Steps toward reproducible research

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Slides: bit.ly/cmp2018

Karl -- this is very interesting, however you used an old version of the data (n=143 rather than n=226).

I'm really sorry you did all that work on the incomplete dataset.

Bruce

The results in Table 1 don’t seem to correspond to those in Figure 2.

Where did we get this data file?

Why did I omit those samples?

How did I make that figure?

Reproducible

vs.

Replicable

Reproducible

vs.

Correct

Steps toward reproducible research

`kbroman.org/steps2rr`

1. Organizing data in spreadsheets

Organize data for computers

Improve this arrangement?

	A	B	C	D	E	F	G
1							
2	1min						
3			Normal			Mutant	
4		10−05−16	10−12−16	10−19−16	10−05−16	10−12−16	10−19−16
5	B6	146.6	138.6	155.6	166	179.3	186.9
6	BTBR	245.7	240	243.1	177.8	171.6	188.1
7							
8	5min						
9			Normal			Mutant	
10		10−05−16	10−12−16	10−19−16	10−05−16	10−12−16	10−19−16
11	B6	333.6	353.6	408.8	450.6	474.4	423.8
12	BTBR	514.4	610.6	597.9	412.1	447.4	446.5

Improved arrangement

	A	B	C	D	E
1	strain	genotype	treatment_time	date	response
2	B6	Normal	1min	2016−10−05	146.6
3	B6	Normal	1min	2016−10−12	138.6
4	B6	Normal	1min	2016−10−19	155.6
5	B6	Mutant	1min	2016−10−05	166
6	B6	Mutant	1min	2016−10−12	179.3
7	B6	Mutant	1min	2016−10−19	186.9
8	BTBR	Normal	1min	2016−10−05	245.7
9	BTBR	Normal	1min	2016−10−12	240
10	BTBR	Normal	1min	2016−10−19	243.1

Fill in all cells

	A	B	C
1	id	date	glucose
2	101	2015−06−14	149.3
3	102		95.3
4	103	2015−06−18	97.5
5	104		117.0
6	105		108.0
7	106	2015−06−20	149.0
8	107		169.4

Make it a rectangle

	A	B	C	D	E	F
1						
2		101	102	103	104	105
3	sex	Male	Male	Female	Female	Male
4						
5		101	102	103	104	105
6	glucose	73.5	101.2	78.0	84.4	141.1
7						
8		101	102	103	104	105
9	insulin	1.22	0.96	1.32	0.89	1.41

No calculations with the raw data

	A	B	C	D	E	F	G
1							
2	Date	11/3/14					
3	Days on diet	126					
4	Mouse #	43					
5	sex	f					
6	experiment		values			mean	SD
7	control		0.186	0.191	1.081	0.49	0.52
8	treatment A		7.414	1.468	2.254	3.71	3.23
9	treatment B		9.811	9.259	11.296	10.12	1.05
10							
11	fold change		values			mean	SD
12	treatment A		15.26	3.02	4.64	7.64	6.65
13	treatment B		20.19	19.05	23.24	20.83	2.17

Use one header row

	A	B	C	D	E	F	G	H	I	J	K
1			week 4			week 6			week 8		
2	Mouse ID	SEX	date	weight	glucose	date	weight	glucose	date	weight	glucose
3	3005	M	3/30/2007	19.3	635	4/11/2007	31	460.7	4/27/2007	39.6	530.2
4	3017	M	10/6/2006	25.9	202.4	10/19/2006	45.1	384.7	11/3/2006	57.2	458.7
5	3434	F	11/22/2006	26.6	238.9	12/6/2006	45.9	378	12/22/2006	56.2	409.8
6	3449	M	1/5/2007	27.5	121	1/19/2007	42.9	191.3	2/2/2007	56.7	182.5
7	3499	F	1/5/2007	19.8	220.2	1/19/2007	36.6	556.9	2/2/2007	43.6	446

1. Organizing data in spreadsheets

- Make it a rectangle (rows = observations, cols=variables)
- Use a single header row; avoid spaces.
- Be consistent.
- Use care about dates.
- Put just one thing in a cell.
- Fill in all cells.
- Explicit code for missing values (e.g. `-` or `N/A`)
- No calculations/graphs in the raw data files.
- Don't use font color or highlighting as data.
- Make backups.
- Use data validation to avoid data entry mistakes.
- Save the data in plain text files.

