MGLC Transferable Skills Workshop: R

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May 27, 2015

1. Introduction

2. UCI ML Repository: Wine Data Set

3. Introduction to R

4. Hands-On Practice

Acknowledgments

- McCormick Graduate Leadership Council (MGLC)
- Eric Earley, Hayley Belli, Paula Straaton, Bruce Lindvall

Schedule

1. Introduction & Lecture
2. Dinner
3. Hands-on Practice

Icebreaker

Introduce yourself to your immediate neighbors and tell them:

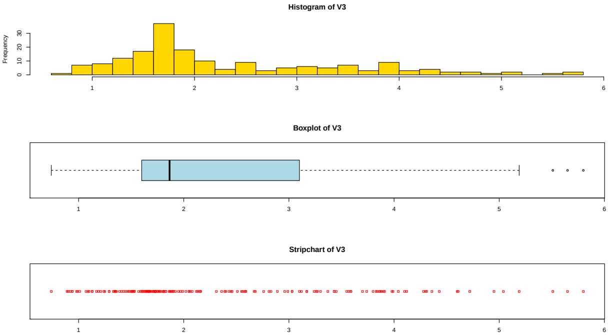
- Your department and/or research interests
- Your favorite programming language
- Your level of experience with R

Wine Data Set

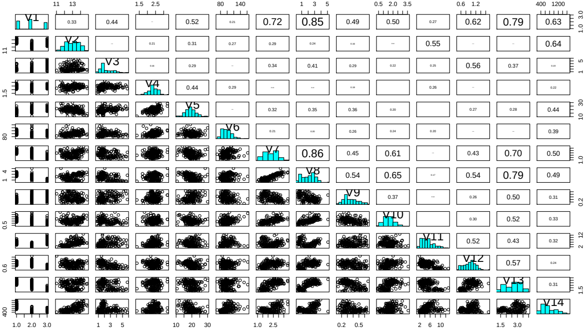
The UCI ML Repository: Wine Data Set:
`https://archive.ics.uci.edu/ml/index.html`

- Chemical analysis of wine from three different cultivators
- 178 samples, 13 attributes (+ CLASS)

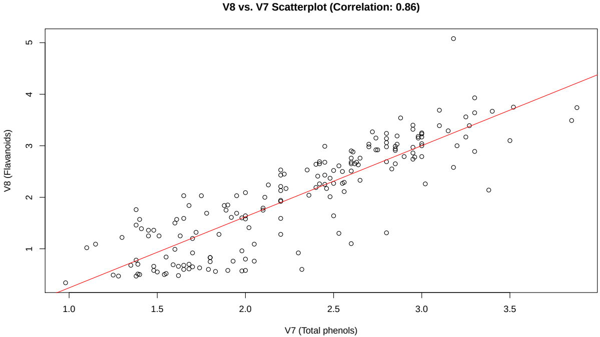
Wine Data Set: V3 (Malic acid)



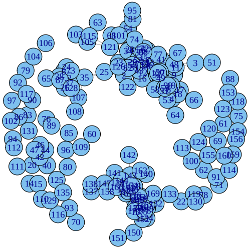
Wine Data Set: Scatterplot Matrix



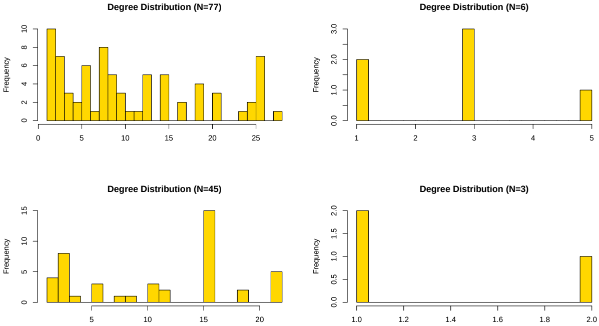
Wine Data Set: Total phenols vs Flavanoids



Wine Data Set: Network ($\rho \geq 0.99$)



Wine Data Set: Graph Components ($N \geq 3$)


Degree Distribution (N=77)

Degree Distribution (N=6)

Degree Distribution (N=45)

Degree Distribution (N=3)

Packages

Repositories

- CRAN (as of today) has **6690** packages for modeling, visualization, etc.
- Bioconductor (as of today) has **1024** packages for analysis of high-throughput genomic data

Download and load packages with

- `install.packages()`
- `library()`

Importing Data

Import data from a CSV file or install packages to **directly** import form Excel, Stata, etc.

- **CSV**: `read.table()` : NB. The default separator is a white space
- **Excel**: `read.xlsx()`
- **Stata**: `read.dta()`

Sweave

Create dynamic reports (i.e. reproducible research) with Sweave

- Combine both LaTeX and R code in one document
- Part of every installation

`*.rnw` → `*.tex` →`*.pdf`

- Begin with a LaTeX document, but with the extensions `*.rnw`
- R commands start with $\ll\gg=$ and end with `@`
- Process the Sweave file in R with `Sweave()` and compile the resulting `*.tex` file

Quest

- `R` is installed on Quest
- Install packages by logging in and using `install.packages()`
- Submit a job by creating a submission script and `*.R` script

Working with R

- `?` : pop-out help for stated function
- `str()` : short description of any R data structure
- `getwd()`
- `setwd()`
- `ls()` : returns a vector of strings giving names of objects
- `rm()` : pass in either an object or (with the `list` argument) character vector naming the object

How do you clear your workspace?

