Scientific Data Analysis Team

Exploratory Data Analysis in R

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Graphics in R

Scientific Data Analysis Team

- Exploratory Data Analysis (EDA)
- Powerful environment for visualizing scientific data
- Fully programmable
- An example of Exploratory Data Analysis will be performed with the Iris data set.

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`, `matplot`: display of multivariant data Help on these functions

Iris Data

The iris data set is available at the UCI Machine Learning Repository.

The data set was created by statistician Douglas Fisher. The data consists of 3 classes of flower types:

- *setosa*
- *virginica*
- *versicolor*

The Iris Attributes

The data has 4 attributes:

- sepal width
- sepal length
- petal width
- petal length

Load Data

The data needs to be loaded into R.

```
head(iris)
```

```
##   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
## 5          5.0         3.6          1.4         0.2  setosa
## 6          5.4         3.9          1.7         0.4  setosa
```

```
names(iris)
```

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

Summary Statistics

The summary function can be used to assess the statistical properties of each attribute.

```
summary(iris[,-5])
```

```
##   Sepal.Length    Sepal.Width     Petal.Length    Petal.Width   
##  Min.   :4.300   Min.   :2.000   Min.   :1.000   Min.   :0.100  
##  1st Qu.:5.100   1st Qu.:2.800   1st Qu.:1.600   1st Qu.:0.300  
##  Median :5.800   Median :3.000   Median :4.350   Median :1.300  
##  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  
```

other statistics may be calculated as described in the introduction to R examples.

Visualizations

Plot

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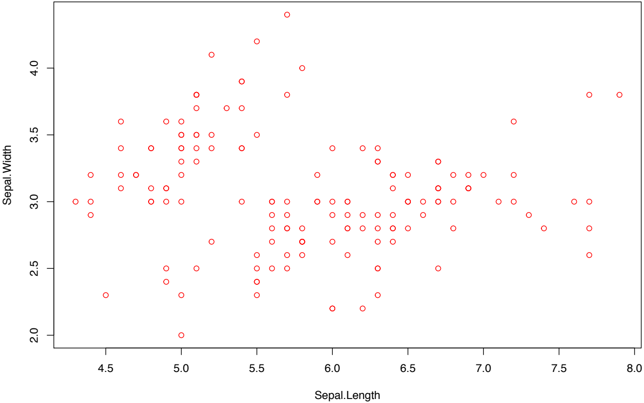
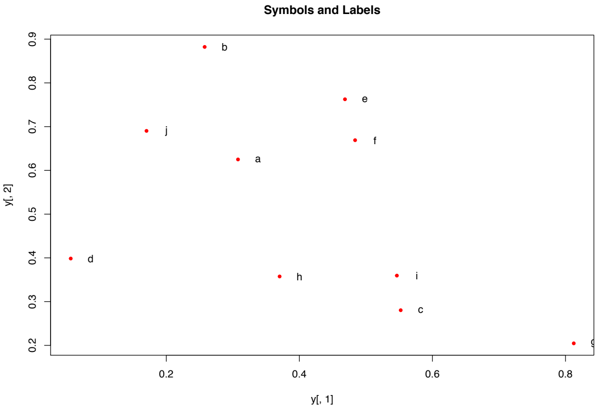
- plot x versus y

```
plot(iris[,1], iris[,2],xlab=names(iris)[1],ylab=names(iris)[2],col=2)
```



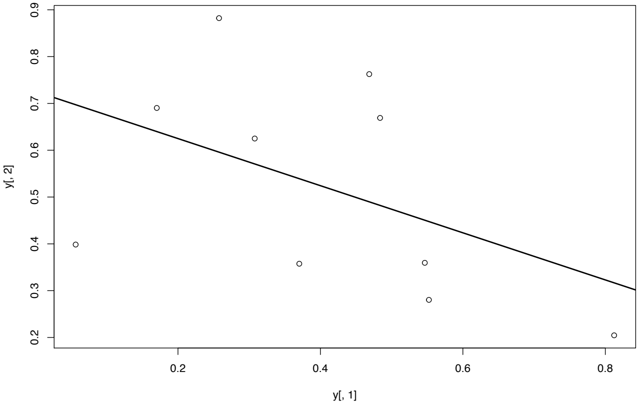
Some more techniques in plot

```
set.seed(100)
y <- matrix(runif(30), ncol=3, dimnames=list(letters[1:10], LETTERS[1:3]))
plot(y[,1], y[,2], pch=20, col="red", main="Symbols and Labels")
text(y[,1]+0.03, y[,2], rownames(y))
```



