Steps toward reproducible research

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Course web: kbroman.org/AdvData



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?

Which image goes with which experiment?

How did I make that figure?

In what order do I run these scripts?

"Your script is now giving an error."

"The attached is similar to the code we used."

Reproducible

VS.

Replicable

Reproducible

VS.

Correct

kbroman.org/steps2rr

A little bit reproducible is better than not reproducible.

A little bit open is better than not open.

Strive to make each project a bit better organized than the last.

File organization and naming are powerful weapons against chaos.

Jenny Bryan

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

(paraphrasing Mark Holder)

Have sympathy for your future self.

```
RawData/
                        Notes/
                        Refs/
DerivedData/
Python/
                        ReadMe.txt
R/
                        ToDo.txt
Ruby/
                        Makefile
Analysis/
Figures/
```

Chaos

```
AimeeNullSims/
                  Deuterium/
                                         Ping/
AimeeResults/
                  ExtractData4Gary/
                                         Ping2/
                  FromAimee/
                                         Ping3/
AnnotationFiles/
                  GoldStandard/
                                         Ping4/
Brian/
Chr6_extrageno/
                  Human GWAS /
                                         Plav/
                                         Prdm9/
Chr6 segdis/
                  Insulin/
ChrisPlaisier/
                  Int2_for_Mark/
                                         RBM_PlasmaUrine_2012-03-08/
Code4Aimee/
                  Islet 2011-05/
                                         Slco1a6/
                  MappingProbes/
CompAnnot/
                                         StudvLineupMethods/
CondScans/
                  MultiProbes/
                                         kidney_chr6.R
D20 2012-02-14/
                  NewMap/
                                         pck2 sucla2.R
D20 cellcvcle/
                  Notes/
                                         penalties.txt
D2Ocorr/
                  NullSims/
                                         transeQTL4Lude/
Data4Aimee/
                  NullSims 2009-09-10/
Data4Tram/
                  PepIns_2012-02-09/
```

```
betw tissue corr.R
                       expr scatterplot allprobes.R
                                                      gve similarity alltissues.R
coatcolor_lod.R
                       expr_scatterplots_dup.R
                                                      gve_similarity.R
colors.R
                       expr_scatterplots_mix.R
                                                      gve_supp.R
                       expr_scatterplots_swap.R
cover_fig.R
                                                      insulin_lod.R
eqtl_counts_10.R
                       expr_swaps.R
                                                      local_eqtl_locations.R
eqtl counts.R
                       func R
                                                      my plot map.R
                                                      my_plot_scanone.R
eve hist.R
                       genotype plates.R
eve scheme.R
                       gve hist.R
                                                      sex_vs_X.R
                       gve new.R
eve similarity.R
                                                      xchr fig.R
eve_similarity_supp.R
                                                      xist_and_y.R
                       gve.R
expr_corr_dup.R
                       gve_scheme.R
expr corr mix.R
                       gve_similarity_2ndbest.R
```

```
fig1.png fig5.png
fig10.png fig6.png
fig2.png fig7.png
fig3.png fig8.png
fig4.png fig9.png
```

- ► Machine readable
 - No spaces
 - No special characters except _ and -
- ► Human readable
 - Explain the contents
- Consistent
 - Name similar files in a similar way
- Make use of computer's sorting
 - pad numbers with 0's (e.g., 01, 02, ...)
 - start with general grouping, then more specific
 - dates like 2019-05-14

PUBLIC SERVICE ANNOUNCEMENT:

OUR DIFFERENT WAYS OF WRITING DATES AS NUMBERS CAN LEAD TO ONLINE CONFUSION. THAT'S WHY IN 1988 ISO SET A GLOBAL STANDARD NUMERIC DATE FORMAT.

THIS IS THE CORRECT WAY TO WRITE NUMERIC DATES:

2013-02-27

THE FOLLOWING FORMATS ARE THEREFORE DISCOURAGED:

02/27/2013 02/27/13 27/02/2013 27/02/13 20130227 2013.02.27 27.02.13 27-02-13 27.2.13 2013. $\pm 0.2.27$ 27/2-13 2013. $\pm 0.2.27$ 27/2-13 2013. $\pm 0.2.27$ 27/2-13 2013. $\pm 0.2.27$ 2013. $\pm 0.2.2$

```
0 vcf2db.R
1 prep geno.R
2 prep pheno clin.R
2 prep pheno otu.R
3 prep covar.R
4 prep analysis pheno clin.R
4 prep analysis pheno otu.R
5 scans.R
6 grab peaks.R
7 find nearby peaks.R
```

