



Data manipulation in R

A program to use when size matters

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Todays workshop

- A common scenario
- A friend has emailed you her data in a spreadsheet
- Todays workshop is not about impressing with R code

Why not use a spreadsheet?

- Data manipulation in Excel is VERY risk and time consuming
- A rage of software packages are available for Excel
- Large data sets can exceed the size limits of standard programs
- Spreadsheets don't have the inherent understanding of statistics that R has
- For example handling of NA's
- R is hot!



Why use R?

- Its free
- Its available on most operating systems Windows, OS X, Linux
- There are huge numbers of packages available
- Its becoming the international standard for statistics



James P. Howard. R Cookbook. O'Reilly Media, Inc, 2011.

Phil Spector.
Data Manipulation with R.
Use R series
Springer, 2008



Download it

- Open http://www.r-project.org
- Click CRAN (Under download on Top Left)
- Click http://cran.ms.unimelb.edu.au/ University of Melbourne

Windows

- Select Windows
- Select Base
- Download R (suggest latest version)

OS X

- Select Select OS X
- Select R-3.2.2.pkg (or the version that matches your OS version)



How about RStudio

- https://www.rstudio.com/products/rstudio/download/
- Its also on your thumb drive



```
2+5
## [1] 7
# Create a sequence of numbers
X = 2:10
# Display basic statistical measures
summary(X)
## Min. 1st Qu. Median Mean 3rd Qu. Max.
## 2 4 6 6 8 10
# use q() to quit
```





To access the documentation type

help.start() help(summary) args(summary) example(sd) ??package



To search R documentation

- RSiteSearch("key phrase")
- help(adf.test,package="tseries")
- To search for a tutorial for a package vignette(package="packagename")
- For an intro to vignettes see
 https://cran.r-project.org/web/packages/sos/vignettes/sos.pdf
- Examples on the web http://shiny.rstudio.com/gallery/

Custom Google search focused on R-specific websites

http://rseek.org

Coding Q&A site

http://stackoverflow.com http://stats.stakexchange.com



Research on how to work creatively based on case studies of successful R&D projects developed into Agile

- Keep the manages away
- Work sustainably
- People over process
- Iterative development



Vectors

- Vectors $I \leftarrow c(1, 3, 4, 7, 11)$
- Refer to elements using array I[c(2,5)] 2nd and 5th elements of I

Data Frames

```
a <- c(35,23,24,65)
e <- c("Peter", "John", "Mark", NA)
f <- c(TRUE,TRUE,TRUE,FALSE)
team <- data.frame(a,e,f)
names(team) <- c("Age","Names","Passed") # variable names
str(team)

## 'data.frame': 4 obs. of 3 variables:
## $ Age : num 35 23 24 65
## $ Names : Factor w/ 3 levels "John","Mark",..: 3 1 2 NA
## $ Passed: logi TRUE TRUE TRUE FALSE</pre>
```



Where are we

```
getwd()
setwd("/Users/pcru/SizeDoesMatter1")
dir() #This lists the files
ls() #This lists the variables
```

http://www.statmethods.net/input/contents.html



To read a csv table as a table try

tab1 ← as.matrix(read.csv(file="filetable.csv", sep=",", header=FALSE))

But our table is an excel file

- What about a package?
- http:

//www.thertrader.com/2014/02/11/a-million-ways-to-connect-r-and-excel/

■ Lets use the R package xlsx



Where from

- install command
- install.packages(pkgs)

Citing Packages

- Citing packages
- Getting the bibtex entry into endnote
- http://www.lib.uts.edu.au/question/5955/ how-can-i-import-bibliography-endnote-bibtex-latex-what-about-converting-other

```
x—citation()
x1—citation(package="RSQLite")
toBibtex(x)

sessionInfo()
packages_in_use ← c( sessionInfo()$basePkgs, names( sessionInfo()$loadedOnly ) )
the_citations_list ← lapply( X=packages_in_use, FUN=citation)
the_citations_list
```



```
\label{lem:condition} $$ table1 \leftarrow read.xlsx2 ("1_R Wkshp_dummy data_OTU table.xlsx", sheetName = $$ "Sheet1", header=FALSE, rowNames=FALSE, transpose=TRUE, endRow=18)
```

