Introduction to R

A Short Overview

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Outline

Outline

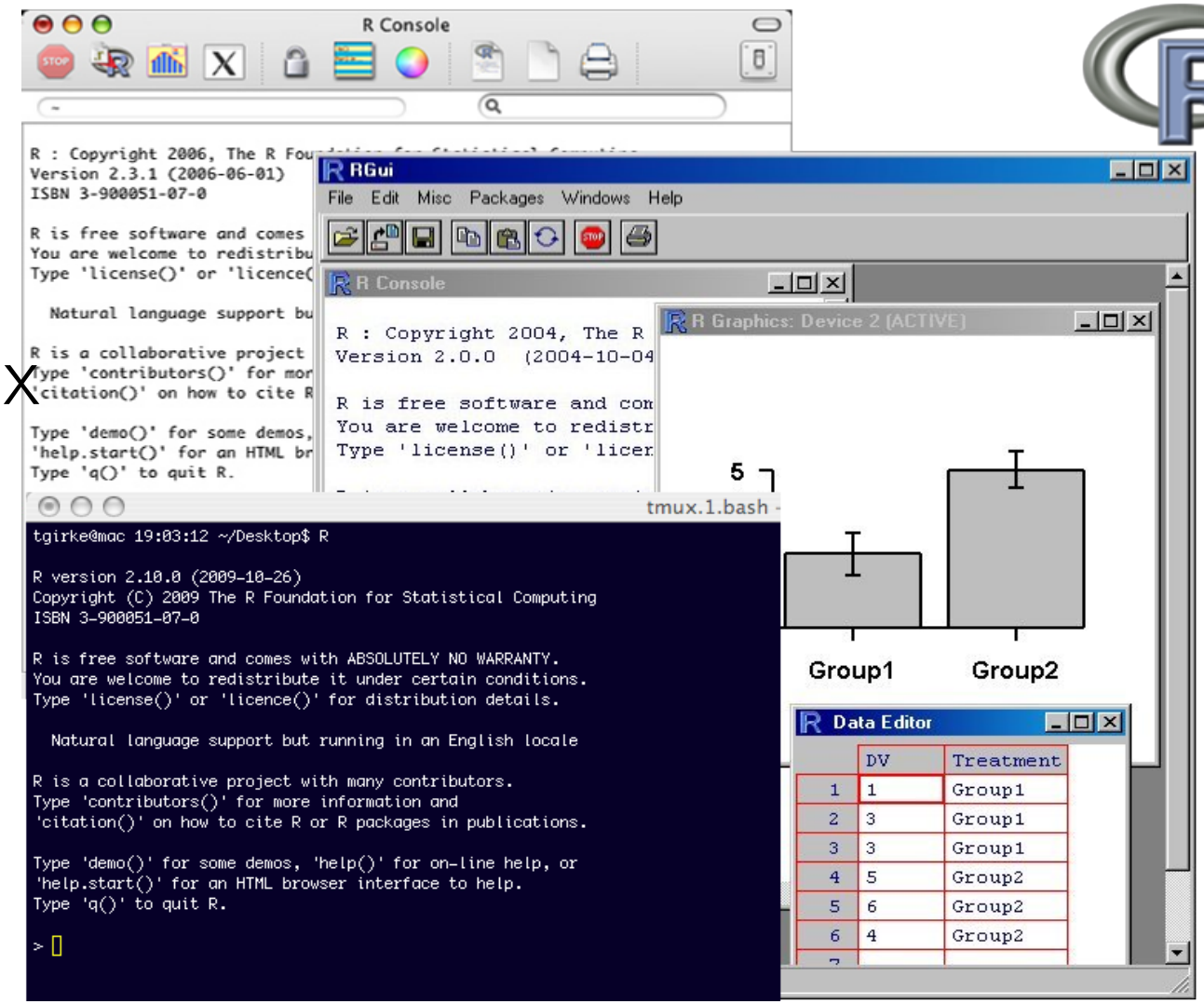
Why Using R?

- Complete statistical environment and programming language
- Efficient functions and data structures for data analysis
- Powerful graphics
- Access to fast growing number of analysis packages
- Most widely used language in bioinformatics
- Is standard for data mining and biostatistical analysis
- Technical advantages: free, open-source, available for all OSs

Books & Documentation

- simpleR - Using R for Introductory Statistics (John Verzani, 2004) Link
- Bioinformatics and Computational Biology Solutions Using R and Bioconductor (Gentleman et al., 2005) Link
- More on this see "Finding Help" section in UCR Manual Link

What You'll Get?



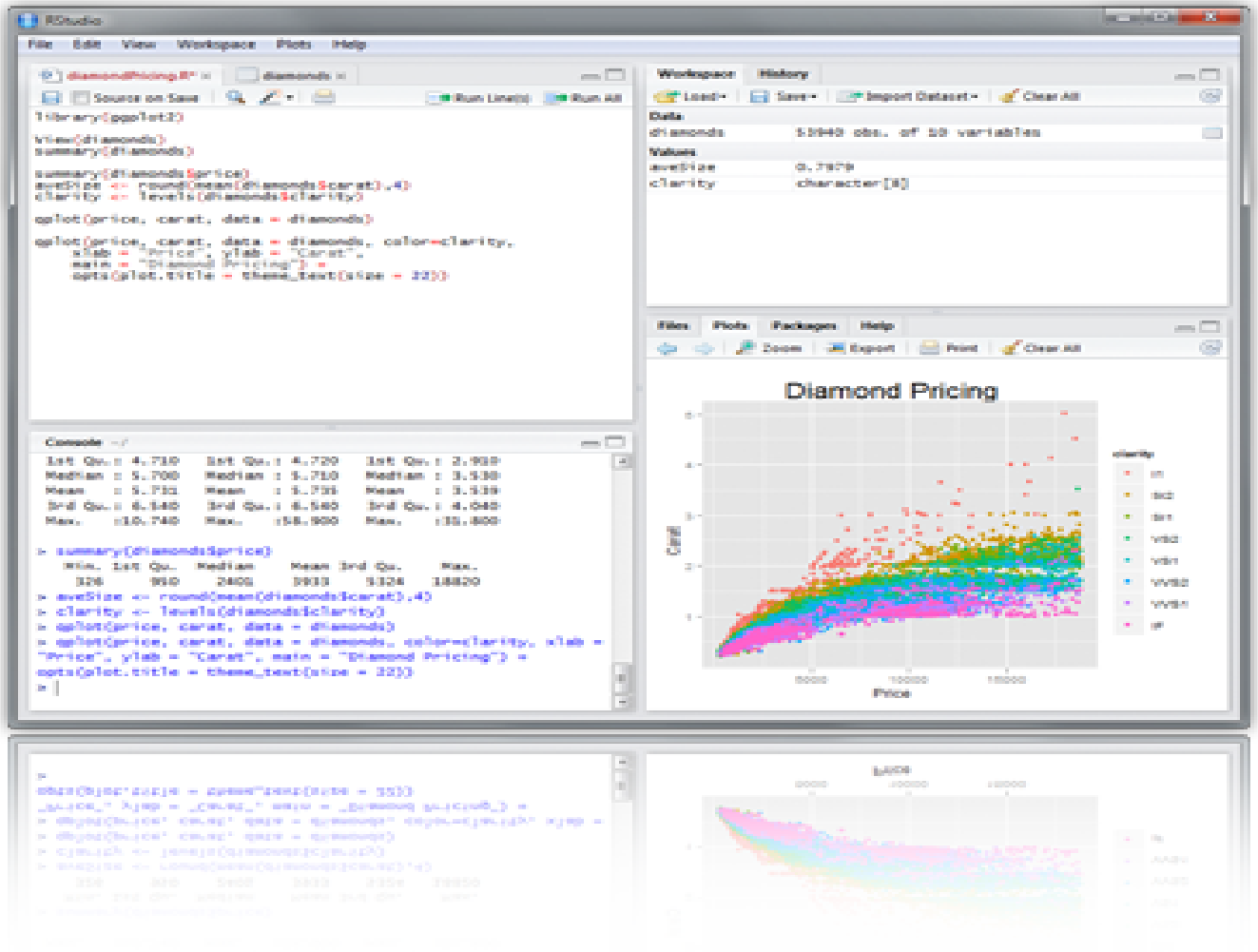
R Gui: OS X

Command-line R: Linux/OS X

R Gui: Windows

RStudio: Alternative Working Environment for R

New integrated development environment (IDE) for R Link that works well for beginners and developers.

