Data management

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Slides at pboesu.github.io/teaching

Why do we care about good data management and reproducibility?

Funder requirement?

NSF, NIH, and many other funders require data management plans

Data Management Planning Tool: https://dmptool.org/

Journal requirement?

An increasing number of journals require deposition of data in public repositories as a condition of publishing

E.g. all ESA and BES journals, Biology Letters, Proceedings B, Ecology and Evolution...

Noble cause?

Opening up data sources and analysis code should make science more transparent and reproducible

Egotism!

You will have to redo most analyses

- because you have new data
- because you made a mistake
- because your advisor wants to change something
- because your committee wants a change
- because reviewer #2 wants a change
- because reviewer #2 didn't want the change anyways
- because every journal has different formatting requirements
- etc
- etc

Computational effort

Ι.	design study	easy
2.	collect data	easy
3.	clean & format data	hard
4.	descriptive statistics	easy
5.	inferential statistics	moderate
6.	reporting	moderate - hard

Start good data and analysis habits now

Organisation starts on your computer

- -- project_folder
 - -- CITATION
 - -- README
 - -- LICENSE
 - |-- requirements.txt
 - |-- data
 - -- birds_count_table.csv
 - -- doc
 - -- notebook.md
 - -- manuscript.md
 - -- changelog.txt
 - -- results
 - -- summarized_results.csv
 - -- src
 - | -- sightings_analysis.py
 - -- runall.py

Resources:

- A Quick Guide to Organizing Computational Biology Projects
 - <u>https://doi.org/10.1371/journal.pcbi.1000424</u>
- British Ecological Society Data Management Guide
 - http://www.britishecologicalsociety.org/publications/guides-to/
- Ten Simple Rules for Creating a Good Data Management Plan
 - <u>https://doi.org/10.1371/journal.pcbi.1004525</u>



Spreadsheets are not going away

- ~I billion use Microsoft Office
- ~650 million use spreadsheets
- >50% use formulas
- 250K I million people use R

Spreadsheets make it easy to enter data

Spreadsheets combine

- data
- figures
- formatting
- interactive calculations
- reactive properties (e.g. "smart" formatting)

often in proprietary data formats

Spreadsheets make it easy to make a mess of data

Use spreadsheets to prepare machine readable data.

Don't use spreadsheets to do your analysis.

Excel analysis

- easy to get started
- easy to be inconsistent
- no logical sequence to your actions
- hard to document your actions
- tweak a detail: usually lots of manual work
- reproducibility limited to impossible

vs R analysis

- hard to start
- inconsistencies can break analysis
- scripts have an order → sequence of analysis steps
- easy to document your actions with comments
- tweak a detail: usually small change in code
- great for reproducibility

Nope

	С	D
1		
2	Comment	
3		
4	In ethonal	
5	In ethonal	
6	In ethanol	
7	In plastic bag. Frozen	
8	IN plastic bag	
9		

Be consistent

	С	D
1		
2	Comment	
3		
4	In ethonal	
5	In ethonal	
6	In ethanol	
7	In plastic bag. Frozen	
8	IN plastic bag	
9		

Nope

	Α	В	С	D	E
32	59	22	1	grass	0
33	40	75	1	М	1
34	64	53	1	Bare/forest	0
35	34	55	1	Bare/forest	0
36	35	72	1	М	0
37	36	38	1	М	0
38	45	47	1	M/grass	0
39	41	44	1	Bushes	0
40	42	30	1	М	0
41	44	25	1	М	0
42	60	50	1	М	0
43	65	25	1	Grass	0
44					0.2195122
45	Average	58.658537			
46	s.e.	22.605876			

Put just one thing in a cell

	А	В	С	D	E
32	59	22	1	grass	0
33	40	75	1	Μ	1
34	64	53	1	Bare/forest	0
35	34	55	1	Bare/forest	0
36	35	72	1	Μ	0
37	36	38	1	Μ	0
38	45	47	1	M/grass	0
39	41	44	1	Bushes	0
40	42	30	1	Μ	0
41	44	25	1	Μ	0
42	60	50	1	Μ	0
43	65	25	1	Grass	0
44					0.2195122
45	Average	58.658537			
46	s.e.	22.605876			

