R for large data and bioinformatics

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Auckland, November 2013
Introduction: Course Aims

- Under the hood of R
  - R essentials, and programming skills
  - Examples implement common genetic analyses, efficiently

- Using R for more sophisticated analyses
  - Using tools, packages produced by others
  - Bioconductor-based bioinformatics

This is not a first course in R – unless you are an experienced programmer. Basic use of R (reading in data, simple manipulation of data, supplying arguments to functions) is assumed. We will review some topics; further background is available here; http://faculty.washington.edu/kenrice/bigr
Introduction: About Prof Lumley

- Professor, Univ of Auckland
- R Core developer
- Genetic/Genomic research in Cardiovascular Epidemiology
- Sings bass
Introduction: About Prof Rice

• Associate Prof, UW Biostat

• Not an author, but a user (and a teacher)

• Genetic/Genomic research in Cardiovascular Epidemiology

• Sang bass (last week)

... and you?

(who are you, what area of genetics, what are you looking for from the course)
Introduction: Course structure

10 sessions over 2.5 days

- Day 1; Review of R, graphics, data-wrangling
- Day 2; Programming (loops), big data, bioconductor

Web page: http://faculty.washington.edu/kenrice/bigr/
Introduction: Session structure

- 45 mins teaching (questions welcome – please interrupt!)
- 30 mins hands-on
- 15 mins summary, discussion

Keys are posted after each session – though there is more than one correct answer
1. Review of R

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What is R?

R is a ‘programming environment for statistics and graphics’

The base R has fewer prepackaged statistics procedure than SPSS or SAS, but it is much easier to extend with new procedures.

There are about 3500 published extension packages for R, many aimed at genetics and genomics research.
Using R

R is a free implementation of S, for which John Chambers won the ACM Software Systems award.

For the S system, which has forever altered how people analyze, visualize, and manipulate data.

The downside is that using R effectively may require changing how you analyze, visualize, and manipulate data.

R is a command-line system, not a point-and-click system.
A calculator

> 2+2
[1] 4
> 1536/317000
[1] 0.004845426
> exp(pi)-pi
[1] 19.9991
> x <- 3
> y <- 2
> x+y
[1] 5
> ls()
[1] "x" "y"
> round(pi, 6)
[1] 3.141593
> round(pi,
+ 6)
[1] 3.141593
Scripts

For longer analyses (and for this course), it’s better to type code into a script and then run it. In base R;

- Windows: File | New script, CTRL-R to run lines or regions

- Mac: File | New Document, command-return to run

- Some other text editors offer this: Emacs, Tinn, WinEDT, JGR, Eclipse. RStudio has a script editor and data viewer

Please note we strongly recommend doing the exercises in pairs
Scripts

Default interface (and how to use it);
Reading data

Ability to read in data is assumed. But to illustrate commands, and show some less-standard approaches, we’ll review reading in:

- Text files
- Other statistics packages datasets
- Web pages

Much more information is in the Data Import/Export manual.
Reading text data

The easiest format has variable names in the first row

<table>
<thead>
<tr>
<th>case</th>
<th>id</th>
<th>gender</th>
<th>deg</th>
<th>yrdeg</th>
<th>field</th>
<th>startyr</th>
<th>year</th>
<th>rank</th>
<th>admin</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>1</td>
<td>F</td>
<td>Other</td>
<td>92</td>
<td>Other</td>
<td>95</td>
<td>95</td>
<td>Assist</td>
<td>0</td>
</tr>
<tr>
<td>2</td>
<td>2</td>
<td>M</td>
<td>Other</td>
<td>91</td>
<td>Other</td>
<td>94</td>
<td>94</td>
<td>Assist</td>
<td>0</td>
</tr>
<tr>
<td>3</td>
<td>2</td>
<td>M</td>
<td>Other</td>
<td>91</td>
<td>Other</td>
<td>94</td>
<td>95</td>
<td>Assist</td>
<td>0</td>
</tr>
<tr>
<td>4</td>
<td>4</td>
<td>M</td>
<td>PhD</td>
<td>96</td>
<td>Other</td>
<td>95</td>
<td>95</td>
<td>Assist</td>
<td>0</td>
</tr>
</tbody>
</table>

and fields separated by spaces. In R, use

```r
salary <- read.table("salary.txt", header=TRUE)
```

to read the data from the file `salary.txt` in the current working directory into the data frame `salary`.**
Syntax notes

• Spaces in commands don’t matter (except for readability), but Capitalisation Does Matter.

