refer to and exchange files

... especially when working in a team! Self-speaking file name:

20240613_RDM_CRC1073_v42.pptx

vs. short file name:





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Avoid special characters



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File Naming Policy Example

• All data files must be stored using this naming scheme:

```
[experiment_datetime] [experiment_name] [experiment_part] [data_type] [executi on_no].[file_extension]
```

• All script files must be stored using this naming scheme:

[experiment_datetime] [experiment_name] [experiment_part] [script_version_no].
[file_extension]

• All analyses files must be stored using this naming scheme:

[experiment_datetime] [experiment_name] [experiment_part] [analysis_datetime] [analysis_type].[file_extension]

- All dates in filenames must be in ISO 8601 format: YYYY-MM-DD
- All data files, script files, analyses files and image files are stored in separate folders: data, scripts, analyses, images
- For publishing datasets, zip archives are created containing the relevant files and according to the following naming scheme:

[experiment_datetime]_[experiment_name]_[experiment_part]_[archiving_date].zip





Versioning

20240613_RDM_CRC1073_v13.pptx
20240613_RDM_CRC1073_v13final.pptx
20240613_RDM_CRC1073_v13new-fine1.pptx
20240613_RDM_CRC1073_v13final-finalv1.pptx
20240613_RDM_CRC1073_revised_v01a.pptx

Best practice:

- Before editing a file, save it under a new name as a new version
- Use consecutive version numbers and eventually author initials
 - No "final" or other unreliable descriptors in filenames
 - Rather **use folders** to mark/sort different purposes and avoid confusion
- If you collaborate, agree on a common naming system for versioning
- **OR:** Use a versioning system
 - e.g. gitlab, ownCloud or GRO.data





Version control with git

- · Mainly used in software development
 - many functionalities for the support of development processes
- Also usable for versioning of documents
- GWDG gitlab
- Web based versioning system
- Advice and support for the establishment of your projects by GWDG
- Connection to the GWDG user administration
- Central monitoring, system stability and backup by the GWDG
- Carpentries workshops on gitlab by SUB

More information: https://info.gwdg.de/docs/doku.php?id=en:services:email_collaboration:gitlab:start







Persistent Identifiers (PIDs)



404 Not Found – 👧

Die angeforderte Seite/Datei konnte nicht gefunden werden.

KONTAKT

Georg-August-Universität Göttin Wilhelmsplatz 1 37073 Göttingen Tel. +49 551 39-0

ONLINE-DIEN

Vortesungsverzeichnis und Personenzuche (UniV2) Prüfungsverwaltung (FlexNow Lemmanagemert (Stud.IP) Studierendenportal (eCampus Mitarbeiterinnenund Mitarbeiterportal (MaP) Stellenausschreibungen Stellenaus (Göttingen

SERVICE Datenschutz Kontakt Notfall Lageplan

1

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What are persistent Identifiers (PIDs)?

Common referrers or links like URLs point directly to the location of an object:

When the storage location of the object changes, the reference points to nothing. The referenced object cannot be found:

The basic idea behind the concept of PIDs is to introduce an **intermediary** between the link and the referenced object:



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This intermediary monitors any movement or changes performed on the object and always directs requests to the current storage location.

Adapted from: Kálmán, Tibor: Nachhaltige Referenzierung von digitalen Objekten mit Hilfe von persistenten Identifikatoren (Persistent Identifiers), nestor/DigCurV School 2012, 22-24 October 2012, <u>http://hdl.handle.net/11858/00-ZZZZ-0000-0007-5E80-3</u>

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What are persistent Identifiers (PIDs) ?

- Prevention of dead links
- Unique naming (referencing) of a digital ressource (e.g. journal articles or research data)
- Assignment of a stable and uniquely referencable code to be resolved on the internet
- Examples:
 - •DOI 10.17192/bfdm.20181.7816
 - •Handle hdl:11304/6eacaa76-c275-11e4-ac7e-860aa0063d1f
 - •EPIC 21.11101/0000-0000-9D43-4
 - •URN urn:isbn:0451450523
 - •PURL http://purl.abcd.org/ABC/DEF/200
 - •ORCID https://orcid.org/0000-0001-2345-6789





How do I get a PID?