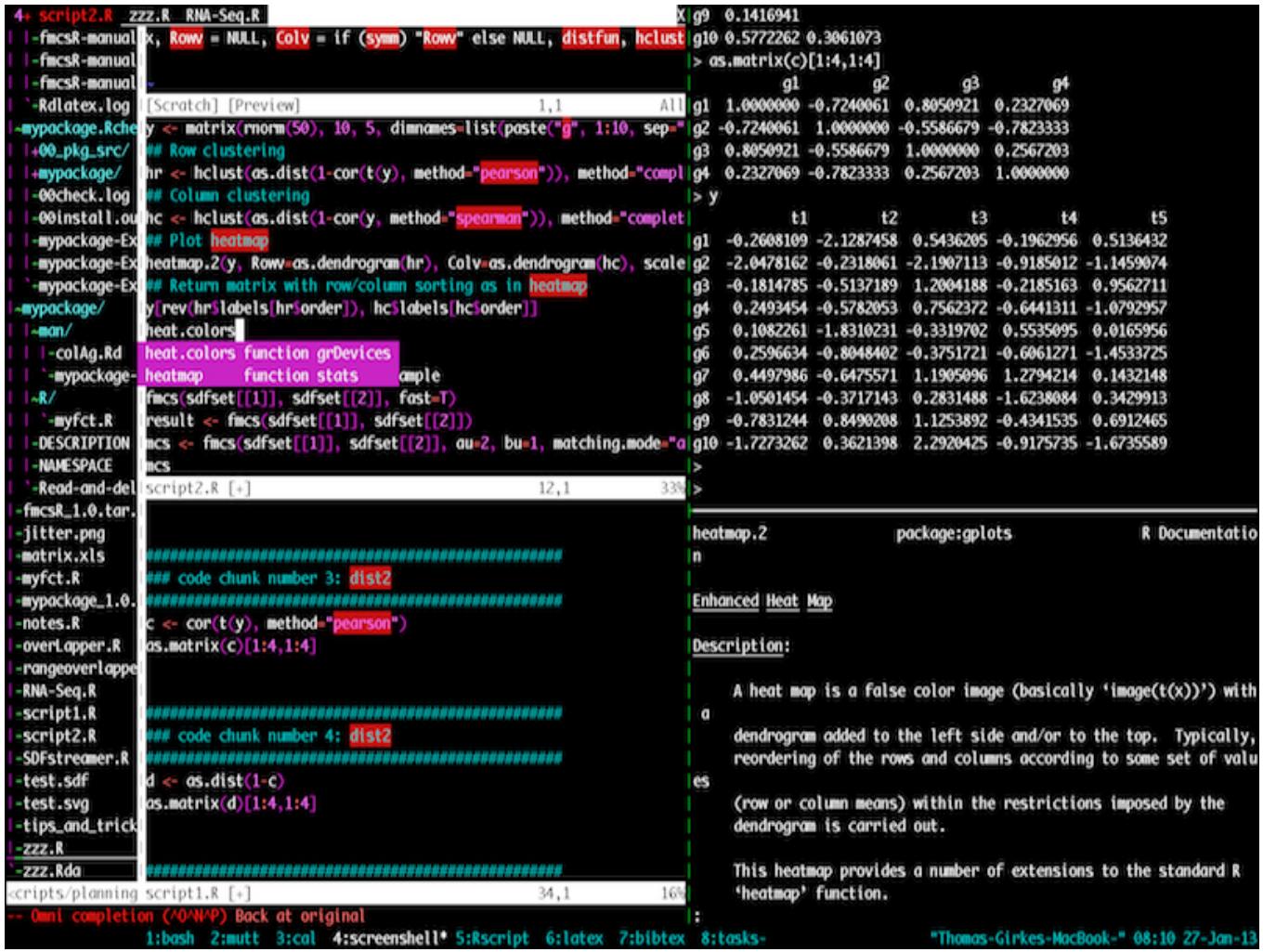


Important shortcuts: `Ctrl+Enter` (send code), `Ctrl+Shift+C` (comment/uncomment), `Ctrl+1/2` (switch window focus)

Vim-R-Tmux: Command-Line IDE for R

Terminal-based Working Environment for R: Vim-R-Tmux

Link



Outline

Package Depositories

- CRAN (>6,000 packages) general data analysis Link
- Bioconductor (>900 packages) bioscience data analysis Link
- Omegahat (>90 packages) programming interfaces Link

Outline

Installation of R and Add-on Packages

Install R for your operating system from:

http://cran.at.r-project.org Link

Install RStudio from:

http://www.rstudio.com/ide/download Link

Installation of CRAN Packages

```
> install.packages(c("pkg1", "pkg2"))
> install.packages("pkg.zip", repos=NULL)
```

Installation of Bioconductor Packages

```
> source("http://www.bioconductor.org/biocLite.R")
> library(BiocInstaller)
> BiocVersion()
> biocLite()
> biocLite(c("pkg1", "pkg2"))
```

For more details see Bioc Install page Link and *BiocInstaller* Link

Outline

Startup and Closing Behavior

Starting R

The R GUI versions, including RStudio, under Windows and Mac OS X can be opened by double-clicking their icons. Alternatively, one can start it by typing 'R' in a terminal (default under Linux).

Startup/Closing Behavior

The R environment is controlled by hidden files in the startup directory: .RData, .Rhistory and .Rprofile (optional).

```
## Closing R
> q()
Save workspace image?  [y/n/c]:
```

Note

When responding with 'y', then the entire R workspace will be written to the .RData file which can become very large. Often it is sufficient to just save an analysis protocol in an R source file. This way one can quickly regenerate all data sets and objects.

Getting Around

Create an object with the assignment operator <- (or =)

```
> object <- ...
```

List objects in current R session

```
> ls()
```

Return content of current working directory

```
> dir()
```

Return path of current working directory

```
> getwd()
```

Change current working directory

```
> setwd("/home/user")
```

Outline

Basic R Syntax

General R command syntax

```
> object <- function_name(arguments)
> object <- object[arguments]
```

Finding help

```
> ?function_name
```

Load a library

```
> library("my_library")
```

Lists all functions defined by a library

```
> library(help="my_library")
```

Load library manual (PDF file)

```
> vignette("my_library")
```

Executing R Scripts

Execute an R script from within R

```
> source("my_script.R")
```

Execute an R script from command-line

```
Rscript my_script.R
R CMD BATCH my_script.R
R --slave < my_script.R
```

Outline

Data Types I

Numeric data: 1, 2, 3

```
> x <- c(1, 2, 3); x
[1] 1 2 3
> is.numeric(x)
[1] TRUE
> as.character(x)
[1] "1" "2" "3"
```

Character data: "a", "b", "c"

```
> x <- c("1", "2", "3"); x
[1] "1" "2" "3"
> is.character(x)
[1] TRUE
> as.numeric(x)
[1] 1 2 3
```

Data Types II

Complex data

```
> c(1, "b", 3)

[1] "1" "b" "3"
```

Logical data

```
> x <- 1:10 < 5
> x

 [1]  TRUE  TRUE  TRUE  TRUE FALSE FALSE FALSE FALSE FALSE FALSE

> !x

 [1] FALSE FALSE FALSE FALSE  TRUE  TRUE  TRUE  TRUE  TRUE  TRUE

> which(x) # Returns index for the 'TRUE' values in logical vector

[1] 1 2 3 4
```

Data Objects: Vectors and Factors

Vectors (1D)

```
> myVec <- 1:10; names(myVec) <- letters[1:10]
> myVec[1:5]

a b c d e
1 2 3 4 5

> myVec[c(2,4,6,8)]

b d f h
2 4 6 8

> myVec[c("b", "d", "f")]

b d f
2 4 6
```

Factors (1D): vectors with grouping information

```
> factor(c("dog", "cat", "mouse", "dog", "dog", "cat"))

[1] dog   cat   mouse dog   dog   cat
Levels: cat dog mouse
```

Data Objects: Matrices, Data Frames and Arrays

Matrices (2D): two dimensional structures with data of same type

```
> myMA <- matrix(1:30, 3, 10, byrow = TRUE)
> class(myMA)

[1] "matrix"

> myMA[1:2,]

     [,1] [,2] [,3] [,4] [,5] [,6] [,7] [,8] [,9] [,10]
[1,]    1    2    3    4    5    6    7    8    9    10
[2,]   11   12   13   14   15   16   17   18   19    20

> myMA[1, , drop=FALSE]

     [,1] [,2] [,3] [,4] [,5] [,6] [,7] [,8] [,9] [,10]
[1,]    1    2    3    4    5    6    7    8    9    10
```

Data Frames (2D): two dimensional structures with variable data types

```
> myDF <- data.frame(Col1=1:10, Col2=10:1)
> myDF[1:2, ]

  Col1 Col2
1    1   10
2    2    9
```

Arrays: data structure with one, two or more dimensions

Data Objects: Lists and Functions

Lists: containers for any object type

```
> myL <- list(name="Fred", wife="Mary", no.children=3, child.ages=c(4,7,9))
> myL

$name
[1] "Fred"

$wife
[1] "Mary"

$no.children
[1] 3

$child.ages
[1] 4 7 9

> myL[[4]][1:2]

[1] 4 7
```

Functions: piece of code

```
> myfct <- function(arg1, arg2, ...) {
+         function_body
+ }
```

General Subsetting Rules

Subsetting by positive or negative index/position numbers

```
> myVec <- 1:26; names(myVec) <- LETTERS
> myVec[1:4]
```

```
A B C D
1 2 3 4
```

Subsetting by same length logical vectors

```
> myLog <- myVec > 10
> myVec[myLog]
```

```
 K  L  M  N  O  P  Q  R  S  T  U  V  W  X  Y  Z
11 12 13 14 15 16 17 18 19 20 21 22 23 24 25 26
```

Subsetting by field names

```
> myVec[c("B", "K", "M")]
```

```
 B  K  M
 2 11 13
```

Calling a single column or list component by its name with the $ sign

```
> iris$Species[1:8]
```

```
[1] setosa setosa setosa setosa setosa setosa setosa setosa
Levels: setosa versicolor virginica
```

Outline

Combining Objects

The c function combines vectors and lists

```
> c(1, 2, 3)
```

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

```
> x <- 1:3; y <- 101:103
> c(x, y)
```

```
[1]   1   2   3 101 102 103
```