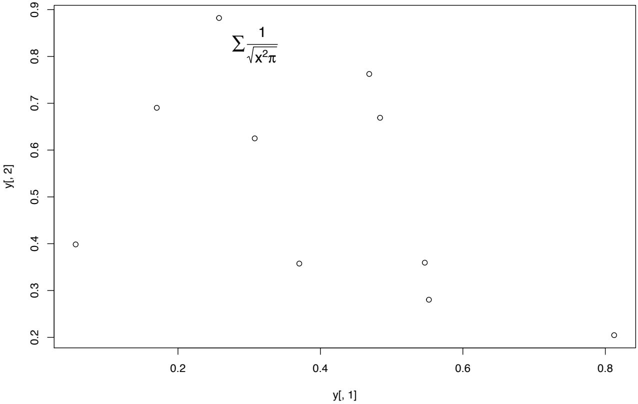
Add a regression line

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



Add a mathematical expression to a plot

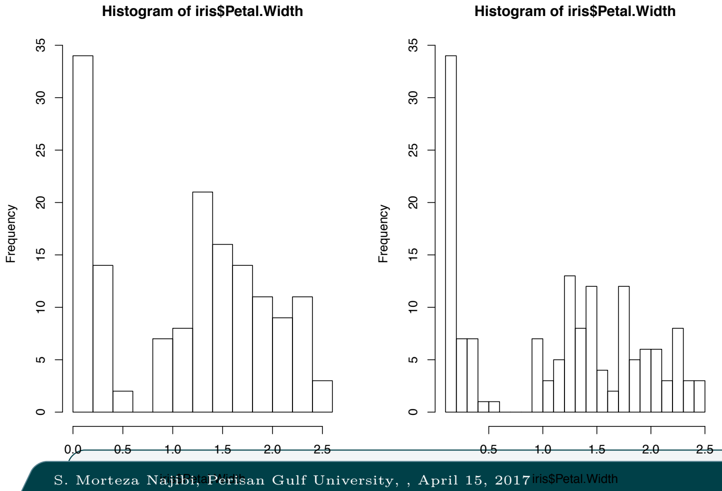
```
plot(y[,1], y[,2])
text(y[1,1], y[1,2]+.2,expression(sum(frac(1,sqrt(x^2*pi)))), cex=1.3)
```



Histograms

- Set the number of breaks to 9, therefore, there will be 10 equal sized bins.

```
par(mfrow=c(1,2))
hist(iris$Petal.Width, breaks=9)
hist(iris$Petal.Width, breaks=19)
```

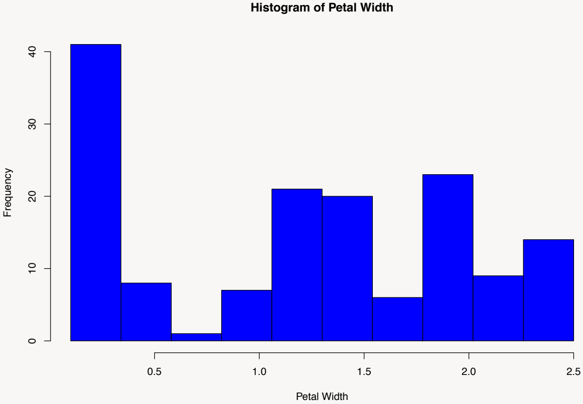

Histogram of iris$Petal.Width

Histogram of iris$Petal.Width

some notes

Note, the number of breaks can be a single number, vector, function to evaluate points or character string.

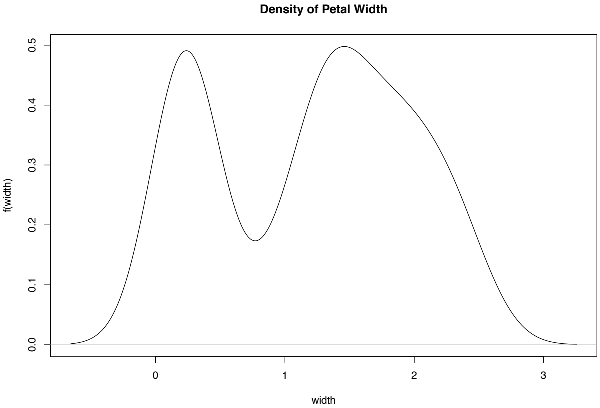
```
b <- seq(min(iris$Petal.Width), max(iris$Petal.Width),
           length=11)
hist(iris$Petal.Width, breaks=b, col="blue", xlab="Petal Width",
     main="Histogram of Petal Width")
```



Density Plots

Density plots can be viewed as smoothed versions of a histogram. We can estimate the density using R's **density** function

```
dens.pw = density(iris$Petal.Width)
plot(dens.pw, ylab = "f(width)", xlab = "width", main= "Density of Petal Width"
```



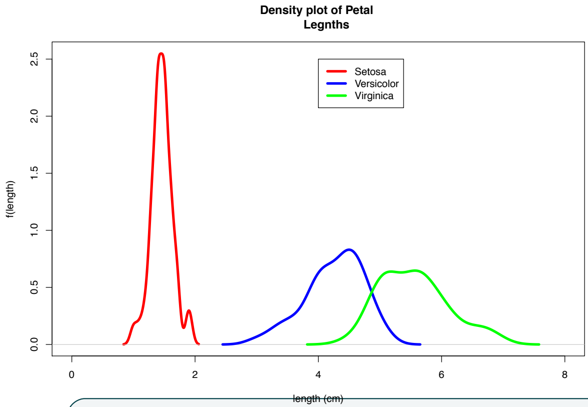
Density plot cont'd

Let's also look at the density function of **`petal.length`** for each of the three classes of irises.

```r
density.setosa = density(iris$Petal.Length[iris$Species == "setosa"])
density.versicolor = density(iris$Petal.Length[iris$Species == "versicolor"])
density.virginica = density(iris$Petal.Length[iris$Species == "virginica"])
```

