Introduction to Bioinformatics

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R

R

R is ‘GNU S’, a freely available language and environment for statistical computing and graphics which provides a wide variety of statistical and graphical techniques: linear and nonlinear modelling, statistical tests, time series analysis, classification, clustering, etc.

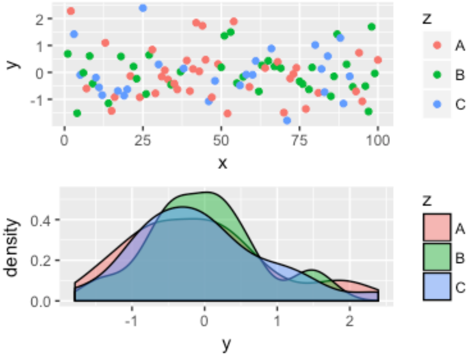
`https://cran.r-project.org/doc/FAQ/R-FAQ.html`

- statistical computation and graphics
- influenced by two existing languages: S (similar appearence) and Scheme (underlying implementation and semantics)
- interpreted
- distributed under a GNU-style copyleft
- Unix-like, Windows and Mac families OS
  - 386, amd64/x86_64, alpha, arm, arm64, hppa, mips/mipsel, powerpc, s390x and sparc CPUs , i386-hurd-gnu, cpu-kfreebsd-gnu for i386 and amd64, i386-pc-solaris, rs6000-ibm-aix, sparc-sun-solaris, x86_64-apple-darwin, x86_64-unknown-freebsd and x86_64-unknown-openbsd

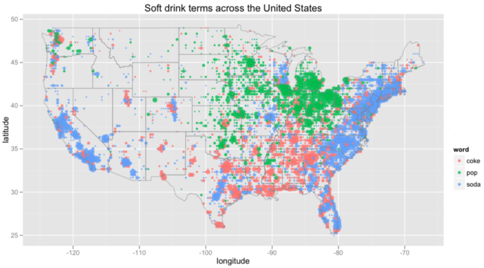
Why R I

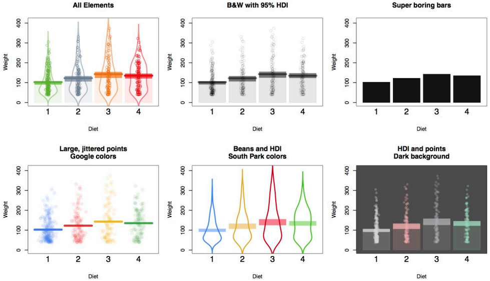
- Free!
- Large user community that contributes packages
- Extremely flexible in abilities
- Graphics capabilities are remarkable
- Fast and efficient
- Interfaces with Microsoft Office Excel
- Can program almost anything AND save and repeat

Why R II



Why R III


Soft drink terms across the United States
latitude
50
45
40
35
30
25
longitude
-120
-110
-100
-90
-80
-70
word
coke
pop
soda


All Elements
B&W with 95% HDI
Super boring bars
Large, jittered points
Google colors
Beans and HDI
South Park colors
HDI and points
Dark background
Weight
0
100
200
300
400
Diet
1
2
3
4

Why R IV

- Requires patience
- Somewhat steep learning curve for R
- Somehow different than other typical programming languages

Operators

Operators	Type of operator
+ − * / %% %/% ^	arithmetic
> >= < <= == ! =	Relational
! & |	logical
< − − > =	assignment
$	reference to list object
:	sequence creation

