Keeping a Computational Lab Notebook & How to Get Programming Help

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- Legal document* to prove patents and defend against accusations of fraud (*requirements vary depending on situation)

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• Lab legacy/institutional memory

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Why do we need to keep \textit{computational} laboratory notebooks?

'Ten Simple Rules for a Computational Biologist's Laboratory Notebook.' S. Schnell, PLOS Computational Biology, 2015.
Why do we need to keep computational laboratory notebooks?

“One of the major hurdles I face as the head of a computational biology laboratory is convincing my research team—particularly those pursuing exclusively mathematical and computational modeling—that they need to keep a laboratory notebook. There seems to be a misconception in the computational biology community that a lab notebook is only useful for recording experimental protocols and their results. **A lab notebook is much more than that. It is an organizational tool and memory aid, which serves as the primary record of scientific research and activity for all scientists. It also serves as a legal record of ownership of the ideas and results obtained by a scientist.”** -S. Schnell

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• Rule 4: Record all* scientific activities in your lab notebook—it is a chronological log of everything scholarly a scientist does (*more wiggle room on this rule)

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• Rule 8: Keep a lab notebook that can serve as a legal record of your work

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• Rule 10: Protect your lab notebook—the original belongs to your institution.

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Example Lab Notebook Entry:

**180410**

**Goal:** I'm trying to understand how many TCGA KIRC samples have each combination of data types

- Working scripts are here: /Data_nonGoogleDrive/TCGAKIRC_TCGBioinks_180314/getTCGAKIRCdata.R
- I set up tcgabiolinks queries for each dataset (except for clinical) and recorded the number of T/N samples for each
- Analyzed the tumor overlap between datasets, including limiting datasets with Reduce(intersect, list()) notation
- Visually examined the results with UpSetR graph (vignette: [https://cran.r-project.org/web/packages/UpSetR/vignettes/basic.usage.html](https://cran.r-project.org/web/packages/UpSetR/vignettes/basic.usage.html))

```
/Data_nonGoogleDrive/TCGAKIRC_TCGBioinks_180314/KIRC_UpSetRPlot_180410.png
```

**Conclusions:** switch from m27 to m450 happened during this dataset so about 25% of tumors have m27k data and rest with m450k data
Example Lab Notebook Entry (continued):

(Partial for Illustrative Purposes) Code to Plot Graph on Previous Slide

```r
#visualize intersections
library(UpSetR)
listInput<-list(GeneEx=strsplit(getResults(query.exp.hg38.KIRC, cols="cases"), 1, 12),
                 DNAm450=strsplit(getResults(query.DNAm450.hg38.KIRC, cols="cases"), 1, 12),
                 DNAm27=strsplit(getResults(query.DNAm27.hg38.KIRC, cols="cases"), 1, 12),
                 microRNA=strsplit(getResults(query.microrna.hg38.KIRC, cols="cases"), 1, 12),
                 #CNVseg=strsplit(getResults(query.CNVseg.hg38.KIRC, cols="cases"), 1, 12),
                 CNVseg_mask=strsplit(getResults(query.CNVsegMasked.hg38.KIRC, cols="cases"), 1, 12),
                 SNV=strsplit(getResults(query.SNV.hg38.KIRC, cols="cases"), 1, 12))
#commented out CNVseg because masked has known germline snps removed
str(listInput)
upset(fromList(listInput), order.by=c("freq"), nsets=7, line.size=0, point.size=5, nintersects = NA,
      text.scale=3)
#KIRC_UpSetRPlot_180410.png
#nsets shows all 7 data sets
#line.size=0 removes vertical lines in plot
#point.size changes circle sizes
#nintersects says number of intersects to plot
#text.scale changes text size
```
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#visualize intersections
library(UpSetR)
listInput<-list(GeneEx=strsplit(getResults(query.exp.hg38.KIRC, cols="cases"), 1, 12),
DNAm450=strsplit(getResults(query.DNAm450.hg38.KIRC, cols="cases"), 1, 12),
DNAm27=strsplit(getResults(query.DNAm27.hg38.KIRC, cols="cases"), 1, 12),
microRNA=strsplit(getResults(query.micro.hg38.KIRC, cols="cases"), 1, 12),
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✓ consistent naming
✓ explain thought process
✓ reproducible
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- Narrow down the problem. Try to create a miniature version of the problem if you can.
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• Be patient and courteous.
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• Google your question/error message/etc.
• Narrow down the problem. Try to create a miniature version of the problem if you can.
• But remember to share what your overall goal is.
• Be patient and courteous.
• Record your troubleshooting in your lab notebook!
Example 1:
want to delete ‘demo1’ directory

```
Brittany-Lasseigne:DemoDir brittany$ pwd
/Users/brittany/GoogleDrive/Teaching/DemoDir
Brittany-Lasseigne:DemoDir brittany$ ls
demo1
Brittany-Lasseigne:DemoDir brittany$ rm demo1
rm: demo1: is a directory
Brittany-Lasseigne:DemoDir brittany$ ls
demo1
Brittany-Lasseigne:DemoDir brittany$
```
Google the error message:

rm: is a directory

About 52,700,000 results (0.37 seconds)

Delete everything. The rm command has a powerful option, -R (or -r), otherwise known as the recursive option. When you run the rm -R command on a folder, you’re telling Terminal to delete that folder, any files it contains, any sub-folders it contains, and any files or folders in those sub-folders, all the way down. Jan 2, 2014

Master the command line: Deleting files and folders | Macworld

People also ask
- How can I force delete a folder?
- What is the function of RM?
- What does RM RF do?
- How do I get rid of files that won’t delete?

How do I remove a full directory in Linux? - Computer Hope
https://www.computerhope.com/issues/ch000798.htm
Jan 24, 2018 - To remove a directory that contains other files or directories, use the following command. In the example above, you would replace "/path/to/directory" with the name of the directory you want to delete. For example, if...
Check the manual: man rm

RM(1)          BSD General Commands Manual          RM(1)

NAME
rm, unlink -- remove directory entries

SYNOPSIS
rm [-dfiPRrvW] file ...
unlink file

DESCRIPTION
The rm utility attempts to remove the non-directory type files specified on
the command line. If the permissions of the file do not permit writing, and the standard input device is a terminal, the user is prompted
(on the standard error output) for confirmation.

The options are as follows:

-R     Attempt to remove the file hierarchy rooted in each file
       argument. The -R option implies the -d option. If the -i
       option is specified, the user is prompted for confirmation
       before each directory's contents are processed (as well as
       before the attempt is made to remove the directory). If the
       user does not respond affirmatively, the file hierarchy
       rooted in that directory is skipped.

-r     Equivalent to -R.
It works!

Brittany-Lasseigne:DemoDir brittany$ pwd
/Users/brttany/GoogleDrive/Teaching/DemoDir
Brittany-Lasseigne:DemoDir brittany$ ls demo1
Brittany-Lasseigne:DemoDir brittany$ rm demo1
rm: demo1: is a directory
Brittany-Lasseigne:DemoDir brittany$ ls demo1
Brittany-Lasseigne:DemoDir brittany$ rm -R demo1
Brittany-Lasseigne:DemoDir brittany$ ls

Brittany-Lasseigne:DemoDir brittany$
Thanks! Slides available at

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