Data management

Fall 2017

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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

1. 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
  - https://doi.org/10.1371/journal.pcbi.1000424
- British Ecological Society Data Management Guide
  - http://www.britishecologicalsociety.org/publications/guides-to/
- Ten Simple Rules for Creating a Good Data Management Plan
  - https://doi.org/10.1371/journal.pcbi.1004525

Spreadsheets

Spreadsheets are not going away

- ~1 billion use Microsoft Office
- ~650 million use spreadsheets
- >50% use formulas
- 250K - 1 million people use R

numbers from Jenny Bryan, UW

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*.

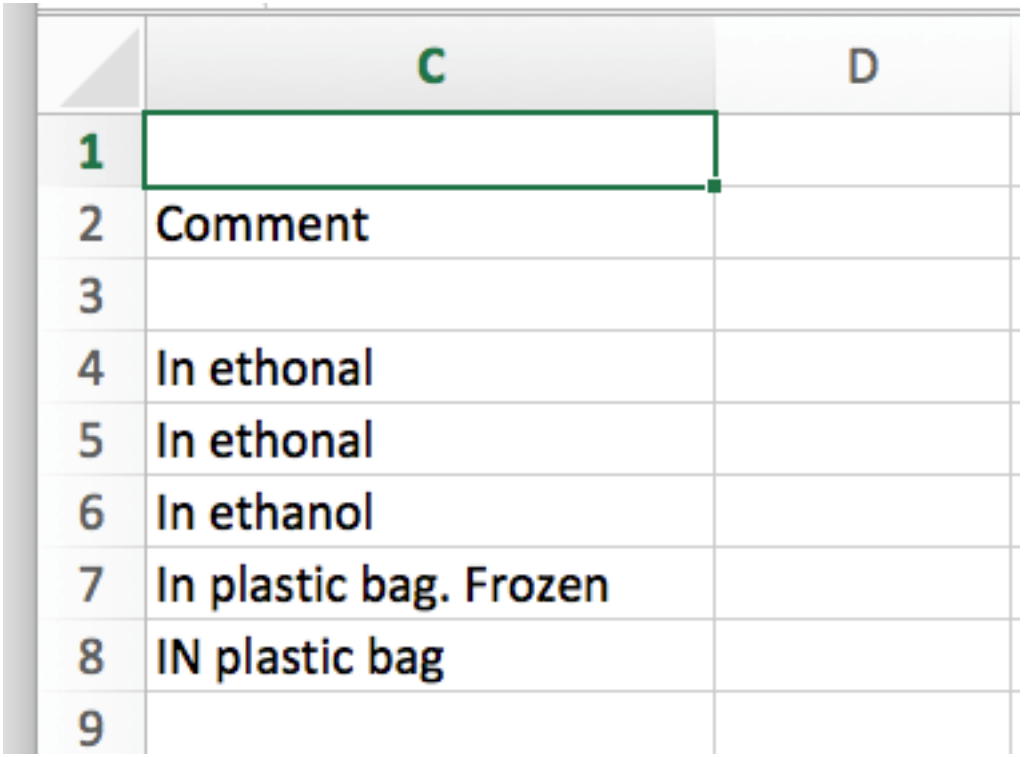
Don’t use spreadsheets to do your analysis.

Excel analysis vs R 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

- 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



	C	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

	C	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

	A	B	C	D	E
32	59	22	1	grass	0
33	40	75	1	M	1
34	64	53	1	Bare/forest	0
35	34	55	1	Bare/forest	0
36	35	72	1	M	0
37	36	38	1	M	0
38	45	47	1	M/grass	0
39	41	44	1	Bushes	0
40	42	30	1	M	0
41	44	25	1	M	0
42	60	50	1	M	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

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

Nope

	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O
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				

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

	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O
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)	
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4	23-Oct	23-Oct							23-Oct						
5	24-Oct	24-Oct							24-Oct						
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9	28-Oct	28-Oct							28-Oct	Down	71				
10	29-Oct	29-Oct							29-Oct	Down	75				
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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				
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31	14-Dec	14-Dec	Down	356					14-Dec	Down	408				
32	15-Dec	15-Dec	Down	328					15-Dec	Down	378				

