# ELEMENTS OF DATA SCIENCE AND STATISTICAL LEARNING

FALL 2017

Week 2

# OUTLINE

- More R
  - Lists, dataframes, factors
  - Conditionals and loops
  - Functions
  - Loading data
- Exploratory analysis
  - Boxplots, scatterplots
- Statistical learning: what is it about?
  - Statistical modes
  - Model bias
  - Prediction vs inference
  - Prediction accuracy

# LISTS IN R

- Vectors and matrices are good for storing homogeneous data (e.g. all values are numeric)
  - Thus vectors/matrices are close to what in most other languages is called an "array" (one- or two-dimensional, respectively). The only difference is that in most languages "raw" arrays have fixed size, while in R vectors/matrices can grow dynamically (e.g. by appending values)
- R also provides a container for storing heterogeneous/arbitrary data, a ***list*** (thus similar to a "list" in Python, List<Object> in Java or array/vector of void * pointers in C/C++)
  - A value of any type can be stored as an element of a list, regardless of what other elements contain: a (vector of) integer, a (matrix of) character, another list, a function, etc

```
> a <- list()
> a[[1]] <- "first el"
> a[[2]] <- 2
> a[[5]] <- 1:3
```

```
> a
[[1]]
[1] "first el"
[[2]]
[1] 2
[[3]]
NULL
[[4]]
NULL
[[5]]
[1] 1 2 3
```

# LIST INDEXING

- There is another indexing operator in R, used for lists: [[ ]]
  - Does *NOT* allow vectors of length > 1 as indexes; single index *ONLY* (technically, it works on vectors/matrices as well, but it is not of much use there)
  - The indexing operator [ ] preserves the mode (type) of the object being indexed. Subsetting a vector/matrix with [ ] returns a vector/matrix; since everything is a vector (even a "single value"), there is nothing to "unwrap": just take a subset of vector elements, it does not matter one or many – it's still a vector
  - Operator [ ] will also work on lists, but will return the object of the same mode, a *list*, even if index has length 1 (will return *list* with one element in that case). Thus: use [ ] on lists when you need to take a *sublist*.
  - Operator [[ ]] *extracts* the value (element) from the list at the specified position.

```
> x=list("first el",2,1:3); x
[[1]]
[1] "first el"

[[2]]
[1] 2

[[3]]
[1] 1 2 3
```

```
> mode(x[1])
[1] "list"
> x[1]
[[1]]
[1] "first el"

> x[1:2]
[[1]]
[1] "first el"

[[2]]
[1] 2
```

```
> mode(x[[1]])
[1] "character"
> x[[1]]
[1] "first el"
```

!!!!!!!!!!

# NAMED LIST ELEMENTS

- Similarly to vectors/matrices, elements of a list can be named
  - Special syntax can be used at the time of list creation;
  - the same function `names()` can be used on lists too!
  - Note that names(x) returns a *vector* of names, which can be further subsetted (even on the left hand side of an assignment as it is done in our example!); this is not unique to lists – works same way on any objects with named elements (vectors, matrices)

```
> x=list(a=1,b=c(5,-3,2),matrix(1:4,ncol=2))
> x
$a
[1] 1

$b
[1]  5 -3  2

[[3]]
     [,1] [,2]
[1,]    1    3
[2,]    2    4
```

```
> names(x)[3]="c"
> x
$a
[1] 1

$b
[1]  5 -3  2

$c
     [,1] [,2]
[1,]    1    3
[2,]    2    4
```

# LIST INDEXING BY NAME

- When list elements are named, those names can be also used for indexing
- Works both with [ ] and [[ ]] operators
- Indexes, either integer or character (element names) can be passed in a variable
- There is an additional operator that can be used ONLY in conjunction with name LITERALS:
  - x$b extracts the element of list x named "b" (SAME as x[["b"]]) – note the lack of quotation marks in expression x$b
  - x$z in the example shown on the left asks for element named "z" (no such thing, NULL is returned). The *value* stored in variable z cannot be used here – one should have used [[z]] instead!

```
> x=list(a=1,b=c(5,-3,2),matrix(1:4,ncol=2))
> x[c("a","b")]
$a
[1] 1

$b
[1]  5 -3  2

> x[["b"]]
[1]  5 -3  2
> z="b"
> x[[z]]
[1]  5 -3  2
> x$b
[1]  5 -3  2
> x$z
NULL
```

# NEED FOR "TABLES"

- Think about a typical data table (e.g. an Excel worksheet or relational database table): a table is usually composed of columns of different data types
  - For instance, employee name (character), SSN (integer), date of hire (date), department (integer id or character name/code), pay rate (integer or float), …
  - Obviously a very ubiquitous data structure. Any relational database supports it (because that's what a relational database is about in the first place) and most languages would have some kind of an extension library – or you would end up writing such class on your own sooner or later
- Matrix type (in R) would not cut it: all elements must have same type; keep all the data in character mode (the most general data type) and convert to integer/float/date etc as needed? – very inelegant and cumbersome
- List (in R) – sounds like a better solution: each element of a list can store an individual column (a vector), each list element (column) can have its own type, consistency of the type is enforced across each column (so much better than e.g. list of lists in Python, here we have something more similar to list of arrays instead)
  - Still many drawbacks: cannot enforce same length for all columns (a table has N rows → all columns must be of length N!)
  - Awkward access: element at row `i` column `j` is `x[[j]][i]` (yes, at least you can chain access operators in R!), but no easy way to ask for a whole row or a few rows at all!

