R

Bioinformatics Applications (PLPTH813)

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Outline

- R introduction
- Data structure
- Data input and output
- Basic graphics
- String operations
- Functions
- Simple statistical test

R

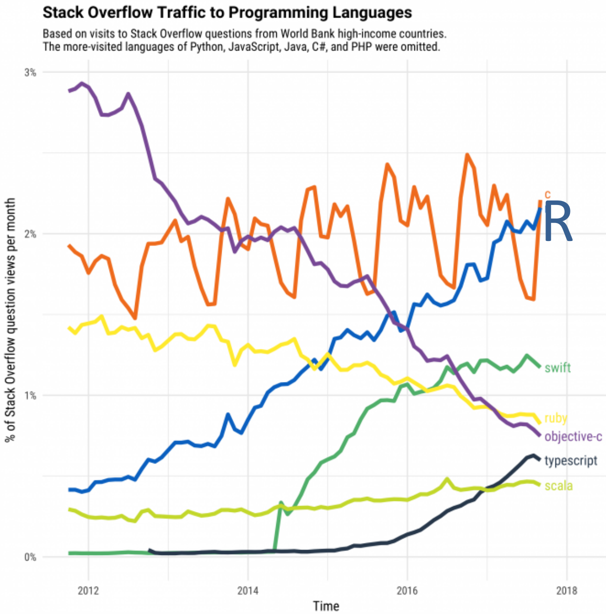
- R is a programming language and a cutting-edge tool for data analysis, especially for **statistical computing** and **graphics**.

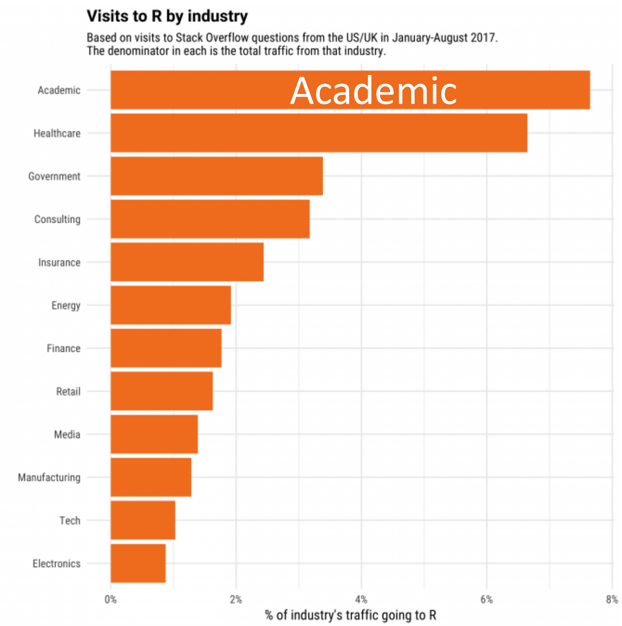
- R is powerful. Applications are easily created by writing new **functions**. Functions are usually distributed through **packages**.

- It has great community supports.

- R is free

www.r-project.org





Example – statistical test

		B	
A	12	36	
	24	70	

- χ^2 test

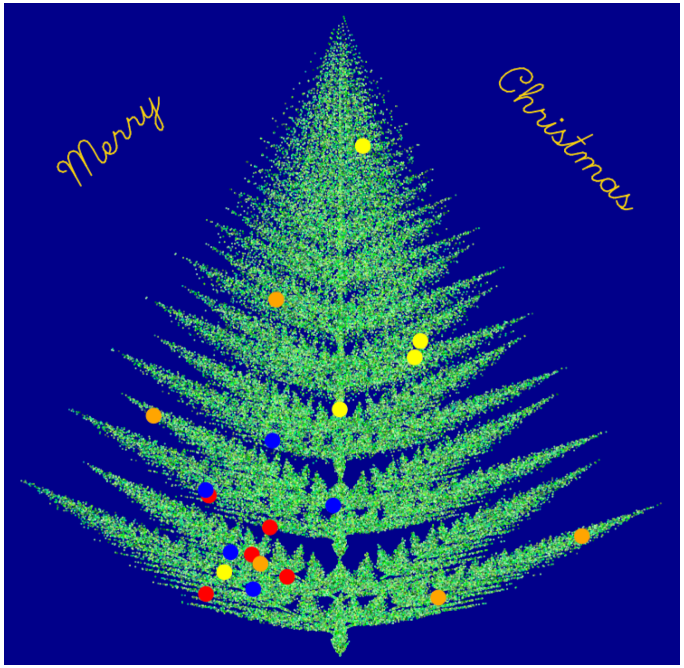
```
d <- c(12, 36, 24, 70)
dm <- matrix(d, nrow=2, byrow=T)
chisq.test(dm)
```

data: dm

X-squared = 0, df = 1, p-value = 1

Example – Christmas tree

```r
# Christmas tree
L <-  matrix(
  c(0.03,  0,     0  ,  0.1,
    0.85,  0.00,  0.00, 0.85,
    0.8,   0.00,  0.00, 0.8,
    0.2,  -0.08,  0.15, 0.22,
    -0.2,   0.08,  0.15, 0.22,
    0.25, -0.1,   0.12, 0.25,
    -0.2,   0.1,   0.12, 0.2),
  nrow=4)
# ... and each row is a translation vector
B <- matrix(
  c(0, 0,
    0, 1.5,
    0, 1.5,
    0, 0.85,
    0, 0.85,
    0, 0.3,
    0, 0.4),
  nrow=2)

prob = c(0.02, 0.6,.08, 0.07, 0.07, 0.07, 0.07)

# Iterate the discrete stochastic map
N = 1e5 #5  #   number of iterations
x = matrix(NA,nrow=2,ncol=N)
x[,1] = c(0,2)   # initial point
k <- sample(1:7,N,prob,replace=TRUE) # values 1-7

for (i in 2:N)
  x[,i] = crossprod(matrix(L[,k[i]],nrow=2),x[,i-1]) + B[,k[i]] # iterate

# Plot the iteration history
#png('card.png')
par(bg='darkblue',mar=rep(0,4))
plot(x=x[1,],y=x[2,],
     col=grep('green',colors(),value=TRUE),
     axes=FALSE,
     cex=.1,
     xlab='',
     ylab='' )#,pch='.')

bals <- sample(N,20)
points(x=x[1,bals],y=x[2,bals]-.1,
       col=c('red','blue','yellow','orange'),
       cex=2,
       pch=19
)
text(x=-.7,y=8,
     labels='Merry',
     adj=c(.5,.5),
     srt=45,
     vfont=c('script','plain'),
     cex=3,
     col='gold'
)
text(x=0.7,y=8,
     labels='Christmas',
     adj=c(.5,.5),
     srt=-45,
     vfont=c('script','plain'),
     cex=3,
     col='gold'
)
```



