DATA7001 - Introduction to Data Science Basic R programming

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Email: xin.guo@uq.edu.au Office: **Priestley Building (67), Room 447** Office Hours: **Tuesday 10–11 AM** R is a programming language. R also refers to a free software environment for statistical computing and visualization. It compiles and runs on a wide variety of UNIX platforms, Windows and MacOS. R was originally designed for statistical computing, and now people also use it to do numerical analysis. It is stable, powerful, and widely used.



Figure: the R logo.

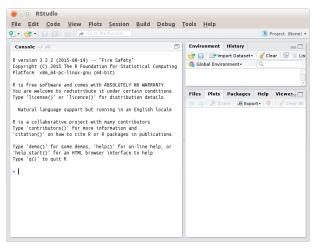
- An interpreter-based programming, graphics and statistics package.
- Free, stable, can be extended.
- Can easily perform standard statistical and numerical analysis.
- Can be programmed to handle non-standard cases.
- For complex tasks, it is often used as a first step to interface with C or FORTRAN.
- Almost all new statistical methodologies are published with ready-to-use packages built with **R**.

R is free in the sense of "free beer", so that you can download it, run it, and re-distribute it with no cost. R is free also in the sense of "free speech", so that you can modify it, and release your modified version (called "fork") of R (for minimizing confusion, R requires that if you modify and release your version of R, you must use some different name). R is usually used in the command-line mode, which already offers a lot of features and freedom. However, there is a graphical user interface (GUI) shell available for R, called RStudio, available for download at https://www.rstudio.com.

```
🙁 – 🗊 xin@xin-tc-M91p: ~
xin@xin-tc-M91p:~$ R
R version 3.2.2 (2015-08-14) -- "Fire Safety"
Copyright (C) 2015 The R Foundation for Statistical Computing
Platform: x86 64-pc-linux-gnu (64-bit)
R is free software and comes with ABSOLUTELY NO WARRANTY.
You are welcome to redistribute it under certain conditions.
Type 'license()' or 'licence()' for distribution details.
  Natural language support but running in an English locale
R is a collaborative project with many contributors.
Type 'contributors()' for more information and
'citation()' on how to cite R or R packages in publications.
Type 'demo()' for some demos, 'help()' for on-line help, or
'help.start()' for an HTML browser interface to help.
Type 'q()' to quit R.
>
```

The welcome message of R environment on Linux system.

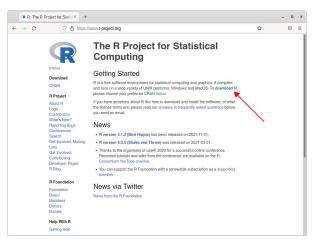
If you launch RStudio, you get the following welcome message. RStudio did nothing but just call R.



The welcome message of RStudio.

Downloading and installing R

visit https://www.r-project.org/

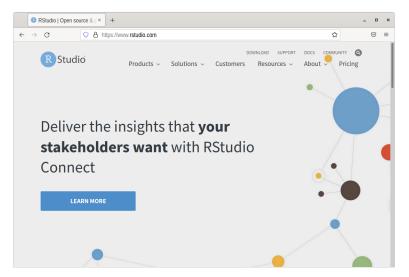


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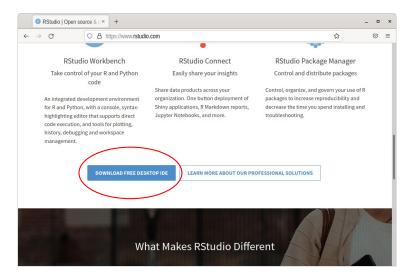
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RStudio is an integrated development environment (IDE) for R, which is optional and may provide some help. RStudio is available at https://www.rstudio.com/



On the homepage of RStudio, scroll down to find the download link.



You may explore the "RStudio Server" but the basic "RStudio Desktop" is good enough.

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Select the package that matches your operating system.

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Some simple commands

• You can directly type commands at the prompt:

```
> 2 + 3
[1] 5
> 5 * pi
[1] 15.70796
> rnorm(20)
[1] -0.57442492 1.68545014 -0.01613824 -0.14110880 0.59271169
[6] 0.08165454 0.16220551 -0.53236657 -0.11977163 0.56726110
[11] -0.19887324 -0.77690512 -1.10581382 -0.70444775 -0.03470233
[16] -0.92088930 -2.95547369 0.22873348 -0.30088267 -0.27960355
```

- If you hit enter before completely entering a command, you will get a + prompt. You must complete the command or type CTR+C (Esc in MSW) to continue.
 - > 3 + + 5 [1] 8
- All arithmetic operations are represented via standard symbols (+ -

```
* /) and have the usual order of precedence.
```

```
> 3 + 4 * 2
[1] 11
> sin(pi / 6)
[1] 0.5
> exp(log(2) + log(3))
[1] 6
> atan(Inf)/pi
[1] 0.5
```

Vectors

• R has six common types of atomic vectors: integer, double, logical, character, complex, and raw¹.

```
> a <- c(1, 3, 5. 7. 9)
                                                  > v <- c("hello". "world". "!")</pre>
                                                  > typeof(v)
> a
[1] 1 3 5 7 9
                                                  [1] "character"
> typeof(a)
                                                  > length(y)
[1] "double"
                                                  [1] 3
> length(a)
                                                  > nchar(y)
[1] 5
                                                  [1] 5 5 1
> b <- 1:5
                                                  > z <- 3 + 5i
> typeof(b)
                                                  > typeof(z)
[1] "integer"
                                                  [1] "complex"
> x <- (a >= 5)
                                                  > 7^2
                                                  [1] -16+30i
> X
[1] FALSE FALSE TRUE TRUE TRUE
                                                  > sin(z)
> typeof(x)
                                                  [1] 10.47251-73.46062i
[1] "logical"
                                                  > exp(z)
> x[2]
                                                  [1] 5.69751-19.26051i
[1] FALSE
```

• In each vector, all the elements must have the same atomic data type.

¹In this course we will not expand complex and raw.