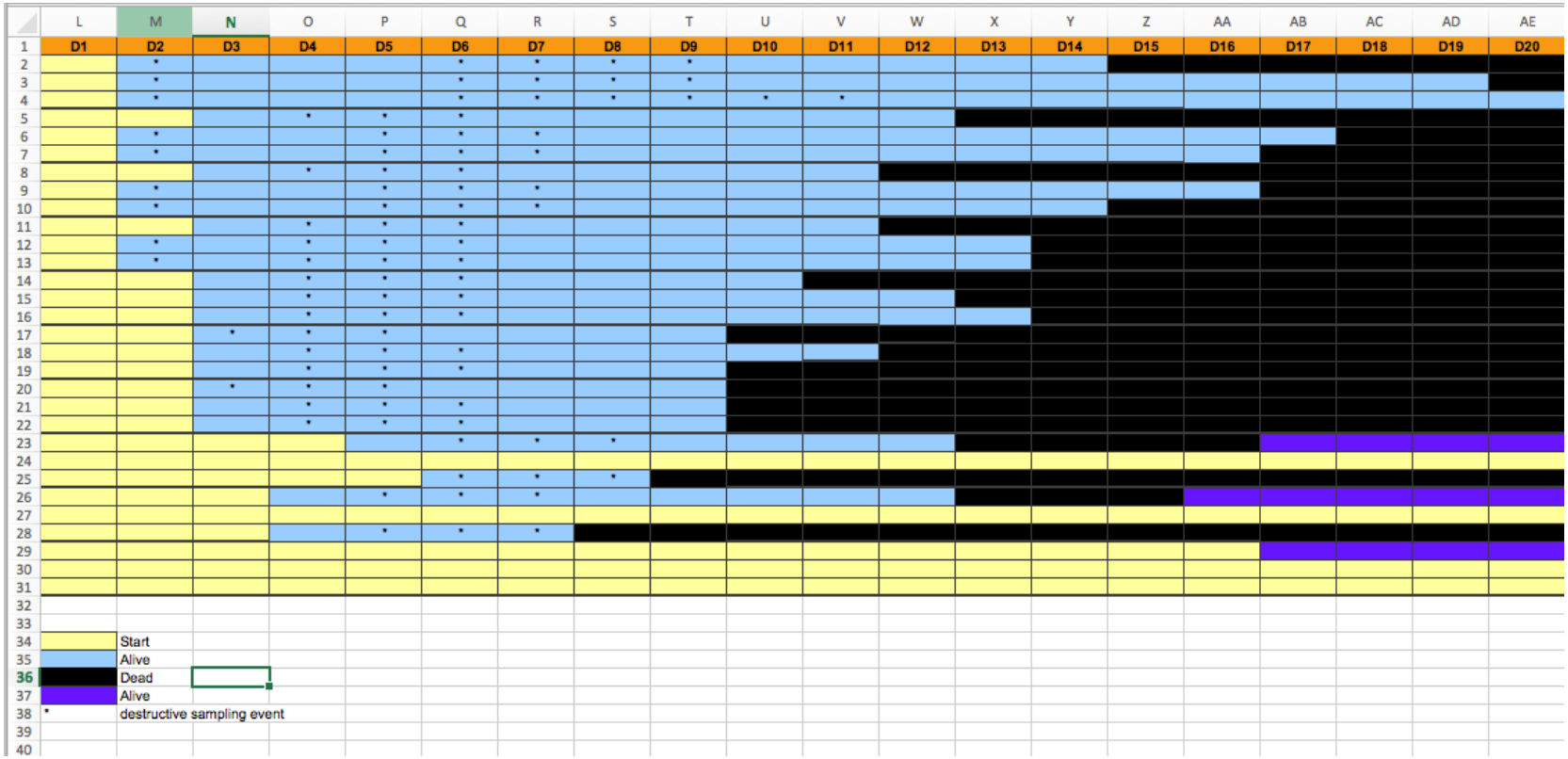
Nope

	V	W	X	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												

Write dates as YYY-MM-DD

	V	W	X	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	O	P	Q	R	S	T	U	V	W	X	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		*			*	*	*													
8				*	*	*														
9		*			*	*	*													
10		*			*	*	*													
11				*	*	*														
12		*		*	*	*														
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14				*	*	*														
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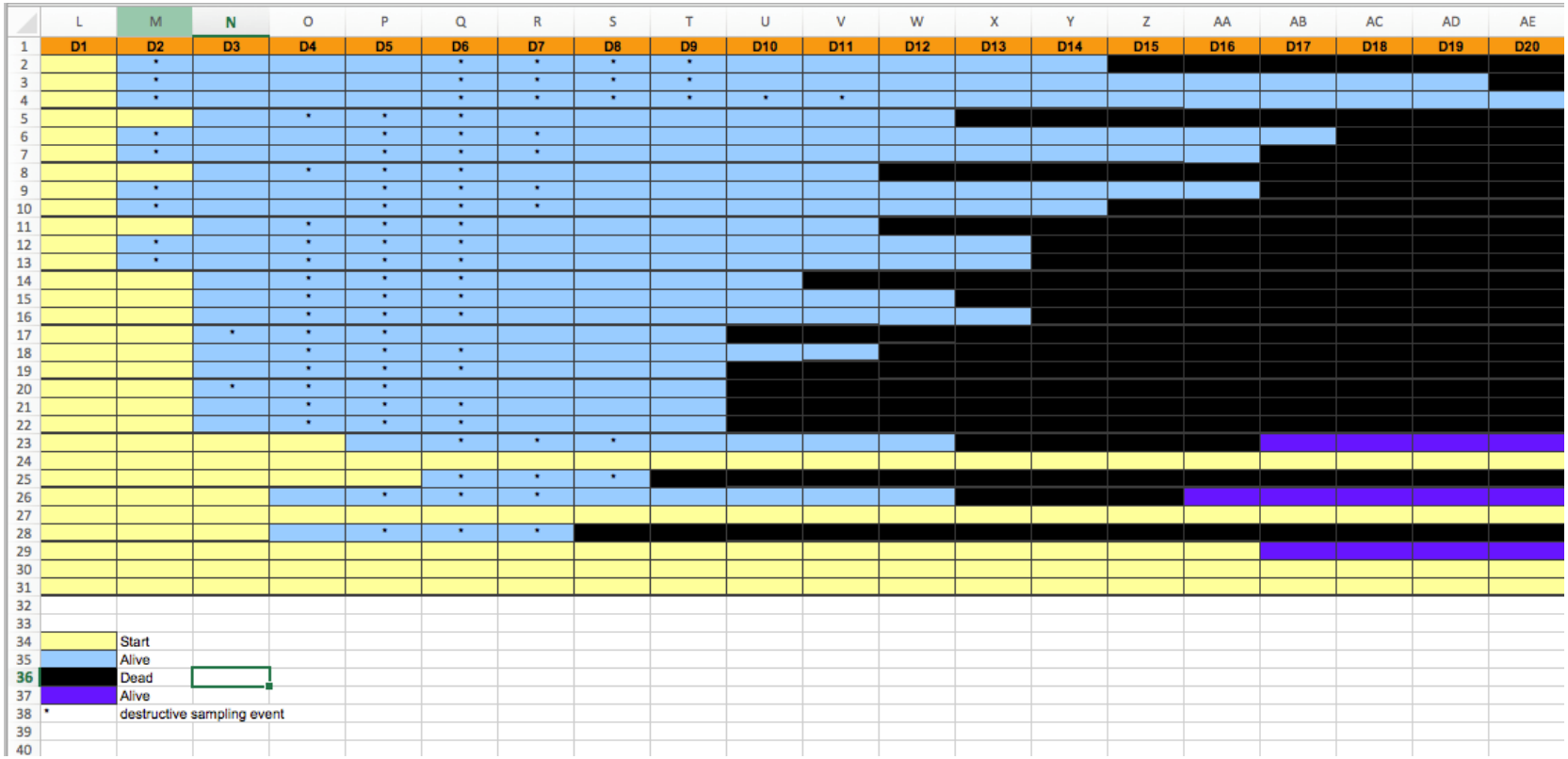
28					*	*	*													
29																				
30																				
31																				
32																				
33																				
34		Start																		
35		Alive																		
36		Dead																		
37		Alive																		
38	*	destructive sampling event																		
39																				
40																				

Do not use font or cell color as data



	L	M	N	O	P	Q	R	S	T	U	V	W	X	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
34		Start																		
35		Alive																		
36		Dead																		
37		Alive																		
38	*	destructive sampling event																		

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 1.png
  - fig 2.png
  - JW7d^(2sI@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	w.
cell_type	CellType	Cell type
Observation_01	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?