• **TRUE** (and **FALSE**) are logical constants

• Unlike many systems, R does not distinguish between commands that do something and commands that compute a value. Everything is a function: i.e. it returns a value.

• Arguments to functions can be named (**header=TRUE**) or unnamed (**"salary.txt"**) 

• A whole data set (called a data frame) is stored in a variable (**salary**), so more than one dataset can be available at the same time.
Did it work?

The `head()` function shows the first few lines of the data frame:

```r
> head(salary)
case id gender deg yrdeg field startyr year rank admin salary
1 1 1 F Other 92 Other 95 95 Assist 0 6684
2 2 2 M Other 91 Other 94 94 Assist 0 4743
3 3 2 M Other 91 Other 94 95 Assist 0 4881
4 4 4 M PhD 96 Other 95 95 Assist 0 4231
5 5 6 M PhD 66 Other 91 91 Full 1 11182
6 6 6 M PhD 66 Other 91 92 Full 1 11507
```

It *should* look like this!

The `View()` command similarly shows your data frame, in a manageable way.
Where’s my file?

- Find out your current directory with `getwd()`

- Change directory with the menus

- or with `setwd("I:/like/this/directory/better")`

- `file.choose()` pops up a dialog for choosing a file and returns the name, so

  ```r
  salary <- read.table(file.choose(), header=TRUE)
  ```
Sometimes columns are separated by commas (or tabs)

Ozone,Solar.R,Wind,Temp,Month,Day
41,190,7.4,67,5,1
36,118,8,72,5,2
12,149,12.6,74,5,3
18,313,11.5,62,5,4
NA,NA,14.3,56,5,5

Use

```r
ozone <- read.table("ozone.csv", header=TRUE, sep="","")
```

or

```r
ozone <- read.csv("ozone.csv")
```
Syntax notes

- Forgetting `header=TRUE` in `read.table()` is bad (try it!)

- Functions can have optional arguments (`sep` wasn’t used the first time). Use `help("read.table")` or `?read.table` for a complete description of the function and all its arguments.

- There’s more than one way to do it.

- `NA` is the code for missing data. Think of it as “Don’t Know”. R handles it sensibly in computations: eg `1+NA`, `NA & FALSE`, `NA & TRUE`. You cannot test `temp==NA` (Is temperature equal to some number I don’t know?), so there is a function `is.na()`.
Reading text data

Sometime the variable names aren’t included

<p>| | | | | | | | | |</p>
<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0.2</td>
<td>115</td>
<td>90</td>
<td>1</td>
<td>3</td>
<td>68</td>
<td>42</td>
<td>yes</td>
</tr>
<tr>
<td>2</td>
<td>0.7</td>
<td>193</td>
<td>90</td>
<td>3</td>
<td>1</td>
<td>61</td>
<td>48</td>
<td>yes</td>
</tr>
<tr>
<td>3</td>
<td>0.2</td>
<td>58</td>
<td>90</td>
<td>1</td>
<td>3</td>
<td>63</td>
<td>40</td>
<td>yes</td>
</tr>
<tr>
<td>4</td>
<td>0.2</td>
<td>5</td>
<td>80</td>
<td>2</td>
<td>3</td>
<td>65</td>
<td>75</td>
<td>yes</td>
</tr>
<tr>
<td>5</td>
<td>0.2</td>
<td>8.5</td>
<td>90</td>
<td>1</td>
<td>2</td>
<td>64</td>
<td>30</td>
<td>yes</td>
</tr>
</tbody>
</table>

and you have to supply them

```
psa <- read.table("psa.txt", col.names=c("ptid","nadirpsa", "pretxpsa", "ps","bss","grade","age", "obstime","inrem"))
```

or

```
psa <- read.table("psa.txt")
names(psa) <- c("ptid","nadirpsa","pretxpsa", "ps", "bss","grade","age","obstime","inrem")
```
Syntax notes

• Assigning a single vector (or anything else) to a variable uses the same syntax as assigning a whole data frame.