The cbind and rbind functions can be used to append columns and rows, respecively.

```
> ma <- cbind(x, y)
> ma
```

```
     x   y
[1,] 1 101
[2,] 2 102
[3,] 3 103
```

```
> rbind(ma, ma)
```

```
     x   y
[1,] 1 101
[2,] 2 102
[3,] 3 103
[4,] 1 101
[5,] 2 102
[6,] 3 103
```

Accessing Name Slots and Dimensions of Objects

Length and dimension information of objects

```
> length(iris$Species)

[1] 150

> dim(iris)

[1] 150   5
```

Accessing row and column names of 2D objects

```
> rownames(iris)[1:8]

[1] "1" "2" "3" "4" "5" "6" "7" "8"

> colnames(iris)

[1] "Sepal.Length" "Sepal.Width"  "Petal.Length" "Petal.Width"  "Species"
```

Return name field of vectors and lists

```
> names(myVec)

 [1] "A" "B" "C" "D" "E" "F" "G" "H" "I" "J" "K" "L" "M" "N" "O" "P" "Q" "R" "S

> names(myL)

[1] "name"         "wife"         "no.children" "child.ages"
```

Sorting Objects

The function `sort` returns a vector in ascending or descending order

```
> sort(10:1)

 [1]  1  2  3  4  5  6  7  8  9 10
```

The function `order` returns a sorting index for sorting an object

```
> sortindex <- order(iris[,1], decreasing = FALSE)
> sortindex[1:12]

 [1] 14  9 39 43 42  4  7 23 48  3 30 12

> iris[sortindex,][1:2,]

   Sepal.Length Sepal.Width Petal.Length Petal.Width Species
14          4.3         3.0          1.1         0.1  setosa
9           4.4         2.9          1.4         0.2  setosa

> sortindex <- order(-iris[,1]) # Same as decreasing=TRUE
```

Sorting on multiple columns

```
> iris[order(iris$Sepal.Length, iris$Sepal.Width),][1:2,]

   Sepal.Length Sepal.Width Petal.Length Petal.Width Species
14          4.3         3.0          1.1         0.1  setosa
9           4.4         2.9          1.4         0.2  setosa
```

Outline

Basic Operators and Calculations

Comparison operators: ==, ! =, <, >, <=, >=

```
> 1==1
```

```
[1] TRUE
```

Logical operators: AND: &, OR: |, NOT: !

```
> x <- 1:10; y <- 10:1
> x > y & x > 5
```

```
 [1] FALSE FALSE FALSE FALSE FALSE  TRUE  TRUE  TRUE  TRUE  TRUE
```

Calculations: to look up math functions, see Function Index Link

```
> x + y
```

```
 [1] 11 11 11 11 11 11 11 11 11 11
```

```
> sum(x)
```

```
[1] 55
```

```
> mean(x)
```

```
[1] 5.5
```

```
> apply(iris[1:6,1:3], 1, mean)
```

```
       1        2        3        4        5        6
3.333333 3.100000 3.066667 3.066667 3.333333 3.666667
```

Outline

Reading and Writing External Data

Import data from tabular files into R

```
> myDF <- read.delim("myData.xls", sep="\t")
```

Export data from R to tabular files

```
> write.table(myDF, file="myfile.xls", sep="\t", quote=FALSE, col.names=NA)
```

Copy and paste (e.g. from Excel) into R

```
> ## On Windows/Linux systems:
> read.delim("clipboard")
> ## On Mac OS X systems:
> read.delim(pipe("pbpaste"))
```

Copy and paste from R into Excel or other programs

```
> ## On Windows/Linux systems:
> write.table(iris, "clipboard", sep="\t", col.names=NA, quote=F)
> ## On Mac OS X systems:
> zz <- pipe('pbcopy', 'w')
> write.table(iris, zz, sep="\t", col.names=NA, quote=F)
> close(zz)
```

Exercise 1: Object Subsetting Routines and Import/Export

Task 1 Sort the rows of the `iris` data frame by its first column and sort its columns alphabetically by column names.

Task 2 Subset the first 12 rows, export the result to a text file and view it in Excel.

Task 3 Change some column titles in Excel and import the result into R.

Structure of `iris` data set:

```
> class(iris)
[1] "data.frame"
> dim(iris)
[1] 150   5
> colnames(iris)
[1] "Sepal.Length" "Sepal.Width"  "Petal.Length" "Petal.Width"  "Species"
```

Outline

Some Great R Functions I

The unique() function to make vector entries unique

```
> length(iris$Sepal.Length)
[1] 150
> length(unique(iris$Sepal.Length))
[1] 35
```

The table() function counts the occurrences of entries

```
> table(iris$Species)

    setosa versicolor  virginica
        50         50         50
```

The aggregate() function computes statistics of data aggregates

```
> aggregate(iris[,1:4], by=list(iris$Species), FUN=mean, na.rm=TRUE)

     Group.1 Sepal.Length Sepal.Width Petal.Length Petal.Width
1     setosa        5.006       3.428        1.462       0.246
2 versicolor        5.936       2.770        4.260       1.326
3  virginica        6.588       2.974        5.552       2.026
```

Some Great R Functions II

The %in% function returns the intersect between two vectors

```
> month.name %in% c("May", "July")
```

```
 [1] FALSE FALSE FALSE FALSE  TRUE FALSE  TRUE FALSE FALSE FALSE FALSE FALSE
```

The merge() function joins two data frames by common field entries, here row names (by.x=0). To obtain only the common rows, change all=TRUE to all=FALSE. To merge on specific columns, refer to them by their position numbers or their column names.

```
> frame1 <- iris[sample(1:length(iris[,1]), 30), ]
> frame1[1:2,]
```

```
   Sepal.Length Sepal.Width Petal.Length Petal.Width Species
17          5.4         3.9          1.3         0.4  setosa
39          4.4         3.0          1.3         0.2  setosa
```

```
> dim(frame1)
```

```
[1] 30  5
```

```
> my_result <- merge(frame1, iris, by.x = 0, by.y = 0, all = TRUE)
> dim(my_result)
```

```
[1] 150  11
```

Graphics in R

- Powerful environment for visualizing scientific data
- Integrated graphics and statistics infrastructure
- Publication quality graphics
- Fully programmable
- Highly reproducible
- Full LaTeX Link & Sweave Link support
- Vast number of R packages with graphics utilities

Documentation on Graphics in R

General

- Graphics Task Page Link
- R Graph Gallery Link
- R Graphical Manual Link
- Paul Murrell's book R (Grid) Graphics Link

Interactive graphics

- rggobi (GGobi) Link
- iplots Link
- Open GL (rgl) Link

Graphics Environments

Viewing and saving graphics in R

- On-screen graphics
- postscript, pdf, svg
- jpeg, png, wmf, tiff, ...

Four major graphic environments

- Low-level infrastructure
  - R Base Graphics (low- and high-level)
  - *grid*: Manual Link, Book Link
- High-level infrastructure
  - *lattice:* Manual Link, Intro Link, Book Link
  - *ggplot2:* Manual Link, Intro Link, Book Link

Outline

Outline

Base Graphics: Overview

Important high-level plotting functions

- `plot`: generic x-y plotting
- `barplot`: bar plots
- `boxplot`: box-and-whisker plot
- `hist`: histograms
- `pie`: pie charts
- `dotchart`: cleveland dot plots
- `image, heatmap, contour, persp`: functions to generate image-like plots
- `qqnorm, qqline, qqplot`: distribution comparison plots
- `pairs, coplot`: display of multivariant data

Help on these functions

- `?myfct`
- `?plot`
- `?par`

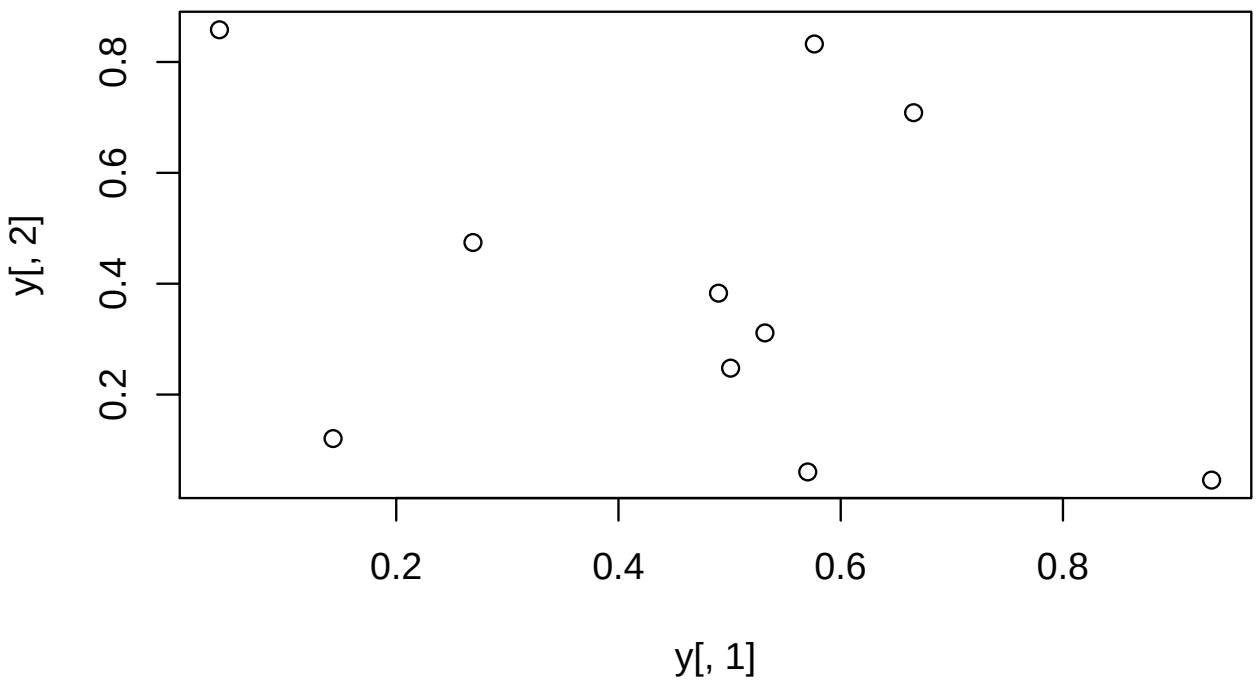
Base Graphics: Preferred Input Data Objects

