





Data manipulation in R

A program to use when size matters

Peter Shaw

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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

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 range 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!

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O'Reilly Media, Inc, 2011.

Phil Spector.

Data Manipulation with R. Use R series Springer, 2008

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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

Window

- 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)

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```
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
```





low about RStudio

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

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To access the documentation type

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

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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

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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>
```



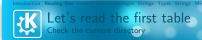


Research on how to work creatively based on case studies of successful R&D projects developed into Agile

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

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Where are we

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

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

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To read a csv table as a table tr

 $\texttt{tab1} \leftarrow \texttt{as.matrix}(\texttt{read.csv}(\texttt{file} = \texttt{"filetable.csv"}, \texttt{sep} = \texttt{"}, \texttt{"}, \texttt{header} = \texttt{FALSE}))$

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/

- Installing the R package xlsx
- CRAN mirror http://cran.csiro.au
- Change in preferences

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table1-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
```





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-way

 $\begin{tabular}{ll} \times-citation() \\ xit-citation(package="RSQLite") \\ to Bibtex(x) \\ sessionInfo() \\ packages_in_use \leftarrow c(sessionInfo()\$basePkgs, names(sessionInfo()\$loadedOnly)) \\ the_citations_list \leftarrow lapply(X=packages_in_use, FUN=citation) \\ the_citations_list \leftarrow lapply(X=packa$

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	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

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Transposing

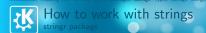
We need to transpose the table and set the column names correctly

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

 $\label{lem:http://rgm3.lab.nig.ac.jp/RGM/R_rdfile?f=Ecdat/man/read.transpose.Rd&d=R_CC http://stackoverflow.com/questions/17288197/reading-a-csv-file-organized-horizontally$

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require(stringr)

A look at the stringer 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>
```

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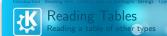


TDD – First do it the easy way first

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

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Levels: 1 2 3 4 FALSE TRUE ## X6 ## 2





- 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

```
library (foreign)
mydata ← read.dta("c:/mydata.dta")
```

Levels: 1 2 3 4 FALSE TRUE

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Let's read the next table

Reading a table using xxs

Need coffee !!



Oh NO

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

First read a few rows only

```
str(table2[,1:11])
## 'data.frame': 48 obs. of 11 variables:
## $ Group
                            : Factor w/ 2 levels "Contaminated",..: 1 1 1 1 1 1 1 1 1 1 ...
                            : Factor w/ 4 levels "1", "2", "3", "4": 1 1 1 2 2 2 1 1 1 2 ...
## $ Site
## $ Sample.ID
                            : Factor w/ 18 levels "10000", "10001", ...: 1 2 3 4 5 6 7 8 9 1 ...
## $ Rep
                            : Factor w/ 9 levels "1", "2", "3", "A", ...: 1 2 3 1 2 3 7 8 9 7 ...
                            : Factor w/ 2 levels "14-May-14", "N/A": 1 1 1 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 1 2 2 2 2 ...
                            : Factor w/ 36 levels "2000", "2001", ...: 1 2 3 4 5 6 7 8 9 19 ...
## $ labnum
## $ phosphate..ppb.
                            : Factor w/ 39 levels "10", "105", "108", ...: 27 30 28 26 25 27 12 15 13 7
                            : Factor w/ 41 levels "10","103","1042",..: 10 14 15 6 7 4 31 34 32 28 .
## $ ammonia..ppb.
## $ chlorophyll..ug.L.
                           : Factor w/ 38 levels "1", "10", "11", ...: 20 23 21 25 17 18 16 14 15 12 ...
## $ DO....
                            : Factor w/ 31 levels "100", "120", "31", ...: 5 4 3 7 6 5 8 7 9 11 ...
Break it down
```

table2<-read.xlsx2("2_R Wkshp_dummy data_Env Data_incl2outliersMK.xlsx", sheetName = "Sheet2",headersapply(table2,mode)</pre>