R commands, case sensitivity

- **Expression:** Print the value and not save the value in the environment

2 + 4
68 * 0.15

- **Assignment:** Assign values to a **variable**

y <- 2
y = 2
assign("y", 2)
Y <- 2 + 4

- **Comments (#)**

Notes/explanation to the scripts, starting with a hashtag ('#'), everything to the end of the line is a comment.

y <- 2 + 4 # an example of the assignment
y <- 2 + 4

Data structure – vector (I)

A vector is a single entity consisting of an ordered collection of numbers, characters, logical quantities, etc.

- **Numeric vector**

x <- c(10.4, 5.6, 3.1, 6.4, 21.7)

sum(x)

y <- 2

2*x + y

c(10.4, 5.6, 3.1, 6.4, 21.7)

↑ 1st ↑ 2nd ...

x[2]

- **Logical vector**

lv <- c(TRUE, FALSE, TRUE, TRUE)

lv == FALSE

sum(lv)

The logical operators are <, <=, >, >=, ==, and !=.

== for exact equality and != for inequality.

x <- c(10.4, 5.6, 3.1, 6.4, 21.7)

lv2 <- x > 10

Data structure – vector (II)

- **Character vectors**

cv <- c("a", "b", "c")

cv2 <- paste(cv, 1:3, sep="")

- **Missing values: NA, not available**

mvv <- c("a", "b", "c", NA)

is.na(mvv)

Select a subset and modify a vector

- **Select a subset of a vector**

```
x <- c(4, 5, 7, 3, 9)
x[c(2, 3)]
x[x>10]
x[-c(1,5)]
```

- **Modify a vector**

```
x[3] <- 23.1
x <- c(x, 10.9)
names(x) <- c("a", "b", "c", "d", "e", "f")
```

mode and length of a vector

- **Mode**

Vectors must have their values with the same mode, either numeric, character, logical, or other types.

```
z <- 0:9
is.numeric(z)
digits <- as.character(z) # convert to character
d <- as.integer(digits) # convert to integer
```

- **Length**

```
length(z)
length(z) <- 5  # retain just the first 5 values
```

factor

Definition: A factor is a vector object used to specify a discrete classification (grouping) of the components of other vectors with the same length.

- **factor = regular vector + Levels**

```
state <- c("tas", "sa", "qld", "nsw",
           "nsw", "nt", "wa", "wa",
           "qld", "vic", "nsw", "vic")
statef <- factor(state)
> statef
[1] tas sa qld nsw nsw nt wa wa qld vic nsw vic
Levels: nsw nt qld sa tas vic wa
> levels(statef)
[1] "nsw" "nt" "qld" "sa" "tas" "vic" "wa"
```

```
state2 <- as.character(statef)
```

matrix

- matrix: a collection of data elements arranged in a two-dimensional rectangular layout

$\begin{bmatrix} 1 & 2 & 3 \\ 4 & 5 & 6 \end{bmatrix}$ 2 rows and 3 columns

```
num <- 1:6
numm <- matrix(num, nrow=2, byrow=T)
```

matrices can be built up by using the functions cbind() and rbind():

cbind(): binding together horizontally, or column-wise
rbind(): binding together vertically, or row-wise.

data.frame

name	age	>30?	gender
Josh	23	FALSE	male
Rose	35	TRUE	female
Jone	18	FALSE	male
Molly	21	FALSE	female
Lisa	36	TRUE	female

- **Data frame**

A data frame may be regarded as a matrix with columns possibly of differing modes and attributes. The data of a matrix are of the same type or mode.

- **Making data frames**

```
df <- data.frame(name=c("Josh", "rose"), age=c(23, 35))
```

- **Working with data frames**

```
> df$name
[1] Josh rose
Levels: Josh rose
> df[, 1]
[1] Josh rose
Levels: Josh rose
```

```
> df[[1]]
[1] Josh rose
Levels: Josh rose
> df[1]
  name
1 Josh
2 rose
```

```
head(df); tail(df); summary(df); str(df)
```

list

A list is a general form of vector in which the various elements need not be of the same type.

- **Objects can be any types or modes**

```
lst <- list(name="Fred", wife="Mary", nkids=3, kid.ages=c(4,7,9))

> lst[1]  # sublist
$name
[1] "Fred"

> lst[[1]] # first element in the list
[1] "Fred"

> lst$name # the element named "name"
[1] "Fred"
```

Problem

```
df <- data.frame(name=c("Josh","rose","John"),
age=c(23, 35, 18))
```

What are the values of

name	age
Josh	23
Rose	35
Jone	18

df[2, 1]
df[3, 2]
df[2]
df[, 2]

What is the difference between the last two?

Data import

```
lisa Jone
28 21
```

- **scan()**: to read data from a file to a vector or list

```
cat("lisa Jone", "28 21", file = "hrdb.txt", sep = "\n")
hr <- scan("hrdb.txt", what=character())
hr
"lisa" "Jone" "28"   "21”
```

- **read.table()**: to read a data frame (table) directly

read.delim, read.csv

```
d <- read.table(data)
```

Input file form with names and row labels:

	Price	Floor	Area	Rooms	Age	Cent.heat
01	52.00	111.0	830	5	6.2	no
02	54.75	128.0	710	5	7.5	no
03	57.50	101.0	1000	5	4.2	no
04	57.50	131.0	690	6	8.8	no
05	59.75	93.0	900	5	1.9	yes

...

