Advanced Scientific Computing with R

5. Simulating Data

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Introduction

Simulated ("random") data is used in many areas:

- gambling
- statistical sampling
- computer simulation
- cryptography
- simulations (Monte Carlo experiments)

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Sampling

'sample' takes a sample of the specified size from the elements of 'x' using either with or without replacement.

```
R> sample(1:100, size=10)
 [1] 12 62 60 61 83 97  1 22 99 47
R> sample(1:10, size=100, replace=TRUE)
  [1]  7  6  3 10  3  9  3  3  2  3  4  4  2  1  3  9  6 10
 [19]  9  1  5  3  4  6  2  8  3  3 10  9  6  7  4  7  4  6
 [37]  7  5  3  8  1  4  8  6  2  6  5  8  2  9  9  1  4  1
 [55]  3  8  4  6  1  6  2  9  1  8  1  6  4  1  4  7 10  5
 [73]  2  6  2  9  4  4  2  9  2 10  2  2  2  6  4  1  4  8
 [91]  1  6  3  3  2  4  2  2  5  1
```

sample can be used to sample from data.frames and matrices.

```
R> data(iris)
R> dim(iris)
[1] 150   5
R> s <- iris[sample(1:nrow(iris), size=50), ]
R> dim(s)
[1] 50  5
```

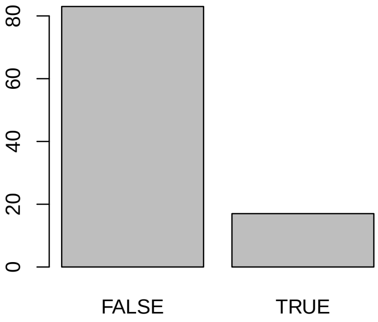
Simple Coin Tossing

We can specify the probability for each outcome.

```
R> x <- sample(c(TRUE, FALSE), 100, replace=TRUE,
prob=c(0.2,0.8))
R> x
  [1] FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE  TRUE
 [10] FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE
 [19] FALSE FALSE FALSE FALSE FALSE FALSE  TRUE FALSE  TRUE
 [28] FALSE FALSE FALSE FALSE  TRUE FALSE  TRUE  TRUE  TRUE
 [37]  TRUE FALSE  TRUE FALSE FALSE FALSE FALSE FALSE FALSE
 [46] FALSE FALSE FALSE FALSE  TRUE FALSE FALSE FALSE FALSE
 [55] FALSE  TRUE FALSE FALSE FALSE  TRUE FALSE FALSE FALSE
 [64] FALSE FALSE FALSE  TRUE FALSE FALSE FALSE FALSE FALSE
 [73] FALSE  TRUE FALSE FALSE FALSE FALSE FALSE  TRUE FALSE
 [82] FALSE FALSE FALSE  TRUE FALSE FALSE FALSE  TRUE FALSE
 [91] FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE
[100] FALSE
R> table(x)
x
FALSE  TRUE
   83    17
```

Simple Coin Tossing II

```
R> barplot(table(x))
```



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Distributions

Functions for all distributions in R come in 4 variants. For example for the normal distribution we have:

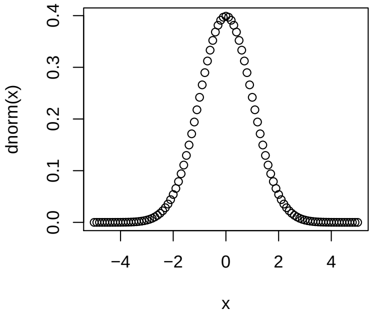
```
dnorm(x, mean = 0, sd = 1, log = FALSE)
pnorm(q, mean = 0, sd = 1, lower.tail = TRUE, log.p = FALSE)
qnorm(p, mean = 0, sd = 1, lower.tail = TRUE, log.p = FALSE)
rnorm(n, mean = 0, sd = 1)
```

Probability density function (d), distribution function (p), quantile function (q) and random deviates (r).