Broman & Woo, Am Stat 78:2–10, 2018

2. Organizing projects

File organization and naming
are powerful weapons against chaos.

– Jenny Bryan

2. Organizing projects

Your closest collaborator is you six months ago,
but you don’t reply to emails.

(paraphrasing Mark Holder)

2. Organizing projects

Have sympathy for your future self.

How to organize these files?

```
Raw phenotype data

    CPL_Rosetta_Lipids_FINAL.xlsx
    Complete F2 Liver TG Set.xlsx
    D2O_Summary_of_All_F2_Samples_MF_30July2009.xlsx
    FINAL_RBM_DATA_102989_26Sep2007.xlsx
    Mapped_Urine_Plasma_Data_to_Statgen.xlsx
    Necropsy_Tracking_Report_rk61412.xlsx
    Necropsy_Tracking_Report_rk_052912_atb.xlsx
    Necropsy_Tracking_Report_rk_2011-04-26.xlsx
    Original_Necropsy_Tracking_Report_rk.xlsx
    RBM_Tube_Number_Key.xlsx

Raw genotype data

    Final Fit1_Filtered_Assay_Allele_Signals_and_Genotypes_18Sep.txt

Converted data

    clinpheno.csv
    detailed_genotypes.csv
    genotypes4rqtl.csv
    genotypes_karl.csv
```

```
R scripts to organize data

    check_necropsy_files.R
    check_necropsy_files_2012-06-02.R
    combine_pheno.R
    combine_pheno2.R
    combine_pheno3.R
    compareData.R
    func.R
    prepData.R

Analysis

    fig1.png
    fig2.png
    fig3.png
    fig4.png
    fig5.png
    fig6.png
    fig7.png
    fig8.png
    scanone_clinphe.Rmd
    scanone_clinphe.html
```

Be consistent

```
RawData/                    Notes/
CleanData/                  Refs/

Python/                     ReadMe.txt
R/                          ToDo.txt
Ruby/
```

Chaos

```
AimeeNullSims/     Deuterium/              Ping/
AimeeResults/      ExtractData4Gary/       Ping2/
AnnotationFiles/   FromAimee/              Ping3/
Brian/             GoldStandard/           Ping4/
Chr6_extrageno/    HumanGWAS/              Play/
Chr6_segdis/       Insulin/                Prdm9/
ChrisPlaisier/     Int2_for_Mark/          RBM_PlasmaUrine_2012-03-08/
Code4Aimee/        Islet_2011-05/          Slco1a6/
CompAnnot/         MappingProbes/          StudyLineupMethods/
CondScans/         MultiProbes/            kidney_chr6.R
D2O_2012-02-14/    NewMap/                 pck2_sucla2.R
D2O_cellcycle/     Notes/                  penalties.txt
D2Ocorr/           NullSims/               transeQTL4Lude/
Data4Aimee/        NullSims_2009-09-10/
Data4Tram/         PepIns_2012-02-09/
```

Naming files

- Concise
- Meaningful
- No spaces or special characters except underscores and hyphens
- Dates like 2018-09-05 (or 20180905)
- Sortable
- Be consistent

Also

- Documentation
  - Detailed electronic notes
  - Have sympathy for your future self
  - Maintained to match the material
- Meta-data
  - Data about the data
  - Yet another spreadsheet
  - Data dictionary: explain variables, abbreviations, units, codes

3. Everything with a script

If you do something once,
you'll do it 1000 times.