List is a data structure like vector, but can have components of mixed data types.

```
> a <- list(1:4, sin, "hello", TRUE, 1+3i)</pre>
> a[[1]]
[1] 1 2 3 4
> a[[2]](pi/6)
[1] 0.5
> a[[3]]
[1] "hello"
> a[[4]]
[1] TRUE
> Arg(a[[5]])
[1] 1.249046
> Arg(a[[5]]) -> e
> Mod(a[[5]]) -> r
> r * (cos(e) + 1i * sin(e))
[1] 1+3i
> names(a) <- letters[1:5]</pre>
> a$a
[1] 1 2 3 4
> a$b
function (x) .Primitive("sin")
> aŚc
[1] "hello"
```

Reading documentation

Documentation is important for learning **R**. Type ?log, or ?"log", for example, to see the help page of the function log. Why quoting? Because sometimes we need the help page of operators. Try ?"+" and ?+ separately. Press q to quit the help page.

8 - D xin@	Pxin-tc-M91p: ~	
log	package:base	R Documentation
Logarithms	and Exponentials	
Description	3:	
comput	computes logarithms, by default na tes common (i.e., base 10) logarith y (i.e., base 2) logarithms. The g tes logarithms with base 'base'.	ms. and 'log2' computes
'log1p	o(x)' computes log(1+x) accurately	also for x << 1.
'exp'	computes the exponential function.	
'expn:	l(x)' computes exp(x) - 1 accuratel	y also for x << 1.
Usage:		
log1p	(x)	
exp(x) expml		
Arguments:		
×: 6	a numeric or complex vector.	
	a positive or complex number: the b logarithms are computed. Defaults	

Help page of the logarithm functions.

Save your commands in a file

- Each R session works under a directory ("folder"). To see the current working directory, type the following command
 getwd()

 [1] "/home/xin/Downloads"
- To change the current working directory, use the function "setwd".
 > setwd("/home/xin/Documents")
 > getwd()
 [1] "/home/xin/Documents"
- For example, one can make a file "a.R" (different filename extensions are OK, for example you can use the text file "a.txt") under the working directory. Save the following code to the file a.R. print("hello, world")

```
    Then in the R session, "source" it.
    source("a.R")
    [1] "hello, world"
```

Loops

• The following for loop is used to find $e = 2.71828 \cdots = \sum_{i=0}^{\infty} \frac{1}{i!}$. There are two key words: for and in.

```
a <- 0

for(i in 0:18){

    a <- a + 1/factorial(i)

}

### below are the results:

> a

[1] 2.718282

> 0:18

[1] 0 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18

> typeof(0:18)

[1] "integer"
```

• One more example:

```
for(i in c("Brisbane", "New York")){
  print(paste("I love", i))
}
### below are the results:
[1] "I love Brisbane"
[1] "I love New York"
```

```
R also provides the while loop
  a <- 0
  while(a < 4){
    a <- a + 1
    print(a)
  3
  ### below are the results:
  [1] 1
  [1] 2
  [1] 3
  [1] 4
• The keyword "break" is used to break from a loop. Save the
  following code to "a.R".
  a <- 0
  repeat{
    a <- a + 1
    if(a > 4) break
    print(a)
  }
  In the R session.
  > source("a.R")
  [1] 1
  [1] 2
  [1] 3
  [1] 4
```

Note that, for practicing programming, the best way is to program, especially on some problems well motivated.

Example

Use the for loop to find

$$\sum_{k=1}^{100} k.$$

If you get the answer 5050, your code is probably correct.

Example

Recall the definition of the Fibonacci numbers: $a_1=a_2=1$ and for any $i\geq 3,$

$$a_i = a_{i-1} + a_{i-2}.$$

Find the first 100 Fibonacci numbers.

Vectors (mathematical concept)

An array x of n real numbers x_1, \ldots, x_n is called a *vector*, and it is written as

$$\boldsymbol{x} = \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix}, \quad \text{or} \quad \boldsymbol{x}' = [x_1, x_2, \cdots, x_n].$$

- Here the prime denotes the operation of transposing a column to a row.
- The number *n* is referred to as the *dimension* of the vector *x*.
- The coordinates x_1, \ldots, x_n can also be complex numbers, in which case x is a complex vector. However in this course we consider ONLY real numbers and real vectors.

- The set of all the real vectors of dimension n, is denoted by \mathbb{R}^n .
- One can scale a vector x by multiplying it by a constant c.

• Vectors can be added.

• inner product: if vectors x and y have the same dimension n,

$$\langle \boldsymbol{x}, \boldsymbol{y} \rangle := \sum_{i=1}^n x_i y_i = \langle \boldsymbol{y}, \boldsymbol{x} \rangle.$$

• length, or norm:

$$\|\boldsymbol{x}\| := \sqrt{\langle \boldsymbol{x}, \boldsymbol{x} \rangle} = \sqrt{x_1^2 + x_2^2 + \dots + x_n^2}.$$

• For any constant c,

$$\langle c \boldsymbol{x}, \boldsymbol{y}
angle = c \langle \boldsymbol{x}, \boldsymbol{y}
angle;$$

 $\|c \boldsymbol{x}\| = \sqrt{\langle c \boldsymbol{x}, c \boldsymbol{x}
angle} = \sqrt{c^2 \langle \boldsymbol{x}, \boldsymbol{x}
angle} = |c| \sqrt{\langle \boldsymbol{x}, \boldsymbol{x}
angle} = |c| \|\boldsymbol{x}\|.$

• triangle inequality: (proof left as a warming up exercise)

$$||x + y|| \le ||x|| + ||y||.$$

There are several ways to generate a vector in R.

```
> a <- 1:5
> a
[1] 1 2 3 4 5
> b <- 5:1
> b
[1] 5 4 3 2 1
> x < - seg(1, 5, length = 10)
> X
[1] 1.000000 1.444444 1.888889 2.333333 2.777778 3.222222 3.666667
 [8] 4.111111 4.555556 5.000000
> runif(5)
[1] 0.1664853 0.6454725 0.3244731 0.4217759 0.3419001
> rep(1, times = 5)
[1] 1 1 1 1 1
> rep(1:5, each = 3)
 [1] 1 1 1 2 2 2 3 3 3 4 4 4 5 5 5
> rep(1:5, times = 3)
[1] 1 2 3 4 5 1 2 3 4 5 1 2 3 4 5
> rep(1:5, length = 14)
[1] 1 2 3 4 5 1 2 3 4 5 1 2 3 4
```