No "final" in file names



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 ngrank final.RData adipose mlratio ngrank 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 kidney mlratio ngrank final.RData batches raw final.RData cpl final.RData kidney prcomp.RData d2o final.RData lipomics final rev2.RData liverTG final.RData gastroc int1 final.RData gastroc int2 final.RData liver int1 final.RData gastroc mlratio final.RData liver int2 final.RData gastroc mlratio ngrank final.RData liver mlratio final.RData gastroc prcomp.RData liver mlratio ngrank final.RData hypo_int1_final.RData liver prcomp.RData mirna final.RData hypo int2 final.RData necropsy_final_rev2.RData hypo mlratio final.RData hypo_mlratio_final_old.RData plasmaurine final rev.RData hypo mlratio ngrank final.RData pmark.RData hypo mlratio ngrank 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 ngrank final.RData adipose mlratio ngrank 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 kidney mlratio ngrank final.RData batches raw final.RData cpl final.RData kidney prcomp.RData d2o final.RData lipomics final rev2.RData liverTG final.RData gastroc int1 final.RData gastroc int2 final.RData liver int1 final.RData gastroc mlratio final.RData liver int2 final.RData gastroc mlratio ngrank final.RData liver mlratio final.RData gastroc prcomp.RData liver mlratio ngrank final.RData hypo_int1_final.RData liver prcomp.RData mirna final.RData hypo int2 final.RData hypo mlratio final.RData necropsy final rev2.RData hypo_mlratio_final_old.RData plasmaurine final rev.RData hypo mlratio ngrank final.RData pmark.RData hypo mlratio ngrank final old.RData rbm final.RData hypo omit.RData

batches raw v1.rds batches v1.rds clinical_cpl_v2.rds clinical d2o v2.rds clinical lipomics v4.rds clinical liverTG v2.rds clinical mirna v2.rds clinical necropsy v4.rds clinical_plasmaurine_v3.rds clinical rbm v2.rds Deprecated/ geneexpr_int1_adipose_v2.rds geneexpr int1 gastroc v2.rds geneexpr int1 hypo v2.rds geneexpr int1 islet v2.rds geneexpr int1 kidney v2.rds geneexpr int1 liver v2.rds geneexpr_int2_adipose_v2.rds geneexpr int2 gastroc v2.rds geneexpr_int2_hypo_v2.rds geneexpr_int2_islet_v2.rds geneexpr int2 kidnev v2.rds geneexpr int2 liver v2.rds geneexpr mlratio adipose v2.rds

geneexpr mlratio gastroc v2.rds geneexpr_mlratio_hypo_v1.rds geneexpr mlratio hypo v2.rds geneexpr_mlratio_islet_v2.rds geneexpr mlratio kidney v2.rds geneexpr mlratio liver v2.rds geneexpr mlratio ngrank adipose v2.rds geneexpr mlratio ngrank gastroc v2.rds geneexpr_mlratio_ngrank_hvpo_v1.rds geneexpr mlratio ngrank hypo v2.rds geneexpr mlratio ngrank islet v2.rds geneexpr mlratio ngrank kidney v2.rds geneexpr_mlratio_nqrank_liver_v2.rds geneexpr omit hypo.rds geneexpr prcomp adipose v2.rds geneexpr prcomp gastroc v2.rds geneexpr prcomp hypo v2.rds geneexpr prcomp islet v2.rds geneexpr prcomp kidney v2.rds geneexpr prcomp liver v2.rds geno_aligned_w_pmap.rds geno pmark.rds ReadMe tyt

Document your work

- ▶ What is all of this stuff?
- ► What was your analysis process?

 \rightarrow ReadMe files

Organizing data in spreadsheets

	А	В	С	D	E	F	G
1	1MIN						
2			Normal			Mutant	
3	В6	146.6	138.6	155.6	166	179.3	186.9
4	BTBR	245.7	240	243.1	177.8	171.6	188.1
5							
6	5MIN						
7			Normal			Mutant	
8	В6	333.6	353.6	408.8	450.6	474.4	423.8
9	BTBR	514.4	610.6	597.9	412.1	447.4	446.5

Organizing data in spreadsheets

	А	В	С	D
1	ttt_min	strain	mutation	response
2	1	B6	normal	146.6
3	1	B6	normal	138.6
4	1	B6	normal	155.6
5	1	B6	mutant	166
6	1	B6	mutant	179.3
7	1	B6	mutant	186.9
8	1	BTBR	normal	245.7
9	1	BTBR	normal	240
10	1	BTBR	normal	243.1
11	1	BTBR	mutant	177.8
12	1	BTBR	mutant	171.6
13	1	BTBR	mutant	188.1
14	5	B6	normal	333.6
15	5	B6	normal	353.6

Organizing data in spreadsheets

- ► Make it a rectangle
- Individual measurements as rows; variables as columns
- Single header row
- One item per cell
- No empty cells
- No calculations in the raw data
- ▶ No highlighting or coloring as data

"What the heck is 'FAD_NAD SI 8.3_3.3G'?"