Density plot cont'd

```
plot(density.setosa, ylab="f(length)", xlab="length (cm)", main="Density plot o
     Legnths", xlim = c(0,8), lwd=4, col="red")
lines(density.versicolor, col="blue", lwd=4)
lines(density.virginica, col="green", lwd=4)
legend(4, 2.5, c("Setosa", "Versicolor", "Virginica"), lwd=rep(4,3),
       col=c("red", "blue", "green"))
```



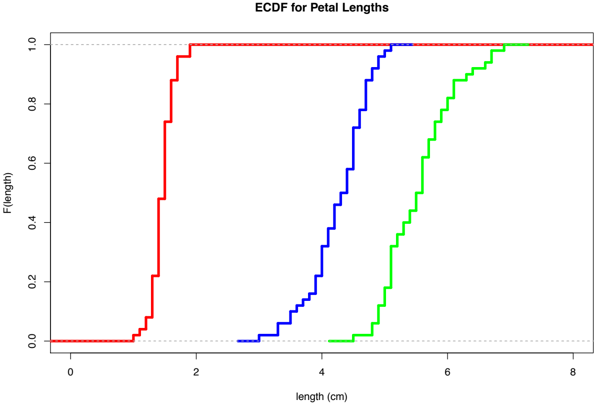
Empirical Cumulative Distribution Functions

The cumulative area under the density function is the cumulative distribution function. Looking at this function using a sample of points gives use the empirical cumulative distribution function (ECDF). Let's start by calculating the cumulative areas

```
ecdf.setosa = ecdf(iris$Petal.Length[iris$Species == "setosa"])
ecdf.versicolor = ecdf(iris$Petal.Length[iris$Species == "versicolor"])
ecdf.virginica = ecdf(iris$Petal.Length[iris$Species == "virginica"])
```

The functions may also be plotted (notice the step function patterns)

```
plot(ecdf.setosa, ylab = "F(length)", xlab = "length (cm)", col.h = "red",
     main = "ECDF for Petal Lengths",
      verticals = T, col.v = "red", do.p = F, lwd = 4, xlim = c(0, 8))
lines(ecdf.versicolor, col.h = "blue", col.v = "blue", verticals = T, lwd = 4,
        do.p = F)
lines(ecdf.virginica, col.h = "green", col.v = "green", verticals = T, lwd = 4,
        do.p = F)
```


ECDF for Petal Lengths
F(length)
0.0
0.2
0.4
0.6
0.8
1.0
0
2
4
6
8
length (cm)

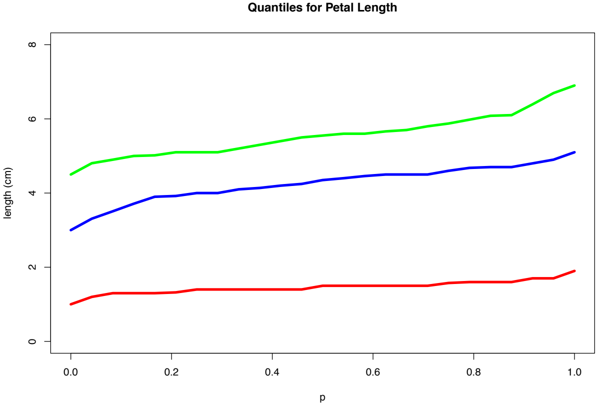
Quantile Plots

The inverse of the ECDF is the quantile function.

```
ps = seq(0,1,length=25)
quantile.setosa = quantile(iris$Petal.Length[iris$Species == "setosa"], probs=p
quantile.setosa
```

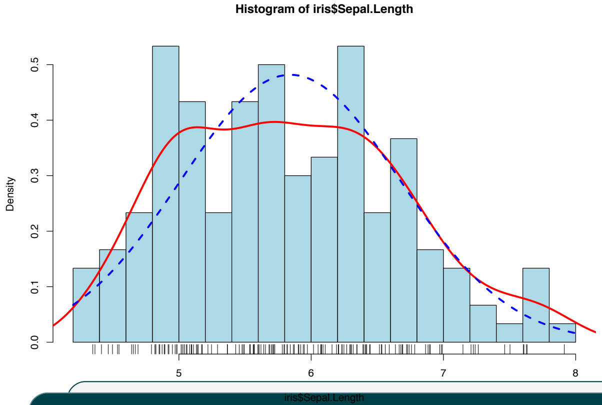
```
##        0% 4.166667% 8.333333%     12.5% 16.66667% 20.83333%       25%
##  1.000000  1.200000  1.300000  1.300000  1.300000  1.320833  1.400000
## 29.16667% 33.33333%     37.5% 41.66667% 45.83333%       50% 54.16667%
##  1.400000  1.400000  1.400000  1.400000  1.400000  1.500000  1.500000
## 58.33333%     62.5% 66.66667% 70.83333%       75% 79.16667% 83.33333%
##  1.500000  1.500000  1.500000  1.500000  1.575000  1.600000  1.600000
##     87.5% 91.66667% 95.83333%      100%
##  1.600000  1.700000  1.700000  1.900000
```

```
quantile.versicolor = quantile(iris$Petal.Length
                               [iris$Species == "versicolor"],probs=ps)
quantile.virginica = quantile(iris$Petal.Length
                              [iris$Species == "virginica"], probs=ps)
plot(ps, quantile.setosa, xlab = "p", ylab = "length (cm)",
     main = "Quantiles for Petal Length",
     type="l", lwd = 4, col="red", ylim=c(0,8))
lines(ps, quantile.versicolor, col = "blue", lwd = 4)
lines(ps, quantile.virginica, col = "green", lwd = 4)
```