Loading the xlsx package

```
## Loading required package: xlsx
## Warning: package 'xlsx' was built under R version 3.1.3
## Loading required package: rJava
## Warning: package 'rJava' was built under R version 3.1.3
## Loading required package: methods
## Loading required package: xlsxjars
## Loading required package: xtable
```



	X1	X2	X3	X4	X5	X6	X7
1	Group	Contaminated					
2	Site	1			2		
3	Sample ID	10000	10001	10002	10003	10004	10005
4	Rep	1	2	3	1	2	3
5	phormidiaceae	24872	24872	5822	7538	7201	7538
6	streptococcaceae	11	7	14	8	10	8



Transposing

We need to transpose the table and set the column names correctly

```
table1t=setNames(data.frame(t(table1[,-1])),table1[,1])
```

 $\label{lem:man_read_transpose_Rd&d=R_CC} $$ $$ http://stackoverflow.com/questions/17288197/$$ reading-a-csv-file-organized-horizontally$



Lets do it the easy way first

```
ctridx<-which(table1t$Group=="Control")</pre>
table1t$Group[1:48] <- "Contaminated"
table1t$Group[(ctridx+1):48]<-"Control"
   ttt ←table1t$Site
   for(i in c(2:length(table1t$Site)))
      temp \( as.character(table1t\)Site[i])
      tempb \leftarrow as.character(ttt[i-1])
      if (table1t $Site[i]=="")
          ttt[i]←tempb
      if (! table1t $ Site [( i )]=="")
          ttt[i]←temp
   table1t $Site ←ttt
## X3
## 1
## Levels: 1 2 3 4 FALSE TRUE
## X4
##
## Levels: 1 2 3 4 FALSE TRUE
## X5
```



- require(stringr)
- Lets look at this package
- stri_c(str1,str2)
- concatenates two string
- str_len(str)

```
require(stringr)
## Loading required package: stringr

table1t$Rep<-str_replace(table1t$Rep,"[rep]{3}?","\\1")
table1t$Rep<-str_replace(table1t$Rep,"A","1")
table1t$Rep<-str_replace(table1t$Rep,"B","2")
table1t$Rep<-str_replace(table1t$Rep,"C","3")
table1t$Rep<-as.factor(table1t$Rep)</pre>
```



- http://www.statmethods.net/input/importingdata.html
- http://stackoverflow.com/questions/17288197/ reading-a-csv-file-organized-horizontally
- http://rgm3.lab.nig.ac.jp/RGM/R_rdfile?f=Ecdat/man/read. transpose.Rd&d=R_CC
- Input files from Stata

```
\begin{array}{l} \textbf{library} \ ( \ \texttt{foreign} \ ) \\ \texttt{mydata} \ \leftarrow \ \textbf{read} \ . \ \texttt{dta} \ ( \ " \ \texttt{c} : \ / \ \texttt{mydata} \ . \ \texttt{dta} " \ ) \end{array}
```



Need coffee!!



setwd("/Users/pcru/SizeDoesMatter1")

#dir()

table2<-read.xlsx2("2_R Wkshp_dummy data_Env Data_incl2outliersMK.xlsx", sheetName

	Group	Site	Sample.ID	Rep	Spill.date	Sample.collection.date
1	Contaminated	1	10000	1	14-May-14	15.5.14
2	Contaminated	1	10001	2	14-May-14	15.5.14
3	Contaminated	1	10002	3	14-May-14	15.5.14
4	Contaminated	2	10003	1	14-May-14	15.5.14
5	Contaminated	2	10004	2	14-May-14	15.5.14
6	Contaminated	2	10005	3	14-May-14	15.5.14