Advantages of code

- More transparent
- Can be automated and repeated
- Less tedious and error prone (in principle)
- More flexible
- Necessary for high-dimensional data

4. Automate the process (GNU Make)

```
R/analysis.html: R/analysis.Rmd Data/cleandata.csv
    cd R;R -e "rmarkdown::render('analysis.Rmd')"

Data/cleandata.csv: R/prepData.R RawData/rawdata.csv
    cd R;R CMD BATCH prepData.R

RawData/rawdata.csv: Python/xls2csv.py RawData/rawdata.xls
    Python/xls2csv.py RawData/rawdata.xls > RawData/rawdata.csv
```

kbroman.org/minimal_make

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```
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    Python/xls2csv.py RawData/rawdata.xls > RawData/rawdata.csv
```

kbroman.org/minimal_make

5. Turn scripts into reproducible reports

Gough project diagnostics

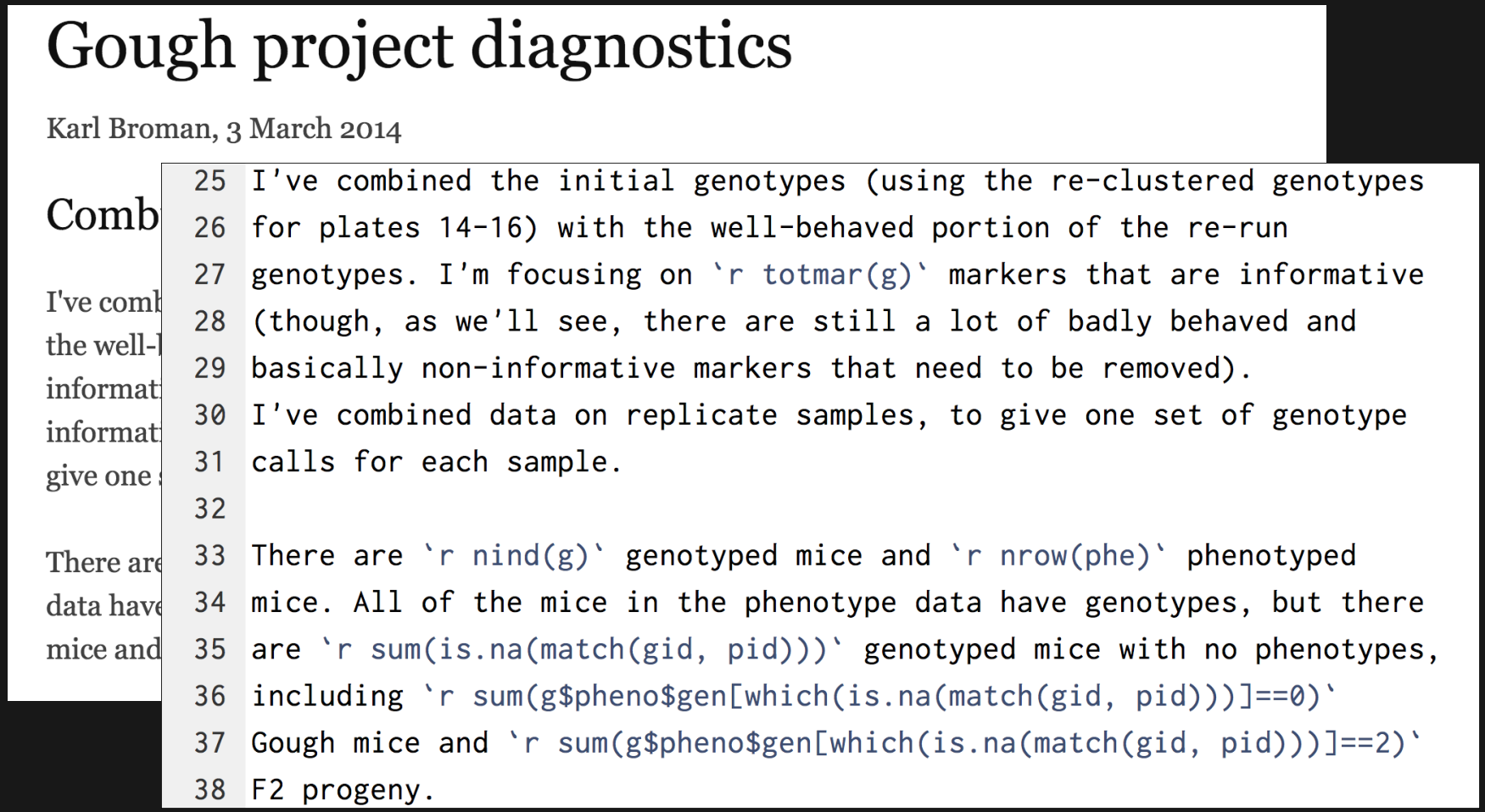
Karl Broman, 3 March 2014

Combine genotypes and phenotypes

I've combined the initial genotypes (using the re-clustered genotypes for plates 14-16) with the well-behaved portion of the re-run genotypes. I'm focusing on 36813 markers that are informative (though, as we'll see, there are still a lot of badly behaved and basically non-informative markers that need to be removed). I've combined data on replicate samples, to give one set of genotype calls for each sample.

There are 1497 genotyped mice and 1464 phenotyped mice. All of the mice in the phenotype data have genotypes, but there are 33 genotyped mice with no phenotypes, including 3 Gough mice and 30 F2 progeny.

5. Turn scripts into reproducible reports



Gough project diagnostics

Karl Broman, 3 March 2014

Comb

I've comb
the well-b
informat
informat
give one

There are
data have
mice and

