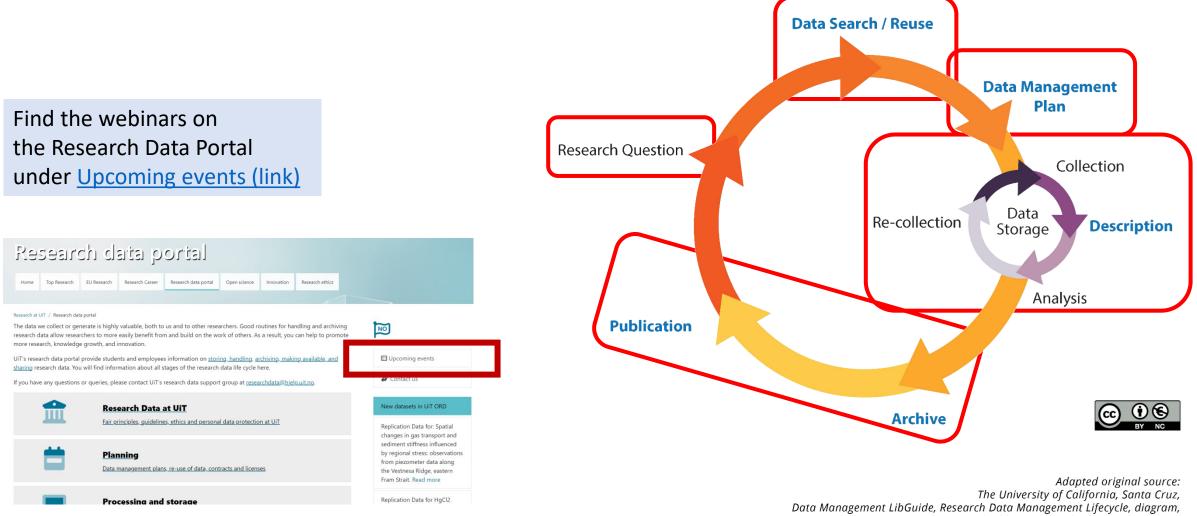


How to structure and document research data

Noortje Haugstvedt, PhD Adrian Verhoef, PhD 17.04.2023 – University Library

Research data @ UIT 😳 🕦 CC BY 4.0

The research data management lifecycle & webinars at UiT



viewed May 2, 2016 at <http://guides.library.ucsc.edu/datamanagement>

Learning objectives for this webinar

Why is it important to **structure** and **document** your data? How to do it in a **persistent** way? Where to find more **information** and **help**?

Please feel free to interrupt for questions or comments! Or use the chat to post questions and comments.

Why?

Do you know where your data are?



👤 Følg

I can't send you the original data because I don't remember what my excel file names mean anymore #overlyhonestmethods

retweets liker **129 80**

📽 🌃 🕼 🕄 🌒 🔊 🖉

09.11 - 8. jan. 2013

A STORY TOLD IN FILE NAMES:					
Location: 😂 C:\user\research\data			~		
Filename 🔺	Date Modified	Size	Туре		
🖁 data_2010.05.28_test.dat	3:37 PM 5/28/2010	420 KB	DAT file		
👸 data_2010.05.28_re-test.dat	4:29 PM 5/28/2010	421 KB	DAT file		
U data_2010.05.28_re-re-test.dat	5:43 PM 5/28/2010	420 KB	DAT file		
U data_2010.05.28_calibrate.dat	7:17 PM 5/28/2010	1,256 KB	DAT file		
data_2010.05.28_huh??.dat data_2010.05.28_WTF.dat	7:20 PM 5/28/2010 9:58 PM 5/28/2010	30 KB 30 KB	DAT file DAT file		
I data_2010.05.28_w1F.dat I data_2010.05.29_aaarrrgh.dat	12:37 AM 5/29/2010	30 KB	DAT file		
ata_2010.05.29_datangn.dat	2:40 AM 5/29/2010	0 KB	DAT file		
8 data_2010.05.29_crap.dat	3:22 AM 5/29/2010	437 KB	DAT file		
ata_2010.05.29_notbad.dat	4:16 AM 5/29/2010	670 KB	DAT file		
data_2010.05.29_woohoo!!.dat	4:47 AM 5/29/2010	1,349 KB	DAT file		
🛿 data_2010.05.29_USETHISONE.dat	5:08 AM 5/29/2010	2,894 KB	DAT file		
🕙 analysis_graphs.xls	7:13 AM 5/29/2010	455 KB	XLS file		
ThesisOutline!.doc	7:26 AM 5/29/2010	38 KB	DOC file		
Notes_Meeting_with_ProfSmith.txt	11:38 AM 5/29/2010	1,673 KB	TXT file		
	2:45 PM 5/29/2010	100.100	Folder		
😝 data_2010.05.30_startingover.dat	8:37 AM 5/30/2010	420 KB	DAT file		
<			>		
Type: Ph.D Thesis Modified: too many times Copyright: Jorge Cham www.phdcomics.com					