- Publications: From the publishing journal or repository
- Data: Public depositing in a repository
- At the Göttingen Campus:
 - GRO.data (Campus-Repositorium), GRO.publications
 - SUB Göttingen: GOEDOC, University press
 - GWDG: ePIC PID-Service

More information:

https://www.eresearch.uni-goettingen.de/knowledge-base/howto/getting-an-identifier/





Metadata



Studies in Conservation

2012

VOL 57

NO. 1

24



Explain these data

	-	0		0.0		0	0.40	0.0		0.04		
AOC	Caesalpinia sappan	2	Dyed silk A	8.0 9.8		3	0.12	2.1		0.61 0.46		3.8 4.9
		2	Dyed wool A	9.8	0.8	25	0.16	5.4	0.1	0.46		3.6
	Carthamus tinctorius	2	Pigment A Dyed silk A	19.6	0.0	2.5	0.06	2.9	- W. I	0.46		6.6
	Cartnamus tinctonus	2		12.2		2.5	0.11	2.8		0.73		4.3
		2	Dyed wool A Prepigment on paper	19.7	0.4	2.5	0.05	3.2	0.1	0.40		6.2
	Curcuma longa	2	Dyed silk A	8.7	0.4	3	0.12	6.6	0.1	0.18		1.3
	Curcuma longa	2	Dyed silk N	8.5		3	0.18	3.8		0.61		22
		2	Dyed wool A	12.3		2.5	0.09	7.7		0.09		1.6
		2	Pigment A	8.6	0.4	3	0.20	4.2	0.9	0.37		2.1
	Gardenia augusta	2	Dved silk A	6.4	0.4	3	0.18	1.1	0.0	0.80		5.6
	Gardenia augusta	2	Dyed silk N	9.2		3	0.30	2.8		0.42		3.3
		2	Dyed wool A	7.2		3	0.26	3.1		0.43		2.3
		2	Pigment A	16.3	0.4	2.5	0.10	11.4	0.3	0.16		1.4
	Laccifer lacca	2	Dyed wool A	5.1	0.4	3	0.29	0.9	0.0	1.24	1.1	4.5
	Laccheriacca	2	Pigment A	6.1	0.3	3	0.32	0.8	0.6	9.99	3.0	2.0
	Lithospermum erythrorhyzon	2	Dyed silk A	6.5	0.0	3	0.29	5.4	0.0	0.40	0.0	12
	Linospernum eryanomyzon	2	Dyed silk N	8.6		3	0.18	4.0		0.40		22
		2	Pigment A	16.9	1.6	2.5	0.17	4.3	0.3	0.49		4.0
	Philodendron amurens	2	Dved silk N	4.7	1.0	3.5	0.34	3.7	0.0	0.39		1.3
	Prinodeniaron amarens	2	Pigment A	7.2	0.1	3	0.18	0.7	0.4	1.72	1.0	7.0
	Rhamnus catharticus, immature	2	Dyed silk A	5.2		3	0.31	0.7		1.83	1.2	4.4
	Andrinus capitarious, ininature	2	Pigment A	11.2	0.1	2.5	0.15	1.7	0.4	1.06	1.5	6.5
	R. catharticus, ripe	2	Dved silk A	10.7		3	0.09	4.2		0.60		2.5
	n. casiancus, npe	2	Dyed wool A	7.2		3	0.18	2.9		0.57		2.5
F	Rubia tinctorum	2	Dved silk A	3.9		3.5	0.37	2.7		0.72		1.5
		2	Dyed wool A	5.1		3	0.19	2.7		0.45		1.9
		2	Pigment A	6.8	0.8	3	0.31	1.3	1.2	5.56	2.3	3.0
	Sophora japonica	2	Dved silkA	3.4		3.5	0.54	2.3		0.52	1000	1.5
	oupriora japonica	2	Dyed wool A	5.0		3.5	0.32	22		0.51		22
		2	Pigment A	9.6	1.6	3	0.25	1.2	0.1	1.52	2.0	4.9
EU-Artech	Reseda luteola	2	Dyed wool A	2.0		4	0.51	2.1		0.55		0.9
LO-HILBOIT	THE BEGRA HATE UNA	2	Pigment AC	7.8	0.6	3	0.15	0.9	0.1	1.08	1.0	8.3
		2	Pigment AL	7.5	0.7	3	0.08	0.8	0.1	1.37	1.0	7.4
		2	Pigment AP	5.5	0.5	3	0.28	1.2	1.1	5.67	2.6	22
Schweppe	Rocella tinctoria	2	Dved wool A	12.1		2.5	0.28	3.0		0.72		4.1
ISOBW	ISOBW1	2	Dved wool	30.5		_	0.02	7.0		0.11		4.3
00011	ISOBW2	2	Dyed wool	24.9			0.03	5.9		0.17		42
	ISOBW3	2	Dyed wool	6.6			0.19	0.6		1.45	0.8	8.2
CMN	Acer	1	Leaf	16.4		2.5	0.10	23		1.03	2.4	6.9
	Aster	1	Leaf	23.3		2	0.04	1.6		0.76		14.2
	Dryopteris	1	Leaf	26.4		1.5	0.05	1.3		0.98		20.8
	Scirpus	1	Grass	9.2		3	0.27	0.4		2.48	1.0	9.6
	Trifolium	1	Leaf	17.1		2.5	0.09	0.9		1.46	1.3	13.2