Oh NO

- All columns have been set to factors.
- Dates have different formats

```
str(table2[,1:11])
## 'data.frame': 48 obs. of 11 variables:
                            : Factor w/ 2 levels "Contaminated"...: 1 1 1 1 1 1
##
    $ Group
##
    $ Site
                            : Factor w/ 4 levels "1", "2", "3", "4": 1 1 1 2 2 2 1 1
                            : Factor w/ 18 levels "10000", "10001"...: 1 2 3 4 5 6
##
   $ Sample.ID
    $ Rep
                            : Factor w/ 9 levels "1", "2", "3", "A", ...: 1 2 3 1 2 3
##
                            : Factor w/ 2 levels "14-May-14", "N/A": 1 1 1 1 1 1 1
    $ Spill.date
##
    $ Sample.collection.date: Factor w/ 4 levels "15.5.14","17/5/14",..: 1 1 1 1
##
##
    $ labnum
                            : Factor w/ 36 levels "2000", "2001"...: 1 2 3 4 5 6 7
    $ phosphate..ppb.
                            : Factor w/ 39 levels "10", "105", "108", ...: 27 30 28 2
##
##
   $ ammonia..ppb. : Factor w/ 41 levels "10","103","1042",...: 10 14 15
    $ chlorophyll..ug.L. : Factor w/ 38 levels "1","10","11",...: 20 23 21 25 1
##
##
   $ DO....
                            : Factor w/ 31 levels "100", "120", "31", ...: 5 4 3 7 6
```

Lets break it down

First lets reed a few rows only

table2<-read.xlsx2("2_R Wkshp_dummy data_Env Data_incl2outliersMK.xlsx", sheetNamsapply(table2,mode)



colClasses

- The variable colClasses can be used to specify the row types.
- We need to set stringsAsFactor=FALSE or all columns with be loaded as factors
- The dates are in a non standard format so we need to read them as chars first

table2b<-read.xlsx2("2_R Wkshp_dummy data_Env Data_incl2outliersMK.xlsx", sheetNatsapply(table2,class)</pre>

```
## Group Site Sample.ID Rep Spill.date
## "character" "numeric" "numeric" "character"
## rowNames as.Data.frame
## "logical" "logical"
```



```
table2f<-table2
table2f$Spill.date<-as.Date(table2f$Spill.date,"%d-%b-%v")
table2f$Sample.collection.date<-as.Date(table2f$Sample.collection.date,"%d.%m.%y"
## Error in as.Date.default(table2f$Sample.collection.date,
"%d.%m.%y"): do not know how to convert
'table2f$Sample.collection.date' to class "Date"
#sapply(table2f, mode)
sapply(table2f,class)
##
           Group
                          Site
                                   Sample.ID
                                                       Rep
                                                              Spill.date
     "character"
                     "numeric"
                                   "numeric" "character"
                                                                   "Date"
##
##
       rowNames as.Data.frame
##
       "logical" "logical"
```



colClasses

- The as.Data method can take a format string as the second variable
- The format strings are described in help on strptime
- But Spill.data has two formats
- We can use the if else function to combine them

```
table2bf<-table2b
table2bf$Spill.date<-as.Date(table2bf$Spill.date, "%d-%b-%y")
cdate1<-as.Date(table2bf$Sample.collection.date, "%d.%m.%y")
cdate2<-as.Date(table2bf$Sample.collection.date, "%d/%m/%y")
table2bf$Sample.collection.date<-as.Date(ifelse(!is.na(cdate1),as.Date(cdate1),as
table2bf$Group<-as.factor(table2bf$Group)
table2bf$Rep<-as.factor(table2bf$Rep)</pre>
na_count <-sapply(table2bf, function(y) sum(length(which(is.na(y)))))</pre>
na_count
##
                     Group
                                              Site
                                                                 Sample.ID
##
                                        Spill.date Sample.collection.date
##
                       Rep
##
                                                24
                                   phosphate..ppb.
##
                    labnum
                                                             ammonia..ppb.
##
                                            DO....
                                                                  rowNames
##
       chlorophyll..ug.L.
```



```
require(stringr)
table2bf$Rep<-str_replace(table2bf$Rep, "[rep]{3}?", "\\1")
table2bf$Rep<-str_replace(table2bf$Rep,"A","1")
table2bf$Rep<-str_replace(table2bf$Rep,"B","2")</pre>
table2bf$Rep<-str_replace(table2bf$Rep, "C", "3")
table2bf$Rep<-as.factor(table2bf$Rep)</pre>
str(table2bf)
  'data.frame': 48 obs. of 13 variables:
                            : Factor w/ 2 levels "Contaminated"...: 1 1 1 1 1 1 1
    $ Group
##
                            : num 1 1 1 2 2 2 1 1 1 2 ...
    $ Site
##
##
    $ Sample.ID
                            : num 10000 10001 10002 10003 10004 ...
##
    $ Rep
                            : Factor w/ 3 levels "1", "2", "3": 1 2 3 1 2 3 1 2 3 1
    $ Spill.date
                            : Date, format: "2014-05-14" "2014-05-14" ...
##
    $ Sample.collection.date: Date, format: "2014-05-15" "2014-05-15" ...
##
    $ labnum
                            : nim 2000 2001 2002 2003 2004 ...
##
                            : num 3020 3253 3169 2999 2879 ...
##
    $ phosphate..ppb.
##
    $ ammonia..ppb.
                            : num 13880 14598 14676 10984 11657 ...
    $ chlorophyll..ug.L.
                            : num 302 323 315 352 289 296 254 248 250 220 ...
##
    $ DO....
                            : num 34 33 31 38 36 34 40 38 41 45 ...
##
    $ rowNames
                            : logi FALSE FALSE FALSE FALSE FALSE ...
##
                            : logi FALSE FALSE FALSE FALSE FALSE ...
    $ as.Data.frame
##
```