http://phdcomics.com/comics/archive.php?comicid=1323



Retraction Watch

Tracking retractions

Doing the right thing: Authors retract brain paper with "systematic human error in coding"

with one comment

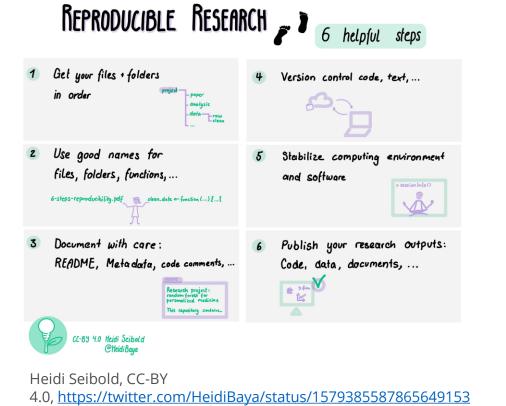
A group of Swiss neurologists have lost their 2013 article in *<u>Frontiers in Human Neuroscience</u>* after reporting that their data were rendered null by coding errors.

frontiers in HUMAN NEUROSCIENCE

"..<u>a systematic human error in coding the name of the files</u> had been made during the extraction of the EEG template topographic maps best differentiating the two experimental conditions at the single subject level." http://retractionwatch.com/2014/01/07/doing-the-right-thing-authors-retract-brain-paper-withsystematic-human-error-in-coding/

Why?







Scriberia, CC-BY 4.0 DOI: 10.5281/zenodo.3332807.

Avoid data loss

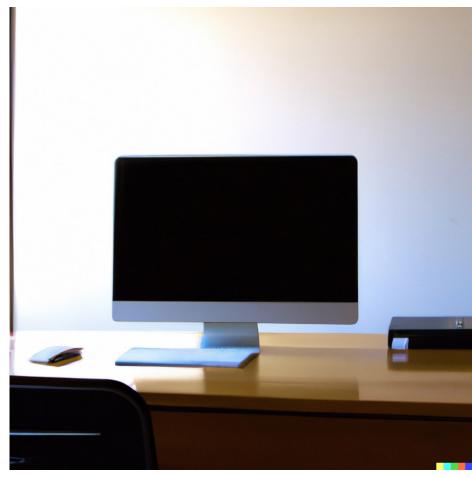
Make sure your data are **understandable** even several years from now

The most important elements:

- Data storage
- Structuring of files and folders
- Names on data files and folders
- Documentation of data: ReadMe and metadata
- The file formats



Plan the data structure early in the project – before you start collecting data.



