

File Management

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Managing your Research Data

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Outline

- Data Management **Principles**
 - Research Data Life-cycle
 - Data Management Checklist
- **Techniques** to help organize your research data
 - File Organization
 - File Naming
 - Version Control
 - Metadata (ReadMe)
 - Running Low on Storage Space?

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Research Data Life-cycle



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Data Management Checklist

- **What** types of data? What format and size?
- **Who** will be responsible for each aspect of DM?
 - Roles & Responsibilities
- **How** – collect/**document**/store/back up/share data

Data Types Recommended by UK Data Archive

Type of data	Recommended formats
Tabular data with extensive metadata variable labels, code labels, and defined missing values	SPSS portable format (.por) delimited text and command ('setup') file (SPSS, Stata, SAS, etc.) structured text or mark-up file of metadata information, e.g. DDI XML file
Tabular data with minimal metadata column headings, variable names	comma-separated values (.csv) tab-delimited file (.tab) delimited text with SQL data definition statements
Geospatial data vector and raster data	ESRI shapefile (.shp, .shx, .dbf, .prj, .sbx, .sbn optional) geo-referenced TIFF (.tif, .tiff) CAD data (.dwg) tabular GIS attribute data Geography Markup Language (.gml)
Textual data	Rich Text Format (.rtf) plain text, ASCII (.txt) eXtensible Mark-up Language (.xml) text according to an appropriate Document Type Definition (DTD) or schema
Image data	TIFF 6.0 uncompressed (.tif)
Audio data	Free Lossless Audio Codec (FLAC) (.flac)
Video data	MPEG-4 (.mp4) OGG video (.ogv, .ogg) motion JPEG 2000 (.mj2)
Documentation and scripts	Rich Text Format (.rtf) PDF/UA, PDF/A or PDF (.pdf) XHTML or HTML (.xhtml, .htm) OpenDocument Text (.odt)

Open and non-proprietary
Information loss during conversion

For a full table including acceptable formats:

<https://ukdataservice.ac.uk/learning-hub/research-data-management/format-your-data/recommended-formats/>

Data Management Checklist

- **What** types of data? Format and size for each.
- **Who** will be responsible for each aspect of DM?
 - Roles & Responsibilities
- **How** – collect/**document**/store/back up/share data
 - Reproducibility & Re-usability
 - Restrictions
 - Ethical Obligations & Copyright/Intellectual Property
 - Privacy and Data-processing Laws

Data Management Checklist – 13 Core Questions to Consider

- **What** data will you collect or create?
- How will the data be **collected** or created?
- What documentation and **metadata** will accompany the data?
- How will you manage any **ethical** issues?
- How will you manage **copyright** and Intellectual Property Rights (IPR) issues?
- How will the data be **stored and backed up** during the research?
- How will you manage **access and security**?
- What is the long-term **preservation** plan for the dataset?
- Which data should be retained, **shared**, and/or preserved?
- How will you **share** the data?
- Are any **restrictions** on data sharing required?
- **Who** will be **responsible** for data management?
- **What resources will you require to deliver your plan? (people, time, hardware)**

Full Checklist with Guidance can be downloaded here:

<https://www.dcc.ac.uk/news/new-checklist-data-management-plan>

https://www.dcc.ac.uk/sites/default/files/documents/resource/DMP/DMP_Checklist_2013.pdf

Data Management Checklist

- **What** types of data? Format and size for each.
 - **Who** will be responsible for each aspect of DM?
 - Roles & Responsibilities
 - **How – collect/document/store/back up/share data**
 - Reproducibility & Re-usability
 - Restrictions
 - Ethical Obligations & Copyright/Intellectual Property
 - Privacy and Data-processing Laws
- Electronic Lab Notebook

Choosing an Electronic Lab Notebook

Needs to think about:

- Cost? One-time or subscription(monthly/yearly)?
- Access control. Other Users? Collaborators?
- Types of information to record and storage space required
- Any specialized functionality you require?
- Protection for sensitive data
- What happens if someone leaves the lab?
- What happens when you stop using this ELN?

