Unix command line; editors Tools for Reproducible Research

Karl Broman

Biostatistics & Medical Informatics, UW-Madison

biostat.wisc.edu/~kbroman github.com/kbroman @kwbroman Course web: bit.ly/tools4rr

My goal in this lecture is to convince you that

- (a) command-line-based tools are the things to focus on,
- (b) you need to choose a powerful, universal text editor (you'll use it a lot),
- (c) you want to be comfortable and skilled with each.

For your work to be reproducible, it needs to be code-based; don't touch that mouse!

Windows vs. Mac OSX vs. Linux

Remote vs. Not

The Windows operating system is not very programmer-friendly.

Mac OSX isn't either, but under the hood, it's just unix.

Don't touch the mouse! Open a terminal window and start typing.

I do most of my work directly on my desktop or laptop. You might prefer to work remotely on a server, instead. But I can't stand having any lag in looking at graphics.

If you're stuck with Windows...

Consider Cygwin (and perhaps Mintty)

Cygwin is an effort to get Unix command-line tools in Windows.

Mintty is a terminal emulator.

If you use a Mac...

Consider Homebrew and iTerm2

Homebrew is a packaging system; iTerm2 is a Terminal replacement.

I do all of my work on a Mac (except really big computational jobs), and there are a lot of different tools that I like and would recommend:

divvy, http://mizage.com/divvy
caffeine, http://lightheadsw.com/caffeine
bartender, http://www.macbartender.com
hazel, http://www.noodlesoft.com/hazel.php
launchbar, http://www.obdev.at/products/launchbar/index.html
simplenote, http://simplenote.com
jumpcut, http://simplenote.com
jumpcut, http://jumpcut.sourceforge.net
color oracle, http://colororacle.org
textexpander, http://smilesoftware.com/TextExpander

The command line is your friend

- ► Don't touch that mouse!
- ► Scriptable
- ► Flexible

In the long run, you'll be happier, having conquered the command line.

Pointing-and-clicking is not reproducible, and every time you take your hands off the keyboard, there's a loss of efficiency.

The command line allows you to piece together multiple tools and so do things that weren't anticipated by the developer of the GUI.

And it's only through scripts that you'll have truly reproducible analyses.

The shell

```
Last login: Wed Jan 29 10:57:07 on ttys003 kbroman@fig ~ $
```

Options: tcsh, bash, zsh

The shell is a program – an interface to the operating system.

There are a number to choose from. I use bash; I've heard great things about zsh.

Basics

- ► Directory structure
 Absolute vs. relative paths

 ls -1 ~/..
- ► Creating, removing, changing directories

```
mkdir
rmdir
cd
cd -
```

► Moving, copying, removing files

```
mv
cp
rm -i
```

This stuff is too boring to spend much time on.

But I should emphasize the importance of using relative paths (e.g., ../Figs/fig1.pdf) in a project; reliance on absolute paths (e.g., ~/Projects/Blah/Figs/fig1.pdf) make life difficult when you move the project to a different system.

-

~/.bash_profile

```
export PATH=.:/usr/local/bin:$PATH
export LD_LIBRARY_PATH=/usr/local/lib
noclobber=1
IGNOREEOF=1
HISTCONTROL=ignoredups
alias cl='clear;cd'
alias rm='rm -i'
alias mv='mv -i'
alias cp='cp -i'
alias ls='ls -GF'
alias 'l.'='ls -d .[a-zA-Z]*'
alias ll='ls -lh'
alias md='mkdir'
alias rd='rmdir'
alias rmb='rm .*~ *~ *.bak *.bk!'
alias Rb='R CMD build --force --resave-data'
alias Ri='R CMD INSTALL --library=/Users/kbroman/Rlibs'
alias Rc='R CMD check --library=/Users/kbroman/Rlibs'
alias Rcc='R CMD check --as-cran --library=/Users/kbroman/Rlibs'
```

Use the .bash_profile file to define various variables and aliases to make your life easier.

The most important variable is PATH: it defines the set of directories where the shell will look for executable programs.

If "." isn't part of your PATH, you'll need to type something like ./myscript.py to execute a script in your working directory. So put "." in your PATH.

My .bash_profile file sources a .bashrc file; I don't quite understand when one is used versus the other. Google ".bashrc vs .bash_profile."

There are links to my .bash_profile and .bashrc files on the resources page at the course web site; some of it might just be total crap.

