Elements of a programming language – 3

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Matrices

A **matrix** is a 2-dimensional data structure, like vector, it consists of elements of the same type. A matrix has *rows* and *columns*.

Say, we want to construct this matrix in R:

$$\mathbf{X} = \begin{bmatrix} 1 & 2 & 3 \\ 4 & 5 & 6 \\ 7 & 8 & 9 \end{bmatrix}$$

```r
X <- matrix(1:9, # a sequence of numbers to fill in
       nrow=3, # three rows (alt. ncol=3)
       byrow=T) # populate matrix by row
X
```

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

Matrices – indexing

Elements of a matrix are retrieved using the '[]' notation, like we have seen for vectors. Here, we have to specify 2 dimensions – the row and the column:

```
X[1,2] # Retrieve element from the 1st row, 2nd column
```

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

```
X[3,] # Retrieve the entire 3rd row
```

```
## [1] 7 8 9
```

```
X[,2] # Retrieve the 2nd column
```

```
## [1] 2 5 8
```

Matrices – indexing cted.

```
X[c(1,3),] # Retrieve rows 1 and 3
```

```
##      [,1] [,2] [,3]
## [1,]    1    2    3
## [2,]    7    8    9
```

```
X[c(1,3),c(3,1)]
```

```
##      [,1] [,2]
## [1,]    3    1
## [2,]    9    7
```

Matrices – dimensions

To check the dimensions of a matrix, use dim():

```
X
```

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

```
dim(X) # 3 rows and 3 columns
```

```
## [1] 3 3
```

Nobody knows why dim() does not work on vectors. . . use length() instead.

Matrices – operations 1

Usually the functions that work for a vector also work for matrices. To order a matrix with respect to, say, 2nd column:

```
X <- matrix(sample(1:9,size = 9), nrow = 3)
ord <- order(X[,2])
X[ord,]
```

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

Matrices – transposition

To **transpose** a matrix use t():

```
X
```

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

```
t(X)
```

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

Nobody knows why dim() does not work on vectors... use length() instead.

Matrices – operations 2

To get the diagonal, of the matrix:

```r
X
```

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

```r
diag(X) # get values on the diagonal
```

```
## [1] 9 7 4
```

Matrices – operations, triangles

To get the upper or the lower triangle use **upper.tri()** and **lower.tri()** respectively:

```
X # print X
```

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

```
upper.tri(X) # which elements form the upper triangle
```

```
##       [,1]  [,2]  [,3]
## [1,] FALSE  TRUE  TRUE
## [2,] FALSE FALSE  TRUE
## [3,] FALSE FALSE FALSE
```

```
X[upper.tri(X)] <- 0 # set them to 0
```

Matrices – multiplication

Different types of matrix multiplication exist:

```
A <- matrix(1:4, nrow = 2, byrow=T)
B <- matrix(5:8, nrow = 2, byrow=T)
A * B # Hadamard product
```

```
##      [,1] [,2]
## [1,]    5   12
## [2,]   21   32
```

```
A %*% B # Matrix multiplication
```

```
##      [,1] [,2]
## [1,]   19   22
## [2,]   43   50
```

```
# A %x% B # Kronecker product
# A %o% B # Outer product (tensor product)
```

Matrices – outer

Outer product can be useful for generating names

```
outer(letters[1:4], LETTERS[1:4], paste, sep="-")
```

```
##      [,1]  [,2]  [,3]  [,4] 
## [1,] "a-A" "a-B" "a-C" "a-D"
## [2,] "b-A" "b-B" "b-C" "b-D"
## [3,] "c-A" "c-B" "c-C" "c-D"
## [4,] "d-A" "d-B" "d-C" "d-D"
```

Expand grid

But **expand.grid()** is more convenient when you want, e.g. generate combinations of variable values:

```
expand.grid(height = seq(120, 121),
            weight = c('1-50', '51+'),
            sex = c("Male","Female"))
```

```
##   height weight    sex
## 1    120   1-50   Male
## 2    121   1-50   Male
## 3    120    51+   Male
## 4    121    51+   Male
## 5    120   1-50 Female
## 6    121   1-50 Female
## 7    120    51+ Female
## 8    121    51+ Female
```

Matrices – apply

Function **apply** is a very useful function that applies a given function to either each value of the matrix or in a column/row-wise manner. Say, we want to have mean of values by column:

```
X
```

```
##      [,1] [,2] [,3]
## [1,]    9    0    0
## [2,]    8    7    0
## [3,]    1    3    4
```

```
apply(X, MARGIN=2, mean) # MARGIN=1 would do it for rows
```

```
## [1] 6.000000 3.333333 1.333333
```

Matrices – apply cted.