How it started How it's going

Images created with DALL*E

Folder naming and organization

Folders can be useful to organize and structure your data

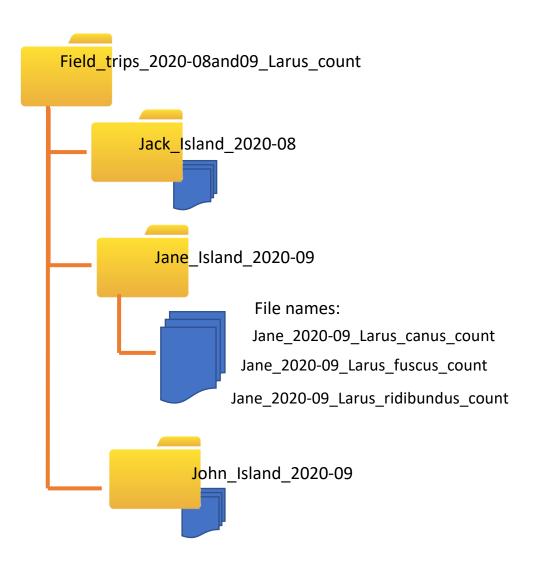
- especially when you have many files

Use a consistent strategy.

Main structure of data should be visible in the **file names**

=> also useful for archiving afterwards

Document file structure and naming convention (in a ReadMe file)



Names for files and folders

- Machine readable
 - Use underscores (_) instead of spaces
 - Avoid special characters
 "/\:*.?'<>[]()&\$ æÆ øØ åÅ
- Human readable
 - Files should be named consistently
 - Descriptive, but short (< 25 signs)
- Use the international dating convention YYYY-MM-DD

X

Joe's notes from today.txt

Tromsø&Ålesund.txt

Mynotes_versjon1.txt

Mine notater ny.txt

figure 1.png

Thesis_DONTdelete_new_draft_final*_last_v2.txt

\checkmark

Joes_filenames_are_getting_better.txt

Tromsoe_og_aalesund.txt

2023-02-10_notes.txt

2023-02-11_notes.txt

Fig01_length-vs-interest.png

PhD_thesis_2023_finalversion.txt

Use file names for sorting files by names

Sorted by date:

2020-08-01_notes_John.pdf 2020-08-31_observations_John.txt 2020-09-01_notes_Jane.pdf 2020-09-30_observations_Jane.pdf

Sorted on data type:

Notes_Jane_2020-09-01.pdf Notes_John_2020-08-01.pdf Observations_Jane_2020-09-30.txt Observations_John_2020-08-31.txt

Sorted by author:

Jane_notes_2020-09-01.pdf Jane_observations_2020-09-30.txt John_notes_2020-08-01.pdf John_observations_2020-08-31.txt

Forced numbering:

01_Notes_John_2020-08-01.pdf 02_Notes_Jane_2020-09-01.pdf 03_Observations_John_2020-08-31.txt 04_Observations_Jane_2020-09-30.txt

Use file names for versioning



The Turing Way Community, & Scriberia. (2020). Illustration from the Turing Way book dashes. Zenodo. https://doi.org/10.5281/zenodo.3695300

Bruk heller:

Larus_canus_counts_RAW Larus_canus_counts_v001 Larus_canus_counts_v002

etc

paper_draft.tex

paper_update.tex

paper_final.tex

paper_final2.tex

paper_final3.tex

paper_please_let_this_be_the_final.tex

paper_please_let_this_be_the_final123.te

paper_ultrafinal.tex

paper_I_will_kill_myself_if_this_will_go_on.tex

CC-BY 4.0 Heidi Seibold

Remember to document your changes in a ReadMe file



Documentation

Why?

To find, understand and re-use your data For yourself - Also many years from now For others – to understand and re-use your data correctly



"Lego Bricks Yard Sale" by JeepersMedia is licensed under <u>CC BY 2.0</u>.





"Lego Tower Bridge" by <u>comedy nose</u> is marked with <u>Public Domain Mark</u> <u>1.0</u>.

Documentation

How?