# DATA FRAMES

- Meet data frame type (this week assignment heavily relies on them!)
  - Based on a list (in many ways data frame still IS a list as we will see shortly)
  - Fixes the drawbacks mentioned early by enforcing rectangular shape and providing matrix-like access operator [ row, column ] (that can take vectors of indices of arbitrary length – consistent with other R data types)
- R is very much about data analysis: data frames are extremely important and expected by many functions

Note that the constructor is very similar to that of a list: the column vectors are passed as arguments, with optional names

```
> m2 <- data.frame(age=c(23,43,32),sex=I(c("M","F","M"))) ; m2
age sex
1  23   M
2  43   F
3  32   M
> class(m2)
[1] "data.frame"
> mode(m2)
[1] "list"
> m2$age # we can use list operator '$' to access dataframe columns
[1] 23 43 32
> mode(m2$age)
[1] "numeric"
> mode(m2$sex)
[1] "character"
```

We will discuss the "magic" of I() later

# ACCESSING DATA IN DATA FRAMES

- Data frame IS a list of columns (as mode() tells us), and the "conventional" list access works for dataframes too
  - `x$column.name` will return the whole column (as a vector!) from the dataframe x
  - `x[["column.name"]]` will do exactly the same, and so will `j="column.name" ; x[[ j ]]`
  - In addition, matrix like operator `[ i , j ]` will extract a subset of rows/columns
  - All the usual indexing options are available with **[ , ]** : integer indexes, character names (if rows/columns have names set), logical vectors of "flags"
  - **IMPORTANT**: when using [ , ] to select elements (one or many) from a *single* column, the result is a vector; when selecting multiple columns (even if the columns have the same mode and even when a single row is selected), the result is always a data frame, never a matrix or a vector!
  - Since dataframe IS a list of columns, `names(x)` will work on dataframes too (and access/set the column names)
  - Additionally, `rownames(x)` and `colnames(x)` can be used to set/retrieve row/column names (just like it works with matrices)
  - Appending an element to a column will expand ALL columns accordingly (filling them with NA)
  - On data frame initialization or column assignment, values may be recycled as usual (if possible), but otherwise an attempt to pass/set columns of different lengths causes an error

# DATA FRAME EXAMPLES

- Continuing with the same data frame m2 defined earlier:

```
# add a new column "weight":
> m2$weight=c(167,135,202)
> m2
  age sex weight
1  23   M    167
2  43   F    135
3  32   M    202
# multiple cols, still a
# dataframe :
> class(m2[1,c(1,3)])
[1] "data.frame"
> mode(m2[1,c(1,3)])
[1] "list"
# but single column is
# returned as a vector:
> mode(m2[ , 3])
[1] "numeric"
> dim(m2)
[1] 3 3
> length(m2)
3
```

```
> m2$healthy=T; m2  # recycling works
  age sex weight healthy
1  23   M    167    TRUE
2  43   F    135    TRUE
3  32   M    202    TRUE
> m2$exercises=c(T,F)
Error in `$<-.data.frame`(`*tmp*`, ...
  replacement has 2 rows, data has 3
# a column is a vector, can use as such:
> sum( m2$age > 30 )
[1] 2
# taking a subset of a data frame:
> m2[ m2$age > 30 , ] # see also docs for subset()
  age sex weight healthy
2  43   F    135    TRUE
3  32   M    202    TRUE
> m2[1,5]="John D"; m2 # fills missing data with NA
  age sex weight healthy      V5
1  23   M    167    TRUE  John D
2  43   F    135    TRUE    <NA>
3  32   M    202    TRUE    <NA>
```

What is the difference?

# PROGRAMMING IN R: IF-ELSE

- If-else is a conventional flow control operator, works the same way as in any other language
  - The condition must evaluate to a logical vector of *length 1* (the condition is either TRUE or FALSE); using a vector of length > 1 will cause a *warning* and only the first element will be used
  - Condition that evaluates to NA causes an *error*
- Compare to ifelse(): not really flow control operator, but a vectorized *function*

```
> x <- c(3,5)
# curly braces optional in one-line form:
> if ( any(x > 4) ) "apples" else "oranges"
[1] "apples"
# multiline form – must use braces:
> if ( any(x > 4) ) {
     x <- x+3
     print(x)
  } else {
     x <- x*2
     print(x)
  }
[1] 6 8
```

```
> x<-c(3,5,1,7)
# note that recycling occurs below. Each arg of ifelse
# has the same length as the first arg (recycled as
# needed) and for each position in the result (also
# same length as the first arg), the corresponding
# element of either 2nd or 3rd arg is taken, depending
# on whether the condition (first arg) is T or F at
# that position:
> ifelse(x>4,"apples","oranges")
[1] "oranges" "apples" "oranges" "apples"
```

# PROGRAMMING IN R: FUNCTIONS

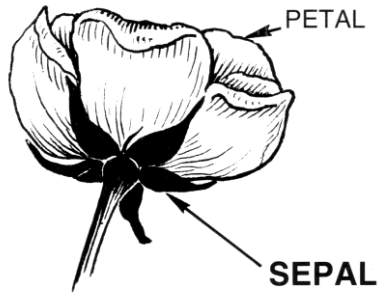
- Function definition in R creates an object that can be assigned to a variable or used as an anonymous function
- Formal parameters allow default values
- In order to pass argument values, function calls can bind formal parameters by name

```
> my.f = function(x,y,option.1=3,option.2="sorted") { # 3rd and 4th args have defaults
      cat("x=",paste(x,collapse=","),"; y=",y,"; option 1=",option.1,
          "; option 2=",option.2,"\n",sep="")
 }
> my.f(c(1,2)) # must specify all args that don't have defaults, error otherwise
Error in cat("x=", paste(x, collapse = ","), "; y=", y, "; option 1=",  :
  argument "y" is missing, with no default
> my.f(c(1,2),NA) # required args specified, remaining parameters use defaults
x=1,2; y=NA; option 1=3; option 2=sorted
> my.f(c(1,2),NA,"test",2) # "traditional" call: all args passed in correct positions
x=1,2; y=NA; option 1=test; option 2=2
> my.f(c(1,2),NA,option.2="unsorted") # binding by name, specify only what you need
x=1,2; y=NA; option 1=3; option 2=unsorted
# can use binding by name even for all args; the order is irrelevant for named args:
> my.f(y=NA,x=10,option.2="unsorted")
x=10; y=NA; option 1=3; option 2=unsorted
```