```
25 I've combined the initial genotypes (using the re-clustered genotypes
26 for plates 14-16) with the well-behaved portion of the re-run
27 genotypes. I'm focusing on `r totmar(g)` markers that are informative
28 (though, as we'll see, there are still a lot of badly behaved and
29 basically non-informative markers that need to be removed).
30 I've combined data on replicate samples, to give one set of genotype
31 calls for each sample.
32
33 There are `r nind(g)` genotyped mice and `r nrow(phe)` phenotyped
34 mice. All of the mice in the phenotype data have genotypes, but there
35 are `r sum(is.na(match(gid, pid)))` genotyped mice with no phenotypes,
36 including `r sum(g$pheno$gen[which(is.na(match(gid, pid)))]==0)`
37 Gough mice and `r sum(g$pheno$gen[which(is.na(match(gid, pid)))]==2)`
38 F2 progeny.
```

6. Turn repeated code into functions

```
# Python
def read_genotypes (filename):
    "Read matrix of genotype data"
```

```
# R
plot_genotypes <-
function(genotypes, ...)
{
}
```

7. Create a package/module

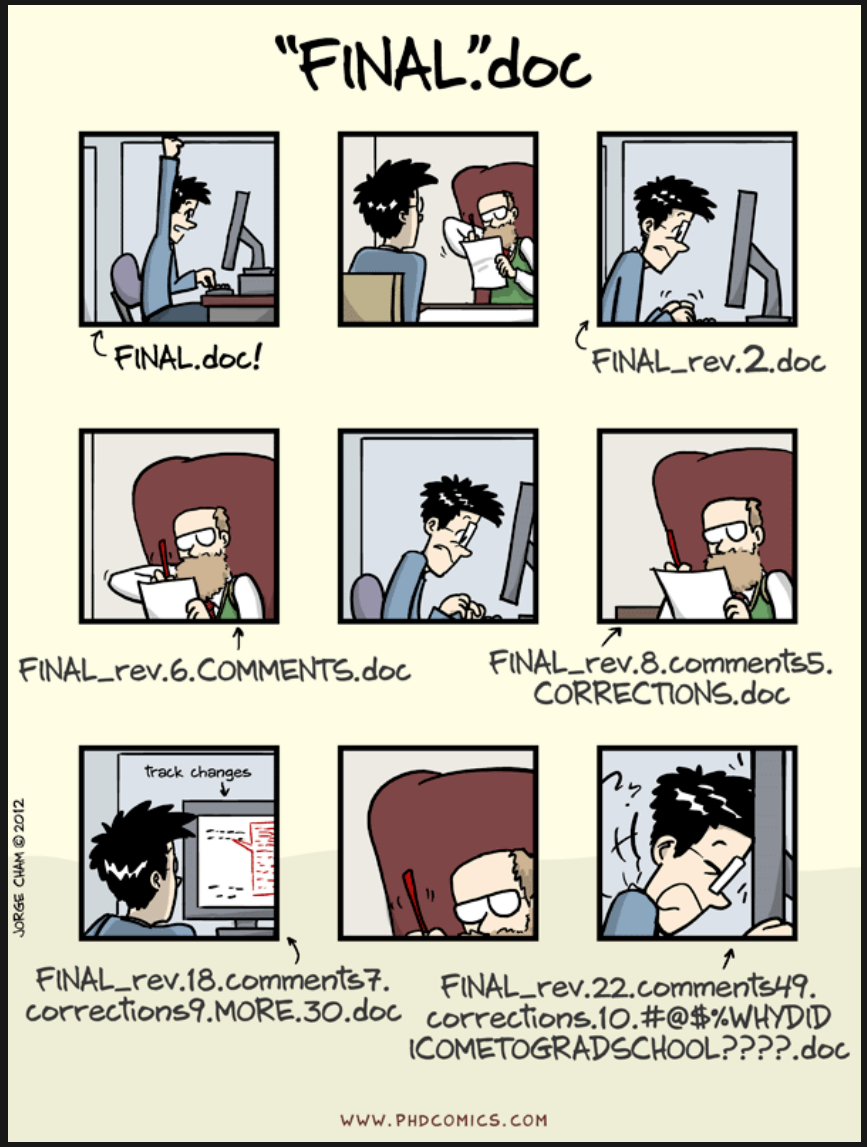
Don’t repeat yourself

7. Create a package/module

Don’t repeat yourself

kbroman.org/pkg_primer

8. Keep track of versions



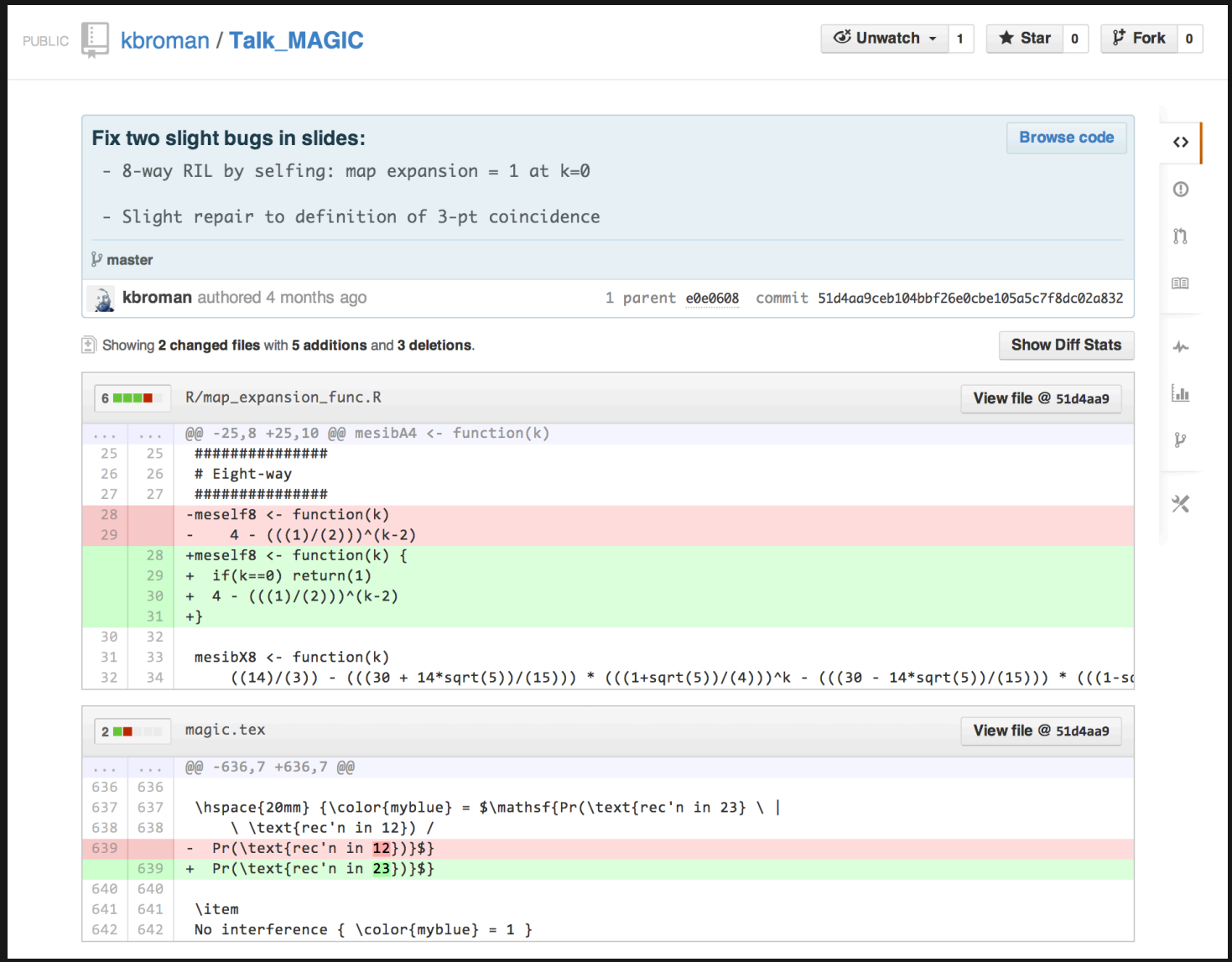
No “final” in file names