Data export

- **write.table()** or **write.csv()**

```
## To write a tab-delimited file:
x <- data.frame(a = "pi", b = pi)
write.table(x, file="foo.txt", sep="\t", row.names=FALSE)

## and to read this file back into R one needs
read.table("foo.txt")

## Alternatively
write.csv(x, file = "foo.csv”, row.names=FALSE)
read.csv("foo.csv")
```

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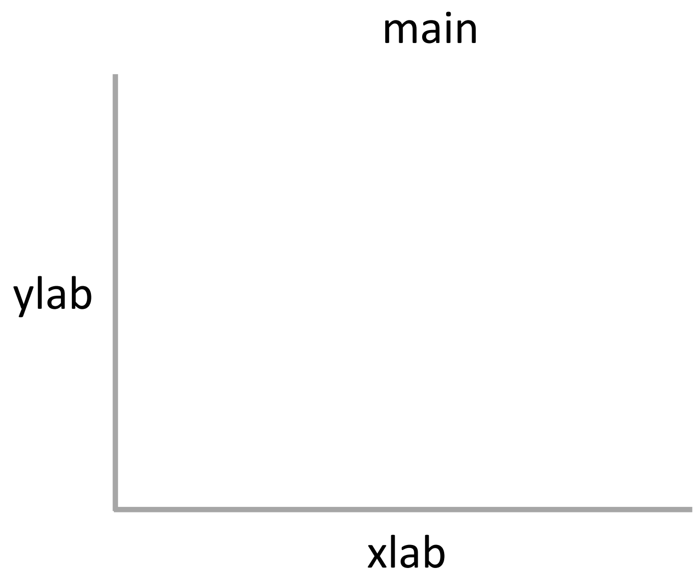
Basic graphics

- **plot(); points(); lines(); abline(); text(); legend()**

High-level plot: create a new plot

```
plot(x, y, xlab, ylab, main, …)
```

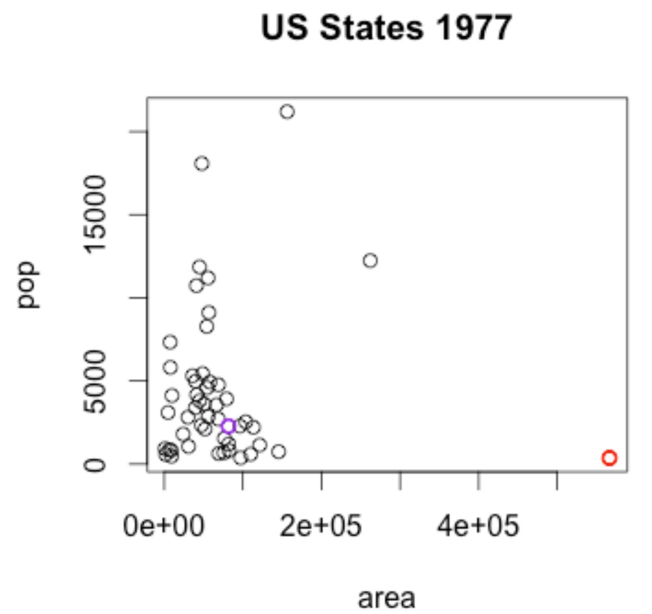


Low-level plot: add to an existing plot

```
# add points
points(x, y)

# add lines
lines(x, y)

# add horizontal or vertical lines
abline(h, v)

# add text or legend
text()
legend()
```

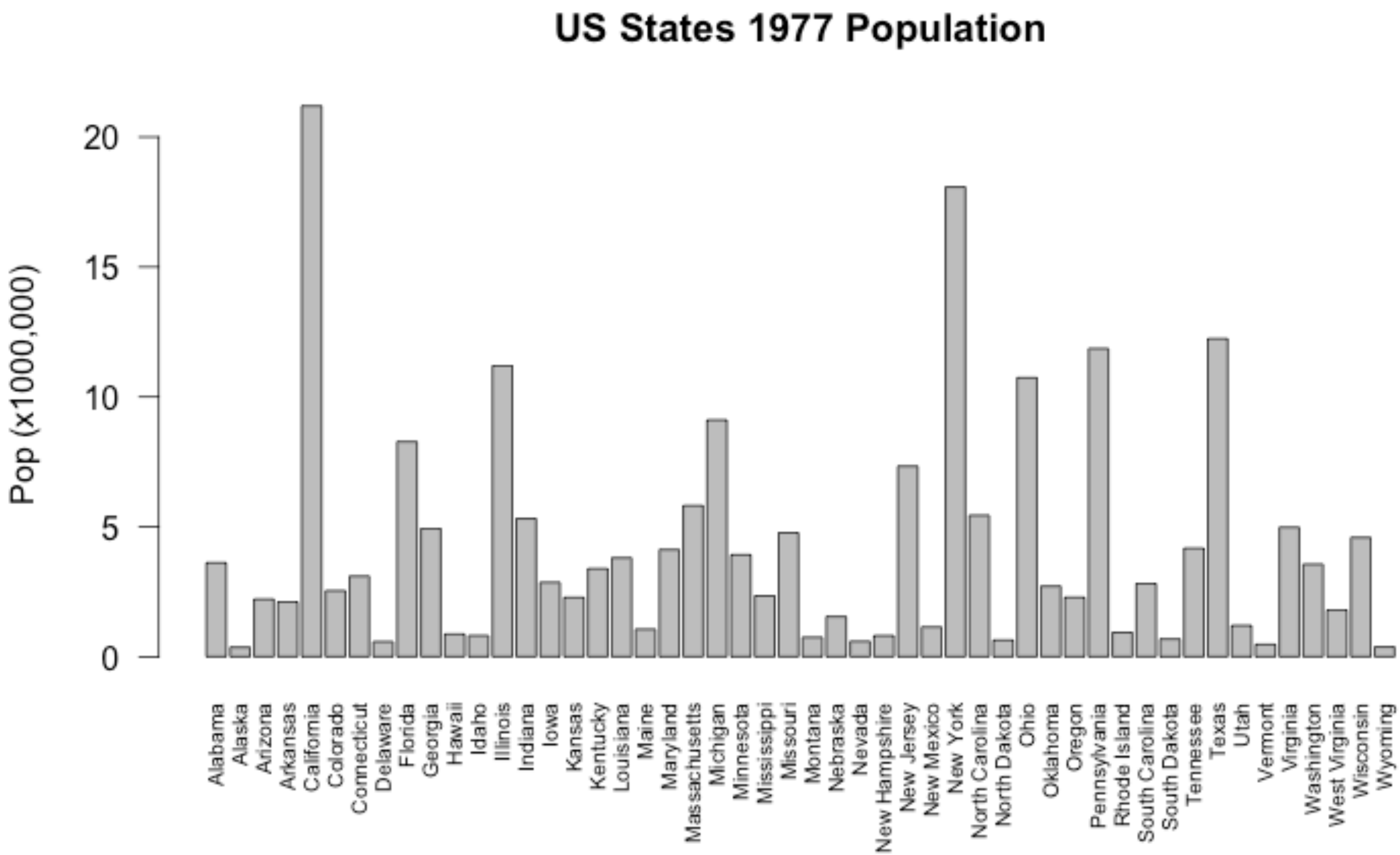
Scatter plot

```
# data
area <- state.x77[, "Area"]
pop <- state.x77[, "Population"]

# scatter plot
plot(area, pop, main="US States 1977")

# label points
state.max.area <- which.max(area)
points(area[state.max.area],
       pop[state.max.area],
       col="red", lwd=2)

points(area["Kansas"], pop["Kansas"],
       col="purple", lwd=2)
```