Quantiles for Petal Length
length (cm)
0
2
4
6
8
0.0
0.2
0.4
0.6
0.8
1.0
p

check Normality plot

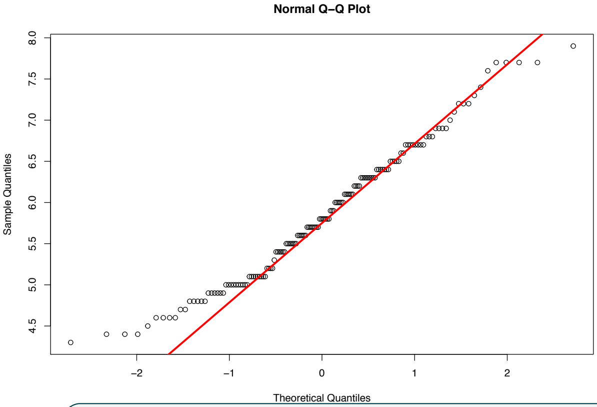
```
hist(iris$Sepal.Length, probability=TRUE, breaks=15, col="light blue")
rug(jitter(iris$Sepal.Length, 5))
points(density(iris$Sepal.Length), type='l', lwd=3, col='red')
f <- function(t) {
  dnorm(t, mean=mean(iris$Sepal.Length), sd=sd(iris$Sepal.Length) )
}
curve(f, add=T, col="blue", lwd=3, lty=2)
```



Q-Q plot

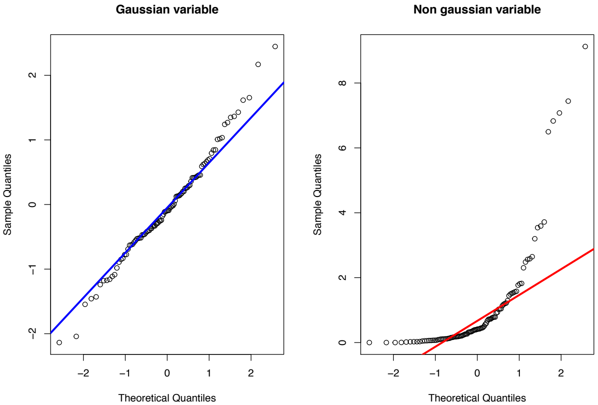
A q-q plot is a plot of the quantiles of the first data set against the quantiles of the second data set.

```
x <- iris$Sepal.Length
qqnorm(x)
qqline(x, col="red", lwd=3)
```



Some more examples

```
par(mfrow=c(1,2))
x <- rnorm(100)
y <- rnorm(100)^2
qqnorm(x, main="Gaussian variable");qqline(x, col="blue", lwd=3)
qqnorm(y, main="Non gaussian variable");qqline(y, col="red", lwd=3)
```

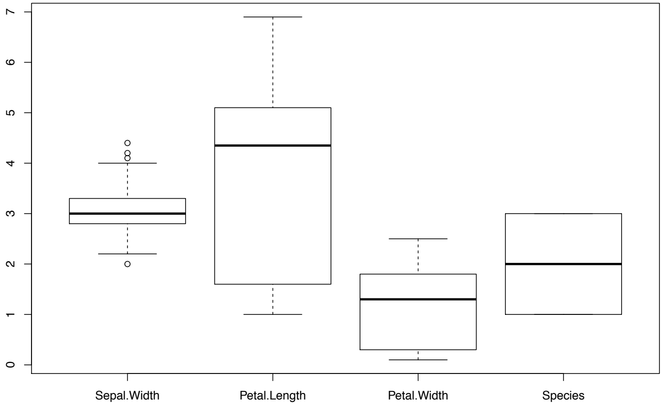


Box Plots

Box plots are used to compactly show many pieces of information about a variables distribution including some summary statistics.