Choosing an Electronic Lab Notebook

Further Reading:

- Kwok, Roberta. 2018. "How to pick an electronic laboratory notebook." *Nature* 560 (7717): 269-270. <https://doi.org/10.1038/d41586-018-05895-3>
- *The Electronic Lab Notebook in 2020: A comprehensive guide with a short list of 5 ELNs.* <https://www.labfolder.com/electronic-lab-notebook-elN-research-guide>
- *A Comprehensive Comparison Grid from Harvard Data Management including over 30 ELNs comparing over 50 features*
<https://datamanagement.hms.harvard.edu/analyze/electronic-lab-notebooks>

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A photograph of a winding asphalt road that curves through a hilly, grassy landscape. The road is dark and has yellow and white painted lines. The hills are covered in dry, golden-brown grass. In the background, there are more hills and a small white building. The sky is a pale blue. The text is overlaid in the center of the image.

No one has
perfect data management habits,
but adopting even a few
goes a long way.

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File Naming – Other Tips

- Use **underscores** “_” to separate elements
 - avoid spaces “ ” and special characters, e.g., “@”
 - Periods “.” only before the file extension

- e.g., compare:

averagetrendclusterearlyonly.png 🥵

average_trend_cluster_early_only.png 😊

File Naming – Other Tips

- Use **underscores** “_” to separate elements
 - avoid spaces “ ” and special characters, *e.g.*, “@”
 - Periods “.” only before the file extension
- Use **leading zero** for consistent sorting

Without Leading Zero

Name

```
datafile_number_1.txt
datafile_number_2.txt
datafile_number_3.txt
datafile_number_4.txt
datafile_number_5.txt
datafile_number_6.txt
datafile_number_7.txt
datafile_number_8.txt
datafile_number_9.txt
datafile_number_10.txt
datafile_number_11.txt
datafile_number_12.txt
datafile_number_13.txt
datafile_number_14.txt
datafile_number_15.txt
datafile_number_16.txt
datafile_number_17.txt
datafile_number_18.txt
datafile_number_19.txt
datafile_number_20.txt
```

```
qw254@qw254-desktop:~/t
datafile_number_10.txt
datafile_number_11.txt
datafile_number_12.txt
datafile_number_13.txt
datafile_number_14.txt
datafile_number_15.txt
datafile_number_16.txt
datafile_number_17.txt
datafile_number_18.txt
datafile_number_19.txt
datafile_number_1.txt
datafile_number_20.txt
datafile_number_2.txt
datafile_number_3.txt
datafile_number_4.txt
datafile_number_5.txt
datafile_number_6.txt
datafile_number_7.txt
datafile_number_8.txt
datafile_number_9.txt
```

Not consistent sorting.

With Leading Zero

Name

```
datafile_number_01.txt
datafile_number_02.txt
datafile_number_03.txt
datafile_number_04.txt
datafile_number_05.txt
datafile_number_06.txt
datafile_number_07.txt
datafile_number_08.txt
datafile_number_09.txt
datafile_number_10.txt
datafile_number_11.txt
datafile_number_12.txt
datafile_number_13.txt
datafile_number_14.txt
datafile_number_15.txt
datafile_number_16.txt
datafile_number_17.txt
datafile_number_18.txt
datafile_number_19.txt
datafile_number_20.txt
```

```
qw254@qw254-desktop:~/t
datafile_number_01.txt
datafile_number_02.txt
datafile_number_03.txt
datafile_number_04.txt
datafile_number_05.txt
datafile_number_06.txt
datafile_number_07.txt
datafile_number_08.txt
datafile_number_09.txt
datafile_number_10.txt
datafile_number_11.txt
datafile_number_12.txt
datafile_number_13.txt
datafile_number_14.txt
datafile_number_15.txt
datafile_number_16.txt
datafile_number_17.txt
datafile_number_18.txt
datafile_number_19.txt
datafile number 20.txt
```

Consistent!

File Naming Examples

How about the following file name?

my Data @DryValley November 15 2010.v2.dat

How would you revise it?