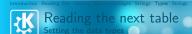
setwd("/Users/pcru/SizeDoesMatter1")

table2<-read.xlsx2("2_R Wkshp_dummy data_Env Data_incl2outliersMK.xlsx", sheetName = "Sheet2

	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

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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", sheetName = "Sheesapply(table2,class)</pre>

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

ses=c("cha

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"character" "numeric" "numeric" "character" "character"

rouNames as Data frame

```
Reading table 2
Setting the Date Type
```



```
table2f<-table2
table2f$Spill.date<-as.Date(table2f$Spill.date,"%d-%b-%y")
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
                                                               Spill.date
                                                                   "Date
##
     "character"
                     "numeric"
                                    "numeric"
                                                "character"
##
       rowNames as.Data.frame
       "logical"
                     "logical"
```

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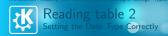
```
Introduction Reading the Course Strings Types Strings Merging Tables Fat or wide Cleaning things up Setting the Relative Abunds

Reading table 2

Just fix the Rep column using the stringer package again
```

```
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:
   $ Group
                           : Factor w/ 2 levels "Contaminated",..: 1 1 1 1 1 1 1 1 1 1 ...
   $ Site
                           : num 1 1 1 2 2 2 1 1 1 2 ...
                           : num 10000 10001 10002 10003 10004 ...
   $ Sample.ID
                           : 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" ...
                           : num 2000 2001 2002 2003 2004 ...
   $ labnum
   $ phosphate..ppb.
                           : num 3020 3253 3169 2999 2879 ...
                           : num 13880 14598 14676 10984 11657 ...
   $ ammonia..ppb.
## $ 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 ...
## $ as.Data.frame
                           : logi FALSE FALSE FALSE FALSE FALSE ...
```

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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$Sample.collection.date,"%d.%m.%y")</pre>
cdate2<-as.Date(table2bf$Sample.collection.date,"%d/%m/%y")</pre>
table2bf$Sample.collection.date<-as.Date(ifelse(!is.na(cdate1),as.Date(cdate1)),as.Date(cdate1)
table2bf$Group<-as.factor(table2bf$Group)</pre>
table2bf$Rep<-as.factor(table2bf$Rep)</pre>
na_count <-sapply(table2bf, function(y) sum(length(which(is.na(y)))))</pre>
na_count
##
                                               Site
                     Group
                                                                   Sample.ID
##
                         0
##
                       Rep
                                         Spill.date Sample.collection.date
##
                         0
                                                 24
                    labnum
                                   phosphate..ppb.
                                                              ammonia..ppb.
##
                         0
                                                  0
                                                                           0
##
                                             DO....
                                                                   rowNames
       chlorophyll..ug.L.
##
##
                         0
```

dated <- table 2 bf \$Sample.collection.date - table 2 bf \$Spill.date





The inbuilt command merge

- R has a command merge
- To begin, start looking at the first 9 lines of the tables and merge them
- Need to use Group, Site, Sample.ID because otherwise it's not uniques

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Provided

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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←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
table3fiii-table3fi[c(1,2,24,3,4:23)]
m3i←m3[c(1:4,19:20,5:18,21:26)]
setdiff(names(m3i),names(table3fii))
m3i←mane(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)] ← sapply(m3ii[,c(7:24)],as.numeric)
m3ii[,c(*Site*")] ←sapply(m3ii[,c(*Site*")],as.character)

table3fiii[,c(*Site*")] ←sapply(table3fiii[,c(1:4)],as.character)

table3fiii[,c(7:24)] ← sapply(table3fiii[,c(1:4)],as.character)
table4←rbind(m3ii,table3fiii)
table4←rbind(m3ii,table3fiii)
table4[,1] ← sapply(table3fiii[,c(7:24)],as.numeric)
table4←rbind(m3ii,table3fiii)
```