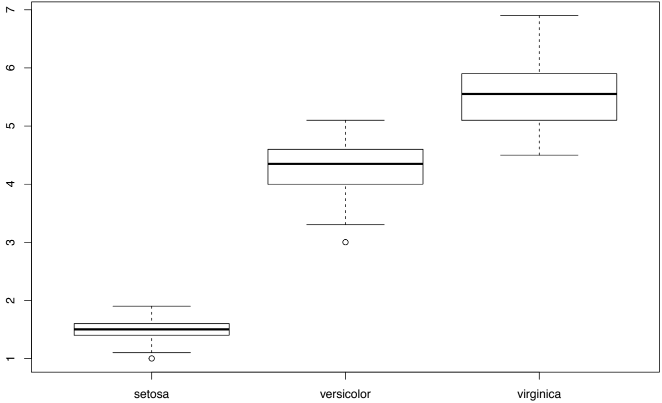
A box plot of each attribute of the iris data set

```
boxplot(iris[,-1])
```



A box plot may also be used for one attribute **petal.length** and show how it varies with the class **Species**

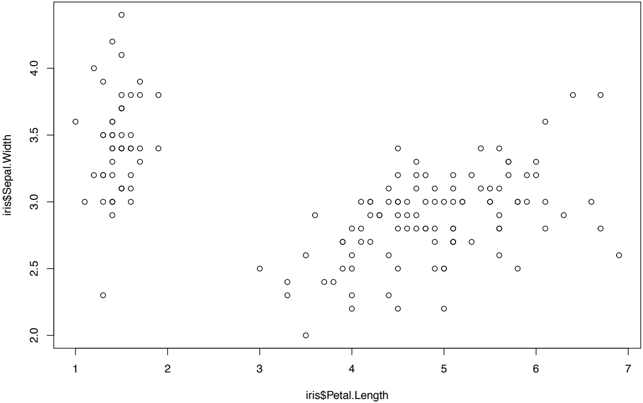
```
boxplot(iris$Petal.Length ~ iris$Species)
```



Scatter Plots

Scatter plots are used to plot two variables against each other (or 3 in the case of 3D plots).

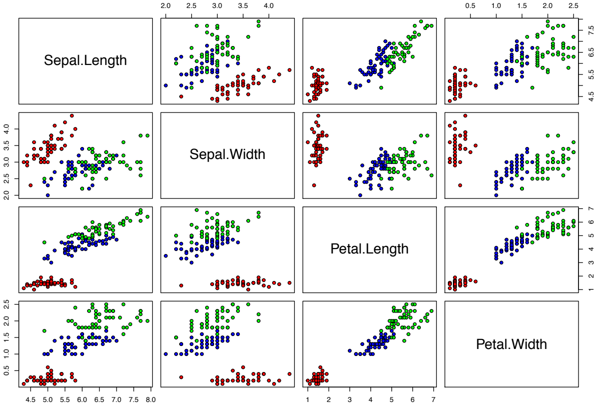
```
plot(iris$Petal.Length, iris$Sepal.Width)
```



Pairwise Plots

For data sets with only a few attributes, all the pairwise scatter plots may be constructed.

```
pairs(as.matrix(iris[,-5]), pch=21, bg=c("red", "blue", "green")[(iris$Species)
```



Color Selection Utilities

Default color palette and how to change it

```
palette()
```

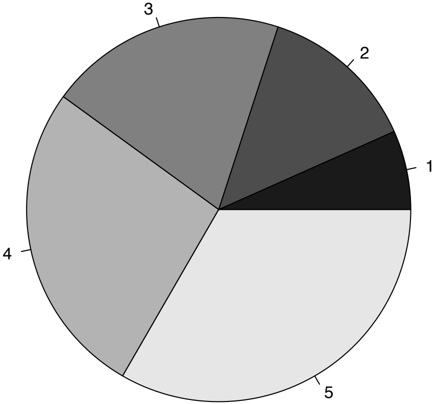
```
## [1] "black"   "red"     "green3"  "blue"    "cyan"    "magenta" "yellow"
## [8] "gray"
```

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

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

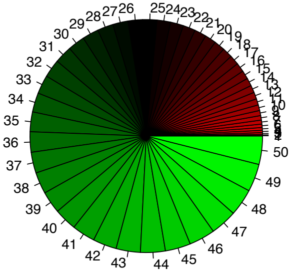
The gray function allows to select any type of gray shades by providing values from 0 to 1

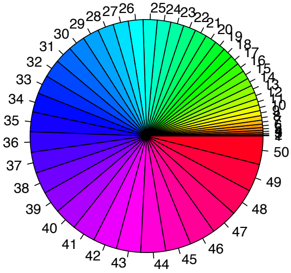
```
pie(1:5,col=gray(seq(0.1, 1, by= 0.2)))
```



Color gradients with colorpanel function from gplots library

```
library(gplots,warn.conflicts = F)
par(mfrow=c(1,2))
pie(1:50, col=colorpanel(50,"red","black","green"))
pie(1:50, col=rainbow(50))
```