```
Deprecated/                              hypo_prcomp.RData
ReadMe.txt                               islet_int1_final.RData
adipose_int1_final.RData                 islet_int2_final.RData
adipose_int2_final.RData                 islet_mlratio_final.RData
adipose_mlratio_final.RData              islet_mlratio_nqrank_final.RData
adipose_mlratio_nqrank_final.RData       islet_prcomp.RData
adipose_prcomp.RData                     kidney_int1_final.RData
aligned_geno_with_pmap.RData             kidney_int2_final.RData
batches_final.RData                      kidney_mlratio_final.RData
batches_raw_final.RData                  kidney_mlratio_nqrank_final.RData
cpl_final.RData                          kidney_prcomp.RData
d2o_final.RData                          lipomics_final_rev2.RData
gastroc_int1_final.RData                 liverTG_final.RData
gastroc_int2_final.RData                 liver_int1_final.RData
gastroc_mlratio_final.RData              liver_int2_final.RData
gastroc_mlratio_nqrank_final.RData       liver_mlratio_final.RData
gastroc_prcomp.RData                     liver_mlratio_nqrank_final.RData
hypo_int1_final.RData                    liver_prcomp.RData
hypo_int2_final.RData                    mirna_final.RData
hypo_mlratio_final.RData                 necropsy_final_rev2.RData
hypo_mlratio_final_old.RData             plasmaurine_final_rev.RData
hypo_mlratio_nqrank_final.RData          pmark.RData
hypo_mlratio_nqrank_final_old.RData      rbm_final.RData
hypo_omit.RData
```

No “final” in file names