(type your proposal in zoom chat window)

Reminder to check:

- **Clear**
 - Objective
 - Meaningful
- **Concise**
- **Consistent**
 - standard

File Naming Examples - revised

Original:

my Data @DryValley November 15 2010.v2.dat

Revised (one of the possibilities):

DV_ICPOES_20101115_JDS_v02.dat

- DV: site code (Dry Valley)
- ICPOES: instrument name
- 20101115: date of data generation
- JDS: initial of the scientist
- V02, second version (leading zero)

Batching Renaming Tools

Windows:

- Ant Renamer: <http://www.antp.be/software/renamer>
- Bulk Rename Utility: <http://www.bulkrenameutility.co.uk/>
- PSRenamer: <http://www.powersurgepub.com/products/psrenamer.html>

Mac:

- PSRenamer: <http://www.powersurgepub.com/products/psrenamer.html>
- Renamer4Mac : <http://renamer4mac.com/>
- Name Mangler: <http://manytricks.com/namemangler/>

Linux/Unix:

- GNOME Commander: <http://www.nongnu.org/gcmd/>
- PSRenamer: <http://www.powersurgepub.com/products/psrenamer.html>
- Use *grep, sed and awk* to search for and change

More details on pros and cons:

https://www.dropbox.com/s/rropbx4ewxlli09/Handout_BatchRenaming.pdf

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Version Control

Why?

- Track changes
- Enable reverting to earlier version

How?

- **File naming** (manually)

- Date

Template_soil_testing_20120319.xlsx

- Author's name

Template_soil_testing_by_AS.xlsx

- Version number

v01, v02 for major edit; v01_0, v01_1, v01_2 for minor edit

Template_soil_testing_v03_02.xlsx

- **Version control tools** (automatic)

- *Wet lab*

Electronic Lab Notebooks(ELN)

Laboratory Information Management System(LIMS)

- *Dry lab*

Git (GitHub/GitLab)

Based on slide from Jing Su

Version Control Example

VERSION CONTROL TABLE FOR A DATA FILE			
Title:		Vision screening tests in Essex nurseries	
File Name:		VisionScreenResults_00_05	
Description:		Results data of 120 Vision Screen Tests carried out in 5 nurseries in Essex during June 2007	
Created By:		Chris Wilkinson	
Maintained By:		Sally Watsley	
Created:		04/07/ 2007	
Last Modified:		25/11/ 2007	
Based on:		VisionScreenDatabaseDesign_02_00	
VERSION	RESPONSIBLE	NOTES	LAST AMENDED
00_05	Sally Watsley	Version 00_03 and 00_04 compared and merged by SW	25/11/2007
00_04	Vani Yussu	Entries checked by VY, independent from SK	17/10/2007
00_03	Steve Knight	Entries checked by SK	29/07/2007
00_02	Karin Mills	Test results 81-120 entered	05/07/2007
00_01	Karin Mills	Test results 1-80 entered	04/07/2007