- Matrices and data frames
- Vectors
- Named vectors

Scatter Plot: very basic

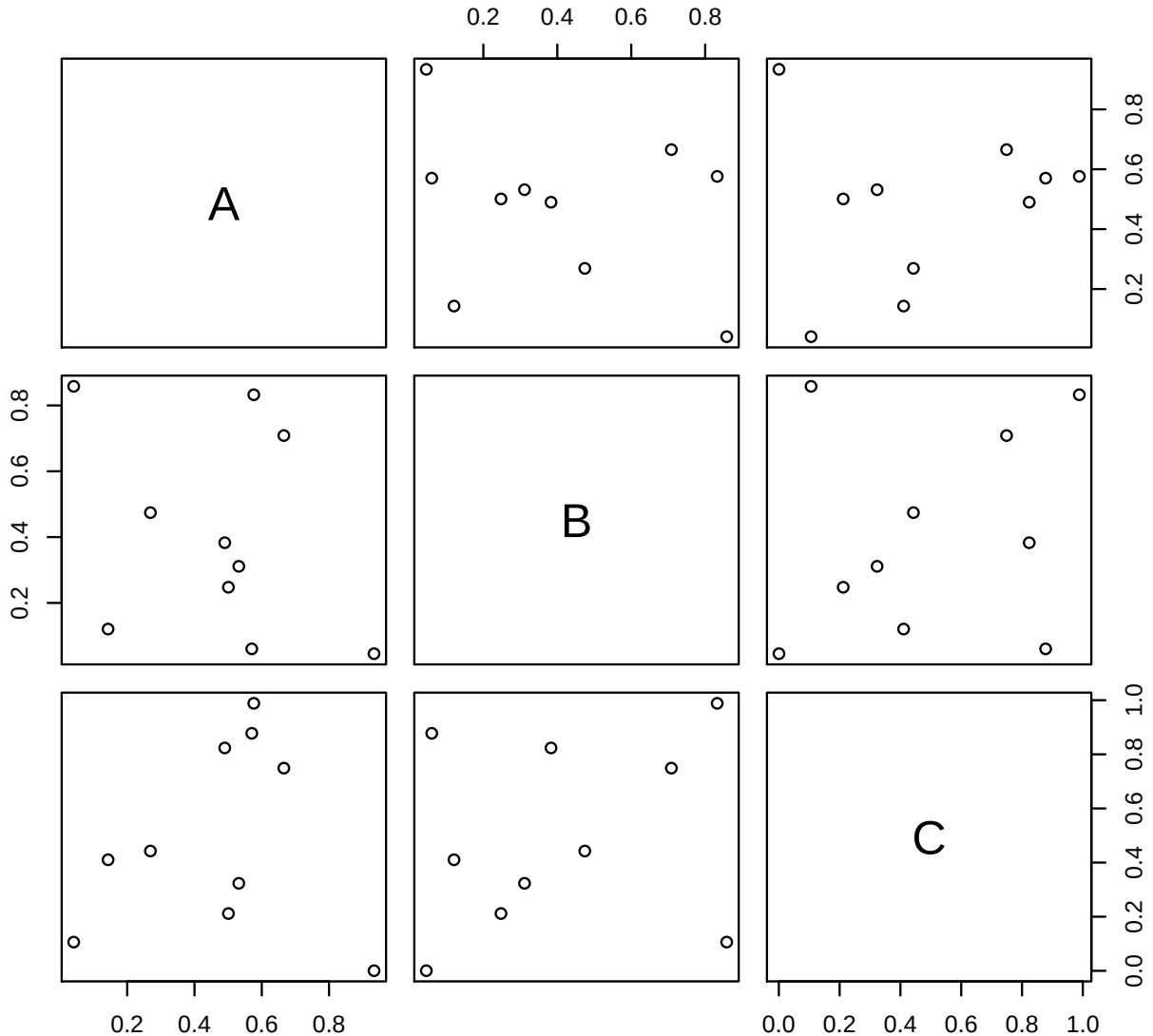
Sample data set for subsequent plots

```
> set.seed(1410)
> y <- matrix(runif(30), ncol=3, dimnames=list(letters[1:10], LETTERS[1:3]))

> plot(y[,1], y[,2])
```



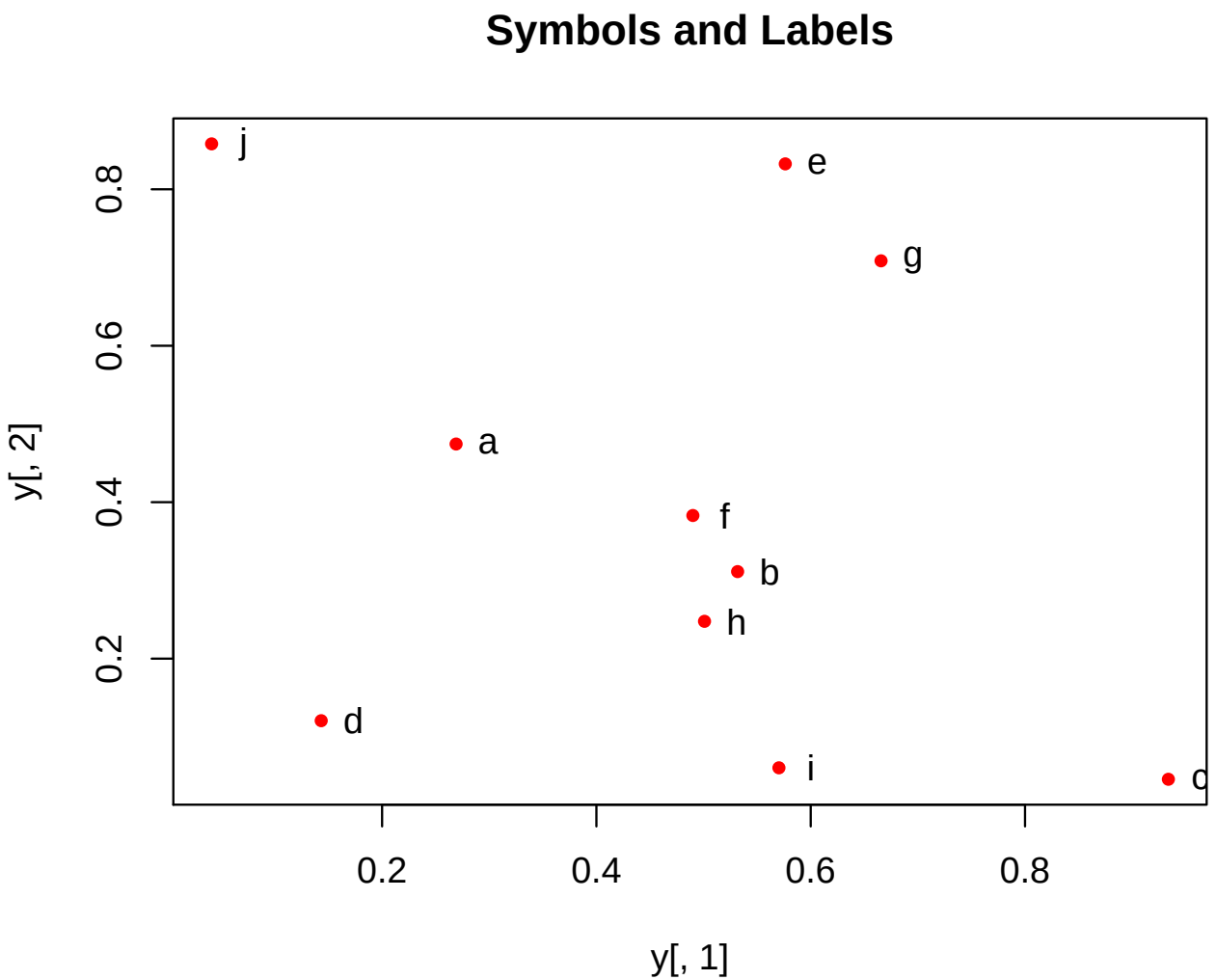
Scatter Plot: all pairs

```
> pairs(y)
```



Scatter Plot: with labels

```
> plot(y[,1], y[,2], pch=20, col="red", main="Symbols and Labels")
> text(y[,1]+0.03, y[,2], rownames(y))
```



Scatter Plots: more examples

Print instead of symbols the row names

```
> plot(y[,1], y[,2], type="n", main="Plot of Labels")
> text(y[,1], y[,2], rownames(y))
```