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Explain these data

	Sample		Туре	ΔE_{Air}		MCDMAir: AEAir	MCDMAir	ΔEAnoxia		MCDMAnox: AEAnox	MCDMAnox		
Source		Trial		Mean	SD	BW	Max	Max	Mean	SD	Max	Max	ΔE_{F}
AOC	Caesalpinia sappan	2	Dved silk A	8.0		3	0.12		2.1		0.61		3.8
		2	Dyed wool A	9.8		3	0.16		2.0		0.46		4.9
		2	Pigment A	19.6	0.8	2.5	0.14		5.4	0.1	0.46		3.6
	Carthamus tinctorius	2	Dved silk A	19.3		2.5	0.06		2.9		0.44		6.6
		2	Dyed wool A	12.2		2.5	0.11		2.8		0.73		4.3
		2	Prepigment on paper	19.7	0.4	2.5	0.05		3.2	0.1	0.40		6.2
	Curcuma longa	2	Dved silk A	8.7		3	0.12		6.6		0.18		1.3
	o si o si na i o i ga	2	Dved silk N	8.5		3	0.18		3.8		0.61		22
		2	Dyed wool A	12.3		2.5	0.09		7.7		0.09		1.6
		2	Pigment A	8.6	0.4	3	0.20		4.2	0.9	0.37		2.1
	Gardenia augusta	2	Dyed silk A	6.4		3	0.18		1.1		0.80		5.6
	ouroonia aogosia	2	Dyed silk N	9.2		3	0.30		2.8		0.42		3.3
		2	Dyed wool A	7.2		3	0.26		3.1		0.43		23
		2	Pigment A	16.3	0.4	2.5	0.10		11.4	0.3	0.16		1.4
	Laccifer lacca	2	Dyed wool A	5.1		3	0.29		0.9		1.24	1.1	4.5*
	Laconeriacia	2	Pigment A	6.1	0.3	3	0.32		0.8	0.6	9.99	3.0	2.0*
	Lithospermum erythrorhyzon	2	Dyed silk A	6.5	0.0	3	0.29		5.4	0.0	0.40	0.0	1.2
	Linospernum erymonryzon	2	Dyed silk N	8.6		3	0.18		4.0		0.40		22
		2	Pigment A	16.9	1.6	2.5	0.17		4.3	0.3	0.49		4.0
	Philodendron amurens	2	Dyed silk N	4.7	1.0	3.5	0.34		3.7	0.0	0.39		1.3
	Filliodeniatori amurens	2	Pigment A	7.2	0.1	3	0.18		0.7	0.4	1.72	1.0	7.0*
	Rhamnus catharticus, immature	2	Dved silk A	5.2	0.1	3	0.31		0.7	0.4	1.83	1.2	4.4*
	Anamnus catharticus, immature	2	Pigment A	11.2	0.1	2.5	0.15		1.7	0.4	1.06	1.5	6.5
	D antibadiana sina	2	Dved silk A	10.7	0.1	3	0.09		4.2	0.4	0.60	1.0	2.5
	R. catharticus, ripe	2		7.2		3	0.18		2.9		0.57		25
	Duble fiester of	2	Dyed wool A	3.9		3.5	0.37		2.7		0.72		1.5
	Rubia tinctorum	2	Dyed silk A	5.1		3.5	0.19		2.7		0.45		1.9
		2	Dyed wool A	6.8	0.8	3	0.31		1.3	1.2	5.56	2.3	3.0*
	0	2	Pigment A	3.4	0.8	3.5	0.54		2.3	1.2	0.52	2.3	1.5
	Sophora japonica	2	Dyed silkA	5.0		3.5	0.32		2.2		0.52		22
		2	Dyed wool A		1.6	3.5	0.32		12	0.1		2.0	4.9*
	Provide Lands		Pigment A	9.6	1.6	4				0.1	1.52	2.0	
EU-Artech	Reseda luteola	2	Dyed wool A	2.0	0.6	4	0.51		2.1	0.1	1.08	1.0	0.9
			Pigment AC				0.15						
		2	Pigment AL	7.5	0.7	3	0.08		0.8	0.1	1.37	1.0	7.4
	2 10010 100	2	Pigment AP	5.5	0.5	3	0.28		1.2	1.1	5.67	2.6	2.2*
Schweppe	Rocella tinctoria	2	Dyed wool A	12.1		2.5	0.28		3.0		0.72		4.1
ISOBW	ISOBW1	2	Dyed wool	30.5		-	0.02		7.0		0.11		4.3
	ISOBW2	2	Dyed wool	24.9			0.03		5.9		0.17		4.2
	ISOBW3	2	Dyed wool	6.6		-	0.19		0.6		1.45	0.8	8.2*
CMN	Acer	1	Leaf	16.4		2.5	0.10		2.3		1.03	2.4	6.9*
	Aster	1	Leaf	23.3		2	0.04		1.6		0.76		14.2
	Dryopteris	1	Leaf	26.4		1.5	0.05		1.3		0.98	2223	20.8
	Scirpus	1	Grass	9.2		3	0.27		0.4		2.48	1.0	9.6*
	Trifolium	1	Leaf	17.1		2.5	0.09		0.9		1.46	1.3	13.2*

