5: EDA, Big Jobs, Automation

bit.ly/SISBID3

Exploratory data analysis

- what were you trying to do?
- what you're thinking about?
- what did you observe?
- what did you conclude, and why?

Avoid

- ”How did I create this plot?”
- ”Why did I decide to omit those six samples?”
- ”Where (on the web) did I find these data?”
- ”What was that interesting gene?”

Basic principles

Step 1: slow down and document.

Step 2: have sympathy for your future self.

Step 3: have a system.

Capturing EDA

- copy-and-paste from an R file
- grab code from the `.Rhistory` file
- Write an informal R Markdown file;
  make use of the “R Notebook” features.
- Write code for use with the KnitR function `spin()`

  Comments like `#' This will become text`
  Chunk options like so: `#+ chunk_label, echo=FALSE`

A file to `spin()`

```
#' This is a simple example of an R file for use with spin().

#' We'll start by setting the seed for the RNG.
set.seed(53079239)

#' We'll first simulate some data with x ~ N(mu=10, sig=5) and
#' y = 2x + e, where e ~ N(mu=0, sig=2)
x <- rnorm(100, 10, 5)
y <- 2*x + rnorm(100, 0, 2)

#' Here's a scatterplot of the data.
plot(x, y, pch=21, bg="slateblue", las=1)
```

Activity

Try out `knitr::spin()`:

- Create an R script using
  - `#'` for text
  - `#+` for chunk options
- Compile the script to HTML using `knitr::spin()`
- Open the resulting HTML file.

Big jobs

- You don't want `knitr` running for a year.
- You don't want to re-run things if you don't have to.

Biggish jobs in knitr

- Manual caching
- Built-in `cache=TRUE`
- Split the work into a separate subdirectory.

Manual caching

```
```{r a_code_chunk}
file <- "cache/myfile.RData"

if(file.exists(file)) {
  load(file)
} else{

  ....

  save(object1, object2, object3, file=file)
}
```
```

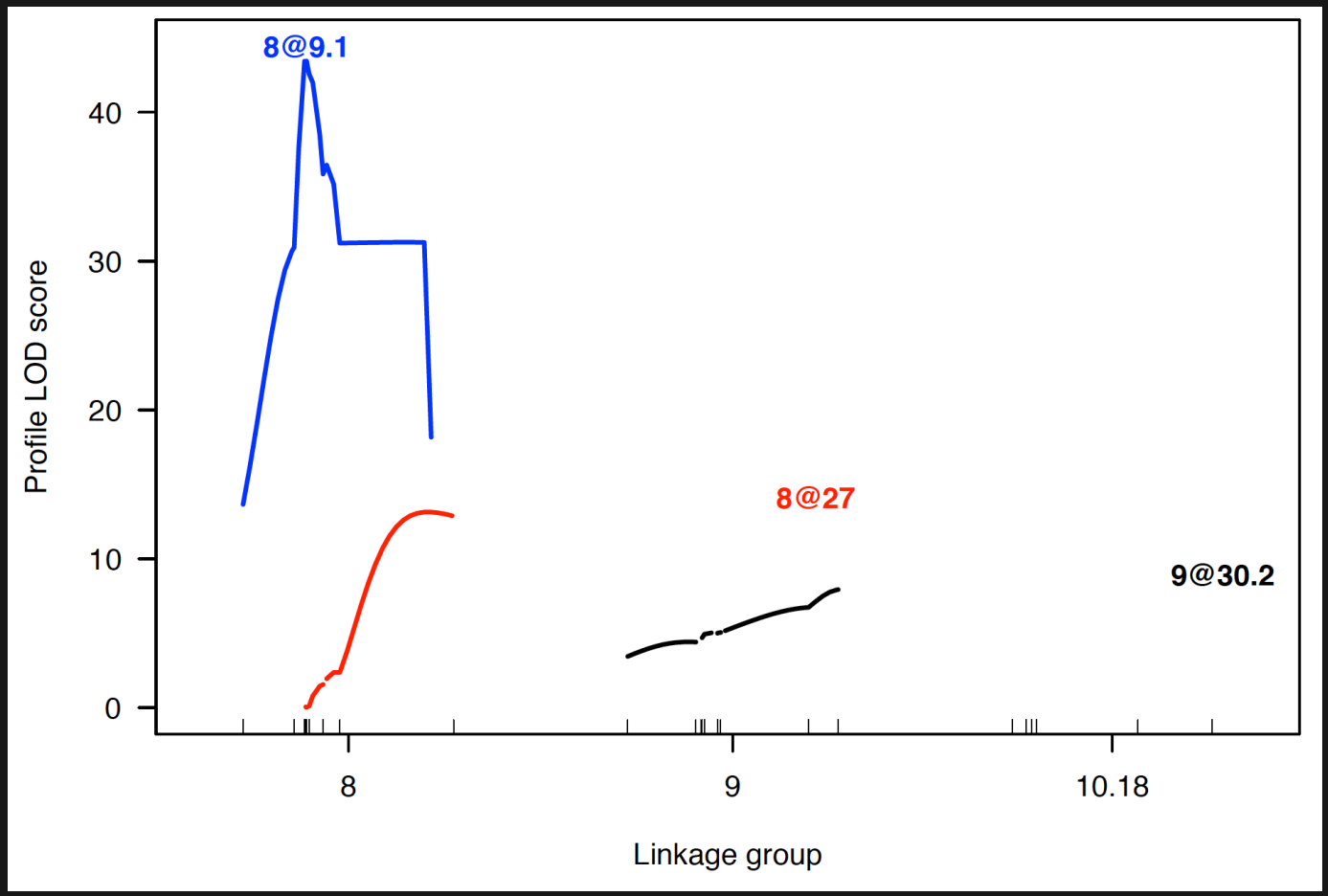
Chunk references

````
```{r not_shown, eval=FALSE}
code_here <- 0
```