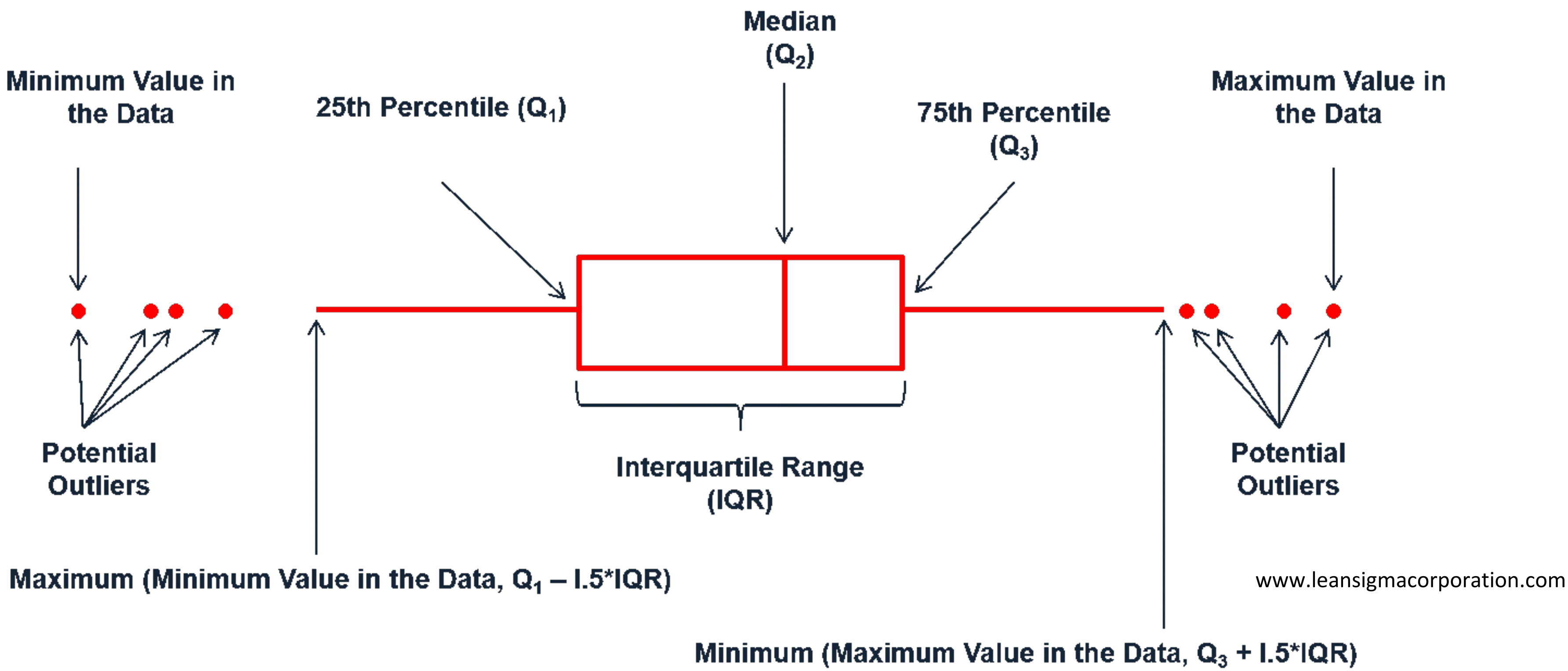


Barplot

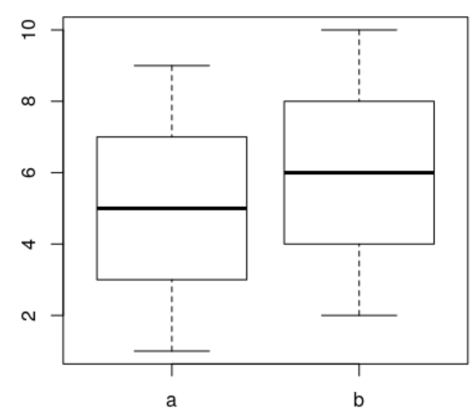
```
barplot(pop/1000, las=2, cex.names=0.65, ylab="Pop (x1000,000)",
        main="US States 1977 Population")
```