<u>ReadMe file</u> = manual for your data

Human readable – important to understand and re-use your data correctly

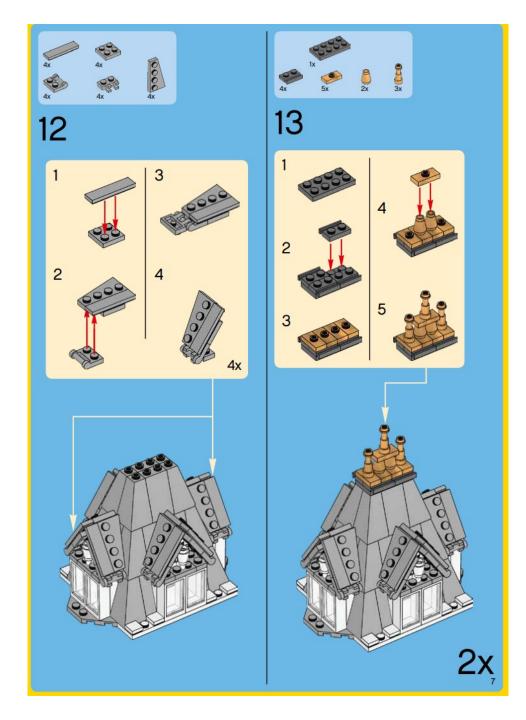
<u>Metadata</u> = data about your data

Computer readable – important for search and discovery of your data

When?

During the entire lifecycle

keep updated methodologies, code descriptions, lab notebooks, experimental protocols, provenance information for data, etc.



ReadMe-file: manual for your data

Enough information to understand and re-use your data

A roadmap for future users that informs how the data was generated, modified, processed and how to use it in the future.

Start documenting early, update continuously, in an open format (e.g. .txt file)

Have a look at ReadMe files in the repository where you are planning to archive your data <u>DataverseNO ReadMe-template (link)</u>

ReadMe-file: manual for your data

General information about the project / dataset:

Title, project period, description, funding sources, project participants, contact information.

Methodology:

Data collection or generation data processing, data quality etc.

Data and file overview:

File overview, file formats, relation between files, version of the dataset.

Data-specific information:

Column headings, abbreviations, units of measure, contextual information **About the dataset:**

Terms of reuse, related datasets, data sources.

0_README.txt

This README file was generated on 2021-01-25 by Thomas Karsten Kilvær. Last updated: 2022-05-20.

GENERAL INFORMATION

// Title of Dataset: Replication Data for: A Pragmatic Machine Learning Approach to Quantify Tumor Infiltrating Lymphocytes in Whole Slide Images

// DOI: https://doi.org/10.18710/4YN9SZ

// Contact Information

<The person to be contacted for questions about the dataset>

// Name: Kilvaer, Thomas K,

// Institution: UiT The Arctic University of Norway

// Email: thomas.k.kilvar@uit.no

// ORCID: https://orcid.org/0000-0003-1669-0117

// Contributors: See metadata field Contributor.

// Kind of data: See metadata field Kind of Data.

// Date of data collection/generation: See metadata field Date of Collection.

// Description of dataset:

This dataset can be used to replicate the findings in "A Pragmatic Machine Learning Approach to Quantify Tumor Infiltrating Lymphocytes in Whole Slide Images".

The motivation for this paper is that increased levels of tumor infiltrating lymphocytes (TILs) indicate favorable outcomes in many types of cancer. Our aim is to leverage computational pathology to automatically quantify TILs in standard diagnostic whole-tissue hematoxylin and eosin stained section slides (H&E slides). Our approach is to transfer an open source machine learning method for segmentation and classification of nuclei in H&E slides trained on public data to TIL quantification without manual labeling of our data.

Our results show that additional augmentation improves model transferability when training on few samples/limited tissue types. Models trained with sufficient samples/tissue types do not benefit from our additional augmentation policy. Further, the resulting TL quantification correlates to patient prognosis and compares favorably to the current state-of-the-art method for immune cell detection in non-small lung cancer (current standard CD8 cells in DAB stained TMAs HR 0.34 95% CI 0.17-0.68 vs TLLs in HE WSIs: HoVer-Net PanNuke Aug Model HR 0.30 95% CI 0.15-0.60, HoVer-Net MoNuSAC Aug model HR 0.27 95% CI 0.14-0.53). Moreover, we implemented a cloud based system to train, deploy and visually inspect machine learning based annotation for H&E slides. Our pragmatic approach bridges the gap between machine learning research, translational clinical implementation. However, validation in prospective studies is needed to assert that the method works in a clinical setting.

The dataset is comprised of three parts: 1) Twenty image patches with and without overlays used by pathologists to manually evaluate the output of the deep learning models, 2) The models trained and subsequently used for inference in the paper, 3) the patient dataset with corresponding image patches used to clinically validate the output of the deep learning models.