Studies

2012

NOL 57





Information Entropy

Time of data development







Explain Your Data

- Why?
 - Make data *FAIR*: Findable, Accessible, Interoperable, Reusable!
 - Not only for others, but also and mainly for yourself!
- How?
 - Directly write down which **methods/materials** you used. Write down what fails and what was successfully analysed.
 - Write down time, place, persons involved in creation of data.
 - Include title, name of primary and processed data.
 - Add a text file with this information to each data file/folder or: keep an overview spreadsheet
 - **Do not change/erase your original notes** but add more infos chronologically (with date of insertion).





Excursion: FAIR data principles



eResearch

Set of guiding principles for research data

- Goal: make data Findable, Accessible, Interoperable and Reusable
- Address data producers and data publishers to promote maximum use of research data
- FAIR refers to both humans and machines
- Published in 2016:

Wilkinson, M., Dumontier, M., Aalbersberg, I. *et al.* The FAIR Guiding Principles for scientific data management and stewardship. *Sci Data* **3**, 160018 (2016). https://doi.org/10.1038/sdata.2016.18

More information: <u>https://www.force11.org/group/fairgroup/fairprinciples</u>





FAIR data Principles

Findable:

- F1. (meta)data are assigned a globally unique and eternally <u>persistent</u> <u>identifier</u>.
- F2. data are described with <u>rich metadata</u>.
- F3. (meta)data are registered or indexed in a <u>searchable resource</u>.
- F4. metadata specify the <u>data identifier</u>.