Boxplot

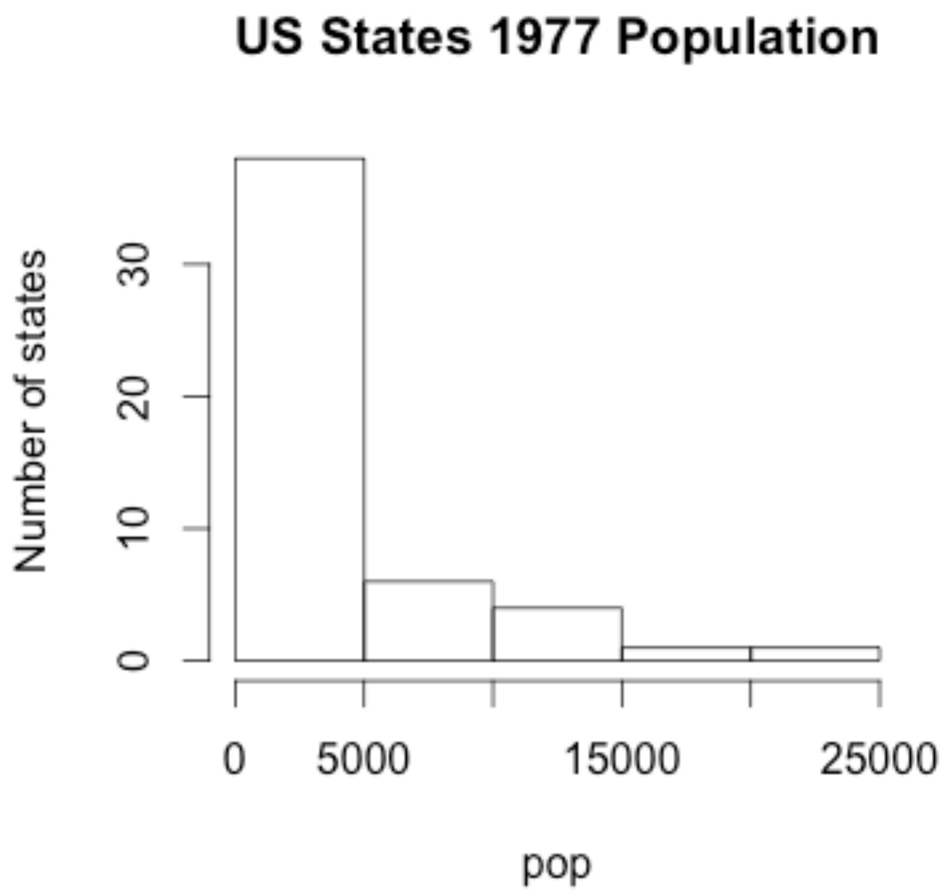



```
y <- 1:10
x <- rep(c("a", "b"), 5)
boxplot(y ~ x)
```



Histogram

```
hist(pop, ylab="Number of states", main="US States 1977 Population")
```



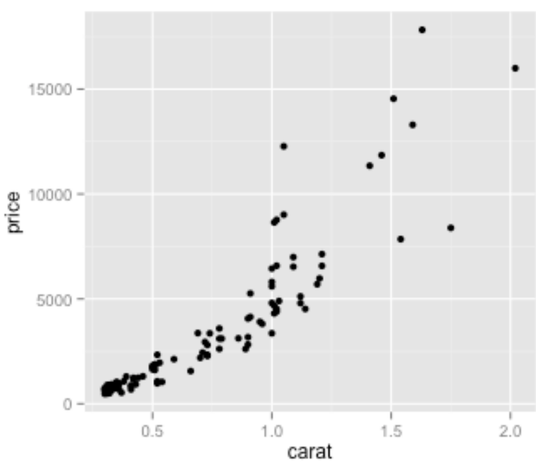
ggplot2 - an easy plotting package

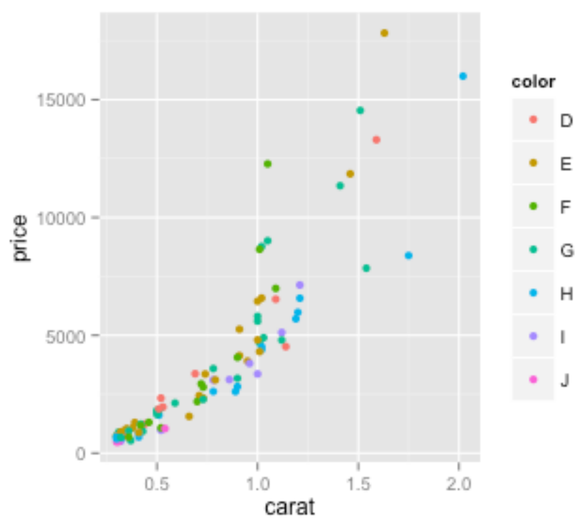
diamonds

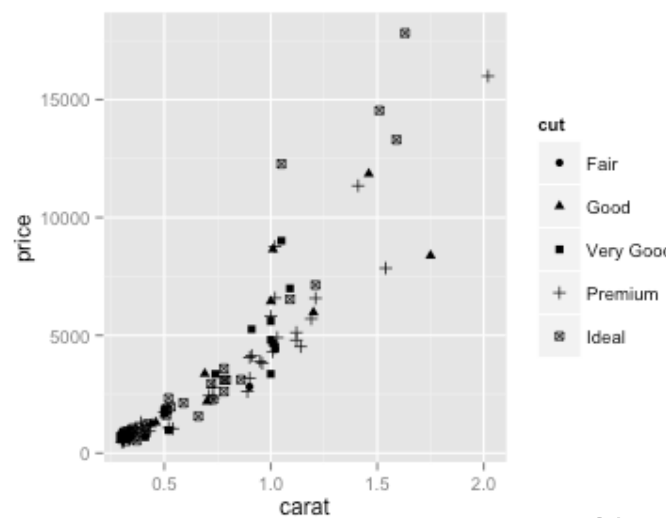
carat	cut	color	clarity	depth	table	price
0.23	Ideal	E	SI2	61.5	55	326
0.21	Premium	E	SI1	59.8	61	326

scatterplots showing the relationship between the price and carats (weight) of a diamond*.

```
qplot(carat, price, data = diamonds)
qplot(carat, price, data = diamonds, colour = color)
qplot(carat, price, data = diamonds, shape = cut)
```







* from http://ggplot2.org/book/qplot.pdf

ggplot2 - geom to control plot type

qplot is not limited to scatterplots, but can produce almost any kind of plot by varying the **geom**. geom has many options:

- "point" draws a scatterplot. This is the default.
- "smooth" fits a smoother to the data
- "boxplot" produces a box-and-whisker plot
- "line" draw lines between the data points.
- "histogram" draws a histogram
- "bar" makes a bar chart

ggplot2 – a flexible tool to plot various plots

diamonds

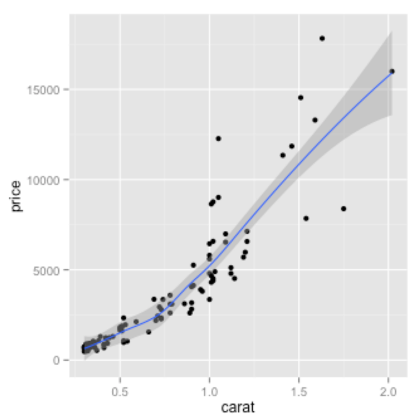
carat	cut	color	clarity	depth	table	price
0.23	Ideal	E	SI2	61.5	55	326
0.21	Premium	E	SI1	59.8	61	326