We may take a look at the properties of a vector

```
> x <- 1:5
> length(x)
[1] 5
> typeof(x)
[1] "integer"
> str(x)
int [1:5] 1 2 3 4 5
> object.size(x)
80 bytes
> object.size(1:10000)
40048 bytes
> object.size(1:100000)
400048 bytes
> object.size(1:1000000)
4000048 bytes
> object.size(as.double(1:10000))
80048 bytes
>
> y <- seq(1, 5, len = 10000)
> head(v)
[1] 1.0000 1.0004 1.0008 1.0012 1.0016 1.0020
> tail(y)
[1] 4.9980 4.9984 4.9988 4.9992 4.9996 5.0000
> length(y)
[1] 10000
> typeof(y)
[1] "double"
> object.size(y)
80048 bytes
```

By default, R takes vectors as column matrices, so a transpose of a vector is a row matrix.

```
> a
[1] 1 2 3 4 5
> t(a)
     [,1] [,2] [,3] [,4] [,5]
[1,]
        1
             2
                   3
                              5
                         Δ
> a <- 1:5
> t(a) # THE TRANSPOSE OF a
     [,1] [,2] [,3] [,4] [,5]
[1,]
              2
                   3
        1
                         Δ
                              5
> t(t(a))
     [,1]
[1,]
        1
[2,]
        2
        3
[3,]
[4,]
        4
[5,]
        5
```

However, vectors do not have the "dimension" attribute, and only matrices have.

```
> dim(a)
NULL
> dim(t(a))
[1] 1 5
> dim(t(t(a)))
[1] 5 1
> attributes(t(a))
$dim
[1] 1 5
```

> attributes(a)
NULL

R does not have handy functions for inner product or vector norms. These operations are usually implemented through functions sum and sqrt.

```
> a <- 1:5
> a * 2
[1] 2 4 6 8 10
> a ^ 2
[1] 1 4 9 16 25
> 2 ^ a
[1] 2 4 8 16 32
> a + rep(10, length = 5)
[1] 11 12 13 14 15
> b <- rep(1, length = 5)
> h
[1] 1 1 1 1 1
> sum(a * b) # INNER PRODUCT
[1] 15
> sqrt(sum(b ^ 2)) # VECTOR NORM
[1] 2.236068
> sqrt(sum((-2 * b) ^ 2))
[1] 4.472136
> 2 * sart(sum(b ^ 2))
[1] 4.472136
```

• Matrix A, of dimension $m \times n$, is just a table of (real) numbers.

$$A = \begin{bmatrix} A_{1,1} & A_{1,2} & \cdots & A_{1,n} \\ A_{2,1} & A_{2,2} & \cdots & A_{2,n} \\ \vdots & \vdots & \ddots & \vdots \\ A_{m,1} & A_{m,2} & \cdots & A_{m,n} \end{bmatrix}$$

٠

- $A_{i,j}$ is called the (i,j)-entry of the matrix A.
- Transpose: A' is a $n \times m$ matrix, defined by

$$A' = \begin{bmatrix} A_{1,1} & A_{2,1} & \cdots & A_{m,1} \\ A_{1,2} & A_{2,2} & \cdots & A_{m,2} \\ \vdots & \vdots & \ddots & \vdots \\ A_{1,n} & A_{2,n} & \cdots & A_{m,n} \end{bmatrix}.$$

Example:
$$\begin{bmatrix} 1 & 2 \\ 3 & 4 \\ 5 & 6 \end{bmatrix}$$
 transpose
$$\begin{bmatrix} 1 & 3 & 5 \\ 2 & 4 & 6 \end{bmatrix}$$

- Write $\mathbb{R}^{m \times n}$ the space of all the $n \times m$ matrices.
- Matrix addition: $A = A_{m \times n}$, $B = B_{m \times n}$, then A + B is an $m \times n$ matrix with $(A + B)_{i,j} = A_{i,j} + B_{i,j}$. Matrix A B is similarly defined.
- Matrix multiplication: $A = A_{m \times n}$, $B = B_{n \times p}$, then AB is a $m \times p$ matrix with

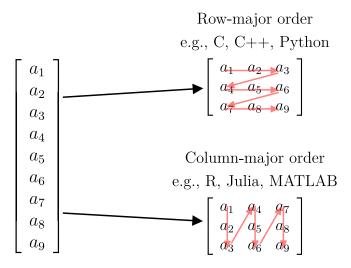
$$(AB)_{i,j} = \sum_{k=1}^{n} A_{i,k} B_{k,j}$$

- Hadamard product: $A, B \in \mathbb{R}^{m \times n}$, $(A \circ B)_{i,j} = A_{i,j}B_{i,j}$.
- Let c be a constant, then cA is an $m \times n$ matrix with $(cA)_{i,j} = cA_{i,j}$.
- Let $A = A_{m \times n}$ be a matrix and $x = x_{n \times 1}$ be a vector, then Ax is an $m \times 1$ vector with $(Ax)_i := A_{i,1}x_1 + A_{i,2}x_2 + \cdots + A_{i,n}x_n$.

Examples

$$\begin{bmatrix} a & b \\ c & d \end{bmatrix} + \begin{bmatrix} \alpha & \beta \\ \gamma & \delta \end{bmatrix} = \begin{bmatrix} a+\alpha & b+\beta \\ c+\gamma & d+\delta \end{bmatrix} \in \mathbb{R}^{2\times 2},$$
$$\begin{bmatrix} a & b \\ c & d \end{bmatrix} \circ \begin{bmatrix} \alpha & \beta \\ \gamma & \delta \end{bmatrix} = \begin{bmatrix} a\alpha & b\beta \\ c\gamma & d\delta \end{bmatrix} \in \mathbb{R}^{2\times 2},$$
$$\begin{bmatrix} a & b & c \\ d & e & f \end{bmatrix} \begin{bmatrix} \alpha \\ \beta \\ \gamma \end{bmatrix} = \begin{bmatrix} a\alpha + b\beta + c\gamma \\ d\alpha + e\beta + f\gamma \end{bmatrix} \in \mathbb{R}^{2},$$
$$\begin{bmatrix} a & b \\ c & d \\ e & f \end{bmatrix} \begin{bmatrix} \alpha & \beta \\ \gamma & \delta \end{bmatrix} = \begin{bmatrix} a\alpha + b\gamma & a\beta + b\delta \\ c\alpha + d\gamma & c\beta + d\delta \\ e\alpha + f\gamma & e\beta + f\delta \end{bmatrix} \in \mathbb{R}^{3\times 2}.$$