The inbuilt command merge

- R has a command merge
- Lets start looking at the first 9 lines of the tables and merge them using the Sample ID
- Because otherwise its not uniques

```
\label{eq:merge} \begin{split} \text{merge}(x,\ y,\ \text{by} &= \text{intersect}\left(\text{names}(x),\ \text{names}(y)\right), \\ \text{by}.x &= \text{by},\ \text{by}.y &= \text{by},\ \text{all} &= \text{FALSE},\ \text{all}.x &= \text{all},\ \text{all}.y &= \text{all}, \\ \text{sort} &= \text{TRUE},\ \text{suffixes} &= \text{c}(".x",".y"), \\ \text{incomparables} &= \text{NULL},\ \dots) \end{split}
```

```
tab1c<-table1t[1:9,]
tab2c<-table2b[1:9,]
m1<-merge(tab1c,tab2c,by.x="Sample ID",by.y="Sample.ID")
m2<-merge(table1t,table2bf,by.x=c("Group","Site","Sample ID"),by.y=c("Group","Site")
m3<-merge(table1t,table2bf,by.x=c("Group","Site","Sample ID","Rep"),by.y=c("Group")</pre>
```



Provided



Follow up data from contaminated site

sapply (table3f, class)

```
 table 3 \leftarrow read. xls x2 \ ("3\_Follow up data from contaminated site\_MK. xls x", sheetName = "Sheet1", head table 3 f \leftarrow table
```



Joining table 3 to are merged tables

- We need to be careful to match everything
- Install the plyr package This has lots of useful functions for renaming var etc
- This means we need columns for corynebacteriaceae and porphyromondaceae
- should these be NA or 0
- we will do one of each. generally we would use NA but in this case 0 is perhaps better

```
require (plyr)
Sample. ID \leftarrow rep(20000,3)
table3fi cbind(table3f.Sample.ID)
#how many columns I can't count
ncol(table3fi)
ncol(m3)
#now get the cols all right
table3fii←table3fi [c(1,2,24,3,4:23)]
m3i \leftarrow m3[c(1:4,19:20,5:18,21:26)]
setdiff(names(m3i),names(table3fii))
m3ii←rename(m3i, c("Sample ID"="Sample.ID"))
corynebacteriaceae←rep(0, nrow(table3fii))
porphyromondaceae←rep(NA, nrow(table3fii))
table3fiii cbind (table3fii, corynebacteriaceae, porphyromondaceae)
setdiff(names(m3ii),names(table3fiii))
m3ii[,c(7:24)] \leftarrow sapply(m3ii[,c(7:24)], as.numeric)
m3ii[,c(1:4)] \leftarrow sapply(m3ii[,c(1:4)], as. character)
#m3ii [, c("Site")] ←sapply (m3ii [, c("Site")], as.character)
table3fiii [c(1:4)] \leftarrow \text{sapply}(\text{table3fiii}[c(1:4)], \text{as.character})
table 3 fiii [, c(7:24)] \leftarrow sapply(table 3 fiii [, c(7:24)], as.numeric)
table4~rbind(m3ii,table3fiii)
table4[,1] \leftarrow sapply(table4[,1], as. factor)
```





reshape2

- vignette(reshape) doesn't work
- try http://had.co.nz/reshape/
- and http://seananderson.ca/2013/10/19/reshape.html