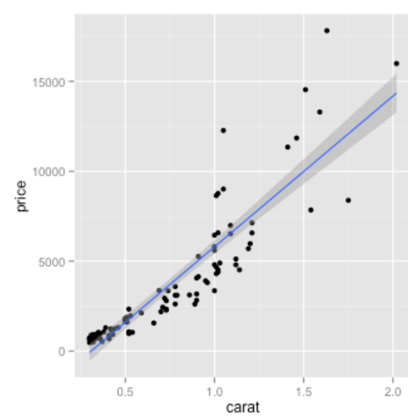
Adding a smooth line or a fitted line

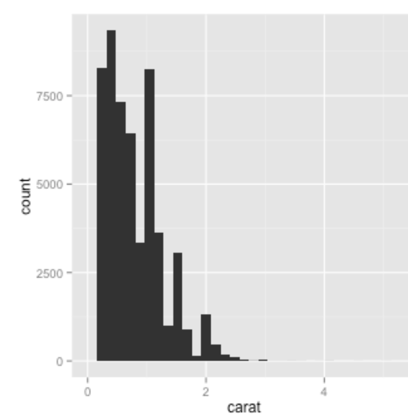
```
qplot(carat, price, data = diamonds, geom = c("point", "smooth"))
qplot(carat, price, data = diamonds, geom = c("point", "smooth"),
      method = "lm")
```

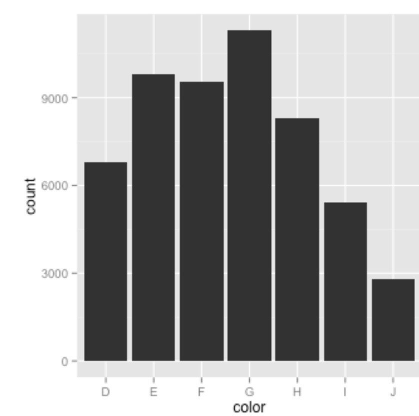
Histogram and barplot

```
qplot(carat, data = diamonds, geom = "histogram")
qplot(color, data = diamonds, geom = "bar")
```









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String operations - nchar

- **nchar()**

nchar the sizes of the corresponding elements of a vector.

nchar(cvec)

```
> cvec
[1] "google" "hello"  "the"    "world"

> nchar(cvec)
[1] 6 5 3 5
```

String operations - grep

- **grep()**

grep searches for matches to argument pattern within each element of a character vector

grep("o", cvec)

```
> cvec
[1] "google" "hello"  "the"    "world"

> grep("o", cvec)
[1] 1 2 4
```

String operations – sub and gsub

- **sub()** and **gsub()**

sub and gsub perform replacement of the *first* and *all* matches respectively.

sub("o", "O", cvec)

gsub("o", "O", cvec)

```
> cvec
[1] "google" "hello"  "the"    "world"


> sub("o", "O", cvec)
[1] "gOogle" "hellO"  "the"    "wOrld"
> gsub("o", "O", cvec)
[1] "gOOgle" "hellO"  "the"    "wOrld"
```

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function/module in R

- If a procedure is repeated multiple times, it would be valuable to convert the procedure to a function/module.

- **Define a function**

```
fun_name <- function(arg_1, arg_2, ...) expression
```

or

```
fun_name <- function(arg_1, arg_2, ...) {
     expressions
}
```

- **Use a function**

```
fun_name(arg_1, arg2, ...)
```

Function example 2

- **Define a function**

name <- function(arg_1, arg_2, ...) expression

```
# example 1
threetimes <- function(x) {
  y <- 3*x
  y
}
```

```
> threetimes(6)
[1] 18

> val <- threetimes(29)
> val
[1] 87
```

Function example 2

```
# return the value of the nth element of the input vector
what_at_n <- function(in_vector, n) {
  # initiate the output value
  nth_val <- NA
  if (n <= length(in_vector)) {
    nth_val <- in_vector[n]
  }
  print_info <- paste("The value of element", n, "is", nth_val, sep=" ")
  print(print_info)
  nth_val
}
```

> what_at_n(c(36, 19, 13), 2)

[1] "The value of element 2 is 19"

[1] 19

> val2 <- what_at_n(c(36, 19, 13), 2)

[1] "The value of element 2 is 19"

> val2

[1] 19

base (build-in) functions in R

- R has many build-in functions
- If you have choices to use a build-in function, do not use your own function (efficiency and code sharing)

"apply" functions

- **apply**
- **lapply**
- **sapply**
- **mapply**
- **tapply**

- vapply
- rapply
- ...

goal: to simplify coding and improve computation efficiency

apply()

- **apply(X, MARGIN, FUN, ...)**

apply a function to margins of an array or matrix.

`apply(d, 1, sum)`

d

3.95	3.98	2.43	10.36
3.89	3.84	2.31	10.04
4.05	4.07	2.31	10.43
4.2	4.23	2.63	11.06
4.34	4.35	2.75	11.44
3.94	3.96	2.48	10.38
24.37	24.43	14.91	

`apply(d, 2, sum)` 24.37 24.43 14.91

```
rowSums
colSums
```

apply - example

```
> head(diamonds)
  carat       cut color clarity depth table price    x    y    z
1  0.23     Ideal     E     SI2  61.5    55   326 3.95 3.98 2.43
2  0.21   Premium     E     SI1  59.8    61   326 3.89 3.84 2.31
3  0.23      Good     E     VS1  56.9    65   327 4.05 4.07 2.31
4  0.29   Premium     I     VS2  62.4    58   334 4.20 4.23 2.63
5  0.31      Good     J     SI2  63.3    58   335 4.34 4.35 2.75
6  0.24 Very Good     J    VVS2  62.8    57   336 3.94 3.96 2.48
```

```
> apply(diamonds[, c("carat", "price")], 2, mean)
     carat        price 
  0.7979397 3932.7997219
```

combine your own function with apply

```
sumsqrt <- function(x) {
   sum(sqrt(x))
}
apply(d, 1, sumsqrt)
```

or

```
apply(d, 1, function(x) sum(sqrt(x)))
```

3.95	3.98	2.43	5.54
3.89	3.84	2.31	5.45
4.05	4.07	2.31	5.55
4.2	4.23	2.63	5.73
4.34	4.35	2.75	5.83
3.94	3.96	2.48	5.55