Nope

	Α	В	С	D	E	F	G	Н	I	J	к	L	М	N	0
1				7	,						9				
2	Date	Date	Sticks	Weight (g)	Bill (mm)	Tarsus (mm)) Wing (mm)		Date	Sticks	Weight (g)	Bill (mm)	Tarsus (mm)	Wing (mm)	
3	22-Oct	22-Oct							22-Oct						
4	23-Oct	23-Oct							23-Oct						
5	24-Oct	24-Oct							24-Oct						
6	25-Oct	25-Oct							25-Oct	Down	40	12.8	18.7	23	
7	26-Oct	26-Oct							26-Oct	Down	55				
8	27-Oct	27-Oct							27-Oct	Down	66				
9	28-Oct	28-Oct							28-Oct	Down	71				
10	29-Oct	29-Oct							29-Oct	Down	75				
11	30-Oct	30-Oct							30-Oct	Down	70				
12	31-Oct	31-Oct							31-Oct	Down	88	14.7	22.9	27	
13	1-Nov	1-Nov							1-Nov	Down	110				
14	2-Nov	2-Nov	Down	43	22.1	18.0	22.1		2-Nov	Down	130				
15	3-Nov	3-Nov	Down	58					3-Nov	Down	123				
16	4-Nov	4-Nov	Down	55					4-Nov	Down	115				
17	5-Nov	5-Nov	Down	63					5-Nov	Down	148				
18	6-Nov	6-Nov	Down	62					6-Nov	Down	157	17.9	28.7	37	
19	7-Nov	7-Nov	Down	113	15.8	22.4	27		7-Nov	Up	163				
20	8-Nov	8-Nov	Down	90					8-Nov	Down	160				
21	9-Nov	9-Nov	Down	120					9-Nov	Down	180				
22	10-Nov	10-Nov	Down	133					10-Nov	Down	188				
23	11-Nov	11-Nov	Down	135					11-Nov	Down	180				
24	12-Nov	12-Nov	Down	145					12-Nov	Down	160	21.3	34	43	
25	13-Nov	13-Nov							13-Nov						
26															
27															
28	11-Dec	11-Dec	Down	338	29.5	45.9	114		11-Dec	Down	358	28.9	41.5	131	
29	12-Dec	12-Dec	Down	320					12-Dec	Down	388				
30	13-Dec	13-Dec	Down	340					13-Dec	Down	388				
31	14-Dec	14-Dec	Down	356					14-Dec	Down	408				
32	15-Dec	15-Dec	Down	328					15-Dec	Down	378				
22	40 Dec	10 D	D	220					10 D	D	270				