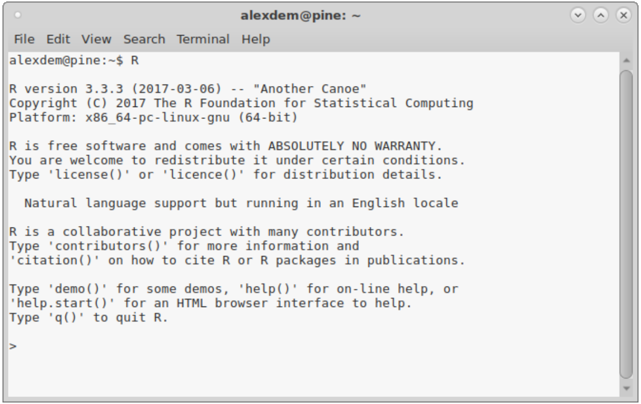
Basic functions

Function	Explanation
log(x)	log to base e of x
exp(x)	antilog of x (e^x)
log(x,n)	log to base n of x
log10(x)	log to base 10 of x
sqrt(x)	$\sqrt{x}$
factorial(x)	$x!$
floor(x)	$\lfloor x \rfloor$
ceiling(x)	$\lceil x \rceil$
round(x, digits=0)	round the value of x to an integer
signif(x, digits=6)	give x to 6 digits in scientific notation
abs(x)	$\|x\|$
cos(x)	cosine of x in radians
sin(x)	sin of x in radians
tan(x)	tan of x in radians

Basic array functions

Function	Explanation
max(x)	maximum value in x
min(x)	minimum value in x
range(x)	vector of min(x) and max(x)
sum(x)	total of all the values in x
mean(x)	arithmetic average of the values in x
median(x)	median value in x
var(x)	sample variance of x
cor(x,y)	correlation between vectors x and y
sort(x)	a sorted version of x
order(x)	an integer vector containing the permutation to sort x into ascending order
quantile(x)	vector containing the minimum, lower quartile, median, upper quartile, and maximum of x
colMeans(x)/rowMeans(x)	column/row means of dataframe or matrix x
colSums(x)/rowSums(x)	column/row totals of dataframe or matrix x

Initial screen I



```
alexdem@pine:~$ R

R version 3.3.3 (2017-03-06) -- "Another Canoe"
Copyright (C) 2017 The R Foundation for Statistical Computing
Platform: x86_64-pc-linux-gnu (64-bit)

R is free software and comes with ABSOLUTELY NO WARRANTY.
You are welcome to redistribute it under certain conditions.
Type 'license()' or 'licence()' for distribution details.

  Natural language support but running in an English locale

R is a collaborative project with many contributors.
Type 'contributors()' for more information and
'citation()' on how to cite R or R packages in publications.

Type 'demo()' for some demos, 'help()' for on-line help, or
'help.start()' for an HTML browser interface to help.
Type 'q()' to quit R.

>
```

- All commands are given after the “>” symbol

Initial screen II

```
> 4+4
[1] 8
> 3*4
[1] 12
> 5/2
[1] 2.5
> 5%%2 #remainder
[1] 1
> 5%/%2 #quotient
[1] 2
```

Initial screen III

```
> log(10)
[1] 2.302585
> log(10,10)
[1] 1
```

Inf & NaN

Inf (Infinity)

```
> 100/0
[1] Inf
> -100/0
[1] -Inf
```

Not a Number (NaN)

```
> 0/0
[1] NaN
>Inf-Inf
[1] NaN
```

Logic values

```
> 10>1
[1] TRUE
> 10<1
[1] FALSE
> 100 == 100
[1] TRUE
```

Vectors I

- Every user input is considered (by default) a vector
- [1] refers to the index of the first object of the (first) row
- One-based numbering is used for the indexes of a vector

```
> 1
[1] 1
> 1:5
[1] 1 2 3 4 5
> 1:25
 [1]  1  2  3  4  5  6  7  8  9 10 11 12 13
[14] 14 15 16 17 18 19 20 21 22 23 24 25
```

Vectors II

- The c(...) function (combine) allows the creation of larger vectors

```
> c(1,3,5,7,9)
[1] 1 3 5 7 9
> c(1,3,5,7,9)+c(2,4,6,8,10)
[1]  3  7 11 15 19
> c(1, 2, 3, 4) + 1
[1] 2 3 4 5
```