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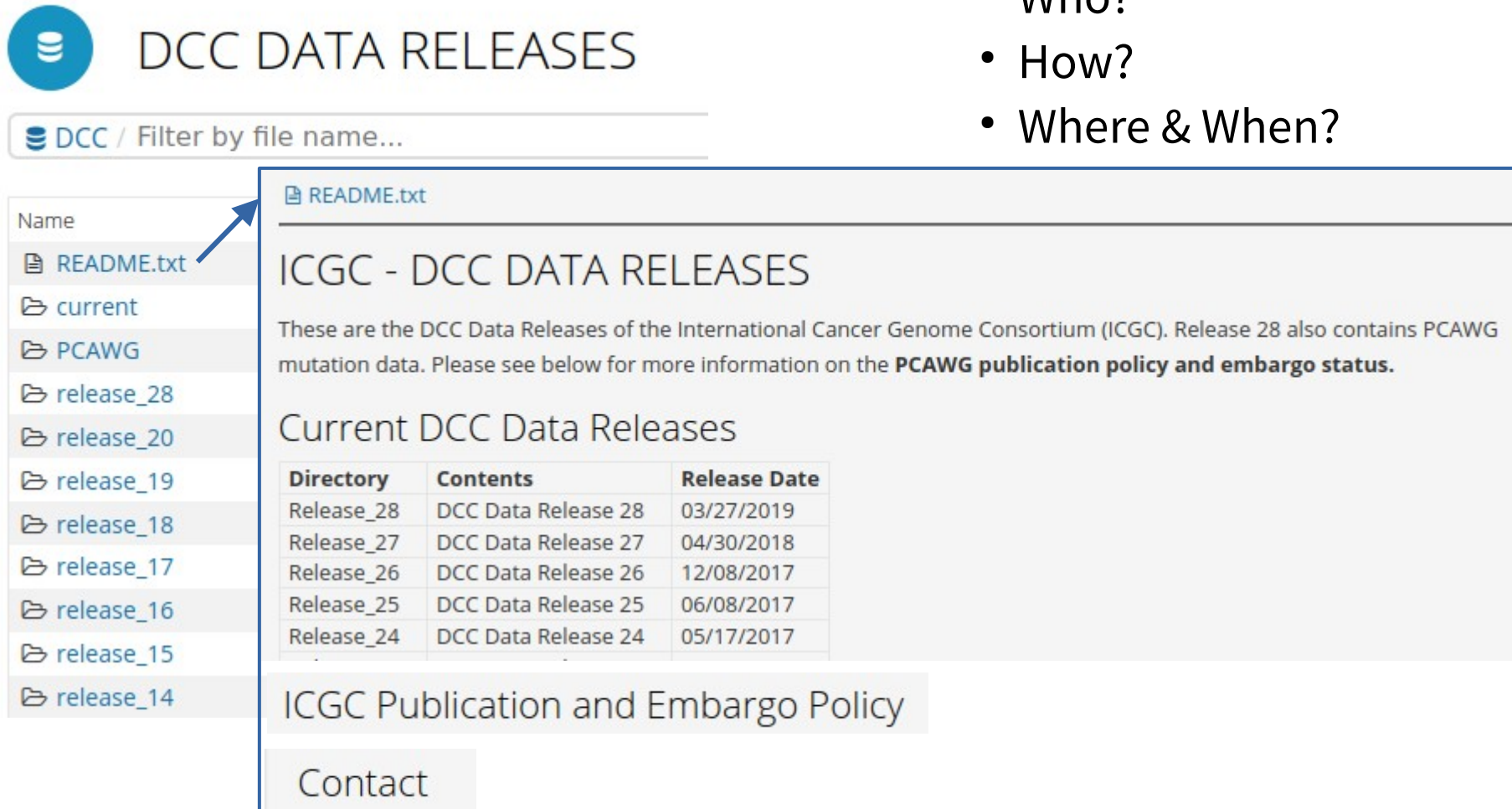
Why metadata?


- What is metadata?
 - Description that helps someone else understand the contents and organization of your files *in your absence*
 - Usually stored in top-level folders
- What should metadata include?
 - What?
 - Who?
 - Where & When?
 - How?


@ Project-level @ Data-level @ File-level

What Is in Metadata? - @Project-Level












- What?
- Who?
- How?
- Where & When?




 DCC DATA RELEASES

 DCC / Filter by file name...

Name

-  README.txt
-  current
-  PCAWG
-  release_28
-  release_20
-  release_19
-  release_18
-  release_17
-  release_16
-  release_15
-  release_14

 README.txt

ICGC - DCC DATA RELEASES

These are the DCC Data Releases of the International Cancer Genome Consortium (ICGC). Release 28 also contains PCAWG mutation data. Please see below for more information on the **PCAWG publication policy and embargo status**.

Current DCC Data Releases

Directory	Contents	Release Date
Release_28	DCC Data Release 28	03/27/2019
Release_27	DCC Data Release 27	04/30/2018
Release_26	DCC Data Release 26	12/08/2017
Release_25	DCC Data Release 25	06/08/2017
Release_24	DCC Data Release 24	05/17/2017

[ICGC Publication and Embargo Policy](#)

[Contact](#)

