Data manipulation in R

A program to use when size matters

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Why use R?

Why not use a spreadsheet?

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?

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

Getting Started

Some References

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

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

Getting Started

Installing R!

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)

Getting Started

Installing a GUI

How about RStudio

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

Getting Started

Basic steps

```
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
```

Getting Started

Help Functions

To access the documentation type

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

Help Functions

Search the Web

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`

Iterative development

Working Creatively

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

R Data types

Lists, frames and tables

Vectors

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

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
```

Lets read the table

Check the current directory

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

Lets read the table

Reading a table

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

R Packages

CRAN

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-othe

```
  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
```

```
sessionInfo()

## R version 3.1.2 (2014-10-31)
## Platform: x86_64-apple-darwin13.4.0 (64-bit)
##
## locale:
## [1] C
```

Lets read the table

An example

```
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
```

Lets read the table

The columns are wrong

	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

Lets read the table

Transpose the table

Transposing

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

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

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

Fields across many columns

Replicating first column

Lets do it the easy way first

```
ctridx<-which(table1t$Group=="Control")
table1t$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←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
##  1
## Levels:  1 2 3 4 FALSE TRUE
## X5
```

How to work with strings

stringer package

- `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)
```

Lets read the table

Reading a table of other types

- 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")
```

Morning Tea Time

Back in 20min

Need coffee !!

Lets read the next table

Reading a table using xlxs

```
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

Lets read the next table

Reading a table

Oh NO

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

```
str(table2[,1:11])

## 'data.frame': 48 obs. of  11 variables:
##  $ Group                 : Factor w/ 2 levels "Contaminated",..: 1 1 1 1 1 1 1
##  $ Site                  : Factor w/ 4 levels "1","2","3","4": 1 1 1 2 2 2 1 1
##  $ Sample.ID             : Factor w/ 18 levels "10000","10001",..: 1 2 3 4 5 6
##  $ Rep                   : Factor w/ 9 levels "1","2","3","A",..: 1 2 3 1 2 3
##  $ Spill.date            : Factor w/ 2 levels "14-May-14","N/A": 1 1 1 1 1 1 1
##  $ 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
##  $ 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
##  $ 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", sheetName
sapply(table2,mode)
```

Lets read the next table

Setting the data types

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", sheetNa
sapply(table2,class)

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

Lets read the next table

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           Rep    Spill.date
##   "character"     "numeric"     "numeric"   "character"        "Date"
##      rowNames as.Data.frame
##     "logical"     "logical"
```

Lets read the next table

Setting the Date Type

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)
na_count <-sapply(table2bf, function(y) sum(length(which(is.na(y)))))
na_count

##                   Group                    Site               Sample.ID
##                       0                       0                       0
##                     Rep              Spill.date  Sample.collection.date
##                       0                      24                       0
##                  labnum         phosphate..ppb.           ammonia..ppb.
##                       0                       0                       0
##      chlorophyll..ug.L.                  DO....                rowNames
##                       0                       0                       0
```

Lets read the next table

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")
table2bf$Rep<-str_replace(table2bf$Rep,"C","3")
table2bf$Rep<-as.factor(table2bf$Rep)
str(table2bf)

## 'data.frame': 48 obs. of  13 variables:
##  $ Group                 : Factor w/ 2 levels "Contaminated",..: 1 1 1 1 1 1 1
##  $ Site                  : num  1 1 1 2 2 2 1 1 1 2 ...
##  $ 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                : num  2000 2001 2002 2003 2004 ...
##  $ phosphate..ppb.       : num  3020 3253 3169 2999 2879 ...
##  $ 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 FALSE ...
##  $ as.Data.frame         : logi  FALSE FALSE FALSE FALSE FALSE FALSE ...
```

How to I merge two data sets

Using the merge command

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

```
merge(x, y, by = intersect(names(x), names(y)),
      by.x = by, by.y = by, all = FALSE, all.x = all, all.y = all,
      sort = TRUE, suffixes = c(".x",".y"),
      incomparables = NULL, ...)
```

```
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"
```

Lunch Time

Back in 30 min

Provided

How to I append two data sets

Lets load a third data set

Follow up data from contaminated site

```
table3←read.xlsx2("3_Follow up data from contaminated site_MK.xlsx", sheetName ="Sheet1",head
table3f←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)
```

How to I append two data sets

Lets load a third data set

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
table3fii←table3fi[c(1,2,24,3,4:23)]
m3i←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)] ← sapply(m3ii[,c(7:24)],as.numeric)
m3ii[,c(1:4)] ←sapply(m3ii[,c(1:4)],as.character)
#m3ii[,c("Site")] ←sapply(m3ii[,c("Site")],as.character)

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

Another Break

Reshaping Tables

reshape2

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

Reshaping Tables

melt and boxplot

The code

```
matable4←melt(table4[,c(1:4,6:25)],variable.name = "microbe",value.name ="abundance", \\
id=c("Group","Site","Sample.ID","Rep"),factorsAsStrings=FALSE,rm.na=TRUE)
```

```
require(reshape2)