# LOADING AND SAVING DATA

- In order to do anything meaningful with data we need to be able to load them
- Here is a classical "iris" dataset (described by R.A.Fisher), the data contain sepal and petal characteristics and types of 150 individual iris plants.

```
sepal.length,sepal.width,petal.length,petal.width,class
5.1,3.5,1.4,0.2,Iris-setosa
4.9,3.0,1.4,0.2,Iris-setosa
4.7,3.2,1.3,0.2,Iris-setosa
…
```




- Download the file and load the data (you'll be doing this twice for this week assignment!):

```
> setwd("C:\\Users\\...\\Week 2") # change dir to where YOUR data are located!
> getwd()  # see what R's current working dir is
[1] "C:/Users/.../Week 2"
> iris=read.table("iris.data.txt",header=T,sep=",") # read data in! Can take full path or even a URL!
> iris[1:3,] # see what we got:
  sepal.length sepal.width petal.length petal.width       class
1          5.1         3.5          1.4         0.2 Iris-setosa
2          4.9         3.0          1.4         0.2 Iris-setosa
3          4.7         3.2          1.3         0.2 Iris-setosa
> write.table(iris,file="C:/Work/iris.data.tsv",sep="\t",col.names=T,row.names=F,quote=F) # write to disk!
```

# FACTORS

- R has yet another basic data type that we ignored so far: factors
  - In statistics, a "factor" is another name for a categorical variable, the one that takes on a finite set of fixed values
  - Thus the 'factor' data type is most similar to what in many other languages is called 'enum' (enumeration type)
  - Very useful and many functions know how to use factors correctly. NOTE: implementation may result in very unexpected consequences if you are not careful when using factors
  - Dataframes convert character vectors (columns) into factors *automatically* – both when explicit constructor data.frame() is used and when a data frame is loaded with read.table – sometimes this is NOT what we want (e.g. patient's gender, M/F is a bona fide categorical variable, while patient's name is probably nothing but just an attribute with no particular statistical significance). If p.names is a character vector, we can either use I() in the constructor (e.g. data.frame(patent.name=I(p.name),…) or set optional parameter stringsAsFactors in order to prevent the conversion; in read.table we can use as.is=TRUE (applies to ALL character columns!)

```
> class(iris)
[1] "data.frame"
> sapply(iris,mode)
Sepal.Length  Sepal.Width Petal.Length  Petal.Width      Species
   "numeric"    "numeric"    "numeric"    "numeric"    "numeric"
> sapply(iris,class)
Sepal.Length  Sepal.Width Petal.Length  Petal.Width      Species
   "numeric"    "numeric"    "numeric"    "numeric"     "factor"
```

# WORKING WITH FACTORS

- A few examples of working with factors:

```
> s<-c("M","F","M")
> f<-as.factor(s); f
[1] M F M
Levels: F M
> as.numeric(s)
[1] NA NA NA
Warning message:
NAs introduced by coercion
> as.numeric(f)
[1] 2 1 2
> levels(f)
[1] "F" "M"
> as.character(f)
[1] "M" "F" "M"
> f[3]<-"Z"; f
Warning message:
In `[<-.factor`(`*tmp*`, 3, value = "Z") :
invalid factor level, NAs generated
[1] M F <NA>
```

# NOTE ON THE DATASETS

- There is a large and very useful collection of various datasets online (it's not the only source of data in this world, of course):
  - http://archive.ics.uci.edu/ml/
  - Visit the website and just browse the collection to get an idea of what's available
  - We will be using some of these datasets for practice!
  - The iris dataset we just looked at was downloaded from that site (in fact, it is also a standard dataset in R, run 'data(iris)' )
  - note that with the data representation chosen on that site, the data table has *only* data; the attribute (column, or variable) meanings and names are defined in a separate file; we chose to edit the downloaded data file by adding column names – slightly "conditioning" your data files is something you might want to consider in general when working with a dataset, especially repeatedly.
  - Always LOOK AT YOUR DATA before loading them (header/no header? Comma or tab-separated? Are text values enclosed in quotation marks? How missing values are represented?)

# OUTLINE

- More R
  - Lists, dataframes, factors
  - Conditionals and loops
  - Functions
  - Loading data
  - Factors
- Exploratory analysis
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- Statistical learning: what is it about?
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# SUMMARY STATISTICS

- ALWAYS explore your data and LOOK at them before jumping into "statistical analysis" let alone "statistical learning"
  - Variables may have funny distributions
  - Data may contain outliers
  - What are the noise levels?
  - Are the (categorical) data well balanced (e.g. your dataset have data for 376 females and 2 males)?
  - What type of trend is present, if any?
  - Is there a batch effect?
- We have discussed mean and variance, but median and interquartile distance may be also useful
  - Convey information similar to mean/variance: the "location" and the "width" of the distribution
  - Non-parametric statistics, much more robust against outliers
- Let us sort all N observations in ascending order
  - Median = the observation in the middle of the list (at position N/2)
  - Z% quantile: a value at the location such that Z% of data are below (N*Z/100) [thus median is simply the 50% quantile]
  - 25% and 75% quantiles are also called Q1 and Q3 quartiles (naturally), *interquartile range or* ***IQR*** is Q3-Q1

