



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 about how to get started.
- It's 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!

Why use R?

- R is free
- R is 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



Workshop files on Github

https://github.com/pechang03/SizeDoesMatter

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

```
wide Cleaning things up S
```

```
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.
##
                                               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

■ Keep the 'manager' away

projects developed into Agile

- 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

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

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



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-converse

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

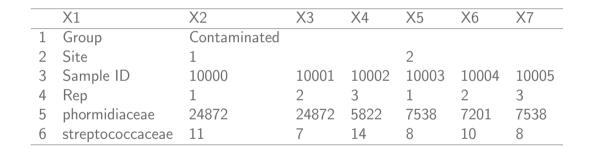
sessionInfo()
packages_in_use ← c( sessionInfo()$basePkgs, names( sessionInfo()$loadedOnly )
the_citations_list ← lapply( X=packages_in_use, FUN=citation)
the_citations_list
```



```
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
```





Transposing

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

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

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



TDD – First 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 \leftarrow as.character(ttt[i-1])
    if (table1t $Site[i]==""")
          ttt [i] ←tempb
    if (! table1t $Site [( i )]=="")
         ttt[i]←temp
table1t $Site ←ttt
```

```
## X3
```

##

Levels: 1 2 3 4 FALSE TRUE

- 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)
```

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")
```

Need coffee!!



setwd("/Users/pcru/SizeDoesMatter1")

#dir()

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

	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:
##
   $ Group
                         : Factor w/ 2 levels "Contaminated",..: 1 1 1 1 1
                         : Factor w/ 4 levels "1", "2", "3", "4": 1 1 1 2 2 2
##
   $ Site
   $ Sample.ID
                         : Factor w/ 18 levels "10000", "10001", ...: 1 2 3
##
##
   $ Rep
                         : Factor w/ 9 levels "1", "2", "3", "A", ...: 1 2 3 1 2
                          : Factor w/ 2 levels "14-May-14", "N/A": 1 1 1 1
##
   $ Spill.date
   $ Sample.collection.date: Factor w/ 4 levels "15.5.14", "17/5/14",...
##
   $ labnum
                         : Factor w/ 36 levels "2000", "2001", ...: 1 2 3 4 5
##
   $ phosphate..ppb. : Factor w/ 39 levels "10","105","108",...: 27 3
##
   $ ammonia..ppb. : Factor w/ 41 levels "10", "103", "1042",..: 10
##
   $ chlorophyll..ug.L. : Factor w/ 38 levels "1","10","11",...: 20 23
##
##
   $ DO....
                         : Factor w/ 31 levels "100", "120", "31", ...: 5 4 3
```

Break it down

First read a few rows only

```
table2 <- read.xlsx2("2_R Wkshp_dummy data_Env Data_incl2outliersMK.xlsx", shee
  header = TRUE, rowNames = FALSE, as.Data.frame = FALSE, colIndex = c(1:5),
  stringsAsFactors = FALSE, colClasses = c("character", "numeric", "numeric",
       rep("character", 2)), endRow = 4)
sapply(table2, mode)
##
       Group Site Sample.ID Rep Spill.date
   "character" "numeric" "character" "character"
##
##
       rowNames as.Data.frame
   "logical" "logical"
##
sapply(table2, class)
##
       Group Site Sample.ID Rep Spill.date
   "character" "numeric" "character" "character"
##
##
       rowNames as.Data.frame
##
    "logical" "logical"
```



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 = "Sheet2",header=TRUE,rowNames=FALSE,as.Data.frame=FALSE,
colIndex=c(1:11),stringsAsFactors=FALSE,
colClasses=c("character",rep("numeric",2),"character",rep("character",2
sapply(table2,class)

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

```
table2f <- table2
table2f$Spill.date <- as.Date(table2f$Spill.date, "%d-%b-%y")
table2f$Sample.collection.date <- as.Date(table2f$Sample.collection.date
## Frror 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$Sample.collection.date<-as.Date(ifelse
(!is.na(cdate1),as.Date(cdate1),as.Date(cdate2)), origin="1970-01-01")
table2bf$Group<-as.factor(table2bf$Group)
table2bf$Rep<-as.factor(table2bf$Rep)
dated<-table2bf$Sample.collection.date-table2bf$Spill.date</pre>
```



Count the NAs

```
na_count <-sapply(table2bf, function(y) sum(length(which(is.na(y)))))</pre>
na_count
##
                 Group
                                       Site
                                                        Sample.ID
##
                     0
##
                                  Spill.date Sample.collection.date
                   Rep
##
                                        24
##
                 labnum
                              phosphate..ppb.
                                                       ammonia..ppb.
##
##
      chlorophyll..ug.L.
                                        DO...
                                                            rowNames
##
##
             as.Data.frame
##
```