METHODOLOGICAL INFORMATION

// Description of sources and methods used for collection/generation of lata:

// Methods for processing the data:

* Models were aguired by running the following scripts from the HoVer-Net pipeline: <extract patches.py>, <train.py>, <export.py>.

Configuration values used for generating config.yml via running ```sh generate.sh``` inside hover docker container

- consep aug linear 2-1.0: https://gist.github.com/nsh23/5e31ee910ca55fcb8c0076973374a717

- consep standard-1.1: https://gist.github.com/nsh23/676a7f7d0d429bf845ac4afa59f6db5f

- pannuke aug p linear 2-1.0: https://gist.github.com/nsh23/3b22307d981760761158c894308025c1

– pannuke_standard-1.0: https://gist.github.com/nsh23/633d4a45523c8c63dbff7b20a8d6ad9b

- monusac standard-1.0: https://gist.github.com/nsh23/34ebaf35d6350145b2809fbb8844eecc

– monuasc aug p linear 2-1.0: https://gist.github.com/nsh23/2c0aa35afcc5908742d844d28522595a

In order to use them copy config file for the target experiment to ```hovernet-pipeline/src``` and rename it as <config.yml>.

* Manual validation images (UiT_TILs/manual_validation.tar/.../) were <u>aquired</u> via HoVer-net inference part by running the following scripts from the HoVer-Net pipeline: <<u>infer.py</u>>, <<u>process.py</u>>. Configuration values used for generating config.ym] via running ```sh generate.sh``` inside hover docker container // Facility-. instrument- or software-specific information needed to interpret the data:

* Transforming patch-level logs to patient-level that you get from HoVer-Net pipeline could be done via running 2 scripts:

First, convert image-level names and select counts for specific cell type with <counts.py> script (hovernet-pipeline/src/metrics/counts.py).

Second, aggregate quantification logs from image-level to patient-level (counts per 1000²) and get (min, max, median, avg) numbers for each patient with <<u>summarize.py</u>> script (<u>hovernet-pipeline</u>/src/metrics/ <u>summarize.py</u>).

DATA & FILE OVERVIEW

// File Lists

Metadata: data about data

Metadata = description of data <u>Examples of metadata:</u> Author, **title**, **description**, ... **Keywords** Geographical information

Standardized general metadata e.g. international date format (e.g. ISO-8601): YYYY-MM-DD (2019-12-09) <u>Dublin Core (link)</u>, <u>Data Documentation</u> <u>Initiative (link)</u>

Domain-specific standardized metadata e.g. <u>Darwin Core(link)</u> = a standard for description of data on biological diversity.

	This field supports only certain HTM	L tags.	
	Text * 😧		-
	Date 🕄		
	YYYY-MM-DD		
Subject * 🕢	Select 💌		
Keyword * 😧	Term * 😧	Vocabulary 🕄	
	Vocabulary URL 📀		4
	Enter full URL, starting with http		
Related Publication ②	Citation 🕢		
			-
			-
			4
	ІД Туре 🕄	ID Number 🕄	4
		ID Number 📀	4
	ІД Туре 3	ID Number 😔	-
	ID Type 3 Select	ID Number 3	4
	ID Type Select • URL ?	ID Number 3	4
	ID Type Select URL Enter full URL, starting with http		4
Distributor 🕄	ID Type 3 Select • URL 3 Enter full URL, starting with http Name 3		4

Metadata : data about data

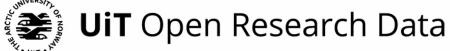
Overview over different standards: <u>Research Data Alliance (link)</u> <u>FAIRSharing.org (link)</u> <u>Digital Curation Centre (link)</u>

Tip: Have a look at metadata in the repository where you are planning on archiving your data. To see how they do it.