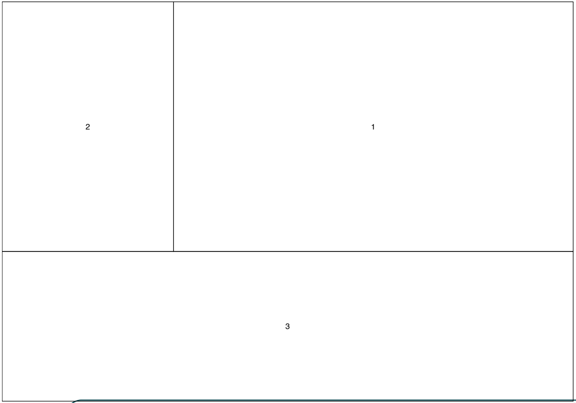




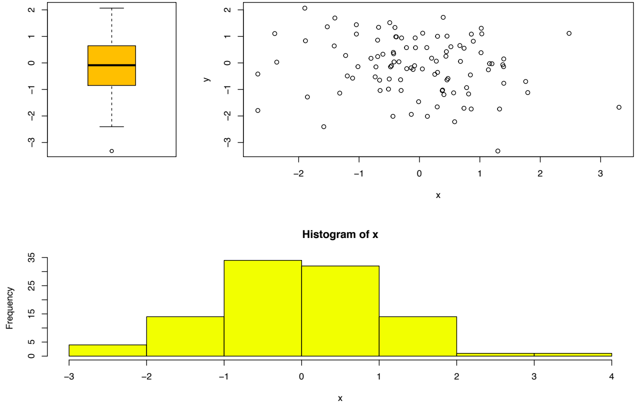
Arranging Plots with Variable Width

The layout function allows to divide the plotting device into variable numbers of rows and columns with the column-widths and the row-heights specified in the respective arguments.

```r
nf <- layout(matrix(c(2,1,3,3), 2, 2, byrow=TRUE), c(3,7), c(5,3))
layout.show(nf)
```

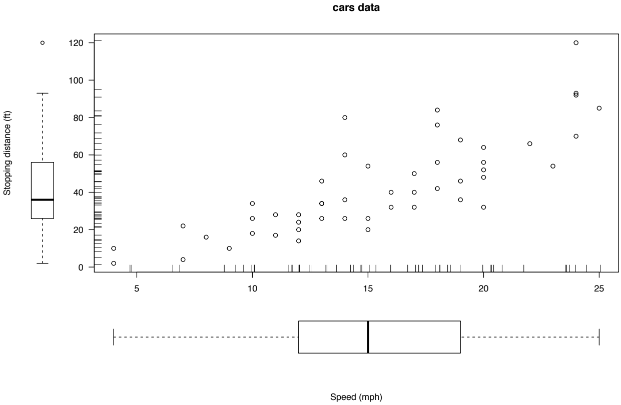


```
x <- rnorm(100) ; y <- rnorm(100)
layout(matrix(c(2,1,3,3), 2, 2, byrow=TRUE), c(3,7), c(5,4))
plot(x,y)
boxplot(y,horizontal = FALSE,col=2)
hist(x,col=4)
```



Margine plots

```
data(cars)
layout( matrix( c(2,1,0,3), 2, 2, byrow=T ),
c(1,6), c(4,1))
par(mar=c(1,1,5,2)); plot(cars$dist ~ cars$speed,xlab='', ylab='',las = 1)
rug(side=1, jitter(cars$speed, 5) );rug(side=2, jitter(cars$dist, 20) );
title(main = "cars data")
par(mar=c(1,2,5,1))
boxplot(cars$dist, axes=F); title(ylab='Stopping distance (ft)', line=0)
par(mar=c(5,1,1,2))
boxplot(cars$speed, horizontal=T, axes=F); title(xlab='Speed (mph)', line=1)
```


cars data
Stopping distance (ft)
0
20
40
60
80
100
120
5
10
15
20
25
Speed (mph)

Exercise: Bar Plots, Pie plot,

- Consider the same approach in this slides for **`barplot`**

Saving Graphics to Files

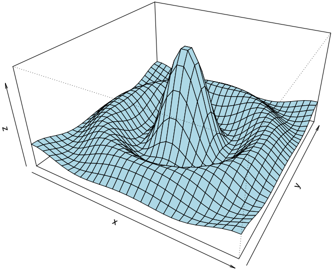
After the pdf() command all graphs are redirected to file test.pdf. Works for all common formats similarly: jpeg, png, ps, tiff, . . .

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

3 Dimesional functions and their plots

persp 3d plot

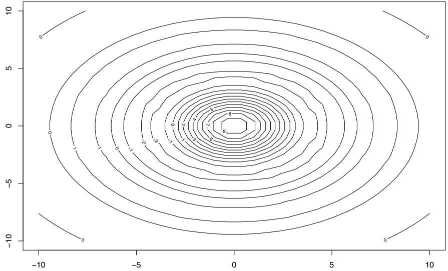
```
x <- seq(-10, 10, length= 30)
y <- x
f <- function(x, y) { r <- sqrt(x^2+y^2); 10 * sin(r)/r }
z <- outer(x, y, f)
persp(x, y, z, theta = 30, phi = 30, expand = 0.5, col = "lightblue")
```



Countour Plots

A contour plot is a graphical technique for representing a 3-dimensional surface by plotting constant z slices, called contours, on a 2-dimensional format.