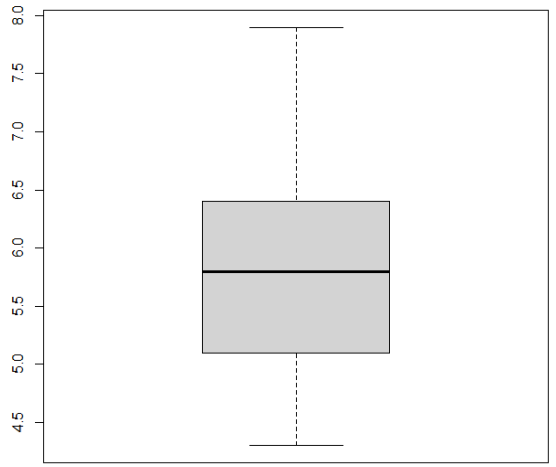
# BOXPLOT

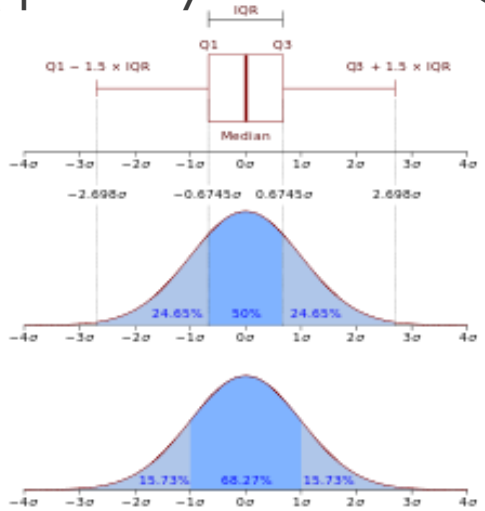
- It is difficult to look at lots of numbers:

```
# summary can be applied to a vector; when applied to a dataframe, it is applied
# to each column separately
> summary(iris)
  Sepal.Length    Sepal.Width     Petal.Length    Petal.Width          Species
 Min.   :4.300   Min.   :2.000   Min.   :1.000   Min.   :0.100   setosa    :50
 1st Qu.:5.100   1st Qu.:2.800   1st Qu.:1.600   1st Qu.:0.300   versicolor:50
 Median :5.800   Median :3.000   Median :4.350   Median :1.300   virginica :50
 Mean   :5.843   Mean   :3.057   Mean   :3.758   Mean   :1.199
 3rd Qu.:6.400   3rd Qu.:3.300   3rd Qu.:5.100   3rd Qu.:1.800
 Max.   :7.900   Max.   :4.400   Max.   :6.900   Max.   :2.500
```

- Boxplot is a very convenient (and custom) way to represent the summary statistics (specifically median and IQR) graphically

```
> boxplot(iris$Sepal.Length,col="lightgrey")
```

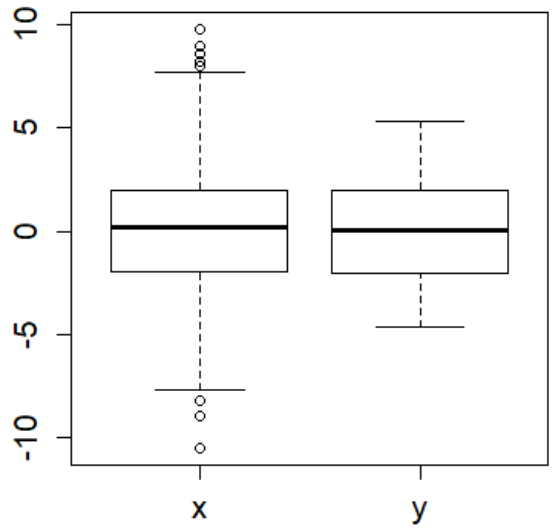


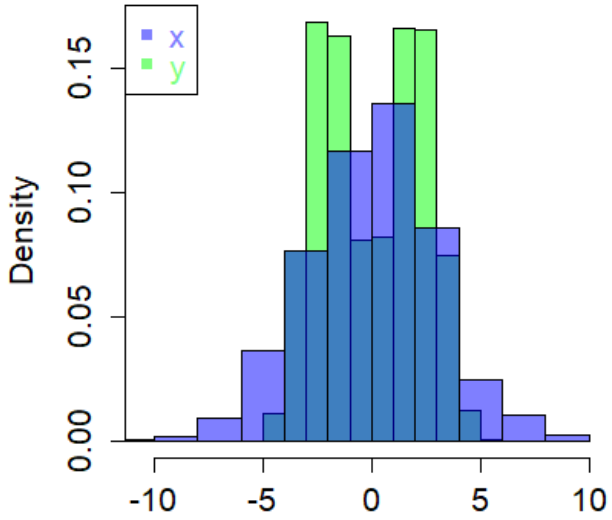




WILL BE USED IN THIS WEEK ASSIGNMENT!

# BOXPLOT VS. HISTOGRAM

```
> x <- rnorm(1000,sd=3)
> y <- c(rnorm(1000,mean=-2),
+        rnorm(1000,mean=2))
> old.par <- par(mfrow=c(1,2),ps=16)
> boxplot(list(x=x,y=y))
> clrsTmp <- c(rgb(0,0,1,0.5),rgb(0,1,0,0.5))
> hist(y,col=clrsTmp[2],freq=FALSE,xlab="",
+                 xlim=range(c(x,y)),main="")
> hist(x,col=clrsTmp[1],add=TRUE,freq=FALSE)
> legend("topleft",c("x","y"),pch=15,
+        col=clrsTmp,text.col=clrsTmp)
> par(old.par)
```