• `c()` is a function that makes a single vector from its arguments.

• `names()` is a function that accesses the variable names of a data frame.

• Some functions, such as `names()`, can be used on the LHS of an assignment.
Other statistical packages

library("foreign")
stata <- read.dta("salary.dta")
spss <- read.spss("salary.sav", to.data.frame=TRUE)
sasxport <- read.xport("salary.xpt")
epiinfo <- read.epiinfo("salary.rec")

Notes:

- Many functions in R live in optional packages. The `library()` function lists packages, shows help, or loads packages from the package library.

- The foreign package is in the standard distribution. It handles import and export of data. Thousands of extra packages are available at [http://cran.r-project.org](http://cran.r-project.org).
The web

Files for `read.table()` can live on the web

```r
fl2000<-read.table("http://faculty.washington.edu/tlumley/data/FLvote.dat", header=TRUE)
```

It’s also possible to read from more complex web services (such as the genome databases)
Operating on data

We assume you know how to use the $ sign, to indicate columns of interest in a dataset, e.g. antibiotics$duration means the variable duration in the data frame antibiotics.

## This is a comment

## Convert temperature to real degrees
antibiotics$tempC <- (antibiotics$temp-32)*5/9

## display mean, quartiles of all variables
summary(antibiotics)
Subsets

Everything in R is a vector (but some have only one element). The re are several ways to use [] to extract subsets

```r
## First element
antibiotics$temp[1]
## All but first element
antibiotics$temp[-1]
## Elements 5 through 10
antibiotics$temp[5:10]
## Elements 5 and 7
antibiotics$temp[c(5,7)]
## People who received antibiotics (note ==)
antibiotics$temp[ antibiotics$antib==1 ]
## or
with(antibiotics, temp[antib==1])
```
Notes

• Positive indices select elements, negative indices drop elements

• 5:10 is the sequence from 5 to 10

• You need == to test equality, not just =

• with() temporarily sets up a data frame as the default place to look up variables.
More subsets

For data frames you need two indices – naming rows and columns can also be useful;

```r
## First row
antibiotics[1,]
## Second column
antibiotics[,2]
## Some rows and columns
antibiotics[3:7, 2:4]
## Columns by name
antibiotics[, c("id","temp","wbc")]
## People who received antibiotics
antibiotics[antibiotics$antib==1, ]
## Put this subset into a new data frame
yes <- antibiotics[antibiotics$antib==1,]
```
Computations

mean(antibiotics$temp)
median(antibiotics$temp)
var(antibiotics$temp)
sd(antibiotics$temp)
mean(yes$temp)
mean(antibiotics$temp[antibiotics$antib==1])
with(antibiotics, mean(temp[sex==2]))
toohot <- with(antibiotics, temp>99)
mean(toohot)
Factors represent categorical variables. You can't do mathematical operations on them (except for `==`)

```r
> table(salary$rank, salary$field)

         Arts Other Prof
    Assist 668 2626   754
    Assoc 1229 4229  1071
    Full  942 6285  1984
> antibiotics$antib<-factor(antibiotics$antib, labels=c("Yes","No"))
> antibiotics$agegp<-cut(antibiotics$age, c(0,18,65,100))
> table(antibiotics$agegp)

       (0,18] (18,65] (65,100]
      2      19       4
```
Help!

- `?fn` or `help(fn)` for help on `fn`

- `help.search("topic")` for help pages related to "topic"

- `apropos("tab")` for functions whose names contain "tab"

- `RSiteSearch("FDR")` to search the R Project website (requires internet access)