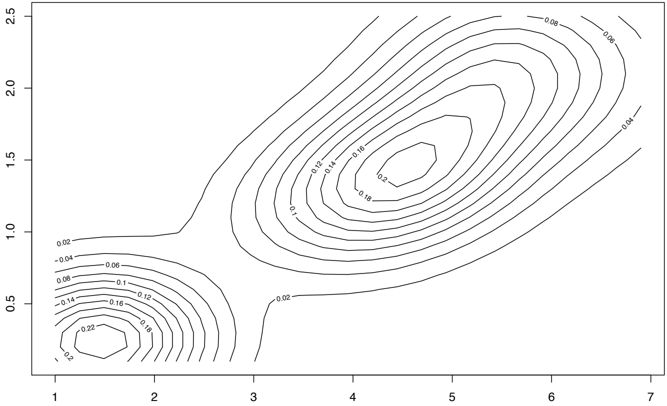
```
contour(x,y,z) # or contour(z)
```



2D Density

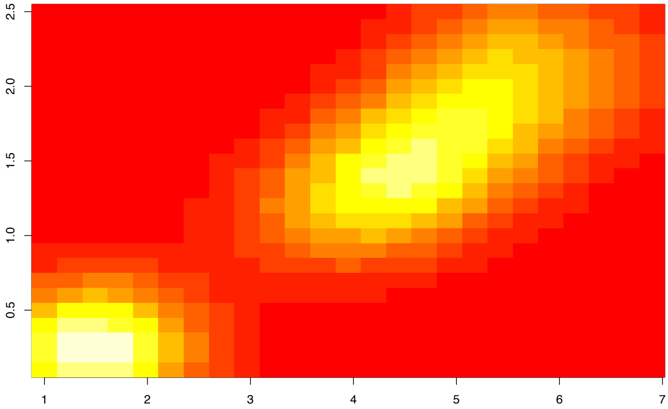
Density estimation is available for higher dimensional data. Use the **MASS** package.

```
library(MASS)
petal.dens = kde2d(iris$Petal.Length, iris$Petal.Width)
contour(petal.dens)
```



The plot may aslo be viewed as an image

```
image(petal.dens)
```



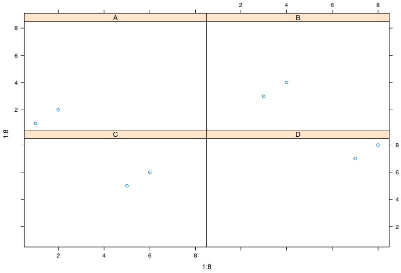
lattice Grapphics

What is lattice?

- High-level graphics system
- Implements Trellis graphics system from S-Plus Simplifies high-level plotting tasks: arranging complex graphical features
- Syntax similar to R's base graphics

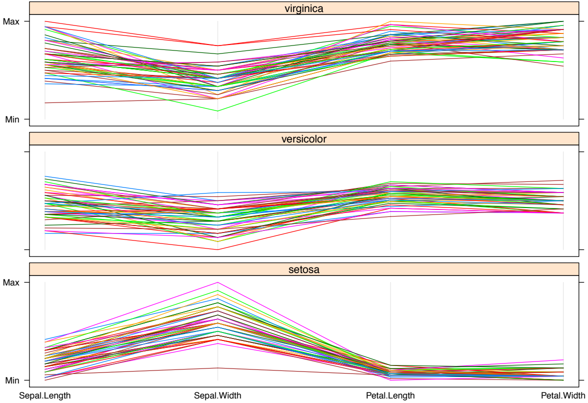
Scatter Plot Sample

```
library(lattice)
xyplot(1:8 ~ 1:8 | rep(LETTERS[1:4], each=2), as.table=TRUE)
```



Line Plot Sample

```
parallelplot(~iris[1:4] | Species, iris, horizontal.axis = FALSE,
             layout = c(1, 3, 1))
```



ggplot2 package (a superfull package in graphic)

ggplot2

- What is ggplot2?
  - High-level graphics system
  - Streamlines many graphics workflows for complex plots
  - Simpler qplot function provides many shortcuts
- ggplot function accepts two arguments
  - Data set to be plotted
  - `Aesthetic` mappings provided by `aes` function
  - Additional parameters such as geometric objects (e.g. points, lines, bars) are passed on by appending them with + as separator.

qplot function

qplot syntax is similar to R's basic plot function Arguments:

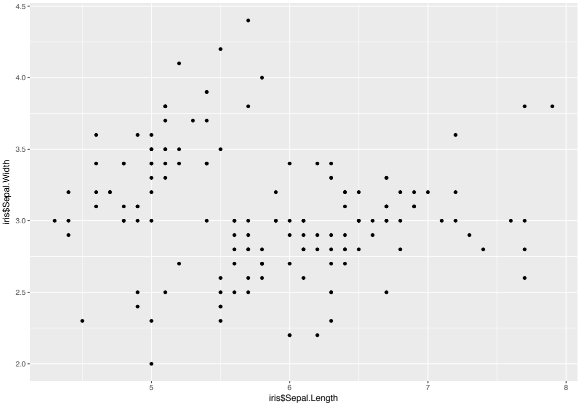
- x: x-coordinates (e.g. col1)
- y: y-coordinates (e.g. col2)
- data: data frame with corresponding column names xlim, ylim: e.g. xlim=c(0,10)
- log: e.g. log="x" or log="xy"
- main: main title; see ?plotmath for mathematical formula xlab, ylab: labels for the x- and y-axes
- color, shape, size
- . . . : many arguments accepted by plot function