tapply

- **tapply()**

Applying *a function* to each element of *a vector* given by the category of each element, provided by *the other vector*.

```
> head(diamonds)
  carat       cut color clarity depth table price    x    y    z
1  0.23     Ideal     E     SI2  61.5    55   326 3.95 3.98 2.43
2  0.21   Premium     E     SI1  59.8    61   326 3.89 3.84 2.31
3  0.23      Good     E     VS1  56.9    65   327 4.05 4.07 2.31
4  0.29   Premium     I     VS2  62.4    58   334 4.20 4.23 2.63
5  0.31      Good     J     SI2  63.3    58   335 4.34 4.35 2.75
6  0.24 Very Good     J    VVS2  62.8    57   336 3.94 3.96 2.48

> tapply(diamonds$price, diamonds$cut, mean)
     Fair      Good Very Good   Premium     Ideal
 4358.758  3928.864  3981.760  4584.258  3457.542
```

table

- **table()**

Determining counts for each category

```
> head(diamonds)
  carat       cut color clarity depth table price    x    y    z
1  0.23     Ideal     E     SI2  61.5    55   326 3.95 3.98 2.43
2  0.21   Premium     E     SI1  59.8    61   326 3.89 3.84 2.31
3  0.23      Good     E     VS1  56.9    65   327 4.05 4.07 2.31
4  0.29   Premium     I     VS2  62.4    58   334 4.20 4.23 2.63
5  0.31      Good     J     SI2  63.3    58   335 4.34 4.35 2.75
6  0.24 Very Good     J    VVS2  62.8    57   336 3.94 3.96 2.48


> table(diamonds$cut)

     Fair      Good Very Good   Premium     Ideal
     1610      4906     12082     13791     21551
```

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t-test

t.test

Performs one and two sample t-tests on vectors of data.

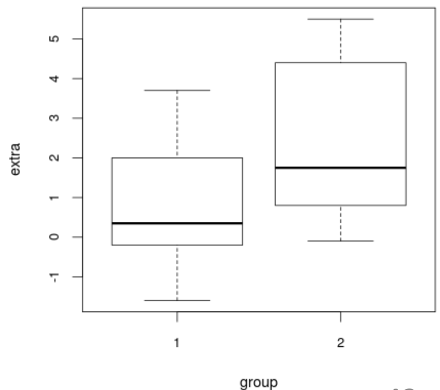
```
# Student's sleep data
plot(extra ~ group, data = sleep)

# t-test
with(sleep, t.test(extra[group == 1],
extra[group == 2]))

# Formula
t.test(extra ~ group, data = sleep)
```

data: sleep

extra	group	ID
0.7	1	1
-1.6	1	2
-0.2	1	3
-1.2	1	4
-0.1	1	5
3.4	1	6
3.7	1	7
0.8	1	8
0.0	1	9
2.0	1	10
1.9	2	1
0.8	2	2
1.1	2	3
0.1	2	4
-0.1	2	5
4.4	2	6
5.5	2	7
1.6	2	8
4.6	2	9
3.4	2	10



Linear models (I)

Fitting a linear model

lm(formula, data = data.frame)

```
pc <- lm(price ~ carat, data=diamonds)
summary(pc)
```

```
Residuals:
     Min       1Q   Median       3Q      Max 
-18585.3   -804.8    -18.9    537.4  12731.7 

Coefficients:
            Estimate Std. Error t value Pr(>|t|)    
(Intercept) -2256.36      13.06  -172.8   <2e-16 ***
carat        7756.43      14.07   551.4   <2e-16 ***
---
Signif. codes:  0 ‘***’ 0.001 ‘**’ 0.01 ‘*’ 0.05 ‘.’ 0.1 ‘ ’ 1

Residual standard error: 1549 on 53938 degrees of freedom
Multiple R-squared:  0.8493,	Adjusted R-squared:  0.8493 
F-statistic: 3.041e+05 on 1 and 53938 DF,  p-value: < 2.2e-16
```

ANOVA (I)

ANOVA

anova(model)

```
pcc <- lm(price ~ carat + cut, data=diamonds)
anova(pcc)
```

```
Analysis of Variance Table

Response: price
             Df     Sum Sq    Mean Sq   F value    Pr(>F)
carat         1 7.2913e+11 7.2913e+11 319162.11 < 2.2e-16 ***
cut           4 6.1332e+09 1.5333e+09    671.17 < 2.2e-16 ***
Residuals 53934 1.2321e+11 2.2845e+06
---
Signif. codes:  0 ‘***’ 0.001 ‘**’ 0.01 ‘*’ 0.05 ‘.’ 0.1 ‘ ’ 1
```

ANOVA (II)

Comparing two models

anova(model1, model2)

```
pc <- lm(price ~ carat, data=diamonds)
pcc <- lm(price ~ carat + cut, data=diamonds)
anova(pc, pcc)
```

```
Analysis of Variance Table

Model 1: price ~ carat
Model 2: price ~ carat + cut
  Res.Df        RSS Df  Sum of Sq      F    Pr(>F)
1  53938 1.2935e+11
2  53934 1.2321e+11  4 6133201436 671.17 < 2.2e-16 ***
---
Signif. codes:  0 ‘***’ 0.001 ‘**’ 0.01 ‘*’ 0.05 ‘.’ 0.1 ‘ ’ 1
```

chi-square test

chisq.test

	B	
A	12	36
	24	70

```
d <- c(12, 36, 24, 70)
dm <- matrix(d, nrow=2, byrow=T)
chisq.test(dm)
```

data: dm

X-squared = 0, df = 1, p-value = 1

Online resources

"apply" function family

- https://www.datacamp.com/community/tutorials/r-tutorial-apply-family#gs.YUI=Luc

Statistical modeling with R

- https://www.datacamp.com/courses/statistical-modeling-in-r-part-1
- http://www.analyticsforfun.com/2014/06/performing-anova-test-in-r-results-and.html

Get help

- help(ls)
- ?ls
- ??colsum: ambiguous search
- R reference card
- stackoverflow
- Google is the best helper!