How do I append two data sets?
To begin load the third data set



Follow up data from contaminated site

```
table3←read.xlsx2("3.Follow up data from contaminated site_MK.xlsx", sheetName = "Sheet1",header=TRUE,row table3fk-table3
table3f$Spill.date←as.Date(table3f$Spill.date,"%d.%m.%y")
table3f$Sample.collection.date←as.Date(table3f$Sample.collection.date,"%d.%m.%y")
sapply(table3f,mode)
sapply(table3f,class)
```

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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

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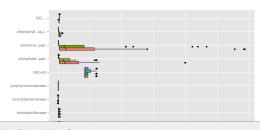
- As we have keys we need to specify the x and y
- Let's make the sites different colors
- The variable names are long so flip it with *coord_flip()*
- Looks like we have outliers...hmm

require(ggplot2)

Loading required package: ggplot2

ggplot(matable4,aes(x=microbe,y=abundance,fill=Site)) + geom_boxplot() + coord_flip()

Warning: Removed 24 rows containing non-finite values
(stat_boxplot).



Reshaping Tables

The code

 $\label{eq:matable4} $$ \mathtt{matable4} = \mathtt{mat$

require(reshape2)

Loading required package: reshape2

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

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Removing Outliers

- Outliers are defined 1.5 times the interquartile range above the upper quartile
- Assume that rows 12 and 14 in phosphate are errors 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>

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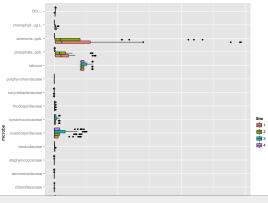




Look again ggplot

matable4<-melt(table4[,c(1:4,7:25)],variable.name = "microbe",value.name = "abundance", id=c("Group"
ggplot(matable4,aes(x=microbe,y=abundance,fill=Site)) + geom_boxplot() + coord_flip()</pre>

Warning: Removed 24 rows containing non-finite values
(stat_boxplot).







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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/

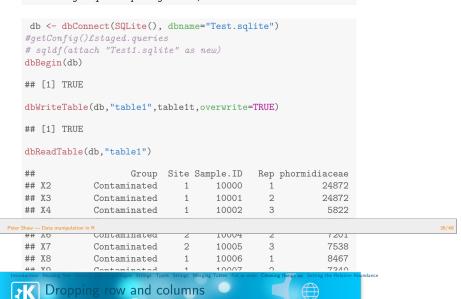
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RSQLite

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

Loading required package: RSQLite



Dropping Row and Columns with too many NAs

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## X39	Control	3	10013	2	72	
## X40	Control	3	10014	3	115	







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

dates4←table4 [, c (5,6)] abundance←table4 [, c (7:25)]

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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=sweep(abundance,2.apply(abundance,2.min,na.rm=TRUE))
afterSweepContinu=sweep(sweepOutContinu,2.apply(sweepOutContinu,2.max,na.rm=TRUE),"/")
tableS=-cbind(table4[,c(1:6)], afterSweepContinu,days)
options(digits=1)
sweep(abundance, 2, colSums(abundance), FUN="/")
scale(abundance, center=FALSE, scale=colSums(abundance))



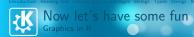


Calculating the number of days

We can just subtract as. Date fields

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

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R has nice graphs

- 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)
- To create a correlation heat map

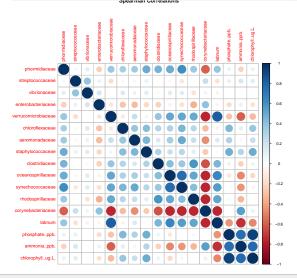
```
library(corrplot)
abuncor~cor(t5lessThan20col[.c(6:22)])
require(corrplot)
corrplot(abuncor, method = "circle")
```

[1] 23

Loading required package: corrplot

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LaTeX Beamer

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

Sharelatex Site

https://www.sharelatex.com

A Data Cleaning Mooc

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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

Peter Shaw — Data manipulation in R



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
##
## 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
```