Make it a rectangle No empty cells No special characters in variable names

	Α	В	С	D	E	F	G	Н	1	J	к	L	M	N	0
1				-	7						9				
2	Date	Date	Sticks	Weight (g)	Bill (mm)	Tarsus (mm)	Wing (mm)		Date	Sticks	Weight (g)	Bill (mm)	Tarsus (mm)	Wing (mm)	
3	22-Oct	22-Oct							22-Oct						
4	23-Oct	23-Oct							23-Oct						
5	24-Oct	24-Oct							24-Oct						
6	25-Oct	25-Oct							25-Oct	Down	40	12.8	18.7	23	
7	26-Oct	26-Oct							26-Oct	Down	55				
8	27-Oct	27-Oct							27-Oct	Down	66				
9	28-Oct	28-Oct							28-Oct	Down	71				
10	29-Oct	29-Oct							29-Oct	Down	75				
11	30-Oct	30-Oct							30-Oct	Down	70				
12	31-Oct	31-Oct							31-Oct	Down	88	14.7	22.9	27	
13	1-Nov	1-Nov							1-Nov	Down	110				
14	2-Nov	2-Nov	Down	43	22.1	18.0	22.1		2-Nov	Down	130				
15	3-Nov	3-Nov	Down	58					3-Nov	Down	123				
16	4-Nov	4-Nov	Down	55					4-Nov	Down	115				
17	5-Nov	5-Nov	Down	63					5-Nov	Down	148				
18	6-Nov	6-Nov	Down	62					6-Nov	Down	157	17.9	28.7	37	
19	7-Nov	7-Nov	Down	113	15.8	22.4	27		7-Nov	Up	163				
20	8-Nov	8-Nov	Down	90					8-Nov	Down	160				
21	9-Nov	9-Nov	Down	120					9-Nov	Down	180				
22	10-Nov	10-Nov	Down	133					10-Nov	Down	188				
23	11-Nov	11-Nov	Down	135					11-Nov	Down	180				
24	12-Nov	12-Nov	Down	145					12-Nov	Down	160	21.3	34	43	
25	13-Nov	13-Nov							13-Nov						
26															
27															
28	11-Dec	11-Dec	Down	338	29.5	45.9	114		11-Dec	Down	358	28.9	41.5	131	
29	12-Dec	12-Dec	Down	320					12-Dec	Down	388				
30	13-Dec	13-Dec	Down	340					13-Dec	Down	388				
31	14-Dec	14-Dec	Down	356					14-Dec	Down	408				
32	15-Dec	15-Dec	Down	328					15-Dec	Down	378				
22	10 D	10 D	D	220					10 D	D	270				

Nope

	V	W	х	Y	Z	AA	AB	AC	AD	AE	AF	AG	AH
1			49							49	1		
2	Date	Weight (g)	Bill (mm)	Tarsus (mm)	Wing (mm)	Comment		Date	Weight (g)	Bill (mm)	Tarsus (mm)	Wing (mm)	Comment
3	28-Dec	295	32.2	43.2	207			Fledged 9 of	January*				
4	Fledged												

Write dates as YYYY-MM-DD

	V	W	Х	Y	Z	AA	AB	AC	AD	AE	AF	AG	AH
1			49							49			
2	Date	Weight (g)	Bill (mm)	Tarsus (mm)	Wing (mm)	Comment		Date	Weight (g)	Bill (mm)	Tarsus (mm)	Wing (mm)	Comment
3	28-Dec	295	32.2	43.2	207			Fledged 9 of	January*				
4	Fledged												

No, no, no, no, no!

	L	M	N	0	Р	Q	R	S	т	U	V	w	х	Y	Z	AA	AB	AC	AD	AE
1	D1	D2	D3	D4	D5	D6	D7	D8	D9	D10	D11	D12	D13	D14	D15	D16	D17	D18	D19	D20
2		•				•	•	•	•											
3		•				•	•	•	•											
4		•				•	•	•	•	•	•									
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34		Start																		
35		Alive																		
36		Dead		1																
37		Alive																		
38	•	destructive	sampling ev	ent																
39																				
40																				

Do not use font or cell color as data

	L	М	N	0	Р	Q	R	S	Т	U	V	w	х	Y	Z	AA	AB	AC	AD	AE
1	D1	D2	D3	D4	D5	D6	D7	D8	D9	D10	D11	D12	D13	D14	D15	D16	D17	D18	D19	D20
2		•				•	•	•	•											
3		•				•	•	•	•											
4		•				•	•	•	•	•	•									
5				•	•	•														
6		•			•	•	•													
7		•			•	•	•													
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9		•			•	•	•													
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37		Alive																		
38	•	destructive	sampling eve	ent																
39																				
40																				

three principles for names

- machine readable
- human readable
- plays well with default ordering

File names

- BAD
 - myabstract.docx
 - Joe's Filenames Use Spaces and Punctuation.xlsx
 - figure I.png
 - fig 2.png
 - JW7d^(2sl@deletethisandyourcareerisoverWx2*.txt