Redirection and pipes

```
$ locate article.cls > output.txt
$ locate book.cls >> output.txt
$ grep texmf output.txt

$ locate article.cls | grep texmf

$ locate article.cls | grep texmf | less

$ locate article.cls | wc -l
$ locate article.cls | grep texmf | wc -l

$ cat file1.txt file2.txt > combined.txt
```

Use > to redirect output "stdout" to a file.

Use >> to redirect output and append to the file.

Use < to have input "stdin" come from a file.

Use | to have the output of one command made the input to another.

A key design principle in Unix is the piecing together of small commands using this sort of technique. There are lots of little commands (often with short, cryptic names) that can be combined together with great flexibility.

Important tools mentioned here: locate (find files matching a pattern), grep (search for patterns in a file), less (look through long files a page at a time), wc (count the number of words, lines and/or characters in a file), cat (print contents of or concatenate text files)

S

Wild cards

```
$ grep blah *.txt

$ ls blah.???

$ ls [a-z]*

$ ls /usr/bin/[auz]*

$ ls /usr/bin/[auz]*.*
```

10

- * stands for anything
- ? stands for a single character

Use [] to match some specific set or range of characters

Suspend/foreground/background

```
$ R CMD BATCH input.R output.txt &

$ R CMD BATCH input.R output.txt
[ctrl-Z]
$ bg

$ emacs afile.txt
[ctrl-Z]
$ fg
```

11

Use & to run a job in the background.

Use ctrl-Z to suspend the current job. Then use bg to then put it in the background or fg to bring it back to the foreground.

I use ctrl-Z and bg if I had forgotten to use &.

I use ctrl-Z with emacs sometimes, to do some command-line things without opening another shell/terminal; I'll then use fg to bring emacs back. Or I'll forget about it and muck a bunch of stuff up.

Other useful tools

```
$ find . -name *.py

$ ps ux

$ top

$ df -hk

$ du -h
$ du -hd2

$ ln -s ~/Projects/SomeFriend/Data
$ ln -s ~/Projects/SomeFriend/Data SomeFriend_Data

$ tar xzvf qtl_1.29-2.tar.gz
$ tar czvf blah.tgz Blah/
$ tar tzvf blah.tgz
$ wget http://kbroman.github.io/Tools4RR/pages/resources.html
```

12

find is like locate

ps ux to see what processes are running.

top gives an interactive view of what processes are running.

df -hk shows disk usage

du -hd2 shows disk usage in a directory and its subdirectories; the d2 bit says go no more than 2 levels down through the subdirectories.

ln -s makes a "soft link" to a file or directory. It acts like there's a copy, but it's not really copied.

tar is used to archive a bunch of files within a single file. x for extract, c for combine, t for test, z for compress/zip, v for verbose, f for "file name to follow."

wget (see also curl) for grabbing something from the web.

Further useful tools

whereis for finding a program.

```
$ whereis bash
$ type rm
$ type emacs

$ pwd

$ head afile.txt
$ tail afile.txt
$ head -n20 afile.txt

$ man head

$ kill 8453
$ kill -9 8453

$ history
$ !!
$ !-2
$ !503

$ ping www.google.com

$ ispell afile.txt
```

```
type for figuring out the location of a program or the definition of an
alias.

pwd - print working directory
head - print first few lines of a file
tail - print the last few lines of a file
man - view manual page
kill - kill a job
history - view command history
! - execute past commands
ping - see if you can connect to some server
ispell - spell checker
```

Moving around the command line

```
ctrl-f, ctrl-b move forward and back
ctrl-a, ctrl-e move to beginning and end of line
ctrl-k, ctrl-u delete rest of line, or to the start
ctrl-l clear the screen
ctrl-c cancel what you've typed
tab autocomplete command or file
ctrl-p, ctrl-n forward and backward in history
ctrl-r search for a previous command
```

These are mostly emacs-like key "bindings".