## Loading required package:  reshape2

matable4<-melt(table4[,c(1:4,6:25)],variable.name = "microbe",value.name ="abunda

## Warning:  attributes are not identical across measure
variables; they will be dropped
## Warning:  cannot avoid coercion of factors when measure
attributes not identical
```

Reshaping Tables

boxplot

Using ggplot

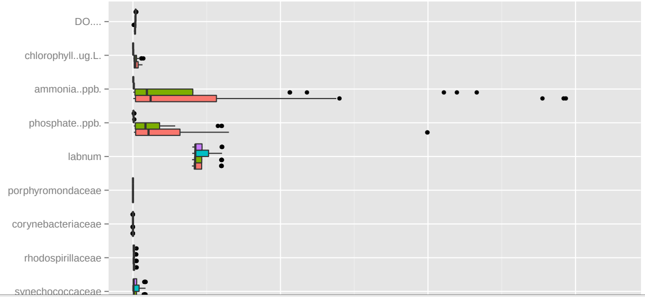
- As we have keys we need to specify the x and y
- lets make the sites different colors
- The variable names are long so lets flit it with $coord_flip()$
- Looks like we have outliers...hmm

```
require(ggplot2)

## Loading required package:  ggplot2

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

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



Reshaping Tables

boxplot

Removing Outliers

- Outliers are defined 1.5 times the interquartile range above the upper quartile

```
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	phosphate..ppb.
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
```

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
## Loading required package:  gsubfn
## Loading required package:  proto
## Warning in doTryCatch(return(expr), name, parentenv,
handler):  unable to load shared object
'/Library/Frameworks/R.framework/Resources/modules//R_X11.so':
##
dlopen(/Library/Frameworks/R.framework/Resources/modules//R_X11.so,
6):  Library not loaded:  /opt/X11/lib/libSM.6.dylib
##  Referenced from:
/Library/Frameworks/R.framework/Resources/modules//R_X11.so
##  Reason:  image not found
## Could not load tcltk.  Will use slower R code instead.
## Loading required package:  chron
## Warning:  package 'chron' was built under R version 3.1.3
```

```
 db <- dbConnect(SQLite(), dbname="Test.sqlite")
#getConfig()£staged.queries
```

R package

svUnit

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

Dropping selected variables

Dropping Row and Columns with too many NAs

```
numNAs_inData4_rows ← apply(rawData4, 1, function(z) sum(is.na(z)))
numNAs_inData4_col ← apply(table4, 2, function(z) sum(is.na(z))) # count NAs in Data4
lessThan20 ← table4[!(numNAs_inData4_rows > 20),]    #only select the rows contain less Than
lessThan20col ← table4[,!(numNAs_inData4_col > 20)]
```

Dropping row and columns

Dropping selected variables

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

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

Adding a new column

Calculating the number of days

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]
```

Setting the Relative abundance

Normalizing data

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),"/")
 table5←cbind(table4[,c(1:6)],afterSweepContinu,days)
 options(digits=1)
 sweep(abundance, 2, colSums(abundance), FUN="/")
scale(abundance, center=FALSE, scale=colSums(abundance))
```

Now lets have some fun

Graphics in R

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")
```

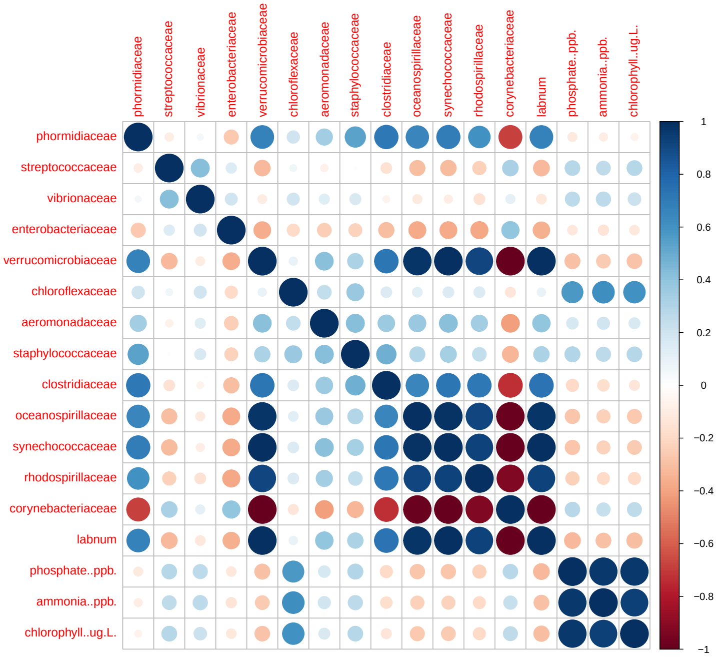
```
## [1] 23

## Loading required package:  corrplot
```

Now lets have some fun

Making a heat map

A heat map



What next

Proposed future talks

Help is on the way

- My 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

Resources

If you want to improve this style

- LaTeX Beamer
  `http://latex-beamer.sourceforge.net/`
- Sharelatex Site
  `https://www.sharelatex.com`
- A Data Cleaning Mooc
  `https://www.sharelatex.com`

The chunk below will not be printed