Usage of important plotting parameters

```
> grid(5, 5, lwd = 2)
> op <- par(mar=c(8,8,8,8), bg="lightblue")
> plot(y[,1], y[,2], type="p", col="red", cex.lab=1.2, cex.axis=1.2,
+      cex.main=1.2, cex.sub=1, lwd=4, pch=20, xlab="x label",
+      ylab="y label", main="My Main", sub="My Sub")
> par(op)
```

Important arguments

- `mar`: specifies the margin sizes around the plotting area in order: `c(bottom, left, top, right)`
- `col`: color of symbols
- `pch`: type of symbols, samples: `example(points)`
- `lwd`: size of symbols
- `cex.*`: control font sizes
- For details see `?par`

Scatter Plots: more examples

Add a regression line to a plot

```
> plot(y[,1], y[,2])
> myline <- lm(y[,2]~y[,1]); abline(myline, lwd=2)
> summary(myline)
```

Same plot as above, but on log scale

```
> plot(y[,1], y[,2], log="xy")
```

Add a mathematical expression to a plot

```
> plot(y[,1], y[,2]); text(y[1,1], y[1,2],
>      expression(sum(frac(1,sqrt(x^2*pi)))), cex=1.3)
```

Exercise 2: Scatter Plots

Task 1 Generate scatter plot for first two columns in `iris` data frame and color dots by its `Species` column.

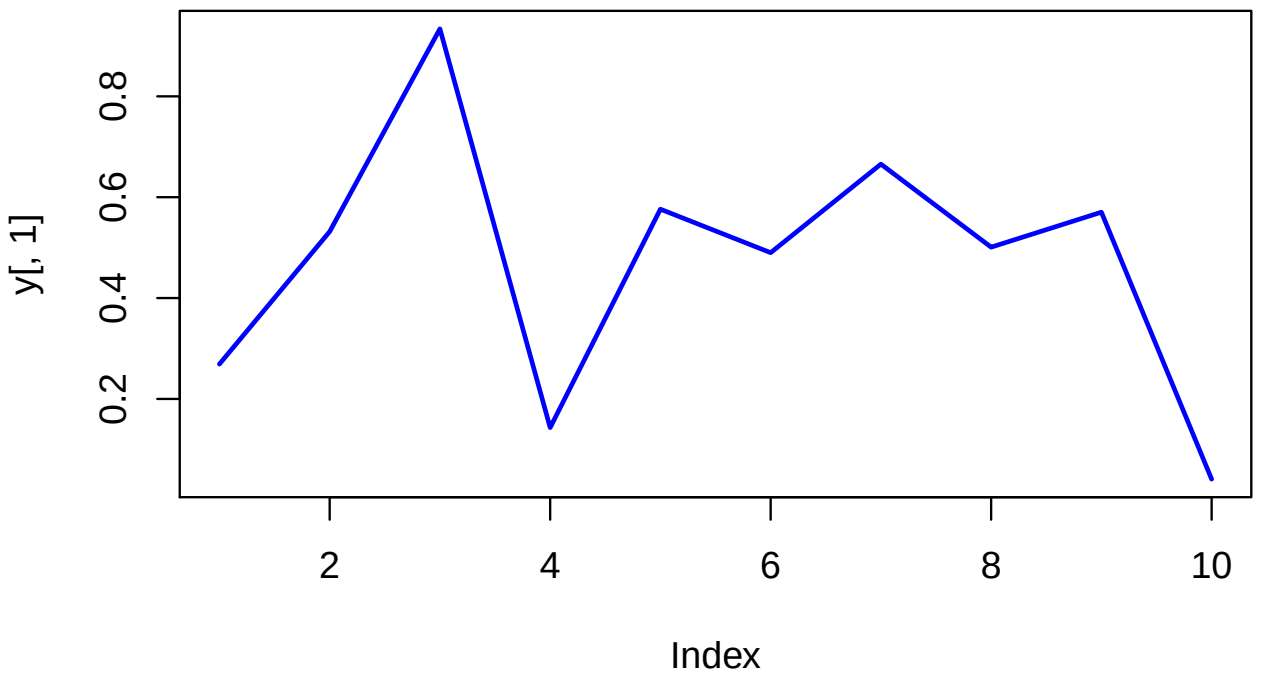
Task 2 Use the `xlim/ylim` arguments to set limits on the x- and y-axes so that all data points are restricted to the left bottom quadrant of the plot.

Structure of iris data set:

```
> class(iris)

[1] "data.frame"

> iris[1:4,]

  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
4          4.6         3.1          1.5         0.2  setosa

> table(iris$Species)

    setosa versicolor  virginica
        50         50         50
```

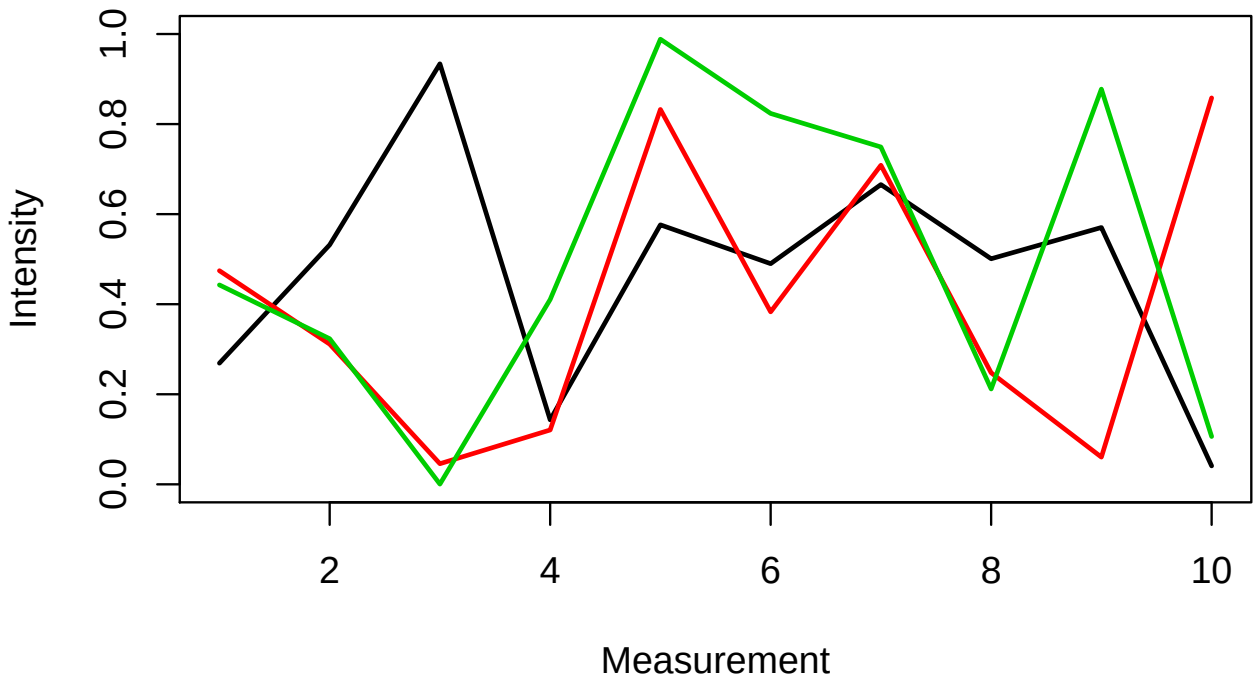
Line Plot: Single Data Set

```
> plot(y[,1], type="l", lwd=2, col="blue")
```



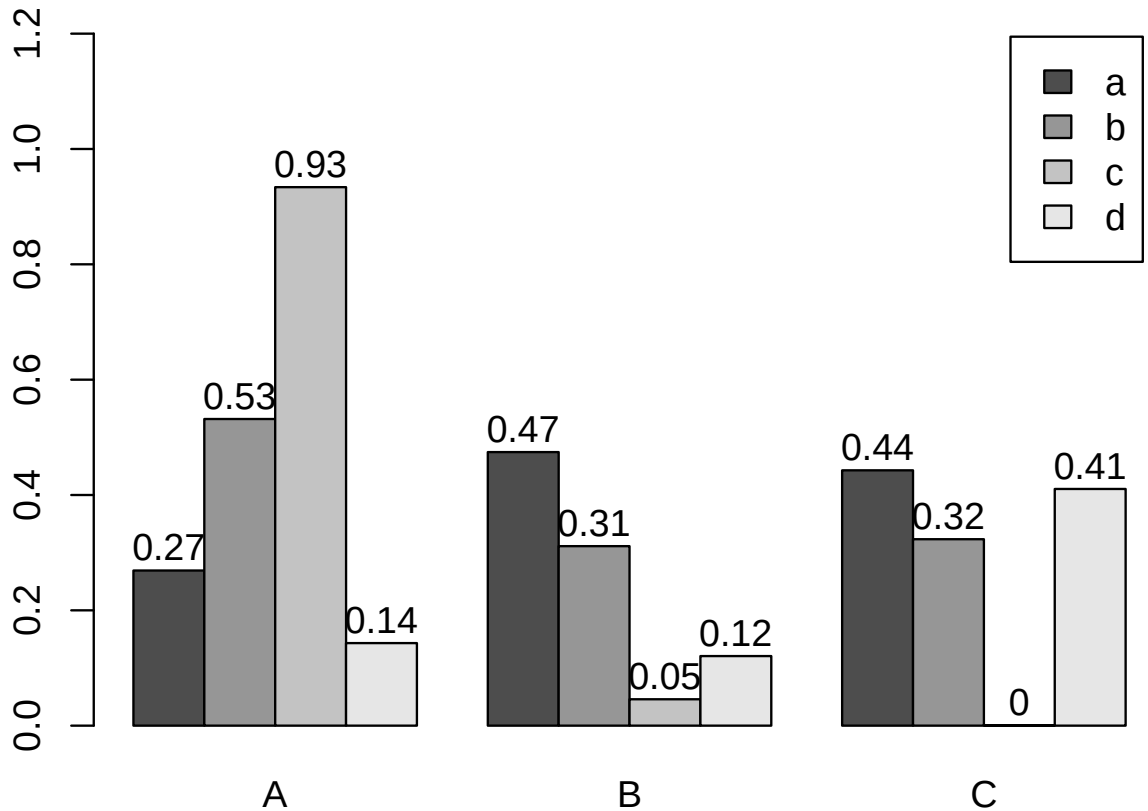
Line Plots: Many Data Sets

```
> split.screen(c(1,1));
[1] 1
> plot(y[,1], ylim=c(0,1), xlab="Measurement", ylab="Intensity", type="l", lwd=2, col=1)
> for(i in 2:length(y[1,])) {
+         screen(1, new=FALSE)
+         plot(y[,i], ylim=c(0,1), type="l", lwd=2, col=i, xaxt="n", yaxt="n", ylab="",
+              xlab="", main="", bty="n")
+ }
> close.screen(all=TRUE)
```