```
Deprecated/                                hypo_prcomp.RData
ReadMe.txt                                 islet_int1_final.RData
adipose_int1_final.RData                   islet_int2_final.RData
adipose_int2_final.RData                   islet_mlratio_final.RData
adipose_mlratio_final.RData                islet_mlratio_nqrank_final.RData
adipose_mlratio_nqrank_final.RData         islet_prcomp.RData
adipose_prcomp.RData                       kidney_int1_final.RData
aligned_geno_with_pmap.RData               kidney_int2_final.RData
batches_final.RData                        kidney_mlratio_final.RData
batches_raw_final.RData                    kidney_mlratio_nqrank_final.RData
cpl_final.RData                            kidney_prcomp.RData
d2o_final.RData                            lipomics_final_rev2.RData
gastroc_int1_final.RData                   liverTG_final.RData
gastroc_int2_final.RData                   liver_int1_final.RData
gastroc_mlratio_final.RData                liver_int2_final.RData
gastroc_mlratio_nqrank_final.RData         liver_mlratio_final.RData
gastroc_prcomp.RData                       liver_mlratio_nqrank_final.RData
hypo_int1_final.RData                      liver_prcomp.RData
hypo_int2_final.RData                      mirna_final.RData
hypo_mlratio_final.RData                   necropsy_final_rev2.RData
hypo_mlratio_final_old.RData               plasmaurine_final_rev.RData
hypo_mlratio_nqrank_final.RData            pmark.RData
hypo_mlratio_nqrank_final_old.RData        rbm_final.RData
hypo_omit.RData
```

8. Use version control (git/GitHub)



PUBLIC kbroman / Talk_MAGIC

Unwatch 1 | Star 0 | Fork 0

Fix two slight bugs in slides:

Browse code

- 8-way RIL by selfing: map expansion = 1 at k=0

- Slight repair to definition of 3-pt coincidence

master

kbroman authored 4 months ago — 1 parent e0e0608 commit 51d4aa9ceb104bbf26e0cbe105a5c7f8dc02a832

Showing **2 changed files** with **5 additions** and **3 deletions**. Show Diff Stats

6 R/map_expansion_func.R — View file @ 51d4aa9

```
...  ...  @@ -25,8 +25,10 @@ mesibA4 <- function(k)
25   25    ###############
26   26    # Eight-way
27   27    ###############
28        -meself8 <- function(k)
29        -    4 - (((1)/(2)))^(k-2)
     28   +meself8 <- function(k) {
     29   +  if(k==0) return(1)
     30   +  4 - (((1)/(2)))^(k-2)
     31   +}
30   32
31   33    mesibX8 <- function(k)
32   34        ((14)/(3)) - (((30 + 14*sqrt(5))/(15))) * (((1+sqrt(5))/(4)))^k - (((30 - 14*sqrt(5))/(15))) * (((1-s
```

2 magic.tex — View file @ 51d4aa9

```
...  ...  @@ -636,7 +636,7 @@
636  636
637  637   \hspace{20mm} {\color{myblue} = $\mathsf{Pr(\text{rec'n in 23} \ |
638  638       \ \text{rec'n in 12}) /
639       -  Pr(\text{rec'n in 12})}$}
     639   +  Pr(\text{rec'n in 23})}$}
640  640
641  641   \item
642  642   No interference { \color{myblue} = 1 }
```

kbroman.org/github_tutorial

9. License your software

Pick a license, any license

– Jeff Atwood

Summary

1. Arrange data to ease analysis
2. Organize your data and code
3. Everything with a script
4. Automate the process
5. Turn scripts into reproducible reports
6. Turn repeated code into functions
7. Create a package/module
8. Use version control
9. License your software

The most important tool is the mindset,
when starting, that the end product
will be reproducible.

– Keith Baggerly

Slides: bit.ly/cmp2018

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