A small example for melt

- Suppose we what a box plot to see if there are outliers
- We will use ggplot2 box plot
- but box plot needs data in long format to use this
- first melt the data
- We need to specify the unique key, the variable name and the value name
- The key is not unique.
- Then plot it



The code

```
require(reshape2)
```

Loading required package: reshape2

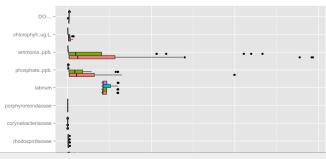
matable4<-melt(table4[,c(1:4,7:25)], variable.name = "microbe", value.name = "abunda"</pre>



Using ggplot

- As we have keys we need to specify the x and y
- lets make the sites different colors
- The variable names are long so lets flit it with *coord_flip()*
- Looks like we have outliers...hmm

```
require(ggplot2)
## Loading required package: ggplot2
ggplot(matable4,aes(x=microbe,y=abundance,fill=Site)) + geom_boxplot() + coord_f:
## Warning: Removed 24 rows containing non-finite values
(stat_boxplot).
```





Removing Outliers

- Outliers are defined 1.5 times the interquartile range above the upper quartile
- lets fix the one with phosphate as the 9 is typed twice
- Still issues with ammonia to explore

```
phosphate<-table4[,"phosphate..ppb."]
upper.limit <- quantile(phosphate)[4] + 1.5*IQR(phosphate)
lower.limit <- quantile(phosphate)[2] - 1.5*IQR(phosphate)
#table4[phosphate> upper.limit,c("Site", "phosphate..ppb.")]
```

	Site	phosphateppb.
1	1	3020.00
2	1	3253.00
3	1	3169.00
12	1	9982.00
14	1	9982.00
16	1	1542.00

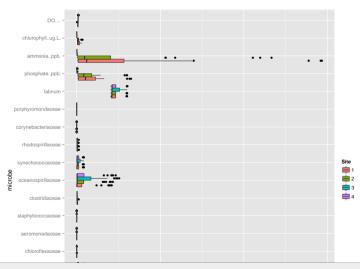
```
table4[12,"phosphate..ppb."]<-982
table4[14,"phosphate..ppb."]<-982</pre>
```



Look again ggplot

(stat_boxplot).

```
matable4<-melt(table4[,c(1:4,7:25)],variable.name = "microbe",value.name = "abundar
ggplot(matable4,aes(x=microbe,y=abundance,fill=Site)) + geom_boxplot() + coord_f
## Warning: Removed 24 rows containing non-finite values</pre>
```





RSQLite

- Suppose merge is not enough? I know about SQL and want to do joins
- Lets Install RSQLite
- We also need to install DBI

Loading required package: RSQLite

```
db <- dbConnect(SQLite(), dbname="Test.sqlite")</pre>
#getConfig()£staged.gueries
# sqldf(attach "Test1.sqlite" as new)
dbBegin(db)
## [1] TRUE
dbWriteTable(db, "table1", table1t, overwrite=TRUE)
## [1] TRUE
dbReadTable(db, "table1")
                           Site Sample.ID
                                            Rep phormidiaceae
##
                    Group
## X2
             Contaminated
                                    10000
                                                         24872
## X3
             Contaminated 1
                                    10001
                                                         24872
             Contaminated
## X4
                                    10002
                                                          5822
```



Another important component of TDD is refactoring and unit tests

- Refactoring http://refactoring.com/
- http://www.r-bloggers.com/
 my-experience-of-learning-r-from-basic-graphs-to-performance-tuning/
- TDD in R http: //www.slideserve.com/andrew/test-driven-development-in-r
- Version Control tortiseSVN http://tortoisesvn.net/
- GitHub https://github.com/



Dropping Row and Columns with too many NAs



Tidy Data

In tidy data:

- Each variable forms a column.
- Each observation forms a row.
- Each type of observational unit forms a table.
- https://cran.r-project.org/web/packages/tidyr/vignettes/tidy-data.html
- http://pj.freefaculty.org/R/Rtips.html#toc-Subsection-1.11

Spit out the dates and numbers

```
\begin{array}{l} \texttt{dates}4 \leftarrow \texttt{table4} \left[ \,, \textbf{c} \left( \, 5 \,, 6 \, \right) \right] \\ \texttt{abundance} \leftarrow \texttt{table4} \left[ \,, \textbf{c} \left( \, 7 \,; 2 \, 5 \, \right) \right] \end{array}
```



Calculating the number of days

We can just subtract as. Date fields

dates4<-table4[,c(5,6)]
abundance<-table4[,c(7:25)]
days<-dates4[,2]-dates4[,1]</pre>



sapply

- Also known as centring the data
- Ecological percentage of the sum of the variables
- We an use sweep to centre the data
- options(digits = 1) Just to make things pretty

```
sweepOutContinu \leftarrow sweep (abundance, 2, apply (abundance, 2, min, na.rm = TRUE)) \\ afterSweepContinu \leftarrow sweep (sweepOutContinu, 2, apply (sweepOutContinu, 2, max, na.rm = TRUE), "/") \\ table 5 \leftarrow cbind (table 4 [, c(1:6)], afterSweepContinu, days) \\ options (digits = 1) \\ sweep (abundance, 2, colSums (abundance), FUN="/") \\ scale (abundance, center = FALSE, scale = colSums (abundance))
```



R has nice graphs

- Lets create a correlation heat map
- Heat map.
- A graphical output
- http://rcharts.io/gallery/
- R Graph gallery currently down try http://rgraphgallery.blogspot.com/
- A reference on where to go R thumbnails
- ggplot2 (scatter plot of 2 var and then 3 plots)

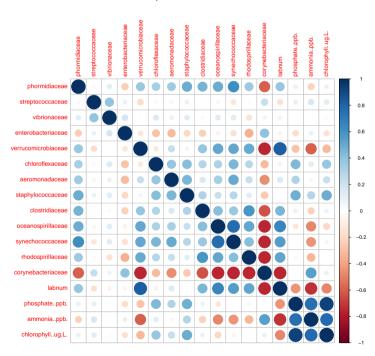
```
library(corrplot)
abuncor←cor(t5lessThan20col[,c(6:22)])
require(corrplot)
corrplot(abuncor, method = "circle")
```

```
## [1] 23
## Loading required package: corrplot
```



A heat map

opearman correlations



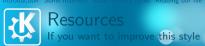


Help is on the way

- Parameterized Complexity Research Unit (PCRU) PhD students
- PhD student in Bioinformatics from Central South Uni

Your feedback on some ideas

- Using Sweave or Knitr
- Advanced Data Cleaning
- Network Centric data analysis





LaTeX Beamer

http://latex-beamer.sourceforge.net/

Sharelatex Site

https://www.sharelatex.com

A Data Cleaning Mooc

https://www.sharelatex.com



Output of sessionInfo

```
sessionInfo()
## R version 3.1.2 (2014-10-31)
## Platform: x86_64-apple-darwin13.4.0 (64-bit)
##
## locale:
## [1] C
##
## attached base packages:
  [1] methods
               stats
                         graphics grDevices utils
                                                    datasets base
##
## other attached packages:
   [1] corrplot_0.73 RSQLite_1.0.0 DBI_0.3.1 ggplot2_1.0.0
##
##
   [5] reshape2_1.4.1 plyr_1.8.1 stringr_0.6.2 xtable_1.7-4
##
   [9] xlsx_0.5.7 xlsxjars_0.6.1 rJava_0.9-7 knitr_1.11
##
## loaded via a namespace (and not attached):
   [1] MASS 7.3-39
##
                       Rcpp_0.11.5
                                      colorspace_1.2-6 digest_0.6.8
   [5] evaluate_0.7.2 formatR_1.2 grid_3.1.2 gtable_0.1.2
##
   [9] highr_0.5 labeling_0.3 munsell_0.4.2 proto_0.3-10
##
## [13] scales 0.2.4 tools 3.1.2
```