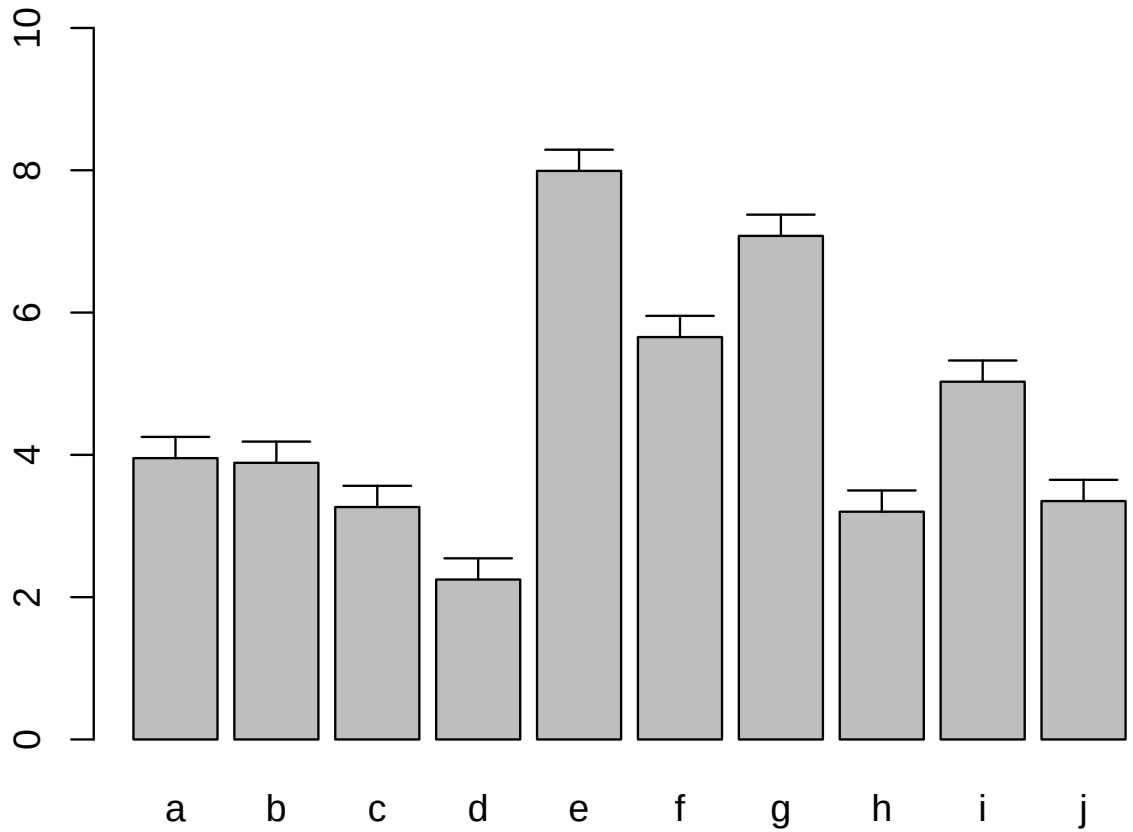
Bar Plot Basics

```
> barplot(y[1:4,], ylim=c(0, max(y[1:4,])+0.3), beside=TRUE,
+         legend=letters[1:4])
> text(labels=round(as.vector(as.matrix(y[1:4,])),2), x=seq(1.5, 13, by=1)
+      +sort(rep(c(0,1,2), 4)), y=as.vector(as.matrix(y[1:4,]))+0.04)
```



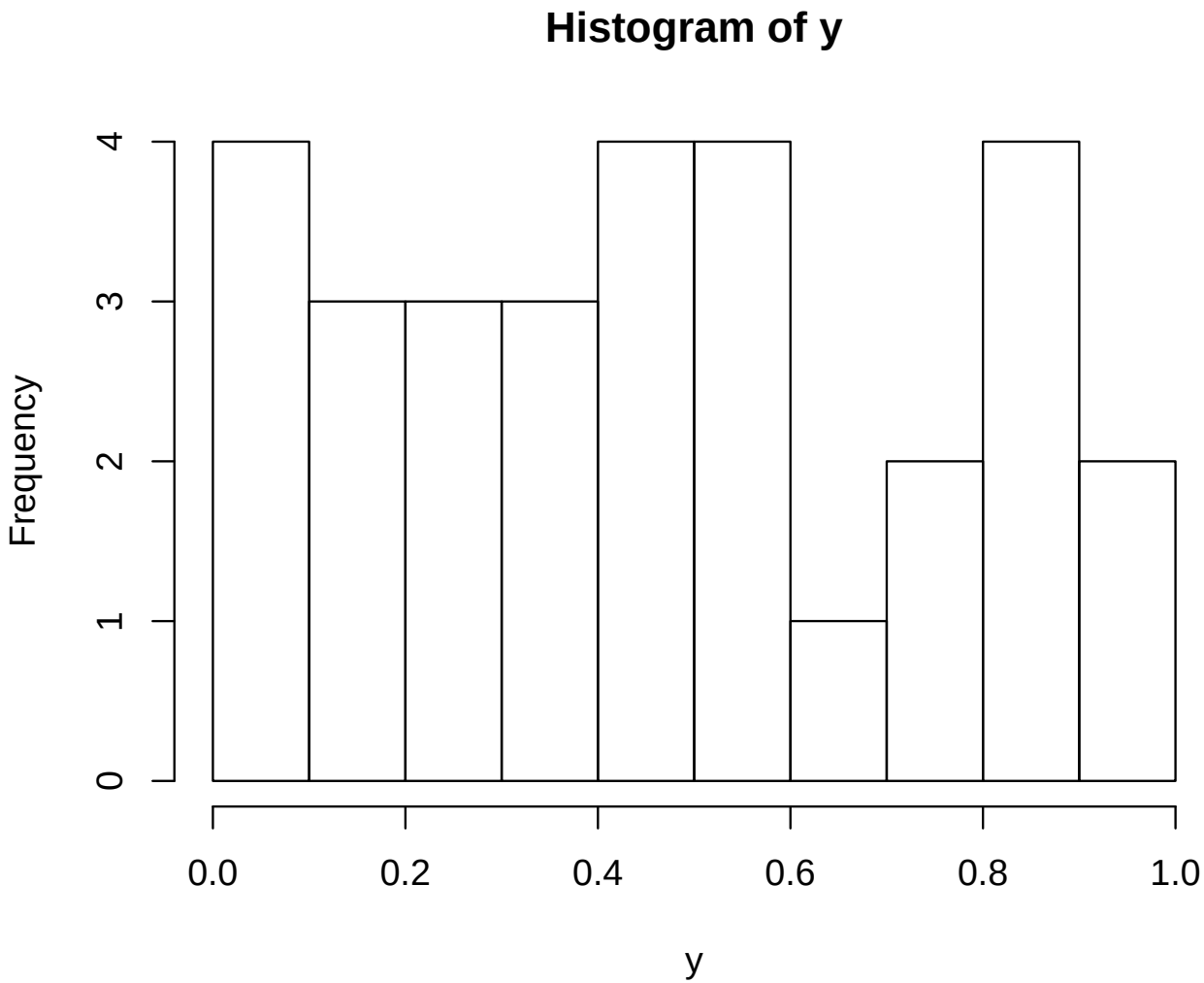
Bar Plots with Error Bars

```
> bar <- barplot(m <- rowMeans(y) * 10, ylim=c(0, 10))
> stdev <- sd(t(y))
> arrows(bar, m, bar, m + stdev, length=0.15, angle = 90)
```