<u>"Metadata Sticks"</u> by <u>Gideon Burton</u> is licensed under <u>CC BY-SA 2.0</u>





DataverseNO > UIT Open Research Data >

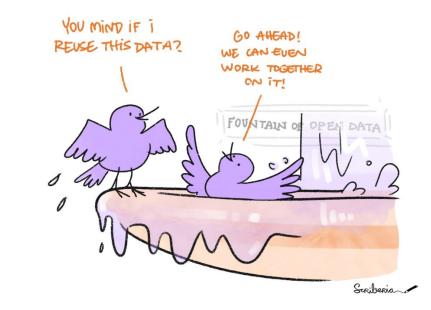
UiT_TILs - Replication Data for "A Pragmatic Machine Learning Approach to Quantify Tumor Infiltrating Lymphocytes in Whole Slide Images"

Version 2.0

	Kilvaer, Thomas K, 2021, "UIT_TILs - Replication Data for "A Pragmatic Machine Learning Approach to Quantify	Access Dataset -	
	Tumor Infiltrating Lymphocytes in Whole Slide Images"", https://doi.org/10.18710/4YN9SZ, DataverseNO, V2	Edit Dataset - Link Dataset	
	Cite Dataset - Learn about Data Citation Standards.		
		Contact Owner	Share
		Dataset Metrics 🕢	
Description 🕄	Description ③ This dataset can be used to replicate the findings in "A Pragmatic Machine Learning Approach to Quantify Tumor Infiltrating Lymphocytes in Whole Slide Images". The motivation for this paper is that increased levels of tumor infiltrating lymphocytes (TILs) indicate favorable outcomes in many types of cancer. Our aim is to leverage computational pathology to automatically quantify TILs in standard diagnostic whole-tissue hematoxylin and eosin stained section slides (H&E slides). Our approach is to transfer an open source machine learning method for segmentation and classification of nuclei in H&E slides trained on public data to TIL quantification without manual labeling of our data. Our results show that improved data augmentation improves immune cell detection in H&E WSIs. Moreover, the resulting TIL quantification correlates to patient prognosis and compares favorably to the properties of the provided to the provided the provided to patient prognosis and compares favorably to the provided to public data to the provided to patient prognosis and compares favorably to the provided to public data.		
	Read full Description [+]		
Subject 🕄	ect Medicine, Health and Life Sciences		
Keyword 😯	eyword 3 machine learning, ML, deep learning, DL, non-small cell lung cancer, NSCLC, immune cell, tissue infiltrating lymphycytes, TIL		
Related Publication	n 📀 submitted for review		
Files Meta	ata Terms Versions		

Preparing for archiving

- Selection
 - Data necessary to understand and replicate the study
 - Do not exclude negative data meaning data that do not support the tested hypothesis
 - Include raw version of the data and processed version(s)
- Anonymization and/or aggregation?
 - Anonymize personal data
- Provide your data in original AND preferred (persistent) file formats
 - ensure the long-term use of your files
- Note: Webinars tomorrow & Wednesday (17 & 18 April 2023): How to archive



Scriberia, CC-BY 4.0 DOI: <u>10.5281/zenodo.3332807</u>.

Preferred file formats

Characteristics of preferred file formats:

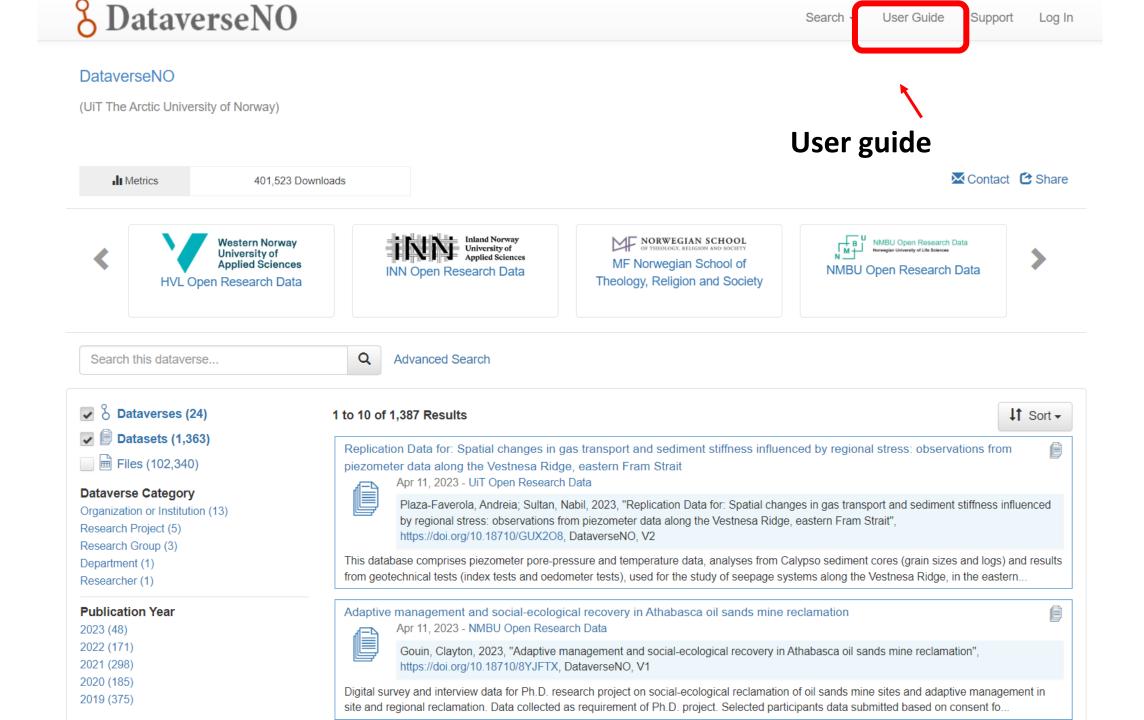
- non-proprietary
- open, with documented international standards
- in common usage by the research community
- using standard character encodings (e.g. ASCII, UTF-8)
- uncompressed (space permitting)



Archiving: Persistent file formats

File type	Preferred file formats (examples)	Non-preferred file formats (examples)
Audio	 → Uncompressed and lossless Wav or AIFF (.wav/.aiff) → Compressed and lossless FLAC (.flac) → Compressed and lossy Mp3 (.mp3) 	 → AAC (.m4a) → Monkey's Audio (.ape) → Ogg Vorbis (.ogg) → Windows Media Audio (.wma)
Container file	Container files are automatically unpacked when uploaded and should only be used to keep the folder structure in your dataset; see more in section Upload data files.	In case container files need to be archived as container files, use .zip. Note! In this case, files must be packed twice. That way, the inner container will be preserved when uploaded.
Image	 → Uncompressed TIFF (.tif or .tiff) → Compressed and lossless PNG (.png) → Compressed and lossy JPEG (.jpg) 	 → Adobe Photoshop (.psd) → Apple Picture File (.pct) → Graphics Interchange Format (.gif) → Raw Image Data File (.raw) → Windows Bitmap (.bmp)
Text (slides, illustrations)	\rightarrow PDF/A (.pdf) combined with original file	→ PowerPoint (.pptx)
Text (tables)	→ Tab separated Unicode plain text (.txt)	→ Excel (.xlsx)
	→ Plain text (.txt)	See the User Guide of DataverseNO for more informatio

on (link)



Two introductory videos

<u>The research data</u> <u>management life cycle</u> <u>(link to Vimeo)</u>

The research data management life cycle



<u>The FAIR data principles</u> (link to Vimeo)



More information and help

<u>UiT Research Data Portal (link)</u>

- Tips
- Overview of webinars/courses

DataverseNO deposit guidelines (link)

• Tips on how to prepare and describe data

Email us! <u>researchdata@hjelp.uit.no</u>



"Help!" by lydia_shiningbrightly is licensed under CC BY 2.0



Are you a Data Steward?

Join our Data Steward Network!

Sign up! Join the Kick-off seminar 3 May!

More information on Tavla (link)



Evaluation

We are constantly working to improve the content of our webinars. Feedback from you will be of great help to us.

Please answer our <u>2 minute questionaire (link)</u>

Date: 16.04.20223

Course code: Research data



researchdata@hjelp.uit.no

Noortje Haugstvedt – Adrian Verhoef