In R, generating a matrix is easy. Note that R is "column-major", i.e., when we feed a vector into a matrix, elements of the vector are fed into the matrix one column after another.



```
> a <- matrix(1:6. nrow = 3)
                                                > b[1:2,] # a submatrix
> b <- matrix((1:6) * 100, ncol = 2)</pre>
                                                     [,1] [,2]
> a
                                                [1,] 100 400
     [,1] [,2]
                                                [2,] 200 500
[1,]
      1 4
                                                > a %*% b[1:2,] # matrix-matrix product
[2,]
     2
            5
                                                     [,1] [,2]
     3
[3,]
            6
                                                [1.] 900 2400
> b
                                                [2.] 1200 3300
     [,1] [,2]
                                                [3,] 1500 4200
[1,]
     100 400
                                                > a
[2,]
     200
          500
                                                     [,1] [,2]
[3,]
     300 600
                                                [1,]
                                                       1
                                                            4
                                                [2,]
                                                        2
                                                             5
> a + b # matrix addition
                                                [3,]
                                                        3
                                                            6
     [,1] [,2]
[1,] 101 404
                                                > a + 10 # adding a scalar to a matrix
[2,] 202 505
                                                     [,1] [,2]
[3.]
     303 606
                                                [1,]
                                                      11 14
> a * b # Hadamard product
                                                [2,]
                                                       12 15
     [,1] [,2]
                                                [3,]
                                                       13 16
[1.] 100 1600
                                                > a * 10 # multiplying a matrix by a scalar
[2,] 400 2500
                                                     [,1] [,2]
[3,] 900 3600
                                                [1,]
                                                      10 40
> x < - c(7, 8)
                                                [2,]
                                                       20 50
> X
                                                [3,] 30
                                                            60
[1] 7 8
> a %*% x # matrix-vector product
     [,1]
[1,]
     39
[2,]
      54
[3,]
      69
```

For linear equation systems where the coefficient matrix is a square matrix of full rank,

$$\begin{bmatrix} A_{1,1} & A_{1,2} & \cdots & A_{1,n} \\ A_{2,1} & A_{2,2} & \cdots & A_{2,n} \\ \vdots & \vdots & \ddots & \vdots \\ A_{n,1} & A_{n,2} & \cdots & A_{n,n} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix} = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix}$$

the solution is $\boldsymbol{x} = A^{-1}\boldsymbol{y}$, where A^{-1} denotes the matrix inverse of A. Then $A^{-1}A = AA^{-1} = I$, which is the identity matrix.

Finding matrix inverse, and solving linear equations are easy in R.

```
> A <- matrix(c(1,2,3,6,5,4,8,7,9), nrow = 3)
> A
     [,1] [,2] [,3]
            6
[1,]
      1
                  8
                                                  > solve(A)
          5
[2,]
       2
                7
                                                             [,1]
                                                                        [,2]
                                                                                   [,3]
          4
                 9
[3,]
        3
                                                  [1,] -0.8095238 1.0476190 -0.0952381
> x <- c(2,3,5)
                                                  [2,] -0.1428571 0.7142857 -0.4285714
> X
                                                  [3,] 0.3333333 -0.66666667 0.3333333
[1] 2 3 5
                                                  > A %*% solve(A)
> y <- A %*% x
                                                                [,1]
                                                                             [,2]
                                                                                          [,3]
> V
                                                  [1.] 1.000000e+00 0.000000e+00 4.440892e-16
     [,1]
                                                  [2.] 1.665335e-16 1.000000e+00 1.665335e-16
[1.]
     60
                                                  [3.] -1.665335e-16 3.330669e-16 1.000000e+00
[2,]
     54
                                                  > solve(A) %*% v # method 2. slower
[3,]
     63
                                                       [,1]
> solve(A, y) # method 1
                                                  [1,]
                                                          2
     [,1]
                                                  [2,]
                                                          3
[1,]
        2
                                                  [3,]
                                                          5
[2,]
        3
                                                  > solve(A) %*% y - x
[3,]
        5
                                                                [,1]
> solve(A, y) - x # numerical errors
                                                  [1,] -1.332268e-15
              [,1]
                                                  [2,] 1.332268e-15
    1.776357e-15
[1.]
                                                  [3,] 8.881784e-16
[2.]
     4.440892e-16
[3.] -8.881784e-16
> 10^(-15)
[1] 1e-15
```

The following example (demonstrated via the Julia language) shows the limit on precision of double. This is also an example that in general, floating-point addition and multiplication are not associative (i.e. one may have $a + b + c \neq a + (b + c)$ and $a \times b \times c \neq a \times (b \times c)$)

There are some other matrix operations.

```
> a <- matrix(1:9, nrow = 3)</pre>
                                                      > b <- matrix(1:6, nrow = 2)</pre>
> a
                                                      > b
                                                            [,1] [,2] [,3]
     [,1] [,2] [,3]
[1,]
         1
              4
                    7
                                                      [1,]
                                                               1
                                                                     3
                                                                          5
[2,]
         2
              5
                                                      [2,]
                                                               2
                    8
                                                                     4
                                                                          6
[3,]
              6
                                                      > apply(b, 1, sum)
         3
                    9
> cbind(1, a, t(a))
                                                      [1] 9 12
     [,1] [,2] [,3] [,4] [,5] [,6] [,7]
                                                      > apply(b, 2, prod)
[1,]
        1
              1
                   4
                         7
                               1
                                    2
                                                      [1] 2 12 30
                                          3
                               4
                                          6
              2
                         8
                                    5
[2,]
        1
                    5
                                                      > sum(1:100)
                               7
                    6
                         9
                                    8
                                          9
[3,]
              3
                                                      [1] 5050
         1
> rbind(sqrt(1:3), a)
                                                      > prod(1:4)
     [,1]
               [,2]
                         [,3]
                                                      [1] 24
[1,]
         1 1.414214 1.732051
[2,]
         1 4.000000 7.000000
[3,]
         2 5.000000 8.000000
[4,]
         3 6.000000 9.000000
```

Example (exercise, Fibonacci sequence, revisited)

Recall the Fibonacci sequence $\{a_n\}_{n=1}^{\infty}$ defined by $a_1 = a_2 = 1$ and then iteratively by $a_{n+2} = a_{n+1} + a_n$ for any integer $n \ge 1$. The iterative relation could be written in the vector form as

$$\left[\begin{array}{c}a_{n+2}\\a_{n+1}\end{array}\right] = \left[\begin{array}{cc}1&1\\1&0\end{array}\right] \left[\begin{array}{c}a_{n+1}\\a_n\end{array}\right], \quad \text{for } n \ge 1.$$

Use the above form to find a_{30} . Do you have a faster way to compute a_{30} ?