Create sample data

```
library(ggplot2,quietly = T)
```

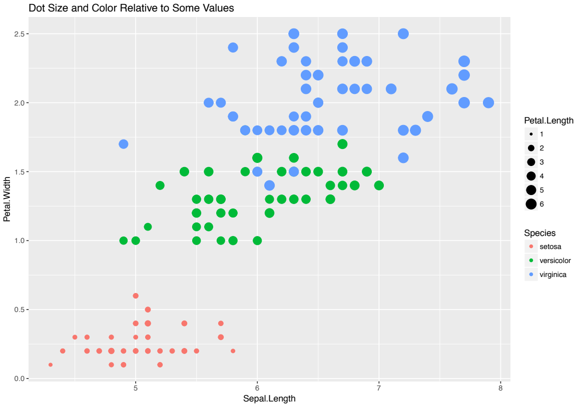
```
## Warning: package 'ggplot2' was built under R version 3.2.5
```

```
#cat <- rep(c("A", "B"), 5)
qplot(iris$Sepal.Length, iris$Sepal.Width, geom="point")
```



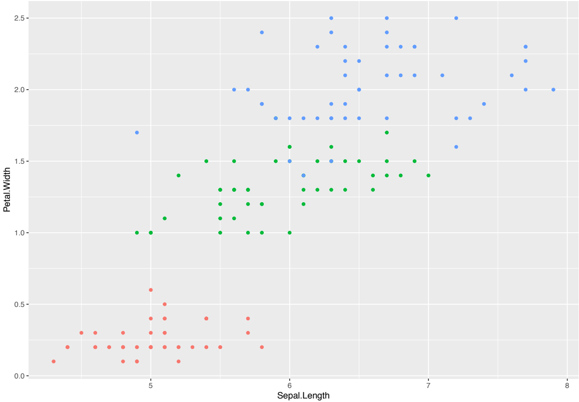
Prints dots with different sizes and colors

```
qplot(Sepal.Length, Petal.Width, data = iris, geom="point",
      size=Petal.Length,col=Species,
      main="Dot Size and Color Relative to Some Values")
```



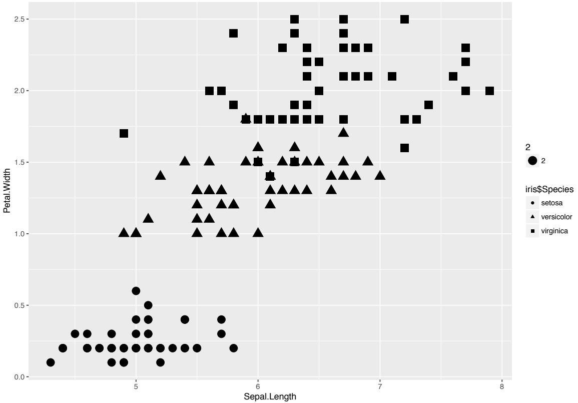
Drops legend

```
qplot(Sepal.Length, Petal.Width, data = iris, geom="point",col=Species)+
      theme(legend.position = "none")
```



Plot different shapes

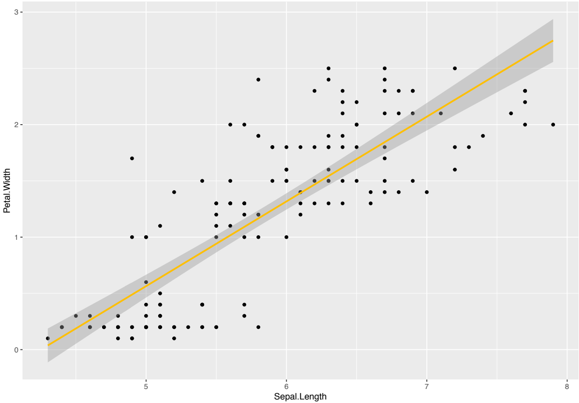
```
qplot(Sepal.Length, Petal.Width, data = iris, geom="point",
      shape=iris$Species,size=2)
```



Scatter Plot with Regression Line

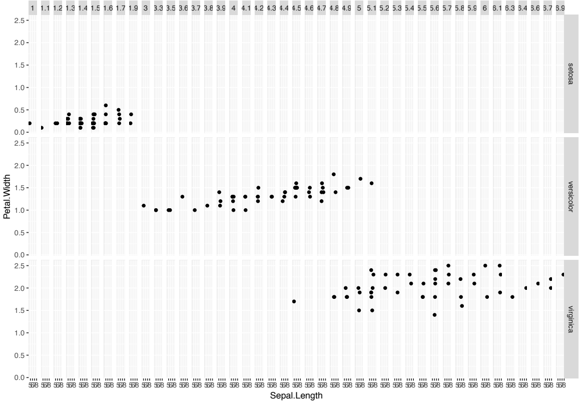
Scientific Data Analysis Team

```
qplot(Sepal.Length, Petal.Width, data = iris, geom = c("point"))+
             geom_smooth(method=lm,col=2)
```



More application of qplot

```
qplot(Sepal.Length, Petal.Width, data = iris, facets = Species ~ Petal.Length)
```


setosa
versicolor
virginica
Petal.Width
Sepal.Length