And now we will use *apply()* to replace each element it a matrix with its deviation from the mean squared:

```
X
```

```
##      [,1] [,2] [,3]
## [1,]    9    0    0
## [2,]    8    7    0
## [3,]    1    3    4
```

```
my.mean <- mean(X)
apply(X, MARGIN=c(1,2),
      function(x, my.mean) (x - my.mean)^2,
      my.mean)
```

```
##           [,1]      [,2]       [,3]
## [1,] 29.641975 12.641975 12.6419753
## [2,] 19.753086 11.864198 12.6419753
```

Matrices – useful fns.

While *apply()* is handy, it is a bit slow and for the most common statistics, there are special functions col/row Sums/Means:

```
X
```

```
##      [,1] [,2] [,3]
## [1,]    9    0    0
## [2,]    8    7    0
## [3,]    1    3    4
```

```
colSums(X)
```

```
## [1] 18 10  4
```

These functions are faster!

Matrices – adding rows/columns

One may wish to add a row or a column to an already existing matrix or to make a matrix out of two or more vectors of equal length:

```
x <- c(1,1,1)
y <- c(2,2,2)
cbind(x,y)
```

```
##      x y
## [1,] 1 2
## [2,] 1 2
## [3,] 1 2
```

```
rbind(x,y)
```

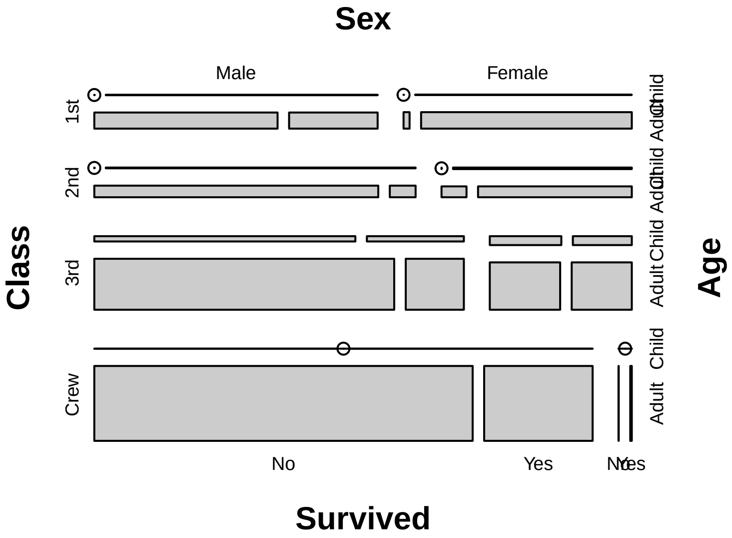
```
##   [,1] [,2] [,3]
## x    1    1    1
## y    2    2    2
```

Matrices – more dimensions

```
dim(Titanic)
```

```
## [1] 4 2 2 2
```

Matrices – more dimensions, example



Lists – collections of various data types

A list is a collection of elements that can be of various data types:

```
name <- c('R2D2', 'C3PO', 'BB8')
weight <- c(21, 54, 17)
data <- list(name=name, weight)
data
```

```
## $name
## [1] "R2D2" "C3PO" "BB8"
##
## [[2]]
## [1] 21 54 17
```

```
data$name
```

```
## [1] "R2D2" "C3PO" "BB8"
```

```
data[[1]]
```

Lists – collections of various data types

Elements of a list can also be different data structures:

```
weight <- matrix(sample(1:9, size = 9), nrow=3)
data <- list(name, weight)
data
```

```
## [[1]]
## [1] "R2D2" "C3PO" "BB8"
##
## [[2]]
##      [,1] [,2] [,3]
## [1,]    5    4    3
## [2,]    7    9    8
## [3,]    6    1    2
```

```
data[[2]][3]
```

```
## [1] 6
```