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:
                        : Factor w/ 2 levels "Contaminated"...: 1 1 1 1 1
##
   $ Group
##
   $ Site
                          : num 1112221112...
##
   $ 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
##
   $ 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 ...
```



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 unique

```
\begin{split} \text{merge}(\textbf{x}, \textbf{ y}, \textbf{ by} &= \textbf{intersect}(\textbf{names}(\textbf{x}), \textbf{ names}(\textbf{y})), \\ \textbf{by}.\textbf{x} &= \textbf{by}, \textbf{ by}.\textbf{y} &= \textbf{by}, \textbf{ all} &= \textbf{FALSE}, \textbf{ all}.\textbf{x} &= \textbf{all}, \textbf{ all}.\textbf{y} &= \textbf{all}, \\ \textbf{sort} &= \textbf{TRUE}, \textbf{ suffixes} &= \textbf{c}(".\textbf{x}",".\textbf{y}"), \\ \textbf{incomparables} &= \textbf{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","Sample.ID"))
m3<-merge(table1t,table2bf,by.x=c("Group","Site","Sample ID","Rep"),
by.y=c("Group","Site","Sample.ID","Rep"))</pre>
```



Provided

Follow up data from contaminated site

```
table3←read.xlsx2("3_Follow up data from contaminated site_MK.xlsx",
    sheetName ="Sheet1", header=TRUE, rowNames=FALSE,
    colClasses=c(rep("character",3),

rep("character",2), rep("numeric",18)))
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)
```

Joining table 3 to the other 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 values be NA or 0?
- We will do one of each.
- Generally we would use NA but in this case 0 is better as its likely the rows were missing as none were detected

```
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)]
set diff(names(m3i),names(table3fii))
m3ii\(\rightarrow\)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 sapply(table3fiii [, c(1:4)], as.character)
table3fiii [, c(7:24)] \leftarrow sapply(table3fiii [, c(7:24)], as.numeric)
table4←rbind(m3ii,table3fiii)
table4[,1] \leftarrow sapply(table4[,1], as.factor)
```

```
## Loading required package: plyr
```

[1] 24



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
- The 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

```
\label{eq:matable4} $$ \mathtt{matable4} \leftarrow \mathtt{melt(table4[,c(1:4,6:25)], variable.name} = "microbe", value.name = "abundance", id=c("Group", "Site", "Sample.ID", "Rep"), factors AsStrings=FALSE, $rm.na=TRUE() $$
```

require(reshape2)

Loading required package: reshape2

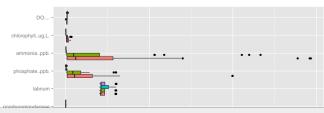
```
matable4<-melt(table4[,c(1:4,7:25)],variable.name = "microbe",
value.name = "abundance", id=c("Group", "Site", "Sample.ID", "Rep"),
factorsAsStrings=FALSE,rm.na=TRUE)</pre>
```

Using ggplot

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



values (stat_boxplot).



Finding 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>

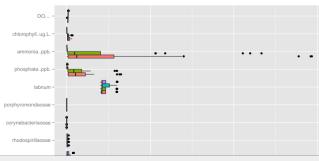


Look again ggplot

```
matable4<-melt(table4[,c(1:4,7:25)],variable.name = "microbe",
value.name = "abundance", id=c("Group","Site","Sample.ID","Rep"),
factorsAsStrings=FALSE,rm.na=TRUE)

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

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



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

```
db <- dbConnect(SQLite(), dbname="Test.sqlite")
#getConfig()$staged.queries
# sqldf(attach "Test1.sqlite" as new)
dbBegin(db)
## [1] TRUE

dbWriteTable(db, "table1", table1t, overwrite=TRUE)
## [1] TRUE</pre>
dbReadTable(db, "table1")
```



RSQLite

- Some links to RSQL ideas
- http://stackoverflow.com/questions/12307685/ join-more-than-2-tables-in-r-using-rsqlite
- https://support.rstudio.com/hc/en-us/articles/ 201057987-Quick-list-of-useful-R-packages
- https://cran.rstudio.com/web/packages/dplyr/vignettes/ introduction.html



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

```
dates 4\leftarrow table 4[,c(5,6)]
abundance \leftarrow table 4[,c(7:25)]
```

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) \\ table5 \leftarrow cbind (table4 [, 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

- 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")
```

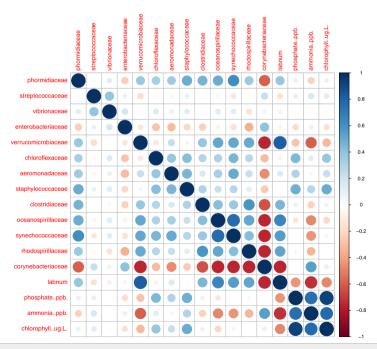
```
## [1] 23
```

Loading required package: corrplot



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 T 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 0.6.820
```