Vectors and Indexing

A vector is an 1-dim array of data of the same *basic data types*. These basic data types include: integer, double, logical, character, complex (complex numbers), etc.

```
> a <- seq(0, 1, bv = 0.1)
> a
[1] 0.0 0.1 0.2 0.3 0.4 0.5 0.6 0.7 0.8 0.9 1.0
> seq(0, 1, len = 5)
[1] 0.00 0.25 0.50 0.75 1.00
> names(a) <- paste0("the", 1:11)</pre>
> a
 the1 the2 the3 the4 the5 the6 the7 the8 the9 the10 the11
 0.0
       0.1
             0.2
                  0.3
                       0.4
                             0.5
                                    0.6
                                          0.7
                                                0.8
                                                      0.9 1.0
> tvpeof(a)
[1] "double"
> str(a)
Named num [1:11] 0 0.1 0.2 0.3 0.4 0.5 0.6 0.7 0.8 0.9 ...
 - attr(*, "names")= chr [1:11] "the1" "the2" "the3" "the4" ...
> a["the3"]
the3
0.2
> a[3]
the3
0.2
> a[-3]
                        the6 the7 the8 the9 the10 the11
 the1 the2 the4 the5
 0.0
       0.1
             0.3
                   0.4
                         0.5
                              0.6
                                    0.7 0.8 0.9 1.0
```

The components of a vector could be retrieved by number indexes, logical indexes, and names. We can even change the vector values in this way.

```
> a <- seq(0, 1, bv = 0.1)
> names(a) <- paste0("the",1:11)</pre>
> a[7]
the7
0.6
> a[1] <- 8
> a > 0.8
the1 the2 the3 the4 the5 the6 the7 the8 the9 the10 the11
TRUE FALSE FALSE FALSE FALSE FALSE FALSE FALSE TRUE
> a[a>0.8] <- 12
> a
the1 the2 the3 the4 the5 the6 the7 the8 the9 the10 the11
12.0 0.1 0.2
                       0.4 0.5 0.6 0.7 0.8 12.0 12.0
                  0.3
> a[a>0.8] <- 1:2
Warning message:
In a[a > 0.8] <- 1:2 :
 number of items to replace is not a multiple of replacement length
> a
the1 the2 the3 the4 the5 the6
                                 the7 the8 the9 the10 the11
 1.0 0.1 0.2
                  0.3 0.4 0.5
                                  0.6
                                        0.7
                                             0.8
                                                   2.0 1.0
> a[a>0.8] <- 1:5
Warning message:
In a[a > 0.8] <- 1:5 :
 number of items to replace is not a multiple of replacement length
> a
the1 the2 the3 the4 the5 the6 the7 the8 the9 the10 the11
 1.0
     0.1
            0.2
                  0.3
                       0.4
                             0.5
                                  0.6 0.7
                                             0.8
                                                   2.0 3.0
```

We now try number indexes

```
> a <- 4:9
> names(a) <- paste0("ID", 1:6)</pre>
> a
ID1 ID2 ID3 ID4 ID5 ID6
 4 5 6 7
               8
                    9
> a[-1]
ID2 ID3 ID4 ID5 ID6
 5 6 7 8
               9
> a[1]
ID1
  4
> a[-(3:5)]
ID1 ID2 ID6
  4 5 9
```

We now try logical indexes

```
> a <- c("Tom", "John", "Xin", "Kosaku", "Rukawa")</pre>
> b <- c("Kosaku", "Xin", "Rukawa", "Barack", "Vladimir")</pre>
> a[a %in% b]
[1] "Xin"
            "Kosaku" "Rukawa"
> a %in% b
[1] FALSE FALSE TRUE TRUE TRUE
> b[b %in% a]
[1] "Kosaku" "Xin" "Rukawa"
> b[!(b %in% a)]
[1] "Barack" "Vladimir"
> ?setdiff
> union(a,b)
[1] "Tom" "John" "Xin" "Kosaku" "Rukawa" "Barack" "Vladimir"
> intersect(a,b)
[1] "Xin" "Kosaku" "Rukawa"
```

We now try name indexes

```
> scores <- runif(5)
> names(scores) <- c("Tom", "John", "Xin", "Kosaku", "Rukawa")
> scores
        Tom        John        Xin        Kosaku        Rukawa
0.28629591 0.31875371 0.03418924 0.51401365 0.49811182
> names(scores)[scores > 0.5]
[1] "Kosaku"
> names(sort(scores, decreasing=T))
[1] "Kosaku" "Rukawa" "John" "Tom" "Xin"
```

Example

Use the following code to generate a score table for 100 students. Now the president plans to locate the best two students. Write code to find their names.

```
> set.seed(123)
> scores <- runif(100)
> names(scores) <- paste0("student", 1:100)
> head(scores)
student1 student2 student3 student4 student5 student6
0.2875775 0.7883051 0.4089769 0.8830174 0.9404673 0.0455565
```

Example

Use the following code to generate a sequence $\{x_n\}_{n=1}^{100}$. Define

$$y_n = \sum_{k=1, k \neq n}^{100} x_k.$$

Write your code to find the vector $(y_n)_{n=1}^{100}$.