Accessible:

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

Interoperable:

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

Re-usable:

R1. meta(data) have a plurality of accurate and relevant <u>attributes</u>.
R1.1. (meta)data are released with a clear and accessible <u>data usage license</u>.

R1.2. (meta)data are associated with their <u>provenance</u>.

R1.3. (meta)data meet domain-relevant <u>community standards</u>.





FAIR Data ≠ Open Data !

- FAIR Data aims at maximum reusability of data, this includes:
 - specific licensing of data to specify the usage conditions
 - possibility of authentication and authorization
 - metadata and identifiers for findability and reusability
- Open Data (just) means that the data are freely accessible and available, but usually makes no claim regarding
 - findability
 - retrievability
 - interoperability
 - reusability
 - metadata
 - licensing and citation requirements





What are metadata?



- Different definitions, depending on the perspective
- Practical approach: Metadata...
 - describe objects in a structured and standardized way
 - can help in the selection and identification of resources
 - can describe how to use data correctly or how to reproduce it
 - can describe everything: literature, a painting, places, a set of data...
 - can be digitally linked to objects (embedded) or added separately





What are metadata?

Who created what,



DFG FOR 552

Timo Henne henne@sub.uni-goettingen.de

r x y abs 35 0.4 34 36 535 0.5 2 777 63 2.6 67 4 1.3 61 5

Excel spreadsheet Used with test data for gene training purposes orig

how,

Used random number generator to modify original field data

when,







At my office Windows PC

where and

To be used in training workshop

why?

Include:

- Description of the item
- Methodology and instrumentation
- Units of measurement
- References to related data
- Definitions of jargons, acronyms, code
- Technical information about the file



"Metadata describes objects in a structured and standardised way..."

Many existing metadata standards, e.g.:

Dublin Core Metadata Element Set (15 optional elements)



Can be extended to 55 elements (DCMI Metadata Terms):

abstract, accessRights, accrualMethod, accrualPeriodicity, accrualPolicy, alternative, audience, available, bibliographicCitation, conformsTo, created, dateAccepted, dateCopyrighted, dateSubmitted, educationLevel, extent, hasFormat, hasPart, hasVersion, instructionalMethod, isFormatOf, isPartOf, isReferencedBy, isReplacedBy, isRequiredBy, issued, isVersionOf, license, mediator, medium, modified, provenance, references, replaces, requires, rightsHolder, spatial, tableOfContents, temporal, valid

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DFG FOR 5522 -<oai_dc:dc>

- <dc:title> Sociology of Religion: Exercises Using General Social Surveys, 2000-2002 [Instructional Materials] <dc:title>

<dc:treator>Nelson, Edward E.</dc:creator> <dc:subject>Bible</dc:subject>

<dc:subject>Christianity</dc:subject>

<dc:subject>church attendance</dc:subject> <dc:subject>instructional materials</dc:subject>

<dc:subject>instructional materials</dc:subject> <dc:subject>instructional modules</dc:subject>

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<dc:subject>religious fundamentalism</dc:subject>

<dc:subject>social issues</dc:subject> <dc:subject>sociology</dc:subject>

<dc:subject>ICPSR.X.A.3</dc:subject>

<dc:subject>ICPSR.XVI.A</dc:subject>

- <dc:description>

These instructional materials were developed from GENERAL SOCIAL SURVEYS, 1972-2002: [CUMULATIVE FILE], compiled by James A. Davis, Tom W. Smith, and Peter V. Marsden. The data file (an SPSS portable file) and accompanying documentation are provided to assist educators in instructing students about religion and social issues in the United States in the late 20th and early 21st centuries. An instructor's handout has also been included. This handout contains the following sections, among others: (1) an exercise using General Social Surveys data to create and validate a measure of religiosity, and then to relate the measure to other social variables, (2) an exercise using General Social Surveys data to explore the relationship between religiosity and other social variables using crosstabulation (focusing on two- and three-variable relationships) and to explore the concepts of explanation, spuriousness, and replication, and (3) an exercise using General Social Surveys data to create a measure of religious fundamentalism and to explore the relationship between this measure and various forms of religious behavior and opinions on social issues. The data contain information on the attitudes of a national probability sample of adults 18 years of age and older on a range of social and political issues. For this instructional subset, some variables were recoded and some new variables were created to facilitate analysis. Variables in the dataset include responses to questions on family and gender roles, abortion, sex and sexual materials, personal morals and social mores, social control, general political attitudes, and social control, general political attitudes, and social control.