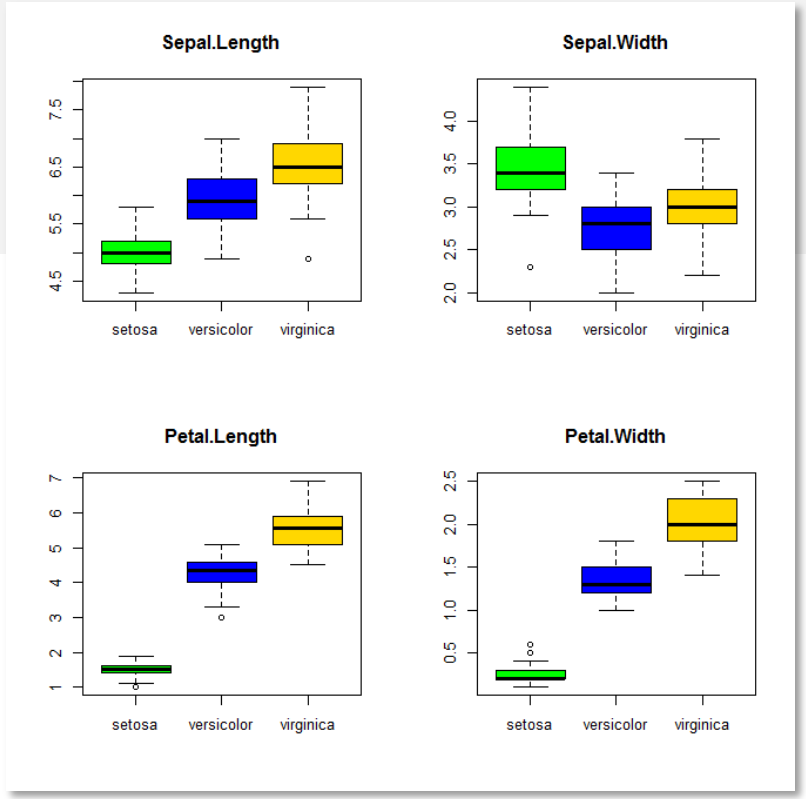




- Of course, similar looking boxplots do not imply "the same" distributions
- In the above, artificially generated, example two samples from a bimodal and a unimodal distributions, although noticeably different when represented as histograms, look very similar as boxplots
- But then, two random samples, especially when relatively small in size, can look fairly different when plotted as histograms also

# STRATIFIED (CONDITIONAL) DISTRIBUTIONS

- Boxplots are very useful to comparing different distributions side by side
- Let us stratify our continuous variables (lengths and widths) by the categorical one (species):

```
# set graphical parameters - in this case, split drawing canvas into 4 separate panels,
# each subsequent plotting command will draw into the next panel (in this case by row).
# we want to save the old set of graphical parameters if we need to restore them later:
> oldpar=par(mfrow=c(2,2))
> for ( i in 1:4 ) {
      # note the "formula interface" in the boxplot call:
    boxplot(iris[[i]] ~ iris$Species,
       main=names(iris)[i],col=c("green","blue","gold"))
 }
> par(oldpar)
```

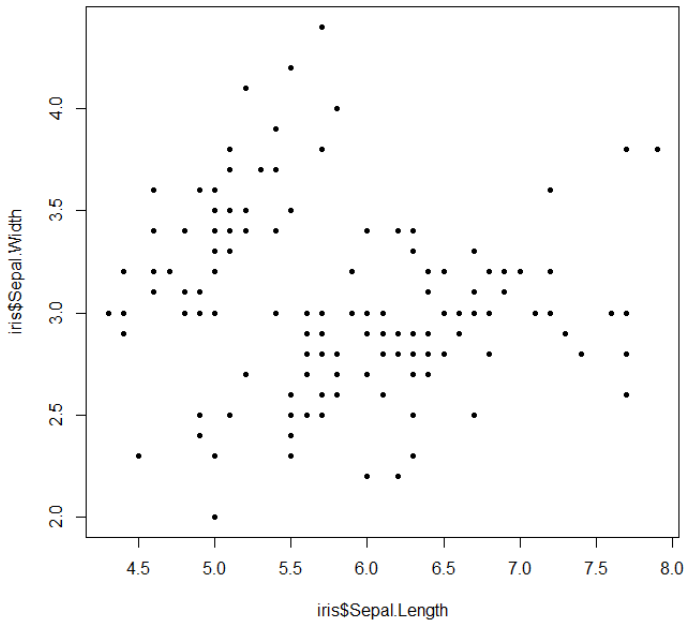


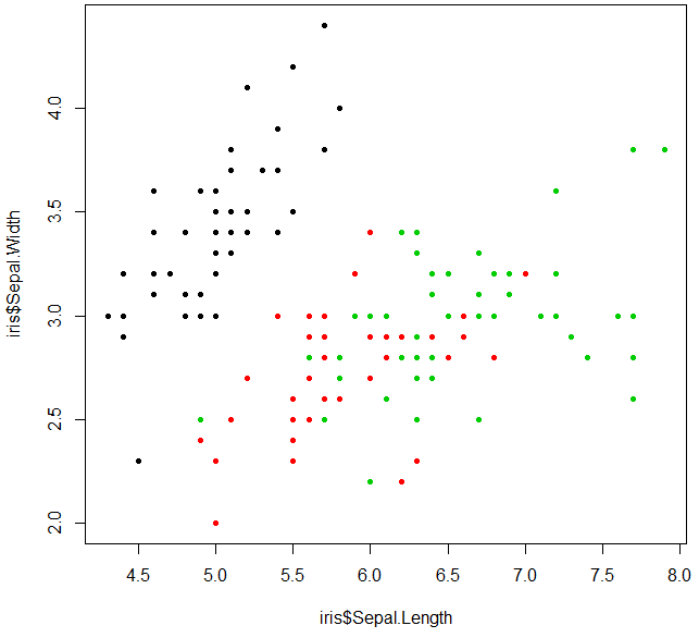

WILL BE USED IN THIS WEEK ASSIGNMENT!

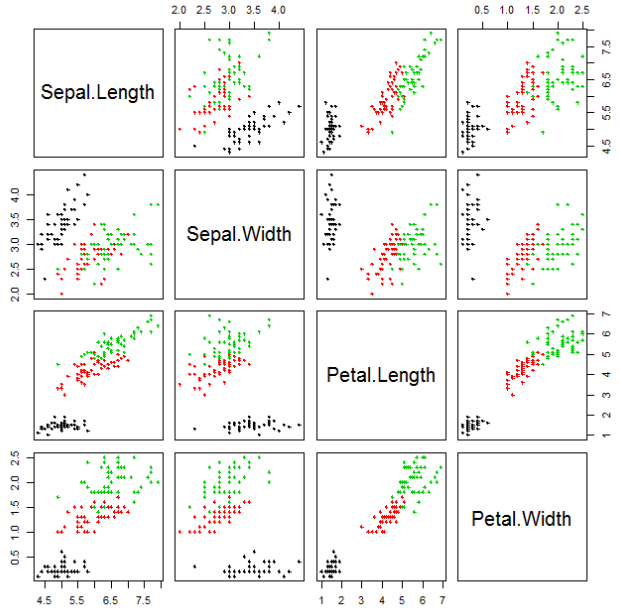
# SCATTERPLOTS

- For continuous variables, it is often useful to generate scatterplots (to see interdependencies/trends, if any)
  - There is also a separate command in R that can generate multiple scatterplots at once, see below

```
> plot(iris$Sepal.Length,iris$Sepal.Width,pch=19,cex=0.7)
> plot(iris$Sepal.Length,iris$Sepal.Width,pch=19,cex=0.7,col=iris$Species)
> pairs(iris[1:4],pch=10,cex=0.5,col=iris$Species)
```