> set.seed(123) > x <- runif(100) > head(x) [1] 0.2875775 0.7883051 0.4089769 0.8830174 0.9404673 0.0455565 Matrix indexing is similar

```
> a <- 1:5 %*% t(2:6)
> a
    [,1] [,2] [,3] [,4] [,5]
[1,]
       2
          3 4 5
                         6
         6 8 10
[2,]
       4
                        12
       6
         9 12 15 18
[3,]
[4,]
       8 12 16 20
                        24
[5,]
      10
           15
               20
                    25
                        30
> rownames(a) <- paste0("Rw", 1:5)</pre>
> colnames(a) <- paste0("Cl", 1:5)</pre>
> a
   cl1 cl2 cl3 cl4 cl5
Rw1 2 3 4
                5
                    6
Rw2 4 6 8 10 12
Rw3 6 9 12 15 18
Rw4
     8 12 16 20 24
Rw5 10 15 20 25 30
> a[Rw3, Cl4]
Error: object 'Rw3' not found
> a["Rw3", "Cl4"]
[1] 15
> a["Rw3", 2:4]
cl2 cl3 cl4
 9 12 15
```

Example

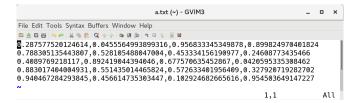
Use the following code to simulate the score table of a class. Find the average score of math, with top 2 and bottom 2 scores removed. Find the math score of the student with highest chem score.

```
> set.seed(123)
> sc <- matrix(runif(75), nrow = 25)
> rownames(sc) <- paste0("Student", 1:25)
> colnames(sc) <- c("bio", "math", "chem")</pre>
```

Reading data from files, and writing data to files

We explain the usage of the functions "read.table" and "write.table".

```
> set.seed(123)
> a <- matrix(runif(20), nrow = 5)
> a
          [,1] [,2] [,3]
                                        [,4]
[1,] 0.2875775 0.0455565 0.9568333 0.89982497
[2.] 0.7883051 0.5281055 0.4533342 0.24608773
[3,] 0.4089769 0.8924190 0.6775706 0.04205953
[4,] 0.8830174 0.5514350 0.5726334 0.32792072
[5,] 0.9404673 0.4566147 0.1029247 0.95450365
> write.table(a, file = "a.txt", col.names = FALSE, row.names = FALSE, sep = ",")
> b <- read.table("a.txt", sep = ",")</pre>
> h - a
                                        V3
             V1
                          V2
                                                      V4
1 -2.220446e-16 4.163336e-17 -1.110223e-16 4.440892e-16
2 3.330669e-16 2.220446e-16 4.996004e-16 8.326673e-17
3 1.110223e-16 -1.110223e-16 4.440892e-16 -3.469447e-17
4 -4.440892e-16 2.220446e-16 -2.220446e-16 3.885781e-16
5 -3.330669e-16 3.330669e-16 -2.775558e-16 -4.440892e-16
```



One may directly store R objects to files.

```
> set.seed(123)
> a <- matrix(runif(20), nrow = 5)</pre>
> save(a, file = "a.RData")
> b <- a
> rm(a)
> a
Error: object 'a' not found
> load("a.RData")
> a
          [.1]
                   [,2] [,3]
                                         [.4]
[1,] 0.2875775 0.0455565 0.9568333 0.89982497
[2,] 0.7883051 0.5281055 0.4533342 0.24608773
[3,] 0.4089769 0.8924190 0.6775706 0.04205953
[4,] 0.8830174 0.5514350 0.5726334 0.32792072
[5,] 0.9404673 0.4566147 0.1029247 0.95450365
> b - a
     [,1] [,2] [,3] [,4]
[1,]
       0
            0
                 0
                      0
            0 0
[2,]
       0
                      0
          0 0 0
[3,]
       0
            0 0
[4,]
       0
                      0
            Θ
                 Θ
                       0
[5,]
       Θ
```

Sometimes, to store a data spreadsheet that contains strings, we use the data type "data frame" in R. It is stored as a list equipped with the data frame structure. We will come back to the dataset "iris" later.

```
> 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
> is.data.frame(iris)
[1] TRUE
> as.matrix(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"
> as.matrix(head(iris)[, 1:4])
  Sepal.Length Sepal.Width Petal.Length Petal.Width
1
           5.1
                        3.5
                                      1.4
                                                   0.2
2
           4.9
                        3.0
                                      1.4
                                                   0.2
3
                        3.2
           4.7
                                      1.3
                                                   0.2
4
           4.6
                        3.1
                                      1.5
                                                   0.2
5
           5.0
                        3.6
                                      1.4
                                                   0.2
6
           5.4
                        3.9
                                      1.7
                                                   0.4
> tvpeof(iris)
[1] "list"
```

Functions

- A function is a fixed sequence of code that takes arguments, and returns output. The following function adds two numbers up.
 add <- function(x, y){ return(x + y) }

 ### we call the function: > add(2,3) [1] 5
- The keyword return terminates the program flow and returns immediately the value of the formula. If a function has no return command, the value of the last formula will be returned.
 add1 <- function(x, y){
 x + y
 }
 ### we call the function:

```
> add1(2,3)
[1] 5
```

Example (Fibonacci sequence, revisited)

The Fibonacci sequence f_1, f_2, \ldots is defined by $f_1 = 1$, $f_2 = 1$, and for any $k \ge 3$, $f_k = f_{k-1} + f_{k-2}$.

1, 1, 2, 3, 5, 8, 13, 21, 34, 55, 89, 144, 233, 377, 610, 987, 1597,...

Make a function which takes argument k and returns f_k . Note that in the code below, we also used the if-else statement.

Note that the above function fibo calls itself! This is called recursion. On the one hand, each call of the function would generate a lot of memory overhead, the efficiency of the program is reduced; on the other hand however, this speeds up programming and saves the programmer's time. We use binomial distributions as an example. Recall that for any positive integer n and real number 0 , a random variable <math>X has the binomial distribution Binomial(n, p) if

$$\operatorname{Prob}(X=k) = \binom{n}{k} p^k (1-p)^{n-k}$$
, for any $X = 0, 1, \dots, n$.

Here $\binom{n}{k} := \frac{n!}{k!(n-k)!}$. The function $f_{n,p}(k) = \binom{n}{k}p^k(1-p)^{n-k}$ of k, is called the probability function (or probability mass function, PMF). In R, $f_{n,p}$ is implemented as

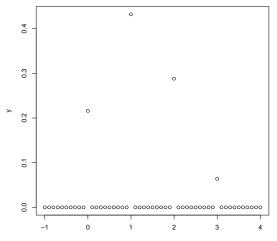
$$f_{n,p}(k) = dbinom(x = k, size = n, prob = p)$$