File modes

```
kbroman@fig ~/Teaching/Tools4RR/Lectures (master) $ 11
total 8
drwxr-xr-x
            27 kbroman
                         staff
                                  918B Jan 27 11:35 01_Intro/
                                  1.0K Jan 29 11:38 02_Unix/
drwxr-xr-x
            30 kbroman
                         staff
             2 kbroman
                         staff
                                   68B Jan 14 06:28 03_KnitrMarkdown/
drwxr-xr-x
            37 kbroman
                         staff
                                  1.2K Jan 20 23:05 04_Git/
drwxr-xr-x
drwxr-xr-x
              2 kbroman
                         staff
                                   68B Jan 14 06:28 05_Organization/
                                   68B Jan 14 06:28 06_EDA/
drwxr-xr-x
              2 kbroman
                         staff
              2 kbroman
                                   68B Jan 14 06:28 07_ClearCode/
drwxr-xr-x
                         staff
                                   68B Jan 14 06:28 08_Rpack/
              2 kbroman
drwxr-xr-x
                         staff
                                   68B Jan 14 06:29 09_TestingDebugging/
              2 kbroman
drwxr-xr-x
                         staff
                                   68B Jan 14 06:29 10_BigJobs/
                         staff
drwxr-xr-x
              2 kbroman
                                   68B Jan 14 06:29 11_KnitrPapers/
              2 kbroman
                         staff
drwxr-xr-x
                                   68B Jan 14 06:29 12_KnitrTalks/
drwxr-xr-x
              2 kbroman
                         staff
                                   68B Jan 14 06:29 13_KnitrPosters/
drwxr-xr-x
              2 kbroman
                         staff
                                   68B Jan 14 06:29 14_Python/
drwxr-xr-x
              2 kbroman
                                   68B Jan 14 06:29 15_Licenses/
drwxr-xr-x
              2 kbroman
-rwxr-xr-x   1 kbroman staff   488B Oct 23 16:18 createVersionWithNotes.rb*
kbroman@fig ~/Teaching/Tools4RR/Lectures (master) $
```

Note the mode, owner, and group for each file.

mode = read/write/executable for owner/group/everyone

r = readable; w = writable; x = executable (for a directory, enter-able)

File modes/owner/group

```
sudo chown kbroman .
chgrp -R staff .
chmod +x createVersionWithNotes.rb
chmod 755 02_Unix
chmod 644 02_Unix/02_unix.tex
chmod 700 Private_stuff
```

16

You don't usually need to change the owner or group assigned to a file or directory, but it's good to be aware of the possibility.

Groups are useful if you want a file accessible by some set of people but not everyone. You need a system admin to set up the group.

You often want to make scripts executable, or make files/directories unreadable or unwriteable.

For example, primary raw data files should not be writable. Large Excel-based data files often contain screwed up cells where someone was typing in some random spot without realizing it. I found myself doing that yesterday!

The octal codes (e.g, 755 and 644) are convenient, once you get the hang of them.

How to solve computing problems

- ► Try stuff!
- man pages and help files
- ▶ blah -h Or blah --help
- ▶ Google
- Stackoverflow and other StackExchange sites
- ► Google with site:stackoverflow.com
- ► email lists and google groups
- ▶ friends or colleagues
- ▶ Twitter
- ▶ Buy a book. Buy all of the books.

You will run into crazy and mysterious errors. Will you give up, or figure them out?

Rule number 1: try stuff. Figure out how something works by trying it out in different ways.

Rule number 2: Google. Google the exact error message, or a part of an error message. You'll often get to a stackexchange site; don't forget to read the comments as well as the answers. Often the best answer is in a comment.

Rule number 3: Ask for help. Talk to your friends. Talk to me. Post a question at a stackexchange site.

I'm a relatively recent convert to Twitter. I focus on just a few things that interest me (mostly academic publishing, reproducible research, and interactive graphics). If you tweet a question, you'll be surprised at how quickly you get an answer.

I do tend to but all possible books on a topic that is of even passing interest to me. I read at least part of each of them.

Examples

- ► How do you suppress warnings in knitr?
- ▶ What symbol corresponds to the unicode \u00B1?
- ► What's the difference between curl and wget?
- ► What does "502 Bad Gateway" mean?
- ▶ "To open gs you need to install X11"
- mclapply isn't working in Windows
- ► How to ping a server in Python?
- ► Font shape `EU1/pplx/m/n' undefined
- ▶ except KeyError, k: raise AttributeError, k

These are examples of things you might search for.

If you don't understand an error message, start by pasting it into google.

Important principle

Learn to code by looking at good code.

Identify programmers that you respect (e.g., Hadley Wickham), and study what they do.

Choose a good editor

- ► Emacs
- ► VIM
- ► RStudio
- ► Textwrangler
- ► Notepad++
- ► Tinn-R

I use emacs; I should probably use vim.

RStudio is increasingly useful, but as a general editor (for things that aren't R), I think it's insufficient.

The choice of editor is very personal.

A good editor

- ► Doesn't require pointing-and-clicking
- ► Easy to get code between R and a script
- ► Syntax highlighting of code
- ► Automatic indentation
- Close parentheses/brackets/braces
- ► Browse code across files
- ► Integrated with other tools (e.g., version control)

I've not figured out how to explore code across a set of files in emacs; otherwise I'm very happy with it.