Vectors III

```
> c(1,3,5,7,9)+c(2,4)
[1]  3  7  7 11 11
Warning message:
In c(1, 3, 5, 7, 9) + c(2, 4) :
  longer object length is not a multiple of shorter object
     length
```

Vectors IV

```
> "Hello world."
[1] "Hello world."
> c("Hello world", "Hello again")
[1] "Hello world" "Hello again"
```

Comments

- Whatever follows the # symbol is considered a comment and is ignored

```
> 1 +2 +3
[1] 6
> 1 +2 #+3
[1] 3
```

Variables I

- As an interpreted language, the variables do not have to be declared prior to usage
- Case-sensitive, i.e. x is considered different to X
- Variable names cannot
  - start with digits (e.g. 1variable) or symbols (e.g. %variable)
  - contain spaces, e.g. variable.name and not variable name

```
> x <- 1
> x
[1] 1
> 1 -> x
> x
[1] 1
```

Variables II

```
> x = 1
> x
[1] 1
```

Variables III

```
> x = 1
> x
[1] 1
> y <- "a"
> y
[1] "a"
> z=c(x,y)
> z
[1] "1" "a"
```

Variables IV

```
> x=11:20
> x
 [1]  11  12 13  14  15  16  17  18  19 20
> x[4]
[1] 14
> x[1:4]
[1] 11 12 13 14
> x[c(4,10)]
[1]  14 20
> x[-c(1:4)]
[1]  15  16  17  18  19 20
```

Variables V

```
> x[x<15]
[1] 11 12 13 14
> x<15
 [1]  TRUE  TRUE  TRUE  TRUE FALSE FALSE FALSE FALSE FALSE
   FALSE
```

Functions

```
> f <- function(x,y) {x + y}
> f(1,2)
[1] 3
> g <- function(x,y) {c(x + y,x * y)}
> g(1,2)
[1] 3 2
```

Factors I

```
> x=c("a","b","a","a","b")
> x
[1] "a" "b" "a" "a" "b"
> x=factor(x)
> x
[1] a b a a b
Levels: a b
```

Factors II

```
> attributes(x)
$levels
[1] "a" "b"
$class
[1] "factor"
```

Factors III

```
> x
[1] a b a a b
Levels: a b
> levels(x)
[1] "a" "b"
> levels(x)=c("0","1")
> x
[1] 0 1 0 0 1
Levels: 0 1
```

Arrays I

```
> a <- array(11:16,dim=c(3,2))
> a
     [,1] [,2]
[1,]   11   14
[2,]   12   15
[3,]   13   16
> a[1,2]
[1] 14
```

Arrays II

```
> a[1:2,1:2]
     [,1] [,2]
[1,]   11   14
[2,]   12   15
```

Arrays III

```
> a>13
      [,1] [,2]
[1,] FALSE TRUE
[2,] FALSE TRUE
[3,] FALSE TRUE
> a[1]
[1] 11
> a[1,]
[1] 11 14
> a[,1]
[1] 11 12 13
```

Arrays IV

```
> which(a>13)
[1] 4 5 6
> which(a>13,arr.ind=T)
     row col
[1,]   1   2
[2,]   2   2
[3,]   3   2
```

Arrays V

```
> b=array(1:12,dim=c(2,2,3))
> b
, , 1
     [,1] [,2]
[1,]    1    3
[2,]    2    4
, , 2
     [,1] [,2]
[1,]    5    7
[2,]    6    8
```

Arrays VI

```
, , 3
     [,1] [,2]
[1,]    9   11
[2,]   10   12
```

Arrays VII

In general in R :

- vector → one dimensional array
- matrix → two dimensional array
- array → array of any dimensional

Lists I

- Lists can contain objects of different types, e.g. numbers and strings

```
> mylist=list(name="alex",id=1234)
> mylist
$name
[1] "alex"

$id
[1] 1234
> mylist$name
[1] "alex"
```