Here, the placeholders x, size, and prob are called formal parameters. When $k \notin \{0, 1, ..., n\}$, one simply takes $f_{n,p}(k) = 0$.

```
Binomial
                         package:stats
                                                        R Documentation
The Binomial Distribution
Description:
     Density, distribution function, guantile function and random
     generation for the binomial distribution with parameters 'size'
     and 'prob'.
     This is conventionally interpreted as the number of 'successes' in
     'size' trials.
Usage:
     dbinom(x, size, prob, log = FALSE)
     pbinom(g, size, prob, lower.tail = TRUE, log.p = FALSE)
     gbinom(p, size, prob, lower.tail = TRUE, log.p = FALSE)
     rbinom(n, size, prob)
Arguments:
    x. g: vector of guantiles.
       p: vector of probabilities.
       n: number of observations. If (length(n) > 1), the length is
          taken to be the number required.
    size: number of trials (zero or more).
    prob: probability of success on each trial.
```

. . .

```
x <- seq(-1, 4, by = 0.1)
y <- dbinom(x = x, size = 3, prob = 0.4)
plot(x, y)</pre>
```



х

The distribution function (also called the cumulative distribution function, CDF) is defined for all $x \in \mathbb{R}$,

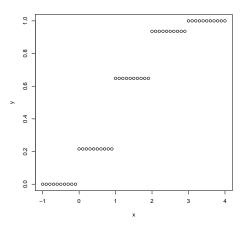
$$F_{n,p}(x) = \sum_{k \le x} f_{n,p}(k).$$

Therefore CDF F for any probability distribution is non-decreasing, and

$$\lim_{x \to \infty} F(x) = 1$$
$$\lim_{x \to -\infty} F(x) = 0$$

The quantile $Q_{n,p}(\xi)$ for $0 < \xi < 1$ is defined as the smallest value $Q = Q_{n,p}(\xi)$ such that $F_{n,p}(Q) \ge \xi$. Here we skip the discussion.

x <- seq(-1, 4, by = 0.1)
y <- pbinom(q = x, size = 3, prob = 0.4)
plot(x, y)</pre>



The function rbinom generates random numbers from a specified binomial distribution.

```
> set.seed(123)
> rbinom(n = 10, size = 3, prob = 0.4)
[1] 1 2 1 2 3 0 1 2 1 1
> x <- rbinom(n = 100000, size = 3, prob = 0.4)</pre>
> table(x)
х
   0
          1
            2
                      3
21659 43256 28703 6382
> table(x) / length(x)
х
      0
              1
                      2
                              3
0.21659 0.43256 0.28703 0.06382
> dbinom(x = 0:3, size = 3, prob = 0.4)
[1] 0.216 0.432 0.288 0.064
```

Continuous probability distributions

We use normal distributions as an example. Recall that for any real number $\mu \in \mathbb{R}$, and any positive variance $\sigma^2 > 0$, a random variable X has the normal distribution $N(\mu, \sigma^2)$ if

$$\operatorname{Prob}(X \le x) = \int_{-\infty}^{x} \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left\{-\frac{(t-\mu)^2}{2\sigma^2}\right\} dt$$

The density function for $-\infty \leq x \leq \infty$

$$f_{\mu,\sigma^2}(x) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left\{-\frac{(x-\mu)^2}{2\sigma^2}\right\}$$

is implemented in R as

$$f_{\mu,\sigma^2}(x) = \operatorname{dnorm}(\mathbf{x}=\!x,\operatorname{mean}=\!\mu,\operatorname{sd}=\!\sigma)$$

The CDF for $-\infty \leq x \leq \infty$

$$F_{\mu,\sigma^2}(x) = \int_{-\infty}^x f_{\mu,\sigma^2}(t)dt = \int_{-\infty}^x \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left\{-\frac{(t-\mu)^2}{2\sigma^2}\right\}dt$$

is implemented in R as

$$F_{\mu,\sigma^2}(x)={ t pnorm}({ t q}=\!x,{ t mean}=\!\mu,{ t sd}=\!\sigma)$$

The quantile $Q_{\mu,\sigma^2}(x) = F_{\mu,\sigma^2}^{-1}(x)$ for $0 \le x \le 1$ is the inverse function of F_{μ,σ^2} , and is implemented in R as

$$Q_{\mu,\sigma^2}(x) = ext{qnorm}(extsf{p}=\!x, extsf{mean}=\!\mu, extsf{sd}=\!\sigma)$$

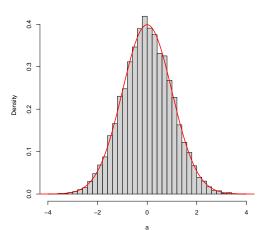
For a comprehensive list of probability distributions (discrete and continuous) implemented in R, see https://CRAN.R-project.org/view=Distributions. The function rnorm generates random numbers from a specified normal distribution.

```
> set.seed(123)
> a <- rnorm(n = 10000) # N(0,1) by default
> head(a) # get the first several (default=6) elements
[1] -0.56047565 -0.23017749 1.55870831 0.07050839 0.12928774 1.71506499
> tail(a) # get the last several (default=6) elements
[1] -0.5896389 -1.0247840 -0.3671164 -0.7574729 1.0793289 -0.6449242
> hist(a, breaks = 30)
```

800 800 Frequency ĝ 200 0 -2 0 2 -4

Histogram of a

```
set.seed(123)
a <- rnorm(n = 10000) # N(0,1) by default
hist(a, breaks = 30, freq = FALSE)
x <- seq(-5, 5, length = 500)
lines(x, dnorm(x), lwd = 2, col = "red")</pre>
```



Histogram of a

Example (exercise)

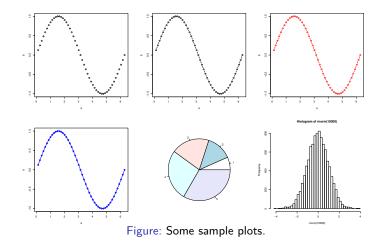
In theory, $Q_{\mu,\sigma^2}(F_{\mu,\sigma^2}(x))\equiv x$ for any real number x. However, the output of the R command

qnorm(p = pnorm(q = 10))

is Inf (infinity, $\infty).$ Please try the command yourself, explain the output, and find a fix.

Plotting

plot is a generic function to plot variables. The default use is plot(x, y) which plots a vector y against another vector x provided they have the same length.



```
> a <- (1:50) / 50 * 2 * pi
> b <- sin(a)
> plot(a,b)
> plot(a,b,type="b")
> plot(a,b,type="b",col="red")
> plot(a,b,type="o",col="blue",pch=23)
> pie(1:5)
> hist(rnorm(10000),breaks=30)
```

For more options, see **?plot** and **?plot.default**. One may save the plot into files.

```
> setEPS()
> postscript("a.eps")
> pie(1:5)
> dev.off()
null device
1
> bmp("a.bmp")
> pie(1:6)
> dev.off()
null device
1
```

R has a simple implementation of optimization function.