</dc:description>

<dc:date>2005-01-07</dc:date>

<dc:type>survey data</dc:type>

<dc:identifier>3719</dc:identifier>

<dc:identifier>10.3886/ICPSR03719.v2</dc:identifier>

<dc:source>personal interviews</dc:source>

<dc:coverage>United States</dc:coverage>

<dc:coverage>2000--2002</dc:coverage>

-<dc:rights>

ICPSR metadata records are licensed under a Creative Commons Attribution-Noncommercial 3.0 United States License

(http://creativecommons.org/licenses/by-nc/3.0/us/).

</dc:rights>

</oai_dc:dc>

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Why Metadata Standards?

- A standard provides a structure with which data can be described:
 - Common terms to ensure consistency
 - Common definitions for easier interpretation
 - Common language to facilitate communication
 - Common structure for quick information retrieval
- For search and retrieval, standards offer:
 - a documentation structure in a reliable and predictable format for computer interpretation
 - a uniform summary description of the data set







Example Metadata standards

• HDF5

HDF5 is a data model, library, and file format for storing and managing data. It supports an unlimited variety of datatypes, and is designed for flexible and efficient I/O and for high volume and complex data. HDF5 is portable and is extensible, allowing applications to evolve in their use of HDF5.

NeXus

NeXus is an international standard for the storage and exchange of neutron, x-ray, and muon experiment data. The structure of NeXus files is extremely flexible, allowing the storage of both simple data sets, such as a single data array and its axes, and highly complex data and their associated metadata, such as measurements on a multi-component instrument or numerical simulations.





Example Metadata standards

• CHEMINF

The Chemical Information Ontology (CHEMINF) aims to establish a standard in representing chemical information. In particular, it aims to produce an ontology to represent chemical structure and to richly describe chemical properties, whether intrinsic or computed.

BioAssay Ontology

The BioAssay Ontology (BAO) describes chemical biology screening assays and their results including high-throughput screening (HTS) data for the purpose of categorizing assays and data analysis.





Data sharing





Data sharing - motivation



Quote from: William E. Demming (1900-1993)



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... but active, open sharing? for free??



Source: Sharing by ryancr via flickr







Reputation

- Get credit for high quality research
- Increased understanding of your methods
- Allows work to be verified by others
- Recognition for contribution to research community
- Extend research beyond your discipline

Funding

- Making data and/or publications available may be a requirement of your funding body
- It may make your funding proposal more attractive when sharing data is not essential
Why share your data?



Impact

- Sharing makes your data:
 - Easier to find
 - Easier to access
- Open data/publications leads to increased citations

Source: Richard Matthews, flickr: dart (2011) online at: https://commons.wikimedia.org/wiki/File:Darts in the middle of a dartboard.jpg?uselang=de

Reuse

- Starting point for a complementary study
- Test data for new software and algorithms
- Teaching purposes
- · Contexts not currently envisioned



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Data Sharing - Credits?

Well documented research data

helps your own (future) research

Shared data may serve as

facilitator for cooperation

- Increased accessibility and usability will enable reuse and citations
- Public data and open access will

extend the range of your data and research





Data Sharing - Real Barriers

• Place

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- No sharing tradition
- No repository
- No expertise
- Funds
 - No money
- Rights
 - No carte blanche



Source: <u>Simatai Great Wall</u> by Arian Zwegers on Wikimedia Commons





Modes of Sharing

Transfer	Access	Use	
Way	Mode	Condition	

peer-to-peer	restricted	none
webspace	on demand	agreement
repository	embargo	license
	open	



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Finding OA journals and repositories

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GRO.data: Research Data Repository

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https://data.goettingen-research-online.de/