Probability density function (pdf)

Probability of a random variable taking certain values: $f(x)$

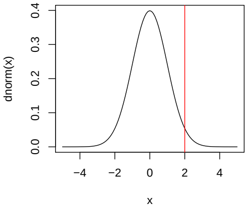
```
R> x <- seq(-5,5, by=.1)
R> plot(x, dnorm(x))
```



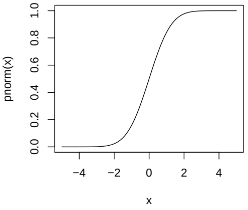
(Cumulative) distribution function (cdf)

Probability that a real-valued random variable X with a given probability distribution will be found at a value less than or equal to x: $F_X(x) = P(X \leq x)$

```
R> plot(x, dnorm(x), "l")
R> abline(v=2, col="red")
```



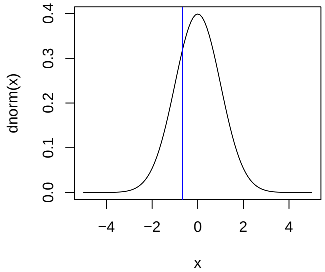

```
R> plot(x, pnorm(x), "l")
```



Quantile function

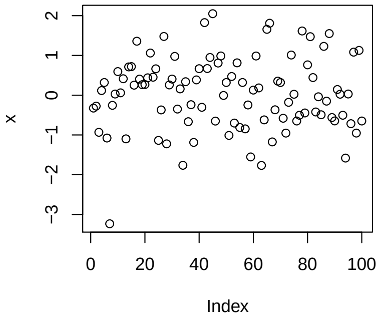
$$Q(p) = \inf\{x \in R : p \leq F(x)\}$$

```
R> qnorm(.25)
[1] -0.674
R> ## 25% quantile
R> plot(x, dnorm(x), type="l")
R> abline(v=qnorm(.25), col="blue")
```



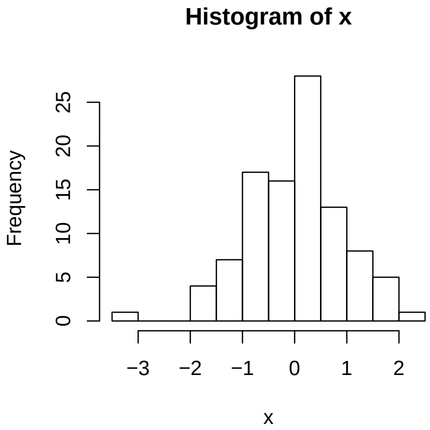
Random deviates

```
R> x <- rnorm(100)
R> head(x)
[1]  1.014  0.253 -1.172  0.669 -1.650 -0.366
R> plot(x)
```



Random deviates II

```
R> hist(x)
```



Some useful distributions

- rnorm
- rlnorm
- runif
- rpois
- rexp
- rbinom
- rnbinom
- rmultinom
- rchisq
- rt
- rbeta
- rweibull

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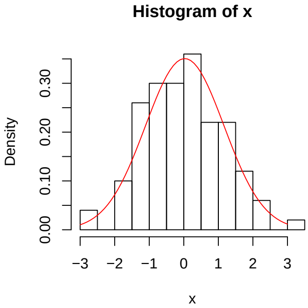
Histogram

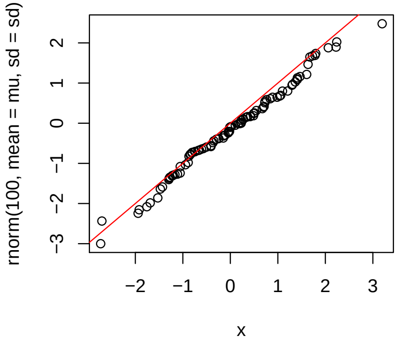
Compare empirical distribution with a fitted theoretical distribution.

```
R> x <- rnorm(100)
R> hist(x, breaks=20, probability=TRUE)
R> mu <- mean(x)
R> sd <- sd(x)
R> r <- seq(-3,3, by =.1)
R> lines(r, dnorm(r, mean=mu, sd=sd), col="red")
```



Quantile-Quantile plot

```
R> qqplot(x, rnorm(100, mean=mu, sd=sd))
R> # use qqnorm for normal distribution
R> abline(0,1, col="red")
```