Lists II I

```
> mylist2=list(list(name="alex",id=1234),
   list(name="alex2",id=1234))
> mylist2
[[1]]
[[1]]$name
[1] "alex"
[[1]]$id
[1] 1234
```

Lists II II

```
[[2]]
[[2]]$name
[1] "alex2"
[[2]]$id
[1] 1234
```

Data frame I

- A list that contains multiple vectors of the same size
- It resembles a spreadsheet

```
> names=c("alex","john","tom")
> ids=c(1,2,3)
> ZipCode=c(5544,2343,1234)
> data=data.frame(names,ids,ZipCode)
> data
  names ids ZipCode
1  alex   1    5544
2  john   2    2343
3   tom   3    1234
```

Data frame II

```
> data$ids
[1] 1 2 3
> data$ZipCode[data$names=="alex"]
[1] 5544
> data$names
[1] alex john tom
Levels: alex john tom
> data[data$names=="alex",]
  names ids ZipCode
1  alex   1    5544
```

Data frame III

```
> colnames(data)
[1] "names"   "ids"     "ZipCode"
> data [ ,2:3]
  ids ZipCode
1   1    5544
2   2    2343
3   3    1234
> colSums(data[,2:3])
    ids ZipCode
      6    9121
> rowSums(data[,2:3])
[1] 5545 2345 1237
```

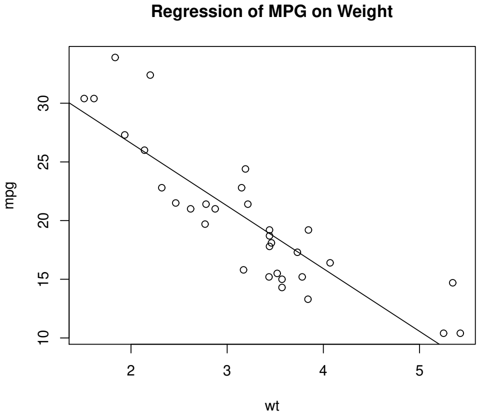
Classes

```
> class(data)
[1] "data.frame"
> class(names)
[1] "character"
> class(ids)
[1] "numeric"
> class(ZipCode)
[1] "numeric"
> class(g)
[1] "function"
```

Creating Plots I

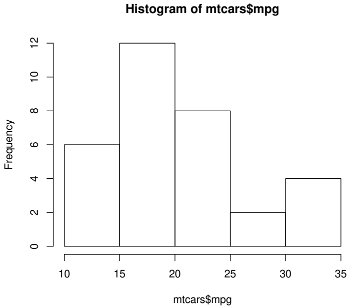
```
# Import data extracted from the 1974 Motor
# Trend US magazine
# mpg   -->     Miles/(US) gallon
# wt    -->     Weight (1000 lbs)
# gear  -->     Number of forward gears
# examples from http://www.statmethods.net/index.html
> attach(mtcars)
> plot(wt, mpg)
> abline(lm(mpg~wt))
> title("Regression of MPG on Weight")
```

Creating Plots II



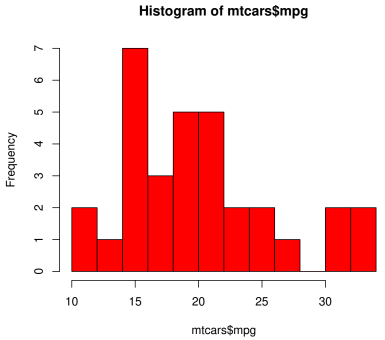
Histograms I

```
> hist(mtcars$mpg)
```



Histograms II

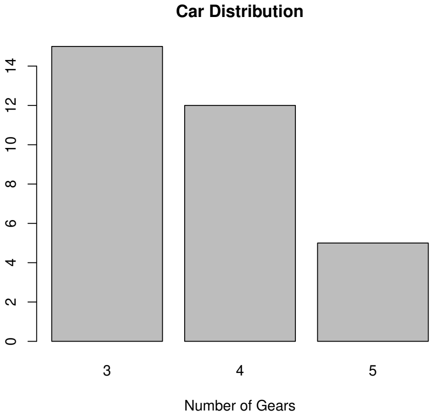
```
> hist(mtcars$mpg, breaks=12, col="red")
```