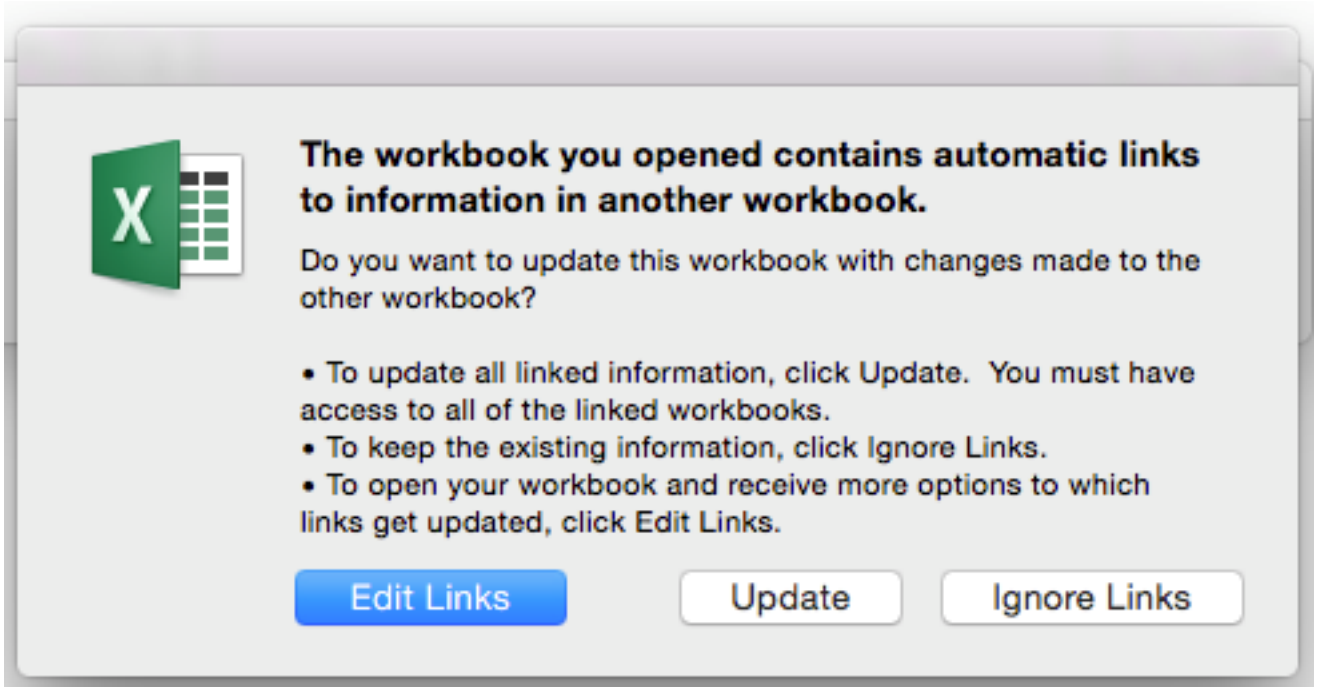
“plays well with default ordering”