Data Manipulation: Data Types

There are four types of data.

1. Logical
2. Integer
3. Double (aka Numeric)
4. Character

NB. Individual numbers or strings are actually vectors of length one

Data Manipulation: Data Structures

Homogenous data structures

- 1d: Atomic vector: `c()`
- 2d: Matrix: `matrix()`
- nd: Array

Heterogeneous data structures

- 1d: List: `list()`
- 2d: Data frame: `data.frame()`

NB. A ‘factor’ is a vector that can contain only predefined values (**cf.** Advanced R by Hadley Wickham)

Data Manipulation: Lists

- Three properties: Type (e.g. Double), Length, Attributes (Arbitrary metadata)
- Attributes include: Names and Dimensions
- The elements of a list can have different types. NB. Lists can contain other lists.
- Under the hood, data frames are lists of equal length vectors
- Linear model objects (`lm()`) are lists

If the columns of a data frame are of different types, can the elements of a column be of different types?

Data Manipulation: Subsetting

With the subsetting operator `[`, you can use

- Positive integers: return elements at specified positions
- Negative integers: omit elements at specified positions
- Logical vectors: select elements where the logical value is `T`
- Nothing: returns the original vector: NB. Very useful for matrices, data frames, and arrays
- Character vectors: return elements with matching names.

Data Manipulation: Subsetting

- Using `[` will always return a list, `[[` pulls out the elements of a list
- ‘If list `x` is a train carrying objects, then `x[[5]]` is the object in car 5; `x[4:6] is a train of cars 4-6`’
- Include `drop=F` when subsetting matrices and data frames
- To modify selected values, values combine subsetting with `<-` (assignment)

If `sample(x)` takes a sample from the elements of `x`, how can you use `sample()` to randomly permute the columns of a data frame?

‘Split-Apply-Combine’

R has standard control structures

- `for (var in seq){ expr }`
- `while (cond){ expr }`
- `if (cond) expr1 else expr2`

but it has built in ‘functionals’ that take in a function apply it to each component and then combine the results

- `lapply` applies a function to each element in a list and returns a list
- `lapply(x,function())`
- Other loop functionals use different types of input and output (**cf.** `dplyr`)

NB. You can loop over the elements, numeric indices, or the names.

Functions

Abstract code into small functions

```
myfunction <- function(arg1,arg2=3,...){
statements return(object)}
```

- Arguments can have default values (e.g. `arg2` above)
- It's not necessary a function return anything (e.g. plotting)
- Use the `source()` to load functions

Plotting

R has strong graphical capabilities and can create for example

- Density plots: `hist()`
- Boxplots: `boxplot()`
- Scatter plots: `plot()`: Use `abline()` to add lines
- Combine plots using the `par` function and `mfrow` or `mfcol` arguments

The `lattice` and `ggplot2` are popular visualization packages

(**cf.** Quick-R: Basic Graphs, Advanced Graphs)

Style

- Use a consistent style
- Strive for names that are concise and meaningful
- Place spaces around all operators
- Use <- not = for assignment
- Comment with #
- Use commented lines to break up your file

References and Resources

References:

- http://adv-r.had.co.nz/
- http://www.statmethods.net/
- http://www.statistik.tuwien.ac.at/public/filz/students/SweaveExa.pdf
- http://nicercode.github.io/

Resources:

- http://google-styleguide.googlecode.com/svn/trunk/Rguide.xml
- http://stackoverflow.com/
- http://www.stat.columbia.edu/~tzheng/files/Rcolor.pdf

Hands-On Practice (Solutions in 'RWorkshop.rnw')

With your neighbors,

- Write a function that returns the first n values of the Fibonacci sequence ($F_1 = F_2 = 1, F_i = F_{i-1} + F_{i-2}$)
- Import the Wine Data Set and create a histogram, boxplot, & stripchart of Malic acid (V3). Combine the plots.
- Create a scatterplot matrix of the data set using `pairs()`. Read its documentation and put histograms on the diagonal and correlations on the upper triangle.
- Create a scatterplot of Total phenols vs Flavanoids. Calculate the Pearson correlation and include it in the title of the plot. Combine `abline` and `lm` to add a regression line on the plot. (cf. Quick-R)

Hands-On Practice (Solutions in ‘RWorkshop.rnw’)

With your neighbors,

- Calculate a 178 × 178 **Spearman** correlation matrix of the wines. (exclude the `CLASS` variable (V1) in your calculation). Create an adjacency matrix by setting all entires of the correlation matrix ≥ 0.99 to 1 and all entries 0.99 to 0
- Install and load the `igraph` package. Use the above adjacency matrix to create an undirected, unweighted, graph without simple loops. Plot the network.
- Use `decompose.graph` and `lapply` to calculate the number of nodes and the degree distribution of each component (with at least three nodes) of the above network. Plot the degree distribution of each of those components. Combine the plots. Include the number of nodes in the component in the title of the plot.