```{r a_code_chunk, echo=FALSE}
file <- "cache/myfile.RData"

if(file.exists(file)) {
  load(file)
} else{
<<not_shown>>
  save(code_here, file=file)
}
```
````

A cache gone bad



Knitr's cache system

```
```{r chunk_name, cache=TRUE}
load("a_big_file.RData")
med <- apply(object, 2, median, na.rm=TRUE)
```
```

- Chunk is re-run if edited.
- Otherwise, objects from previous run are loaded.
- Don't cache things with side effects

  e.g., `options()`, `par()`

Cache dependencies

Manual dependencies

````
```{r chunkA, cache=TRUE}
Sys.sleep(2)
x <- 5
```

```{r chunkB, cache=TRUE, dependson="chunkA"}
Sys.sleep(2)
y <- x + 1
```

```{r chunkC, cache=TRUE, dependson="chunkB"}
Sys.sleep(2)
z <- y + 1
```
````

Cache dependencies

Automatic dependencies

````
```{r setup, include=FALSE}
opts_chunk$set(autodep = TRUE)
dep_auto()
```
````

Parallel computing

If your computer has multiple processors, use `library(parallel)` to make use of them.

- `detectCores()`
- `RNGkind("L'Ecuyer-CMRG")` and `mclapply` (Unix/Mac)
- `makeCluster`, `clustersetRNGStream`, `clusterApply`, and `stopCluster` (Windows)

Systems for distributed computing

- At UW-Madison, we use HTCondor
- There are oddles of similar systems
- ”By hand”

Simulations

- Computer simulations require RNG seeds (`.Random.seed` in R).
- Multiple parallel jobs need different seeds.
- Don't rely on the current seed, or on having it generated from the clock.
- Use something like `set.seed(91820205 + i)`
- An alternative is create a big batch of simulated data sets in advance.

Save everything

- RNG seeds
- input
- output
- version numbers, with `sessionInfo()`
- raw results
- script to combine results
- combined results
- `ReadMe` describing the point

Compartmentalize big jobs

- Separate directory for each batch of big computations.
- Collect the results in ‘.RData‘ or ‘.rds‘ files.
- KnitR-based documents for the analysis/use of those results.

Potential problems

- Forgetting `save()` in your distributed jobs
- A bug in the `save()` command
- Keeping things synchronized
  - Have you re-run the big jobs when upstream data were revised?

Big jobs summary

- Careful organization and modularization.
- Save everything.
- Document everything.
- Learn the basic skills for distributed computing.

Activity

Try out the knitr cache system.

- Create an RMarkdown document with multiple dependent chunks.
- Maybe add `Sys.sleep(5)` to slow things down, as if the jobs were taking a while.
- Compile the document.
- Edit a chunk.
- Re-compile the document and see what was actually run and what was taken from cache.

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
```

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Automation with GNU Make

- `Make` is for more than just compiling software
- The essence of what we're trying to do
- Automates a workflow
- Documents the workflow
- Documents the dependencies among data files, code
- Re-runs only the necessary code, based on what has changed

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
```

Installing Make

- On Macs, Make should be installed. Type `make --version` to check.
- On Windows, probably the easiest is to install Rtools, which includes Make.

  `cran.r-project.org/bin/windows/Rtools`

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`