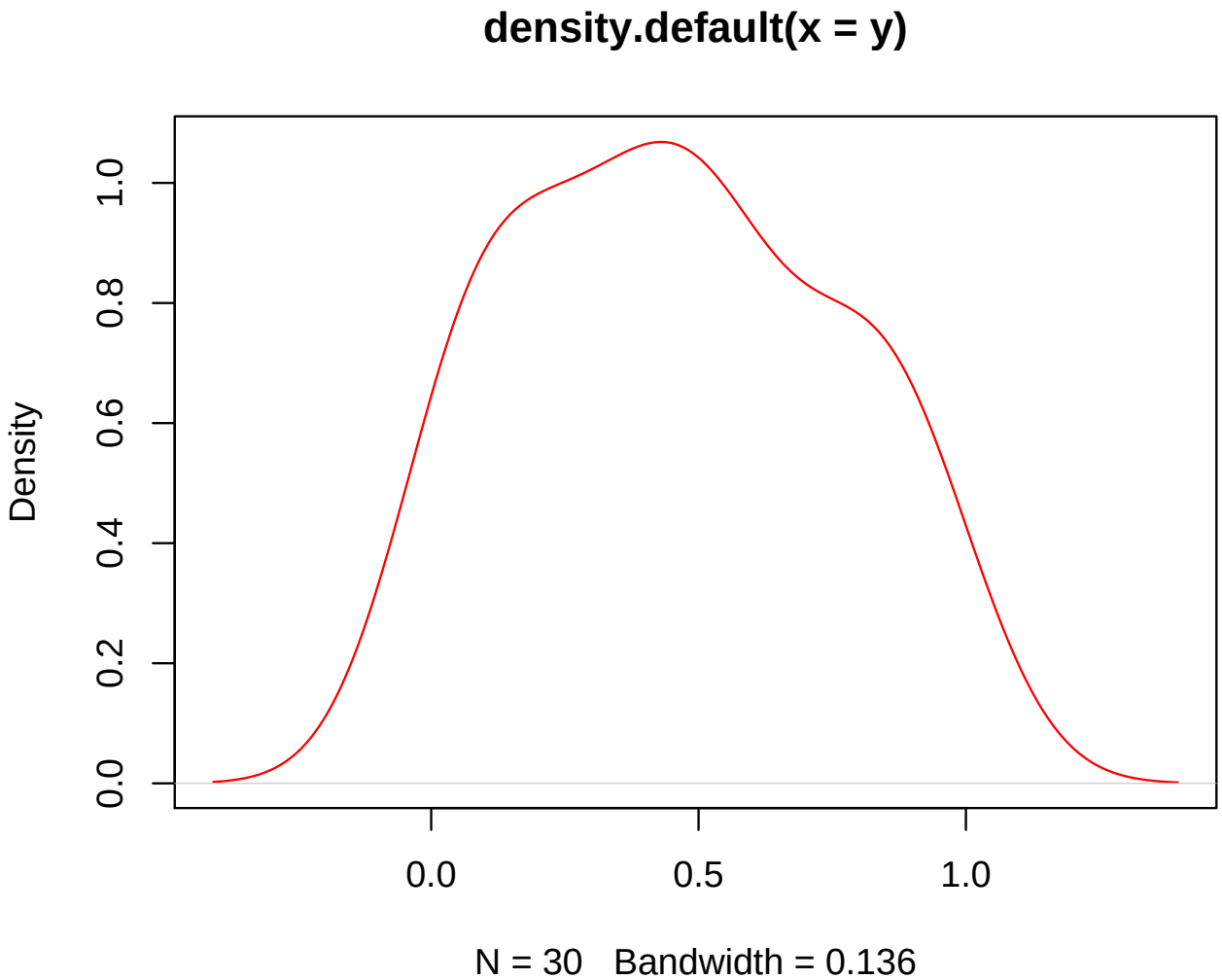
Histograms

```
> hist(y, freq=TRUE, breaks=10)
```



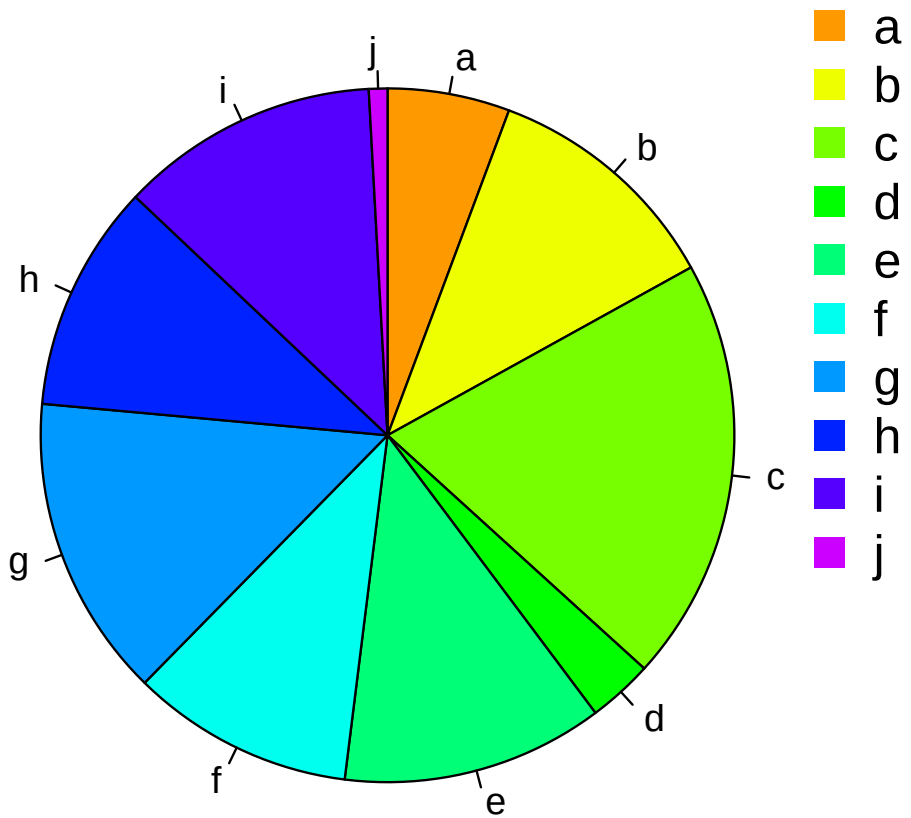
Density Plots

```
> plot(density(y), col="red")
```



Pie Charts

```
> pie(y[,1], col=rainbow(length(y[,1]), start=0.1, end=0.8), clockwise=TRUE)
> legend("topright", legend=row.names(y), cex=1.3, bty="n", pch=15, pt.cex=1.8,
+ col=rainbow(length(y[,1]), start=0.1, end=0.8), ncol=1)
```



Color Selection Utilities

Default color palette and how to change it

```
> palette()

[1] "black"   "red"     "green3"  "blue"    "cyan"    "magenta" "yellow"  "gray

> palette(rainbow(5, start=0.1, end=0.2))
> palette()

[1] "#FF9900" "#FFBF00" "#FFE600" "#F2FF00" "#CCFF00"

> palette("default")
```

The gray function allows to select any type of gray shades by providing values from 0 to 1

```
> gray(seq(0.1, 1, by= 0.2))

[1] "#1A1A1A" "#4D4D4D" "#808080" "#B3B3B3" "#E6E6E6"
```

Color gradients with `colorpanel` function from *gplots* library

```
> library(gplots)
> colorpanel(5, "darkblue", "yellow", "white")
```

Much more on colors in R see Earl Glynn's color chart Link

Saving Graphics to Files

After the `pdf()` command all graphs are redirected to file `test.pdf`. Works for all common formats similarly: jpeg, png, ps, tiff, ...

```
> pdf("test.pdf"); plot(1:10, 1:10); dev.off()
```

Generates Scalable Vector Graphics (SVG) files that can be edited in vector graphics programs, such as InkScape.

```
> svg("test.svg"); plot(1:10, 1:10); dev.off()
```

Exercise 3: Bar Plots

Task 1 Calculate the mean values for the `Species` components of the first four columns in the `iris` data set. Organize the results in a matrix where the row names are the unique values from the `iris Species` column and the column names are the same as in the first four `iris` columns.

Task 2 Generate two bar plots: one with stacked bars and one with horizontally arranged bars.

Structure of iris data set:

```
> class(iris)

[1] "data.frame"

> iris[1:4,]

  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
4          4.6         3.1          1.5         0.2  setosa

> table(iris$Species)

    setosa versicolor  virginica
        50         50         50
```

Outline

Analysis Routine: Overview

- The following exercise introduces a variety of useful data analysis utilities in R.

Analysis Routine: Data Import

Step 1 To get started with this exercise, direct your R session to a dedicated workshop directory and download into this directory the following sample tables. Then import the files into Excel and save them as tab delimited text files.