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# PREDICTION PROBLEM

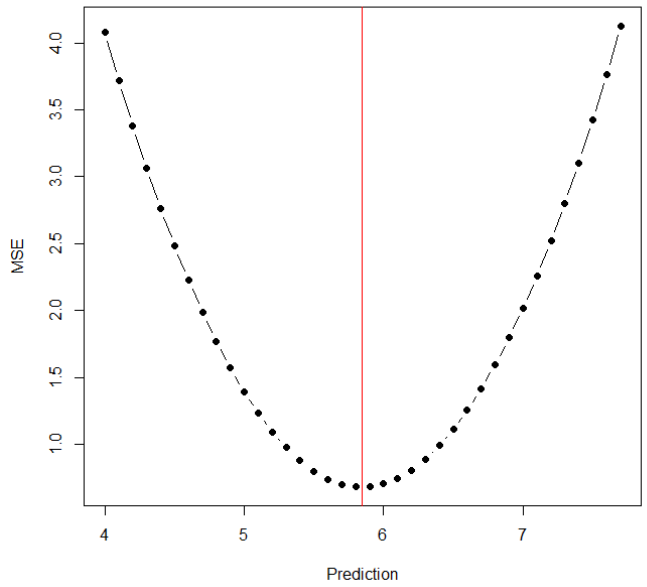
- What does it mean to "predict" anything (in statistical sense)?
  - There is a quantity of interest, an *outcome*, *response*, or *dependent variable* (all interchangeable), often denoted as Y (it is a random variable!)
  - We have some "historical" (previously measured) values (a realization) $y_1, y_2, \ldots, y_k$
  - We want to know what the next measurement is going to be:

    Y = [ prediction generator ]
  - Our "prediction generator" gives some value $\overline{y}$. Ideally, we would like to have $y - \overline{y} = 0$, for all measurements, past and future. Not going to happen, most of the time. We can characterize predictions by their accuracy, i.e. how far they are from true values. For instance, $\frac{1}{k}\sum_i (y_i - \overline{y}_i)^2$ - this quantity is known as mean squared error, or MSE.
  - Our goal is to produce "the best" prediction generator. When we use previously measured data – we are "learning from example"
  - In most (all?) practical settings, we have other variables measured , $X_1, \ldots, X_n$, and we want to use those to help us with prediction

# PREDICTION AND VARIANCE: SINGLE VARIABLE

- Try to predict the following:
  - Will the sun rise tomorrow?
  - What is the result of the next coin toss?
- Probability distribution is all we need to make *a* prediction. What is the best prediction we can make if the distribution P(Y) is all we know (i.e. we do not measure anything else)?
  - Try predicting the height of the next person to come into this room
  - Try predicting the sepal length of the next iris plant you are going to see
  - Note: we are not playing a lottery, we want the prediction strategy that works best long term i.e. *on average*

```
mse=numeric()
for ( x in seq(4,7.7,by=0.1 ) ) {
    mse=c(mse,sum((x-iris$Sepal.Length)^2)/150)
}
plot(seq(4,7.7,by=0.1 ),mse,xlab="Prediction",ylab="MSE",pch=19,type="b")
abline(v=mean(iris$Sepal.Length),col="red")
```



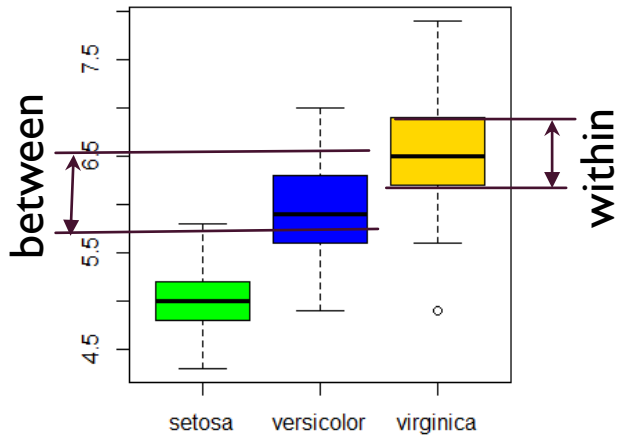

- Note: if we defined the accuracy as $\frac{1}{k}\sum_i |y_i - \overline{y}_i|$ the best prediction would be the median!

# PREDICTION AND VARIANCE: EXPLANATORY VARIABLES

- Now let's recollect that the sepal length seem to depend on the species
- In the presence of an "explanatory variable" we can predict much better!
  - What our predictions are going to be for each species?
- Let us look at sums of squares in different scenarios:

```
v.total = var(iris$Sepal.Length)
levels(iris$Species)
[1] "setosa"     "versicolor" "virginica"
v.setosa = var(iris$Sepal.Length[iris$Species=="setosa"])
v.versi = var(iris$Sepal.Length[iris$Species=="versicolor"])
v.virg = var(iris$Sepal.Length[iris$Species=="virginica"])
m1=mean(iris$Sepal.Length[iris$Species=="setosa"])-mean(iris$Sepal.Length)
m2=mean(iris$Sepal.Length[iris$Species=="versicolor"])-mean(iris$Sepal.Length)
m3=mean(iris$Sepal.Length[iris$Species=="virginica"])-mean(iris$Sepal.Length)
v.total*149
[1] 102.1683
(v.setosa+v.versi+v.virg)*49 + (m1^2+m2^2+m3^2)*50
[1] 102.1683
```