R learning: http://swirlstats.com/

Rstudio

Rstudio is an open source integrated development environment (IDE) for R

- On your own machine (Rstudio Desktop)

Download and install R

Download and install Rstudio

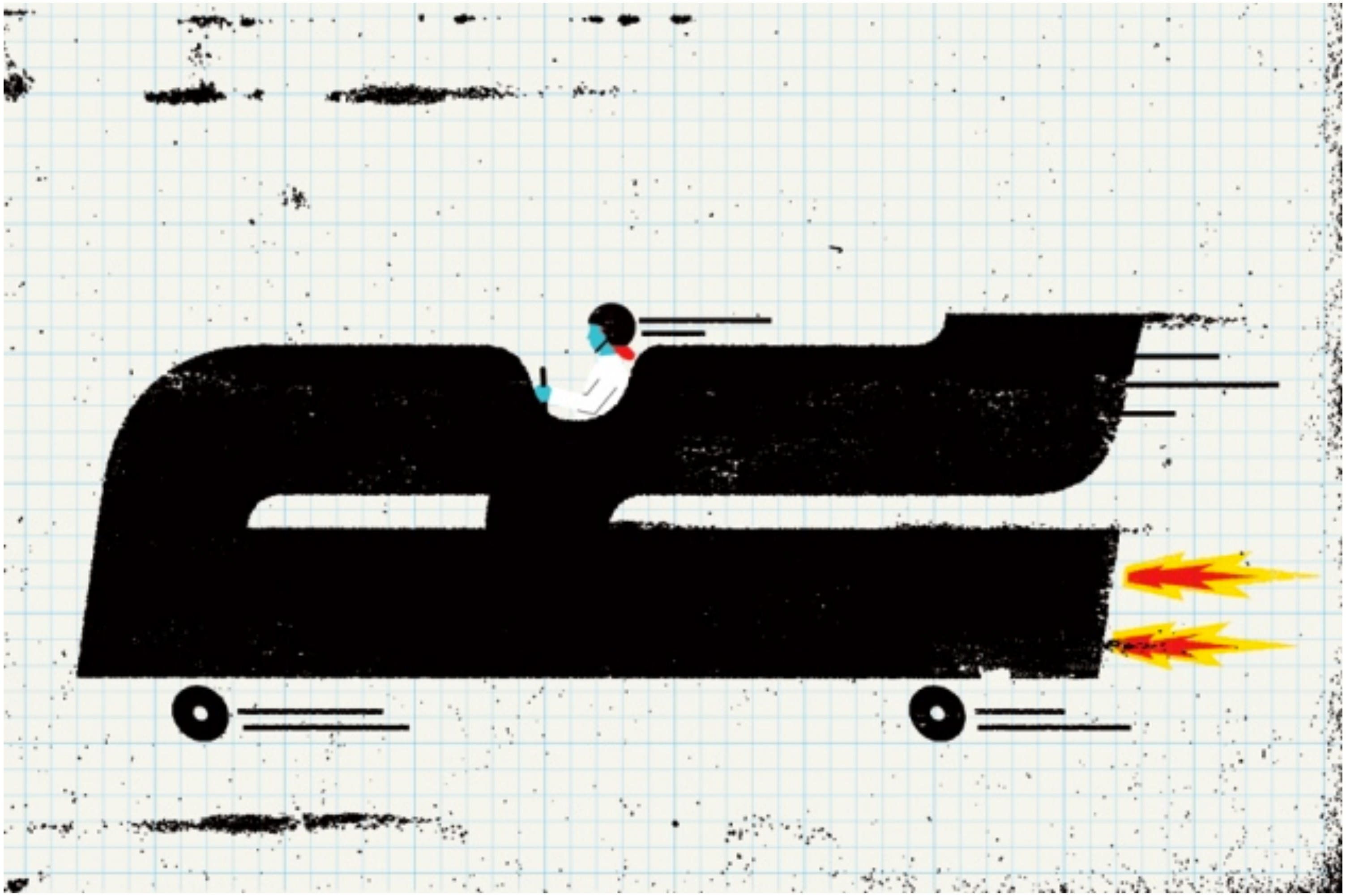
- Use Rstudio at Beocat (Rstudio server)

rstudio.beocat.cis.ksu.edu

https://ondemand.beocat.ksu.edu

Your KSU ID and password to login

Adventures with R



http://www.nature.com/news/programming-tools-adventures-with-r-1.16609

sapply and lapply

`sapply()` and `lapply()`

work in a similar way, calling the specified function for each item of a list or vector.

```
> sapply(1:3, function(x) x^2)
[1] 1 4 9
```

lapply returns a list rather than a vector:

```
> lapply(1:3, function(x) x^2)
[[1]]
[1] 1

[[2]]
[1] 4

[[3]]
[1] 9
```

mapply

`mapply()`

vectorize arguments to a function that is not usually accepting vectors as arguments.

```
> rep(1:3, 3)
[1] 1 2 3 1 2 3 1 2 3

> mapply(rep, 1:3, 3)
     [,1] [,2] [,3]
[1,]    1    2    3
[2,]    1    2    3
[3,]    1    2    3

> mapply(rep, 1:3, 3:1)
[[1]]
[1] 1 1 1
[[2]]
[1] 2 2
[[3]]
[1] 3
```

1. apply each element from the 3rd argument to each element in the 2nd argument using the function specified in the 1st argument

2. combine them by column or organize them in a data frame or list format

aggregate

aggregate(X, by, FUN, ...)

Splits the data into subsets, computes summary statistics for each, and returns the result in a convenient form.

```
carat       cut color clarity depth table price    x    y    z
1  0.23     Ideal     E     SI2  61.5    55   326 3.95 3.98 2.43
2  0.21   Premium     E     SI1  59.8    61   326 3.89 3.84 2.31
3  0.23      Good     E     VS1  56.9    65   327 4.05 4.07 2.31
4  0.29   Premium     I     VS2  62.4    58   334 4.20 4.23 2.63
5  0.31      Good     J     SI2  63.3    58   335 4.34 4.35 2.75
6  0.24 Very Good     J    VVS2  62.8    57   336 3.94 3.96 2.48
```

```
> aggregate(diamonds$price, by=list(diamonds$cut), FUN=mean)
 Group.1        x
1      Fair 4358.758
2      Good 3928.864
3 Very Good 3981.760
4   Premium 4584.258
5     Ideal 3457.542
```

```
> tapply(diamonds$price, diamonds$cut, FUN=mean)
 Fair      Good Very Good   Premium     Ideal
 4358.758  3928.864  3981.760  4584.258  3457.542
```