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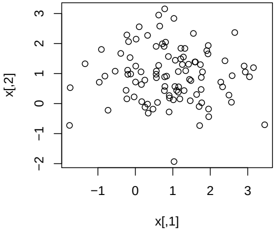
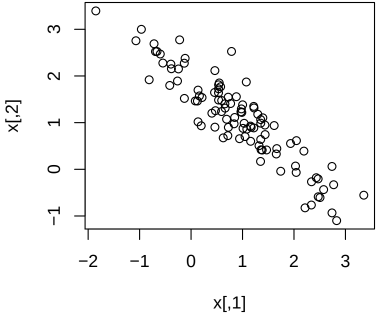
Multivariate Distributions

```
R> library(MASS)
R> Sigma <- rbind(c(1,0), c(0,1)) ## covariance matrix
R> x <- mvrnorm(100, c(1,1), Sigma=Sigma)
R> head(x)
      [,1]  [,2]
[1,] 2.189 0.767
[2,] 2.060 1.156
[3,] 2.337 0.396
[4,] 0.633 1.629
[5,] 0.696 1.714
[6,] 0.650 2.076
R> plot(x)
```



Multivariate Distributions

```
R> Sigma <- rbind(c(1,.9), c(-.9,1)) ## strong correlation
R> x <- mvrnorm(100, c(1,1), Sigma=Sigma)
R> plot(x)
```



More about multivariate data can be found in the Task View "Multivariate"

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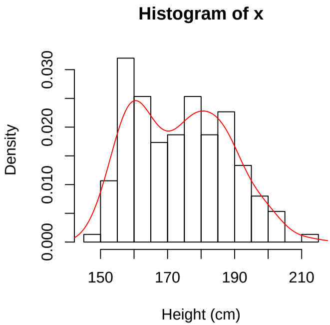
Mixture of two univariate Gaussian

Measurement of height (in centimeters) for subjects from two groups (female/male).

```
R> female <- rnorm(50, 160, 5)
R> male <- rnorm(100, 180, 10)
R> x<-c(female,male)
R> hist(x, prob=TRUE, breaks=20, xlab="Height (cm)")
R> lines(density(x), col="red")
```



Multivariate data

Create a dataset for clustering with two clusters and uniform noise.

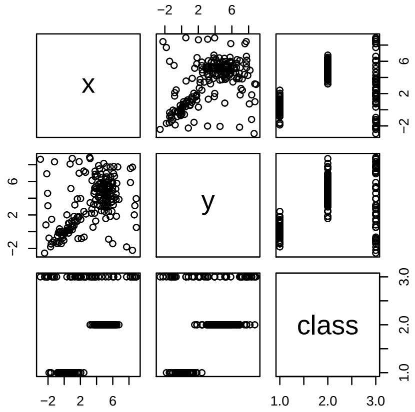
```
R> c1 <- mvrnorm(50, c(0,0), Sigma=rbind(c(1,.9), c(.9,1)))

R> c2 <- mvrnorm(100, c(5,5), Sigma=rbind(c(.5,0),
c(-.3,2)))
R> noise <- cbind(runif(50, -3,9), runif(50, -3,9))
R> x <- rbind(c1,c2,noise)
R> class <- c(rep("c1", nrow(c1)), rep("c2",nrow(c2)),
rep("noise", nrow(noise)))
R> data <- cbind(as.data.frame(x), class)
R> colnames(data) <- c("x", "y", "class")
R> data <- data[sample(1:nrow(data)), ] ## shuffle the data

R> head(data)
       x      y class
51  4.68  4.625    c2
164 5.49 -0.898 noise
86  4.97  4.373    c2
79  5.68  7.728    c2
167 3.91  5.375 noise
71  5.68  1.813    c2
```

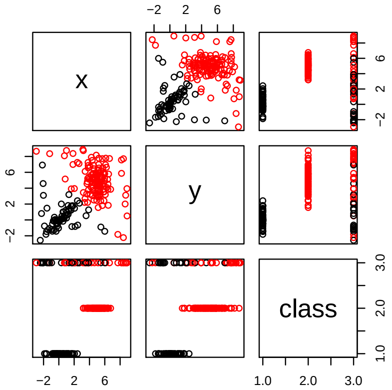
Multivariate data II

```
R> plot(data)
```



Multivariate data III

```
R> cl <- kmeans(data[-3],2)
R> plot(data, col= cl$cluster)
```



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Exercises

1. You use two dice for a party. The first die is fair while the second one has a 10% higher chance of rolling a 6 and a 5% each lower chance to role a 1 or a 4. Each time a player chooses randomly one die and rolls it. Display the distribution of the numbers rolled after 100 times. Hint: use sample for the dice.
2. Create a variable with 100 random values following a Poisson distribution with parameters of your choice. Use a histogram and a Q-Q plot to compare the distribution to a normal distribution and to a Poisson distribution.