Explained variance




We used the fact that variance=sum (squared diff from mean) / (Nobservations-1)

Note: the figure is an illustration only as boxplots show medians/IQRs, not means/variances

# PREDICTION AND VARIANCE: CONTINUED

- What we observed (can be proved, of course!) is that the squared sum of "errors" in the best possible prediction without explanatory variables (which is just the sample's grand mean) is equal to the sum of remaining errors of predictions *with* explanatory variable PLUS the squared differences between new predictions and the sample mean.
- Variation within each species ("within" term) is still unexplained – even if we know the species, we cannot predict better than just the mean *in that subset*
- Variation between different predictions (means of the subsets) and the sample mean ("between" term) is what we *explained* : indeed, this is what we *predict* based on the species!
- Total variation in the dataset = Unexplained (remaining) variation + Explained (predicted) variation
- Or in other words, prediction = reducing remaining unexplained variance!

# STATISTICAL LEARNING

- Previously, we have written the "idea" of prediction down as Y = [ prediction generator ]
- More formal way is to write $Y = f(X)+\varepsilon$
  - Here X are all the explanatory variables we are considering, $X_1,\ldots,X_n$
  - f(X) is the "prediction generator" – it does not necessarily have a closed functional form (e.g. f(x)=Ax+B), but of course it should be computable in some way, e.g. by computer program. For each measurement (realization) $x_1,\ldots,x_n$ of the random processes X, we can substitute those values into the prediction generator and we get back the corresponding predicted value.
  - The predicted value is not going to be always precisely correct – there will be *unexplained* variance remaining, which is described by the noise term $\varepsilon$.
  - Note that we call "noise" everything that our model does not explain: it can be "true" random noise (as in nature throwing a coin) or it can be some effect that *could* be explained if we could (or cared to) include additional variables into our model! Return to our Sepal Length example: if you examine the pairwise scatterplots carefully, you could observe that *within* each species sepal length still correlates pretty well with sepal width. So we could improve our model further and explain a bigger chunk of the total variance in the observations of the sepal length! But for as long as we don't include sepal width, all the remaining, "within" variance in our boxplots is just that: "noise".

# PREDICTION VS INFERENCE

- In prediction problem we are interested in predicting outcome in new cases
  - Stock price
  - Patient survival
- In inference problem we are more interested in describing the data at hand
  - Which parameters are important?
  - Which parameters have positive/negative effect?
- In general, there is no clear distinction between models that can be used for prediction or inference, but the properties of different models may make them more or less desirable in different settings
  - For instance, extremely complex model that does not allow for clear interpretation of the dependencies or relative importance of the variables might be something we are more willing to adopt for prediction but not for inference

# MODEL BIAS AND VARIANCE

- As we have been discussing the prediction generator, or the *model* (which is the proper term) f(X), we ignored the fact that there is a difference between "true" model (or the "best possible one") and the one we explicitly use to explain the observations. This difference is called the *model bias*
  - Again, the true model may or may not have any particular closed functional form. We refer to the best possible model here in statistical sense: the one that gives the most accurate predictions, in the presence of noise
- You will also hear a lot about model bias-variance tradeoff (and/or decomposition)
- We will look closer at bias-variance decomposition and tradeoff later in the course
- For now it suffices to say that model variance in this context refers to variability across models fit to different training datasets (i.e. different random samples from the same population)

# OVERFITTING

- The model can perform great on the training dataset, but does it generalize well?
- We can have so many parameters in the model/so few data points that our model starts fitting the noise!
- If prediction is what we are after, we MUST evaluate our model on a test dataset – a dataset that has NOT been used for training. Accuracy on the *test* dataset is of the greatest importance.
- Data that we are trying to fit a model to are only a *sample* (randomly drawn!). Just like sample mean is a random variable, so is any quantity that is computed from a given sample. Thus, it also includes a model (or rather its *parameters*)
  - Models that are too flexible have high ***variance***: change a lot from one training dataset to the next, i.e. fit noise
- ***Bias*** is the error due to oversimplification of the model, i.e. the (expected value of the) difference between what the prediction could be if we knew the "true" dependence and the prediction that our model makes.
  - For instance, if the true dependence is $Y = a X^2 + b X$, but we are only considering a model $Y = b X$, we are having a bias.
  - Bias-Variance tradeoff: there is a sweet spot where overall accuracy is optimal
  - Note that the "true model" may or may not have any particular closed functional form. We refer to it here, somewhat informally, as some "true underlying dependence".

# SUMMARY

- We have finished the review of basic capabilities of R
  - lists, data frames and factors
  - Flow control, functions
  - Loading and saving data
- Few basic techniques and approaches for preliminary/exploratory data analysis, summary statistics and plots
- "Prediction" interpreted in a sense of expecting the most "likely" outcome (there is a reason for defining the mean of the distribution as *expected value* of x, or E(x))
  - If we have a distribution for outcome Y, the best prediction is the mean (if the accuracy measure is the MSE!)
  - When we have additional variables X measured, we essentially try computing (or estimating) P(Y|X) (this is *exactly* what the stratification we performed in iris dataset represented: we built the distributions of the sepal length for each species *separately*, i.e. we looked at P(Length|Species)!
  - The difference(s) between the predicted values (at different values of X) are the part of total variance in Y that we *explain*. The remaining variance of P(Y|X) at any fixed $X=x_i$ is *unexplained* variance.
- Discussion of statistical modeling: models, their complexity and flexibility, model bias, overfitting (model variance), bias-variance tradeoff.