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Supplementary Data: Status of the scalar singlet dark matter model (arXiv:1705.07931)







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Physics

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- Astrophysics (astro-ph new, recent, search) includes: Astrophysics of Galaxies; Cosmology and Nongalactic Astrophysics; Earth and Planetary A: Instrumentation and Methods for Astrophysics; Solar and Stellar Astrophysics
- Condensed Matter (cond-mat new, recent, search) includes: Disordered Systems and Neural Networks; Materials Science; Mesoscale and Nanoscale Phy Condensed Matter; Statistical Mechanics; Strongly Correlated Electrons; Superconductivity
- General Relativity and Quantum Cosmology (gr-qc new, recent, search)

New arXiv articles are now automatically

assigned DOIs

Update: As of Feb 2022, all arXiv articles now have DOIs.

New articles submitted to arXiv are now automatically assigned DOIs that align with their arXiv ID. This makes research articles more discoverable across search engines because associated metadata is made available to the community in a reusable format.

DOIs (digital object identifiers) are unique and unchanging, just like the original arXiv ID number already assigned to every arXiv article. However, because DOIs are used across many different platforms, they enable greater interoperability with other services.

"Sure, the arXiv papers have had a persistent identifier for years, the arXiv identifier, and that's a very good thing not only for citability. But with the assignment of DOIs, arXiv now becomes even more visible as an important element of the publication ecosystem," said Dr. Irina Sens, Deputy Director and Head of Library Operations at the Technische Informationsbibliothek in Germany, which organizes arXiv's



largest member consortium. "The DataCite metadata schema enables connections to other persistent identifiers, for example researchers' ORCIDs and institutional RORs, and other content like associated research data – and offers easy tracking of research outputs through simple user interfaces. That's a huge step forward."

DOIs align with arXiv IDs



Publishing / sharing research software

- Any scripts, methods implementations or programs that you use or develop in your research can be important to understand, verify, reproduce or reuse your results
- If possible, you should also share or publish such software in a similar way as your research data (including metadata and documentation), in order to:
 - ensure your software is citable, preserved, and accessible to support scientific reproducibility, replication, and transparency.
 - gain appropriate credit for your work
 - help your research community by enabling reuse
 - fulfil increasing requirements by funders and journals
- Where and how do you do that?

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Publishing software: where

	Main purposes	Examples	Pros
Source code repository	Accessibility, cooperation, development	Github, Codeplex, BitBucket, Sourceforge	ongoing development, own organization & structure, workflow integration
Software journal	Scholarly attribution, credit, citation	JOSS (OA), JORS (SSI), RescienceC (OA), PLOS One, Computer Physics Communication, SoftwareX (Elsevier)	Visibility, DOI assignment, review process
General application archive	Transparency, replicability, reuse	Zenodo, Figshare	Versioning, DOI assignment
Disciplinary archive	Reuse	CRAN, NanoHub	Visibility, possibly across communities
Institutional archive	Preservation	GRO.data	Easy access, institution's commitment



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Publishing research software: how

OSI's Open Source Definition

- free redistribution
- source code availability
- derivatives allowed
- no limitations of who may use it or for what
- no additional license in place
- license must not depend on distribution format, technology, presence of other works





Publishing research software: how

- 1. Create a software citation file
 - can be human readable CITATION files or machine readable
 - should include:
 - author(s)
 - title of the software package or code
 - · link to the code location
 - DOI or other unique identifier
 - version number
 - release date
- 2. Choose a license

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Research software licenses

- Why do I need a license?
 - As creator, you are the sole copyright holder of your work
 - Others are legally not allowed to reuse your software, even if it is freely available
 - A license allows you to define *additional rights and obligations* regarding your work that go beyond the copyright you own, and it can protect yourself
- What options are there in licenses?
 - adhere to similar terms: Copyleft (GPL, AGPL, LGPL), CC-BY-SA
 - attribution & protection: MIT, BSD, Apache, CC-BY
 - no commercial use: CC-BY-NC
 - no claims: Public Domain, CC0, Unlicense