- `MolecularWeight_tair7.xls` Link
- `TargetP_analysis_tair7.xls` Link

Import the tables into R

```
> ## Import molecular weight table
> my_mw <- read.delim(file="MolecularWeight_tair7.xls", header=T, sep="\t")
> my_mw[1:2,]
```

```
  Sequence.id Molecular.Weight.Da. Residues
1 AT1G08520.1                83285      760
2 AT1G08530.1                27015      257
```

```
> ## Import subcelluar targeting table
> my_target <- read.delim(file="TargetP_analysis_tair7.xls", header=T, sep="\t")
> my_target[1:2,]
```

```
     GeneName Loc   cTP   mTP    SP other
1 AT1G08520.1   C 0.822 0.137 0.029 0.039
2 AT1G08530.1   C 0.817 0.058 0.010 0.100
```

Analysis Routine: Merging Data Frames

Step 2 Assign uniform gene ID column titles

```
> colnames(my_target)[1] <- "ID"
> colnames(my_mw)[1] <- "ID"
```

Step 3 Merge the two tables based on common ID field

```
> my_mw_target <- merge(my_mw, my_target, by.x="ID", by.y="ID", all.x=T)
```

Step 4 Shorten one table before the merge and then remove the non-matching rows (NAs) in the merged file

```
> my_mw_target2a <- merge(my_mw, my_target[1:40,], by.x="ID", by.y="ID", all.x=T
>    # To remove non-matching rows, use the argument setting 'all=F'.
> my_mw_target2 <- na.omit(my_mw_target2a)
>    # Removes rows containing "NAs" (non-matching rows).
```

Problem 1: How can the merge function in the previous step be executed so that only the common rows among the two data frames are returned? Prove that both methods - the two step version with `na.omit` and your method - return identical results.

Problem 2: Replace all `NAs` in the data frame `my_mw_target2a` with zeros.

Analysis Routine: Filtering Data

Step 5 Retrieve all records with a value of greater than 100,000 in 'MW' column and 'C' value in 'Loc' column (targeted to chloroplast).

```
> query <- my_mw_target[my_mw_target[, 2] > 100000 & my_mw_target[, 4] == "C", ]
> query[1:4, ]
```

	ID	Molecular.Weight.Da.	Residues	Loc	cTP	mTP	SP	other
219	AT1G02730.1	132588	1181	C	0.972	0.038	0.008	0.045
243	AT1G02890.1	136825	1252	C	0.748	0.529	0.011	0.013
281	AT1G03160.1	100732	912	C	0.871	0.235	0.011	0.007
547	AT1G05380.1	126360	1138	C	0.740	0.099	0.016	0.358

```
> dim(query)

[1] 170   8
```

Problem 3: How many protein entries in the `my_mw_target` data frame have a MW of greater then 4,000 and less then 5,000. Subset the data frame accordingly and sort it by MW to check that your result is correct.

Analysis Routine: String Substitutions

Step 6 Use a regular expression in a substitute function to generate a separate ID column that lacks the gene model extensions.

```
> my_mw_target3 <- data.frame(loci=gsub("\\..*", "",
+                             as.character(my_mw_target[,1]), perl = TRUE),
+                             my_mw_target)
> my_mw_target3[1:3,1:8]
```

```
       loci           ID Molecular.Weight.Da. Residues Loc  cTP   mTP    SP
1 AT1G01010 AT1G01010.1                49426      429   _ 0.10 0.090 0.075
2 AT1G01020 AT1G01020.1                28092      245   * 0.01 0.636 0.158
3 AT1G01020 AT1G01020.2                21711      191   * 0.01 0.636 0.158
```

Problem 4: Retrieve those rows in `my_mw_target3` where the second column contains the following identifiers: `c("AT5G52930.1", "AT4G18950.1", "AT1G15385.1", "AT4G36500.1", "AT1G67530.1")`. Use the `%in%` function for this query. As an alternative approach, assign the second column to the row index of the data frame and then perform the same query again using the row index. Explain the difference of the two methods.

Analysis Routine: Calculations on Data Frames

Step 7 Count the number of duplicates in the loci column with the `table` function and append the result to the data frame with the `cbind` function.

```
> mycounts <- table(my_mw_target3[,1])[my_mw_target3[,1]]
> my_mw_target4 <- cbind(my_mw_target3, Freq=mycounts[as.character(my_mw_target3
```

Step 8 Perform a vectorized devision of columns 3 and 4 (average AA weight per protein)

```
> data.frame(my_mw_target4, avg_AA_WT=(my_mw_target4[,3] / my_mw_target4[,4]))[1
```

```
  Loc  cTP   mTP    SP other Freq avg_AA_WT
1   _ 0.10 0.090 0.075 0.925    1  115.2121
2   * 0.01 0.636 0.158 0.448    2  114.6612
```

Step 9 Calculate for each row the mean and standard deviation across several columns

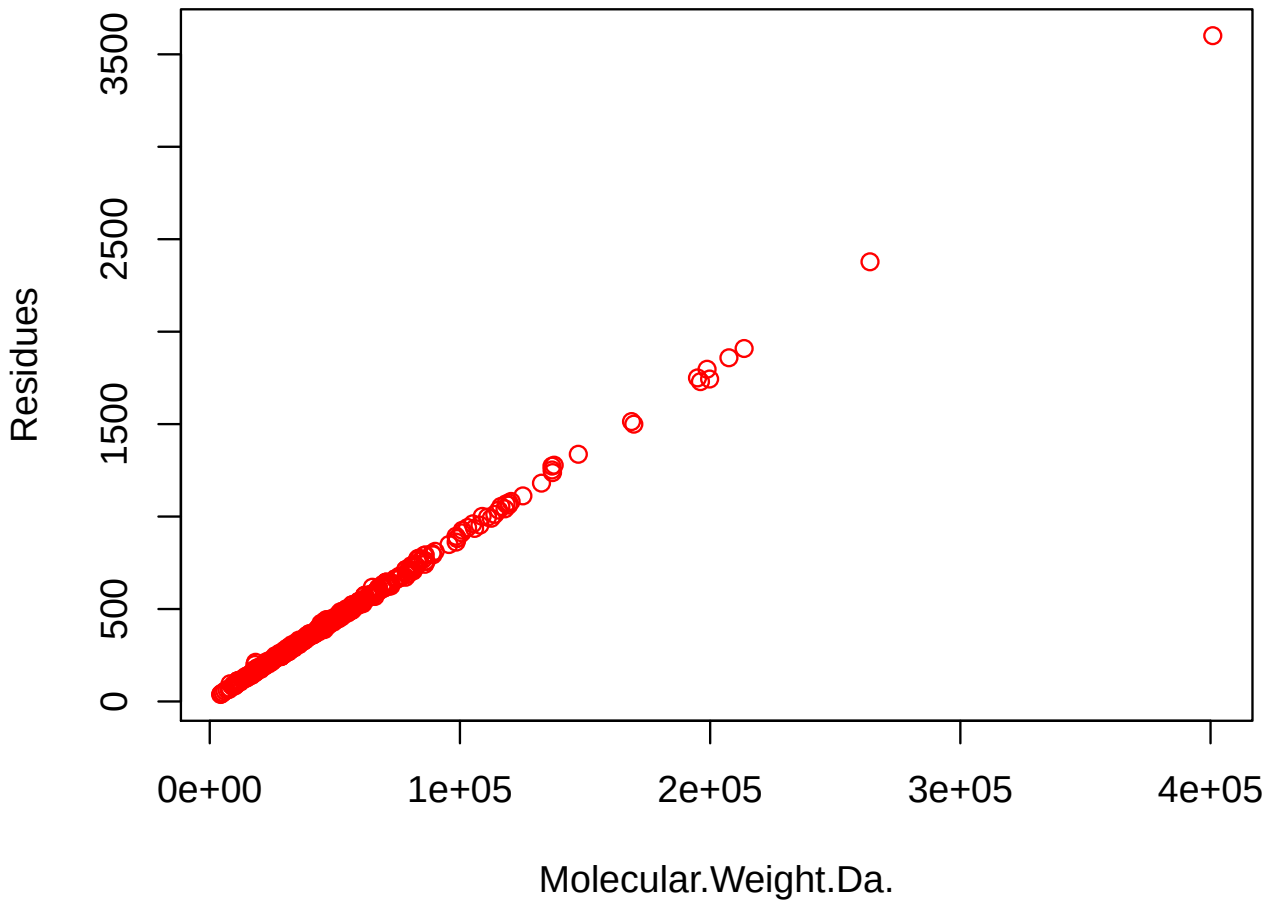
```
> mymean <- apply(my_mw_target4[,6:9], 1, mean)
> mystdev <- apply(my_mw_target4[,6:9], 1, sd, na.rm=TRUE)
> data.frame(my_mw_target4, mean=mymean, stdev=mystdev)[1:2,5:12]
```

```
  Loc  cTP   mTP    SP other Freq   mean     stdev
1   _ 0.10 0.090 0.075 0.925    1 0.2975 0.4184595
2   * 0.01 0.636 0.158 0.448    2 0.3130 0.2818912
```

Analysis Routine: Plotting Example

Step 10 Generate scatter plot columns: 'MW' and 'Residues'

```
> plot(my_mw_target4[1:500,3:4], col="red")
```



Analysis Routine: Export Results and Run Entire Exercise as Script

Step 11 Write the data frame `my_mw_target4` into a tab-delimited text file and inspect it in Excel.

```
> write.table(my_mw_target4, file="my_file.xls", quote=F, sep="\t",
+             col.names = NA)
```

Problem 5: Write all commands from this exercise into an R script named `exerciseRbasics.R`, or download it from here Link. Then execute the script with the `source` function like this: `source("exerciseRbasics.R")`. This will run all commands of this exercise and generate the corresponding output files in the current working directory.

Session Information

```
> sessionInfo()

R version 3.1.2 (2014-10-31)
Platform: x86_64-unknown-linux-gnu (64-bit)

locale:
[1] C

attached base packages:
[1] stats     graphics  utils     datasets  grDevices methods   base

loaded via a namespace (and not attached):
[1] tools_3.1.2
```