Principles of data management and organization

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Where You're From

Date of Presentation

What are data disasters?

(My) Definition

Anything that stops somebody analysing data in the way that they are supposed to be able so to do.

- Total destruction of data
- Inability to find data
- Corruption of data
- Forgetting what the data mean
- Being unable to reproduce your results
- Somebody else being unable to reproduce your results
- Unauthorized access-to/use-of data

Some of these are Computing issues

Principle 1

Ensure you have a secure back up of the raw data

- Vulnerable until you have this - requires care
- Some degree of organization required
- Check that the backup is working
- Need to be clear what the raw data are
- There are costs associated with backing data up
- Check that the backup is future-proofed

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ICGC Hard drive corruption example

Can you/colleagues actually get to the data?

What are raw data?

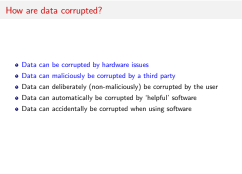
- Probably the data as received
- Possibly a subset of the data received
- What if there are clear errors in the data received?

Could future lab members access it?

- Is it in a proprietary format that might disappear? c.f. my thesis
- Is it protected by a password that only you know?

How are data corrupted?

- Data can be corrupted by hardware issues
- Data can maliciously be corrupted by a third party
- Data can deliberately (non-maliciously) be corrupted by the user
- Data can automatically be corrupted by 'helpful' software
- Data can accidentally be corrupted when using software



Merging/deleting/rearranging data without thinking of long term consequences
Editing raw data thinking that it is a copy.

Will somebody else give the Excel examples or should I add a slide?

gene names that are misinterpreted e.g. SEPT9
dates generally
IDs that are numbers e.g. Karl Broman's example

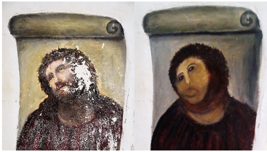
e.g. Shifting cells/rows/columns as per Keith Baggerly's Duke example

mention md5 sum checks?

Don't touch-up a masterpiece

Principle 2

Never work directly on the raw data



Ideally we adopt a practice of having a raw data file and recording the changes made to it

- Even better if the recording is 'automatic'
- This approach naturally makes research reproducible
- It can aid the understanding of the data
- It saves having to backup multiple large datasets

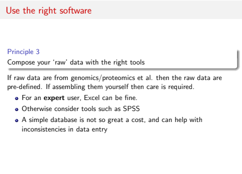
Use the right software

Principle 3

Compose your 'raw' data with the right tools

If raw data are from genomics/proteomics et al. then the raw data are pre-defined. If assembling them yourself then care is required.

- For an **expert** user, Excel can be fine.
- Otherwise consider tools such as SPSS
- A simple database is not so great a cost, and can help with inconsistencies in data entry



SPSS: Similar to Excel, but a number of safeguards built in, and it is also an easy-to-use analysis suite

e.g. If collecting data for a week, but on Thursday you accidentally put dates in a different format...

Use the right format

Format here doesn't mean .csv not .xls, nor fonts, colours etc.

Principle 4

Set up your data with the right shape

You'll see a lot of this later, but:

- Aim for a rectangle
- No blank cells (but be careful how you represent missing data)
- Each row is a case, each column a variable (although not always)
- The key is deciding what constitutes a case
- If it isn't clear what a case is, you might be better off with two tables.

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expression sets often have genes as rows, cases as columns

Naming variables

Principle 5

Give variables and cases sensible names

- A document explaining the primary data is invaluable.
- Variously known as a Data Dictionary (KB), Glossary (GSS), or XXXXX (SPSS),
- For variables that can only take fixed values it can define those levels.

Naming variables 2

Case and variable names need to be

- unique
- lacking in exotic characters
- interpretable
- accurate

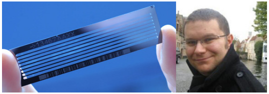

Figure 1: One of these is a person.

(flowcell image from global.fncstatic.com)

METABRIC example 1

In METABRIC we looked at breast cancer samples from ~ 2000 patients

- Each patient had two breasts
- Each breast potentially had multiple tumours
- Each tumour potentially had multiple samples
- Each sample was run on multiple technologies
- Each technology could have been repeated

Two reasons not to label data from a microarray as if it was a person

1. if there are multiple arrays from the same person, then it leads to confusion

METABRIC example 2

2. The only thing you know about the microarray data (i.e. the only metadata that are raw) is that they came from the microarray.

We had a problem with sample mixups within the project.

- Had we had ‘raw’ data where the cases were labelled by array name, we could simply have changed the file that mapped arrays to patients.
- It would have been easy to check that every analyst had the latest version
- By just changing the labels on the raw data, it became much harder to keep track of who was using what

Meta data

Principle 6

Have thorough Meta Data

- Since you now have rectangular data with succinct variable names, you may have lost some detail of what those variables are.
- A document explaining the primary data is invaluable.
- It is variously known as a Data Dictionary (KB), Glossary (GSS), or XXXXX (SPSS),
- For variables that can only take fixed values it can define those levels.

Versioning

Principle 7

Be clear what data are being analysed

- The raw data shouldn't change (probably), but the working data could easily so do
- To reproduce results, it is important to be able to specify the version of the data that was used.
- Some form of versioning is therefore important.

Principle 7
Be clear what data are being analysed

- The raw data shouldn't change (probably), but the working data could easily so do
- To reproduce results, it is important to be able to specify the version of the data that was used.
- Some form of versioning is therefore important.

Beware taunting the gods by calling a data set, "final", "frozen" etc.

Summary

1. Ensure you have a secure back up of the raw data
2. Never work directly on the raw data
3. Compose your ‘raw’ data with the right tools
4. Set up your data with the right shape
5. Give variables and cases sensible names
6. Have thorough meta data
7. Be clear what data are being analysed

Examples

Enjoy the rest of the course.