- 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

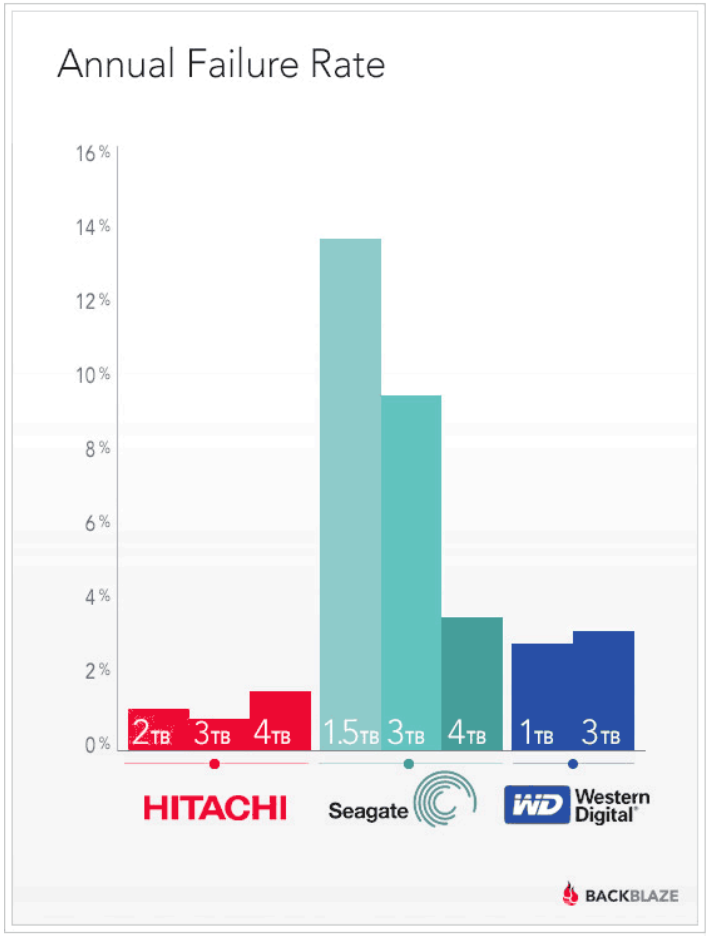
10_final-figs-for-publication.R
1_data-cleaning.R
2_fit-model.R

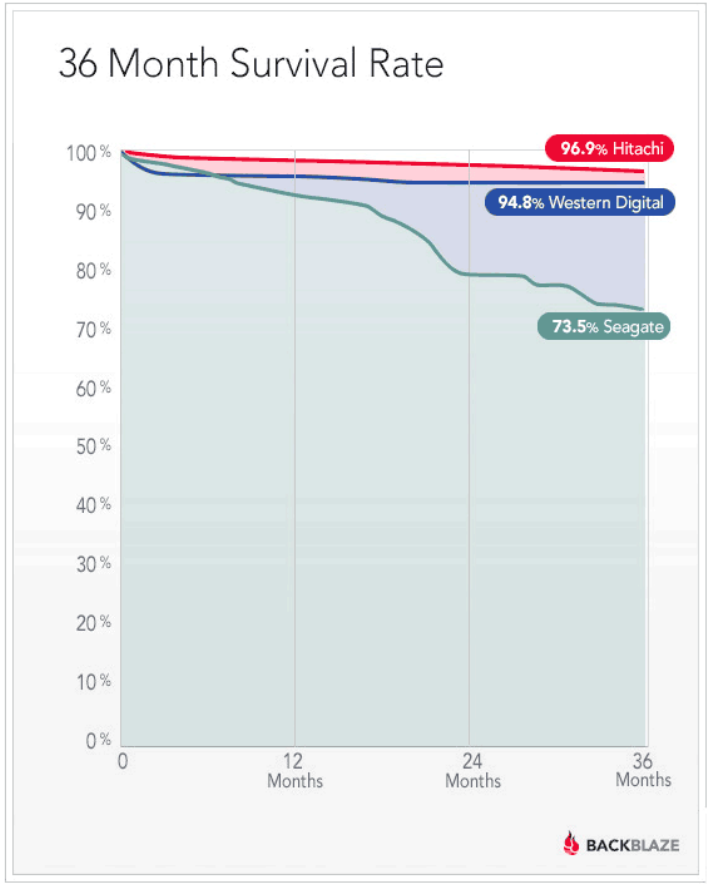
01_data-cleaning.R
02_fit-model.R
10_final-figs-for-publication.R

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
Update
Ignore Links

Make backups





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

Sources: Backblaze, CGS Ph.D. Completion Project

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:

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

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/