• GOOD

- 2014-06-08_abstract-for-sla.docx
- joes-filenames-are-getting-better.xlsx
- fig01_scatterplot-talk-length-vs-interest.png
- fig02_histogram-talk-attendance.png
- 1986-01-28_raw-data-from-challenger-o-rings.txt

Variable names

good name	good alternative	avoid
Max_temp_C	MaxTemp	Maximum Temp (°C)
$Precipitation_mm$	Precipitation	precmm
Mean_year_growth	MeanYearGrowth	Mean growth/year
sex	sex	M/F
weight	weight	Ψ.
cell_type	CellType	Cell type
$Observation_01$	$\texttt{first_observation}$	1st Obs.

"machine readable"

- Search friendly
- Avoid
 - Spaces
 - Punctuation
 - Symbols, accented characters
 - case sensitivity
- easy to compute on
 - deliberate use of delimiters like "-" and "_"

"human readable"

• name contains info on *content*

"human readable"

- 01_marshal-data.md
- 01_marshal-data.r
- 02_pre-dea-filtering.md
- 02_pre-dea-filtering.r
- 03_dea-with-limma-voom.md
- 03_dea-with-limma-voom.r
- 04_explore-dea-results.md
- 04_explore-dea-results.r
- 90_limma-model-term-name-fiasco.md
- 90_limma-model-term-name-fiasco.r
- helper01_load-counts.r
- helper02_load-exp-des.r
- helper03_load-focus-statinf.r
- helper04_extract-and-tidy.r

- 01.md
- 01.r
- 02.md
- 02.r
- 03.md
- 03.r
- 04.md
- 04.r
- 90.md
- 90.r
- helper01.r
- helper02.r
- helper03.r
- helper04.r

Which set of file(name)s do you want at 3a.m. before a deadline?

"plays well with default ordering"

- put something numeric first
 - Sequence number for logical ordering
 - Date/timestamp for chronological ordering
- use the ISO 8601 standard for dates
 - YYYY-MM-DD
- left pad other numbers with zeros

I0_final-figs-for-publication.RI_data-cleaning.R2_fit-model.R

01_data-cleaning.R 02_fit-model.R 10_final-figs-for-publication.R

Also this 🌢 🌢 🌢

	The workbook you opened contains automatic links to information in another workbook.
	Do you want to update this workbook with changes made to the other workbook?
	 To update all linked information, click Update. You must have access to all of the linked workbooks. To keep the existing information, click Ignore Links. To open your workbook and receive more options to which links get updated, click Edit Links.
	Edit Links Updated, click Edit Links.

- Excel offers many features that can trip you up later.
- Use individual sheets for individual datasets.
- Do the crosslinking in your analysis scripts.

Make backups



• Most likely duration of a STEM Ph.D. in the US: 6 years

Recap: spreadsheets

- Be consistent.
- Write dates as YYYY-MM-DD.
- Fill in all of the cells.
- Put just one thing in a cell.
- Make it a rectangle.
- Keep metadata and/or a data dictionary.
- No calculations in the raw data files.
- Don't use font color or highlighting as data.
- Choose good names for things.
- Use data validation to avoid data entry mistakes.
- Save the data in plain text files.
- Make backups.

Resources:

- <u>http://kbroman.org/dataorg/</u>
- Data organization in spreadsheets
 - <u>https://doi.org/10.7287/peerj.preprints.3183v1</u>

Where to get more training?

- The Carpentries teach researchers computing skills they need to get more done in less time & with less pain.
- Data wrangling skills
 - Spreadsheets, OpenRefine, SQL, R, Python
 - http://www.datacarpentry.org/workshops-upcoming/
- Software/programming skills
 - R, SQL, Python, Unix shell, version control
 - https://software-carpentry.org/workshops/
- Usually several workshops per year at UF in Gainesville
- Your lab/BGSO/etc. can organize a workshop locally
 - https://software-carpentry.org/workshops/request/