Barplots I

```
> counts <- table(mtcars$gear)
> counts
 3  4  5
15 12  5
> barplot(counts, main="Car Distribution",
   xlab="Number of Gears")
```

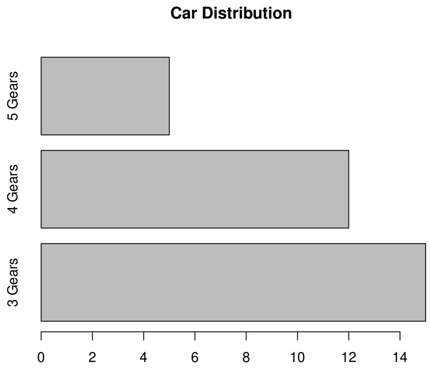
Barplots II



Barplots III

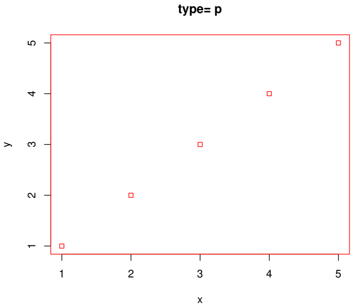
```
> counts <- table(mtcars$gear)
> barplot(counts, main="Car Distribution", horiz=TRUE,
   names.arg=c("3 Gears", "4 Gears", "5 Gears"))
```

Barplots IV



Line Chart

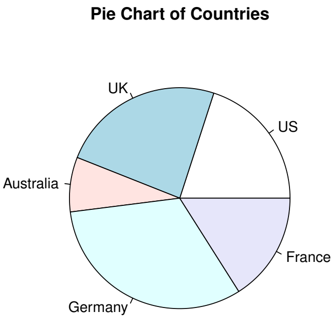
```
> x <- c(1:5); y <- x # create some data
> plot(x, y, type="p", main=heading)
```



Pie Chart I

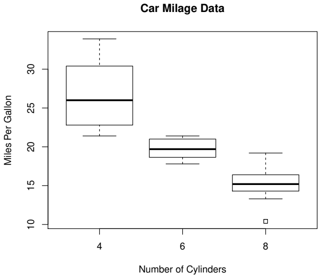
```
> slices <- c(10, 12, 4, 16, 8)
> lbls <- c("US", "UK", "Australia", "Germany", "France")
> pie(slices, labels = lbls, main="Pie Chart of Countries")
```

Pie Chart II



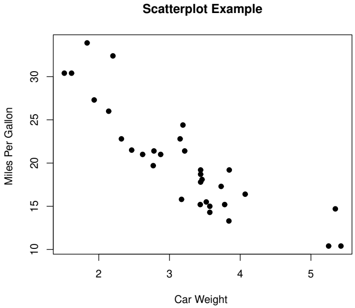
Boxplot

```
# Boxplot of MPG by Car Cylinders
> boxplot(mpg~cyl,data=mtcars, main="Car Milage Data",
   xlab="Number of Cylinders", ylab="Miles Per Gallon")
```



Scatterplot

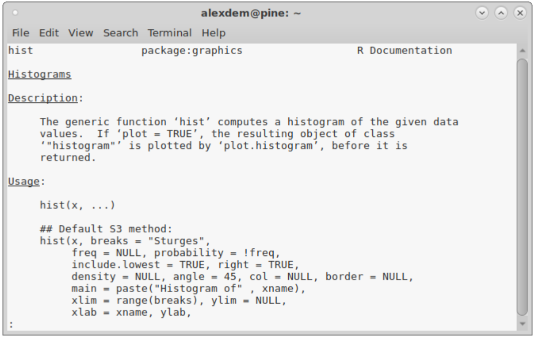
```
> plot(wt, mpg, main="Scatterplot Example", xlab="Car
   Weight ", ylab="Miles Per Gallon ", pch=19)
```