What Is in Metadata? - @Data-Level

```
<EXPERIMENT_SET>
  <EXPERIMENT alias="exp_mantis_religiosa">
    <TITLE>The 1KITE project: evolution of insects</TITLE>
    <STUDY_REF accession="SRP017801"/>
    <DESIGN>
      <DESIGN_DESCRIPTION/>
      <SAMPLE_DESCRIPTOR accession="SRS462875"/>
      <LIBRARY_DESCRIPTOR>
        <LIBRARY_NAME/>
        <LIBRARY_STRATEGY>RNA-Seq</LIBRARY_STRATEGY>
        <LIBRARY_SOURCE>TRANSCRIPTOMIC</LIBRARY_SOURCE>
        <LIBRARY_SELECTION>cDNA</LIBRARY_SELECTION>
        <LIBRARY_LAYOUT>
          <PAIRED NOMINAL_LENGTH="250" NOMINAL_SDEV="30"/>
        </LIBRARY_LAYOUT>
        <LIBRARY_CONSTRUCTION_PROTOCOL>Messenger RNA (mRNA) was isolated using the Dynabeads mRNA Purification Kit (Invitrogen, Carlsbad Ca. USA) and then sheared using divalent cations at 72°C. These cleaved RNA fragments were transcribed into first-strand cDNA using II Reverse Transcriptase (Invitrogen, Carlsbad Ca. USA) and N6 primer (IDT). The second-strand cDNA was subsequently synthesized using RNase H (Invitrogen, Carlsbad Ca. USA) and DNA polymerase I (Invitrogen, Shanghai China). The double-stranded cDNA then underwent end-repair, a single 'A' base addition, adapter ligation, and size selection on agarose gel (250 * 20 bp). At last, the product was indexed and PCR amplified to finalize the library preparation for the paired-end cDNA.</LIBRARY_CONSTRUCTION_PROTOCOL>
      </LIBRARY_DESCRIPTOR>
    </DESIGN>
    <PLATFORM>
      <ILLUMINA>
        <INSTRUMENT_MODEL>Illumina HiSeq 2000</INSTRUMENT_MODEL>
      </ILLUMINA>
    </PLATFORM>
    <EXPERIMENT_ATTRIBUTES>
      <EXPERIMENT_ATTRIBUTE>
        <TAG>library preparation date</TAG>
        <VALUE>2010-08</VALUE>
      </EXPERIMENT_ATTRIBUTE>
    </EXPERIMENT_ATTRIBUTES>
  </EXPERIMENT>
</EXPERIMENT_SET>
```

- What?
- Who?
- How?
- Where & When?

What Is in Metadata? - @File-Level

File Descriptions

Open-access analyzed data:

clinical.[ICGC project code].tsv.gz: contains aggregated clinical donor, specimen and sample information

exp_array.[ICGC project code].tsv.gz: gene expression measured at the transcriptional level (mRNA) using array-based platforms

exp_seq.[ICGC project code].tsv.gz: gene expression measured at the transcriptional level (mRNA) using sequencing-based platforms

3. chr

Chromosome number

4. position

Chromosome position

5. ref

Reference allele

6. alt

Alternate allele

7. gene

Gene name

8. driver



information related to 'mutational' driver type, in particular whether the driver mutation is in [promoters_core, 5utr, 3utr, enhancers, cds, ncRNA, mirna_pre, lncrna_promoters_core, splice_sites]

9. driver_statement



information related to 'mutational' drivers, whether the driver mutation is known_driver, driver_by_rank, driver_by_rule or germline pathogenic variant

Data Dictionary

- What?
- Who?
- How?
- Where & When?

More on data dictionary: <http://kbroman.org/dataorg/pages/dictionary.html>

<https://dcc.icgc.org/releases>

Further reading about metadata:

Cornell University has excellent README file guidelines:

<https://data.research.cornell.edu/content/readme>

Homework

Choose any folder in your research data and write a “ReadMe” file (metadata) for contents in that folder.

What if your file transfer
got **interrupted**
without any warning message?

What Is in Metadata?