Metadata

► Create a data dictionary

- Explain each column
- Include different versions of the variable names (compact vs descriptive)
- Units
- Allowable values

▶ The metadata are data

Make it a rectangle

Data dictionary

	А	В	С	D
1	name	plot_name	group	description
2	mouse	Mouse	demographic	Animal identifier
3	sex	Sex	demographic	Male (M) or Female (F)
4	sac_date	Date of sac	demographic	Date mouse was sacrificed
5	partial_inflation	Partial inflation	clinical	Indicates if mouse showed partial pancreatic inflation
6	coat_color	Coat color	demographic	Coat color, by visual inspection
7	crumblers	Crumblers	clinical	Indicates if mouse stored food in their bedding
8	diet_days	Days on diet	clinical	Number of days on high-fat diet

Everything with a script

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

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.

Reproducible reports

Gough project diagnostics

```
25 I've combined the initial genotypes (using the re-clustered genotypes
Karl
     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
Col
     28 (though, as we'll see, there are still a lot of badly behaved and
I've
     29 basically non-informative markers that need to be removed).
the v
     30 I've combined data on replicate samples, to give one set of genotype
infor
     31 calls for each sample.
info
     32
give
     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
Ther
     35 are 'r sum(is.na(match(gid, pid)))' genotyped mice with no phenotypes.
data
        including `r sum(g$pheno$gen[which(is.na(match(gid, pid)))]==0)`
mice
        Gough mice and `r sum(g$pheno$gen[which(is.na(match(gid, pid)))]==2)`
     38 F2 progeny.
```

```
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
```

```
R/analysis.html: R/analysis.Rmd Data/cleandata.csv
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```

```
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    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
```

Fancier example

```
FIG_DIR = Figs

mypaper.pdf: mypaper.tex ${FIG_DIR}/fig1.pdf ${FIG_DIR}/fig2.pdf
    pdflatex mypaper

# One line for both figures
${FIG_DIR}/%.pdf: R/%.R
    cd R;R CMD BATCH $(<F)

# Use "make clean" to remove the PDFs
clean:
    rm *.pdf Figs/*.pdf</pre>
```

How do you use make?

- ► If you name your make file Makefile, then just go into the directory containing that file and type make
- ► If you name your make file something.else, then type make -f something.else
- ► Actually, the commands above will build the first target listed in the make file. So I'll often include something like the following.

```
all: target1 target2 target3
```

Then typing make all (or just make, if all is listed first in the file) will build all of those things.

► To be build a specific target, type make target. For example, make Figs/fig1.pdf

Write modular code

- ▶ Modular code is easier to understand, maintain, and reuse.
- ► Turn repeated code into functions
- ► Combine useful functions into a package or module

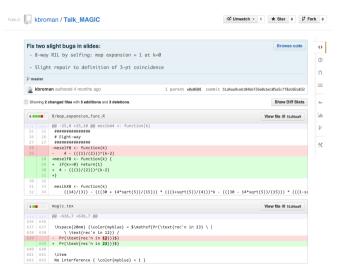
Keeping track of versions

- ► Google drive / Dropbox / Box
- Version numbers in file names
- ► Formal version control (e.g., git/GitHub)
 - Browse changes
 - Try new things without fear of breaking what works
 - Jump to the state of the project at any time point
 - Merge simultaneous changes from multiple people









```
-meself8 <- function(k)
              4 - (((1)/(2)))^{(k-2)}
         +meself8 <- function(k) {
     28
         + if(k==0) return(1)
         + 4 - (((1)/(2)))^{(k-2)}
     30
         +}
30
     32
31
     33
          mesibX8 <- function(k)</pre>
32
     34
               ((14)/(3)) - (((30 + 14*sqrt(5))/(15)))
```

Backups

- ► Multiple places, including off-site
- ► Automatic

License your software

Pick a license, any license

- Jeff Atwood

Share your stuff

▶ Code

- GitHub / BitBucket
- Zenodo (archival, with DOIs)

▶ Data

- Domain-specific repository (e.g., dbGAP)
- General repository (e.g., github, figshare, zenodo, datadryad)
- Institutional repository

Summary

- 1. Organize your project
- 2. Choose good names for things
- 3. Document what's what
- 4. Organize data as a rectangle
- 5. Metadata is data
- 6. Everything with a script
- 7. Even better: reproducible reports
- 8. Automate the process (GNU Make)
- 9. Write modular code (functions and packages)
- 10. Use version control (git/GitHub)
- 11. License your software
- 12. Share your data and code