# ADDITIONAL DETAILS

- Above covers basic necessities to complete this week assignment
- For the remaining time we will cover few more topics closely related to those already discussed

# LISTS: OUT OF BOUNDS ACCESS

- Just like vectors, lists allow out of bounds access without causing an error
  - On access, a NULL will be returned (not an NA!!)
  - On assignment, the list will auto-expand and NULL elements will be inserted as needed.

```
> x=list(1:3);x
[[1]]
[1] 1 2 3

> x$V="new element"; x
[[1]]
[1] 1 2 3

$V
[1] "new element"
```

```
> x[5]=2
> x
[[1]]
[1] 1 2 3

$V
[1] "new element"

[[3]]
NULL

[[4]]
NULL

[[5]]
[1] 2
```

# VARIABLE SCOPING

- The body of if/else, 'while' or 'for' statement does NOT have its own scope (variable first defined inside if/else or a loop is available afterwards)
- Variables defined inside functions (including formal parameters) are local to those functions and will mask variables with the same names in the outer scope
- Outer scope ("global") variables are visible inside function body (unless masked by another variable) but unmodifiable (sort of)
  - Global variables are "copy-on-change"; it *is* possible to modify a global variable (and even the argument passed to a function!) from inside a function, but you really shouldn't!

```
> y=1:3
> f=function() {
    print(y)
    y[2]=5 # now y is local!
    print(y)
 }
> f()
[1] 1 2 3
[1] 1 5 3
> y
[1] 1 2 3
```

```
> y=1:3
> f=function() {
    print(y)
    y[2]<<-5 # assign in outer scope
    print(y)
 }
> f()
[1] 1 2 3
[1] 1 5 3
> y
[1] 1 5 3
```

# LAZY EVALUATION

- Evaluations in R are performed lazily (only when needed)
  - Logical expressions are short-circuited (something you most likely have seen before)
  - Function arguments and even *default values* are not evaluated until they are needed!

```
> x=5
# need to evaluate both expressions:
> ! is.na(x) && x > 0
[1] TRUE
> x=NA
# evaluates only part to the left of &&:
> ! is.na(x) && x > 0
[1] FALSE
# proof: undefined function - no problem!
> ! is.na(x) && some.undefined.fun(x)
[1] FALSE
# Can you explain what happened here:
> F & some.undefined.fun(x)
Error: could not find function
"some.undefined.fun"
```

```
f=function(x,y=sqrt(z)) {
    if ( x == 1 ) print("I need only x")
    else {
       if ( x == 2 ) { y=y+1; print("I need x and y") }
    }
 }
> f(1) # y never used, default not evaluated!
[1] "I need only x"
> f(1,sqrt(W)) # y not used, passed arg not evaluated!
[1] "I need only x"
> f(2) # needs y for y=y+1, cannot evaluate default!
Error in f(2) : object 'z' not found
> z=4 # now z is defined…
> f(2)# and the function can evaluate the default for y!
[1] "I need x and y"
> f(2,y=sqrt(W)) # arg is evaluated since y is needed
Error in f(2, y = sqrt(W)) : object 'W' not found
```

# TRADITIONAL LOOPS VS VECTORIZED CODE

- A word on vectorized arithmetic (cannot be overstated):

```
> x<-numeric(10000000)
> system.time(x[] <- 1)
   user  system elapsed
   0.03    0.00    0.03
> system.time(for(i in 1:length(x)) x[i] <- 1)
   user  system elapsed
  10.44    0.02   10.54
```

- R provides mapping functions (the 'apply' family); contrary to popular belief they are not necessarily faster, but at least they are convenient and fit well into the whole paradigm of vectorized calculations:

```
> y=numeric(length(x))
> system.time(for(i in 1:length(x)) y[i]=x[i]^2)
   user  system elapsed
  16.22    0.00   16.27
> system.time(y <- sapply(x,FUN=function(x) x^2 ))
   user  system elapsed
  18.82    0.06   18.91
> system.time(y <- x^2)
   user  system elapsed
   0.02    0.00    0.02
```

Why can't we use '='?

```
> m=matrix(1:6,ncol=2)
> m
     [,1] [,2]
[1,]    1    4
[2,]    2    5
[3,]    3    6
# apply a function to each row (MARGIN=1);
# to apply to each column we'd use MARGIN=2:
> apply(m,MARGIN=1,sum)
[1] 5 7 9
```

# EXTENDING R

- R can be easily extended by writing functions
  - technically, one can write an efficient implementation in C and wrap is as an R function too – well beyond our scope
- The easiest way to manage a collection of functions (which you most likely will end up having if you continue doing data analysis with R!) is:
  - Save your function definitions into a file (e.g. myCS63library.R)
  - Read the code from the R script file in: `> source("myCS63library.R")`
  - R simply reads and executes the "sourced" code line by line, so you may have a bona fide script too, which not only defines functions (function definitions ARE R commands, of course), but executes some other commands, e.g. performs end-to-end computation, draws plots etc
- Third party libraries are released as "packages" – a more sophisticated way (which we will not go deep into, just use)
  - at the basic level, a package is a library that needs to be (a) installed on your system and (b) loaded into your R session; as the result, additional functions (and maybe variables/data) from the package will become available
  - R GUI offers packages->install packages.. option with graphical package chooser interface
  - Note: on my machine, installing via HTTPS does not always work due to some proxy/security settings, in that case choose 'HTTP mirrors' from the menu, then 0-Clouds, then select package to download and install

# LOADING PACKAGED LIBRARY/DATA

- When the package is installed, you have to load it into your session, for instance:

```
> library(ggplot2)
```

- Note that you do not need the quotation marks
- Some packages also (or only!) provide datasets. Those can be loaded as in the following example:

```
> data(iris)
> iris[1:3,]
  Sepal.Length Sepal.Width Petal.Length Petal.Width Species
1          5.1         3.5          1.4         0.2  setosa
2          4.9         3.0          1.4         0.2  setosa
3          4.7         3.2          1.3         0.2  setosa
```

- Package 'iris' does not need to be loaded, it's part of base R distribution
- When dataset is loaded it creates variable 'iris' in the workspace (so the old value we had from downloading the data file manually is now overridden)