- Avoid pitfalls in data transfer using md5sum check

file name	md5sum
PCAWG16.consensus.virus.genus.normal.2out3.v3.icgc.controlled.tsv.gz	854b6a4dce3b46891c8cc4afc65a40d3
PCAWG16.consensus.virus.genus.normal.3out3.v3.icgc.controlled.tsv.gz	82f20aa61129522672fb8e1d7036cdfc
PCAWG16.consensus.virus.genus.tumour.2out3.v3.icgc.controlled.tsv.gz	1787e28e61651b19701cfbb9c108b908
PCAWG16.consensus.virus.genus.tumour.3out3.v3.icgc.controlled.tsv.gz	054200b756d059fc435c6f39ae9646b3
PCAWG16.consensus.virus.genus.normal.2out3.v3.tcga.controlled.tsv.gz	bba31c95dad98dc3b796c6937969a4e7
PCAWG16.consensus.virus.genus.normal.3out3.v3.tcga.controlled.tsv.gz	af0d91d2be2263f68c40e10a7780aced
PCAWG16.consensus.virus.genus.tumour.2out3.v3.tcga.controlled.tsv.gz	f5c5c6b6b09a2f2eb1372cdfd85077b9
PCAWG16.consensus.virus.genus.tumour.3out3.v3.tcga.controlled.tsv.gz	8e1352617fff430d5bedfcaa8fd3362f

- Md5sum output are “**fingerprints**” to files. They are hash values derived using the whole file as input.
- Changes to a file will cause md5sum output to change. Conversely, if md5sum outputs are the same the files are identical.

Note : If you are worried that the data is maliciously altered instead of accidental corruption, there are more advanced options: SHA-256 (sha256sum), SHA-512 (sha512sum) or BLAKE2(b2sum).

Put It Together

```
Project_20190102_SuJ_BC_RNASeq_5490/
├── README
├── meta/
│   ├── ExperimentalDesign_20190105.doc
│   ├── Platelayout.doc
│   ├── SampleSheet.csv
│   ├── FileList.csv
│   └── MeetingNotes_20190114.doc
├── data/
│   ├── bam/
│   │   ├── Sample1.aligned.bam
│   │   └── Sample2.aligned.bam
│   └── fastq/
│       ├── Sample1_R1.fq
│       ├── Sample1_R2.fq
│       ├── Sample2_R2.fq
│       └── Sample2_R2.fq
├── reference/
│   └── human/
│       ├── Grch38_genome.fa
│       └── Gencode26_genes.gtf
├── scripts/
│   ├── 1.subread_align_grch38.sh
│   ├── 2.featureCounts_mRNA.sh
│   ├── 3.edgeR_DE.R
│   ├── 4.GSEA_mSigDB13.sh
│   └── 5.backup_scratca_to_nas.sh
└── results/
    ├── counts/
    │   └── count_files.txt
    └── DE_genelists
        ├── PrimaryTumour_v_normal_DE_genelist.csv
        └── Metastatic_v_Primary DE_genelist.csv
```

- File Structures/Organization
- File Naming
- Version Control
- Metadata

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Running out of Space – Do we need all the files?

Five steps to decide what data to keep:

1. Identify data that **must** be kept
2. Identify **purposes** that the data could fulfill
3. Identify data that **should** be kept
4. Weight up the **costs** £££
5. Complete the data appraisal

For more details:

<https://www.dcc.ac.uk/guidance/how-guides/five-steps-decide-what-data-keep>

SpaceSniffer http://www.uderzo.it/main_products/space_sniffer/index.html



Running out of Space – for Mac & other Linux?

For Mac:

Disk Inventory X

<http://www.derlien.com/>

Linux command line (bash):

du -sh # shows you how much disk space the current folder takes

du -h -d 1 | sort -h # sort all folders in the current directory by size

Summary

- Principle

Can **someone else** (as well as yourself years from now) understand the contents and organization of your files *in your absence*.

- Data Management Checklist

- **What?**
- **Who?**
- **How?**

- File Structure & File Name (3C)

- Metadata (ReadMe)

- **W W H** + **Where** and **When**

- @Project-level @Data-level @File-level

- Keep track of changes with Version Control

- Avoid pitfalls in data transfer using md5sum check

Further Reading:

Good Practice in Bioinformatics Analysis

Wilson, G. (2017). Good enough practices in scientific computing. PLoS Computational BiologyS Computational Biology.
(<https://doi.org/10.1007/BF02378113>)