Publishing research software: how

- 1. Create a software citation file
- 2. Choose a license
- 3. Include a license in your software
 - a) can be included in citation file
 - b) or create a separate LICENCE.txt
- 4. Choose your channel(s) or place(s) for publication
 - a) Code repository
 - b) Software journal
 - c) Software archive





Publishing software: Further reading

- <u>https://libguides.mit.edu/software</u>
- <u>https://www.software.ac.uk/top-tip/which-journals-should-i-publish-my-software</u>
- <u>https://www.tudelft.nl/en/library/research-data-</u> management/r/publish/publish-research-software
- <u>https://blog.tib.eu/2024/02/29/software-journals-der-einfluss-von-software-auf-die-forschung/</u>
- <u>https://github.com/readme/guides/open-source-licensing</u>
- <u>https://choosealicense.com/</u>
- <u>https://www.tldrlegal.com/</u>





Other services on campus

Name	available through	Purpose/comments
Jupyter notebooks	GWDG	Live editing and execution of text, diagrams, equations and code in a web browser
CodiMD pad	GWDG	Collaborative text editing
Electronic laboratory notebook	UMG	(Re)organisable, searchable and storable research documentation
Self-study online courses on digital competencies	SUB	Courses on literature search, IT basics, data security, data visualization, OER https://www.uni-goettingen.de/en/565228.html
Open Access Publication Fund	SUB	full coverage for up to € 2.000,- for publication in OA journals
Overleaf (ShareLaTeX)	GWDG	Collaborative LaTeX editing in the browser





GWDG services

SERVICES

Storage Services

Data Archiving Backup File Service GWDG ownCloud Cryptshare

E-Mail Collaboration

E-Mail-Service (MS Exchange 2016) Spam and Virus Filtering Mailing Lists MS Sharepoint Managed Services Project Management Service GWDG Pad ShareLaTeX Rocket.Chat GWDG Web-Office GitLab

Server Services

Virtual Server Housing of Servers Web Hosting GWDG Cloud Server FTP-Server

Network Services

IP Address Management System System Monitoring Setting up eduroam Integration into the Active Directory User Management with OpenLDAP Client Management for Windows Client Management for macOS and iOS

Application Services

Persistent Identifier (PID) Library Service Aleph Library Service Koha Databases Application/Event Management Plagiarism Prevention Online Surveys Bioinformatics Programs Statistics Programs Jupyter Pseudonymisation and Data Trusteeship

General Services

Videoconferencing Identity and Access Management [MPG] Identity and Access Management [Uni] Single Sign-on (SSO) /Authentication and Authorization Infrastructure (AAI) URL Shortener Software and Licence Management Computer Lending Pool General Services - Print & Scan Services

IT Consulting

Scientific Data Management IT Security Hardware Purchase Apple Support Centre Establishing Directory Services (AD, LDAP) Planning of Data Transmission Networks

IT Security Services

Vulnerability Scans on Networkattached Equipment Public-Key-Infrastructure (PKI) Virus Protection (Sophos Update Service)

https://www.gwdg.de/services





Further information

https://reproducible-science-curriculum.github.io/rr-jupyterworkshop/

https://www.forschungsdaten.info/

https://www.dfg.de/foerderung/info_wissenschaft/2022/info_ wissenschaft_22_25/index.html

https://www.eresearch.uni-goettingen.de/consulting-andtraining/training-material/



Göttingen eResearch Alliance (eRA)

Team

- Diverse scientific backgrounds
 - Mainly in natural sciences and humanities
- Jointly run by





- Partner: University Research & Transfer Department, Medical Informatics
- High expertise on eResearch topics
- , We are no experts in your discipline, but we can relate to your data management requirements."



Alliance

eResearch





What eRA can do for you

- Consultations / Support
 - Research Data Management
 - Publication strategies
 - Digital methods, software and technologies to enhance a research project
 - Information hub for experts & expertise on the whole campus

- Training
 - Discipline- or projectspecific or general
 - Information material / knowledge base
- Collaboration
 - Liaising project partnership
 - Project as a service

www.eresearch.uni-goettingen.de



The deeper meaning of Research Data Management

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