Example

Using R to find the minimizer of the following function

$$f(x_1, x_2, x_3) = x_1^2 + (x_2 - 2)^2 + (x_3 + 2)^2$$

f <- function(x) x[1]² + (x[2] - 2)² + (x[3] + 2)²

Note

- If the body of a function has only one sentence, the curly bracket {} can be ignored.
- Obviously the minimizer is (0, 2, -2). Knowing the true result helps us to verify the program output.

```
optim(c(1,1,1), f, control = list(reltol = 1e-8))
### below are the results:
$par
[1] 4.366903e-07 2.000140e+00 -2.000049e+00
```

\$value [1] 2.19478e-08

\$counts function gradient 186 NA

\$convergence [1] 0

\$message NULL

Note

- The output item par is the minimizer obtained of the function.
- The output item value is the minimum value of *f*.
- The output item counts gives the time that *f* is called. Roughly speaking, the more times the function is called, the longer the program takes to run. Sine we have never provided the gradient information, we have not called the gradient function.
- The output item convergence has value 0 if the function has confidence that a local minimizer is achieved. The value is not 0 if some potential problems are detected.

Recall

$$f(x_1, x_2, x_3) = x_1^2 + (x_2 - 2)^2 + (x_3 + 2)^2.$$

We feed the optim function below, also with the gradient

$$\nabla f(x_1, x_2, x_3) = \begin{pmatrix} \partial f/\partial x_1 \\ \partial f/\partial x_2 \\ \partial f/\partial x_3 \end{pmatrix} = \begin{pmatrix} 2x_1 \\ 2(x_2 - 2) \\ 2(x_3 + 2) \end{pmatrix}$$

We define

```
gra.f <- function(x){
    2 * c(x[1], x[2] - 2, x[3] + 2)
}</pre>
```

.

```
The updated optimization code is
```

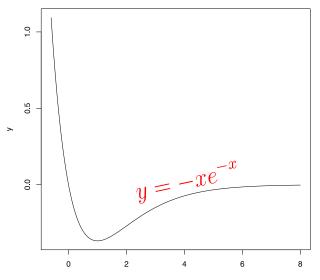
We see that although we call the gradient function 7 times, the times we call the function f is reduced, from 186, to 15. More importantly, the precision is much better than the previous run.

Example

Use R to find the minimizer of the function

$$f(x) = -xe^{-x}.$$

Note that you may use calculus to verify that the minimizer is x = 1 where $f(1) = -e^{-1} = -0.3679$.



х

Example (exercise, Maximum likelihood estimation, MLE)

Let x_1, \ldots, x_n be drawn independently from $\mathsf{Poisson}(\lambda)$. If λ is unknown, one may estimate λ by maximizing the log-likelihood function

$$\ell(\lambda) = \log \prod_{i=1}^{n} e^{-\lambda} \frac{\lambda^{x_i}}{x_i!} = \sum_{i=1}^{n} \left\{ -\lambda + x_i \log \lambda - \log(x_i!) \right\}$$

Set λ and n, and generate data yourself. Then write a function mle to minimize ℓ by the above R function optim. Compare your solution with the analytical minimizer $\hat{\lambda} = \frac{1}{n} \sum x_i$.

Integration, 1-dim

Note that for integration with more than 1 dimension, methods like Monte-Carlo may be better.

Example

Use R to find the value of the integral

$$\int_{-\infty}^{\infty} \exp(-x^2) dx.$$

Note that the true value of the integral is

$$\int_{-\infty}^{\infty} \exp(-x^2) dx = 2 \int_{0}^{\infty} \exp(-x^2) dx$$
$$\stackrel{y=x^2}{=} \int_{0}^{\infty} y^{\frac{1}{2}-1} e^{-y} dy = \Gamma\left(\frac{1}{2}\right) = \sqrt{\pi} = 1.77245385.$$

integrate(function(x) exp(-x^2), lower = -Inf, upper = Inf)
below are the results:
1.772454 with absolute error < 4.3e-06</pre>

Note

- We see that the numerical integration is already very precise. We skip the algorithm behind.
- In R, one uses Inf to denote infinity $\infty.$
- We see that in the above command we have used a function function(x) exp(-x^2)

which is passed to the function integrate immediately after it is generated. We did not even give it a name! This kind of function is called anonymous function.

Example

Use R to evaluate the following function

$$\Phi(x) := \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{x} \exp\left\{-\frac{t^2}{2}\right\} dt.$$

Note that this function is the cumulative distribution function of the standard normal distribution N(0,1). R has a high-performance implementation of this function: pnorm. After writing your function, you may compare it with pnorm.

Numerically, R implements some algorithms to solve nonlinear equations, e.g. Newton's method. It is not therefore guaranteed that all the roots can be found.

Example

Find the solution of the equation f(x) = 0 with

$$f(x) = e^x + x.$$

```
install.packages("nleqslv") # install the package, just for the first time
library("nlegslv")
f <- function(x) exp(x) + x
nleqslv(1, f) # 1: initial guess
   ### below are the results:
                                                           $scalex
   Śχ
                                                           [1] 1
   [1] -0.5671433
                                                           Śnfcnt
   $fvec
                                                           [1] 6
   [1] 8.346891e-10
                                                           $njcnt
   Stermcd
                                                           [1] 1
   [1] 1
                                                           $iter
                                                           [1] 6
   $message
   [1] "Function criterion near zero"
```

So the solution is x = -0.5671433.

Example (exercise)

Find the solution to the equation f(x) = 0 with

$$f(x) = x^3 - x^2 + x - 1.$$

In R, there is a function polyroot specially designed to find the roots of polynomials. Let $a = (a_1, a_2, \ldots, a_{n+1}) \in \mathbb{R}^{n+1}$ be the coefficient vector for the polynomial

$$p(x) = a_1 + a_2 x + a_3 x^2 + \dots + a_{n+1} x^n,$$

then we may use the command polyroot(a) to find ALL the roots of p. For the above example,

```
> polyroot(c(-1,1,-1,1))
[1] 0+1i 0-1i 1+0i
```

We see that some complex roots are also found.