Help I

- R has a help system for built-in functions and installed packages

```
> ?hist
```

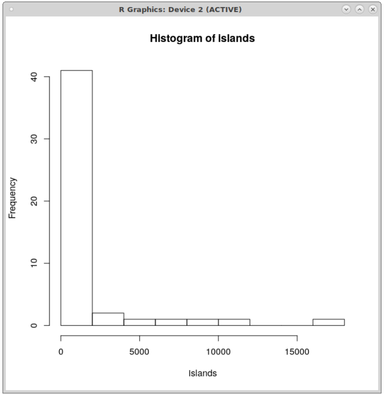


```
hist                     package:graphics                     R Documentation

Histograms

Description:

     The generic function ‘hist’ computes a histogram of the given data
     values.  If ‘plot = TRUE’, the resulting object of class
     ‘"histogram"’ is plotted by ‘plot.histogram’, before it is
     returned.

Usage:

     hist(x, ...)

     ## Default S3 method:
     hist(x, breaks = "Sturges",
          freq = NULL, probability = !freq,
          include.lowest = TRUE, right = TRUE,
          density = NULL, angle = 45, col = NULL, border = NULL,
          main = paste("Histogram of" , xname),
          xlim = range(breaks), ylim = NULL,
          xlab = xname, ylab,
:
```

Help II

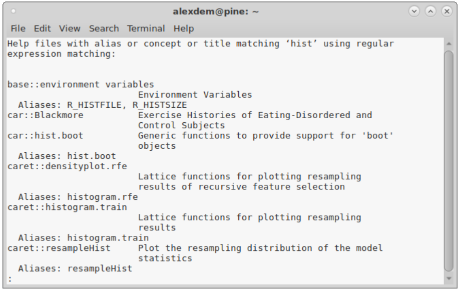
```
> example(hist)
> op <- par(mfrow = c(2, 2))
> hist(islands)
```

Help III


R Graphics: Device 2 (ACTIVE)
Histogram of Islands
Frequency
0
10
20
30
40
0
5000
10000
15000
Islands

Help IV

```
> ??hist
```



```
Help files with alias or concept or title matching ‘hist’ using regular
expression matching:


base::environment variables
                        Environment Variables
  Aliases: R_HISTFILE, R_HISTSIZE
car::Blackmore          Exercise Histories of Eating-Disordered and
                        Control Subjects
car::hist.boot          Generic functions to provide support for 'boot'
                        objects
  Aliases: hist.boot
caret::densityplot.rfe
                        Lattice functions for plotting resampling
                        results of recursive feature selection
  Aliases: histogram.rfe
caret::histogram.train
                        Lattice functions for plotting resampling
                        results
  Aliases: histogram.train
caret::resampleHist     Plot the resampling distribution of the model
                        statistics
  Aliases: resampleHist
:
```

Help V

vignette

A Vignette is a free-form document describing a package usage with examples

```
> vignette("affy")
```

Hands on

- Create a vector (A) of 100 elements, containing the values from 1 to 100
- Create a vector (B) of 100 elements, containing the values from 100 to 1
- Create a data frame (DF) with 2 columns, containing the vectors A and B
- Add a new column to DF, containing the sum of the elements of A and B at each row
- Plot sin(x) for a range of x from -10 to 10 with various steps, e.g. 1, 0.5, 0.01

Exercise 3 - Familiarizing with R

- Filter data
- Create plots
- . . .

Submit via e-class assigment

`https://eclass.uoa.gr/modules/work/index.php?course=DI425&id=46015`

OR by email at alexdem@di.uoa.gr

`https://eclass.uoa.gr/modules/document/file.php/DI425/2023-24/exercises/ITBI2023-exercise3-ACD24102023.zip`

DEADLINE 7/11/23

Questions?

?