Data frames

A **data frame** or a **data table** is a data structure very handy to use. In this structure elements of every column have the same type, but different columns can have different types. Technically, a data frame is a list of vectors...

```
df <- data.frame(c(1:5),
                 LETTERS[1:5],
                 sample(c(TRUE, FALSE), size = 5,
                        replace=T))
df
```

```
##   c.1.5. LETTERS.1.5. sample.c.TRUE..FALSE...size...5..r
## 1      1            A
## 2      2            B
## 3      3            C
## 4      4            D
## 5      5            E
```

Data frames – cted.

As you have seen, columns of a data frame are named after the call that created them. Not always the best option…

```
df <- data.frame(no=c(1:5),
                 letter=c('a','b','c','d','e'),
                 isBrown=sample(c(TRUE, FALSE),
                        size = 5,
                        replace=T))
df
```

```
##   no letter isBrown
## 1  1      a    TRUE
## 2  2      b    TRUE
## 3  3      c    TRUE
## 4  4      d   FALSE
## 5  5      e   FALSE
```

Data frames – accessing.

As you have seen, columns of a data frame are named after the call that created them. Not always the best option...

```
df[1,]  # get the first row
```

```
##   no letter isBrown
## 1  1      a    TRUE
```

```
df[,2]  # the first column
```

```
## [1] a b c d e
## Levels: a b c d e
```

```
df[2:3, 'isBrown'] # get rows 2-3 from the isBrown column
```

```
## [1] TRUE TRUE
```

```
df$letter[1:2] # get the first 2 letters
```

Data frames – factors

An interesting observation:

```
df$letter
```

```
## [1] a b c d e
## Levels: a b c d e
```

```
df$letter <- as.character(df$letter)
df$letter
```

```
## [1] "a" "b" "c" "d" "e"
```

Data frames – factors cted.

To treat characters as characters at data frame creation time, one can use the **stringsAsFactors** option set to TRUE:

```
df <- data.frame(no=c(1:5),
                 letter=c("a","b","c","d","e"),
                 isBrown=sample(c(TRUE, FALSE),
                        size = 5,
                        replace=T),
                 stringsAsFactors = TRUE)
df$letter
```

```
## [1] a b c d e
## Levels: a b c d e
```

Well, as you see, it did not work as expected...

Data frames – names

To get or change row/column names:

```
colnames(df) # get column names
```

```
## [1] "no"       "letter"   "isBrown"
```

```
rownames(df) # get row names
```

```
## [1] "1" "2" "3" "4" "5"
```

```
rownames(df) <- letters[1:5]
rownames(df)
```

```
## [1] "a" "b" "c" "d" "e"
```

```
df['b', ]
```

```
##   no letter isBrown
```

Data frames – merging.

A very useful feature of R is merging two data frames on certain key using **merge**:

```r
df1 <- data.frame(no=c(1:5),
                  letter=c("a","b","c","d","e"))
df2 <- data.frame(no=c(1:5),
                  letter=c("A","B","C","D","E"))
merge(df1, df2, by='no')
```

```
##   no letter.x letter.y
## 1  1        a        A
## 2  2        b        B
## 3  3        c        C
## 4  4        d        D
## 5  5        e        E
```

Objects – type vs. class

An object of class **factor** is internally represented by numbers:

```
size <- factor('small')
class(size) # Class 'factor'
```

```
## [1] "factor"
```

```
mode(size) # Is represented by 'numeric'
```

```
## [1] "numeric"
```

```
typeof(size) # Of integer type
```

```
## [1] "integer"
```

Objects – structure

Many functions return **objects**. We can easily examine their **structure**:

```
his <- hist(1:5, plot=F)
str(his)
```

```
## List of 6
##  $ breaks  : num [1:5] 1 2 3 4 5
##  $ counts  : int [1:4] 2 1 1 1
##  $ density : num [1:4] 0.4 0.2 0.2 0.2
##  $ mids    : num [1:4] 1.5 2.5 3.5 4.5
##  $ xname   : chr "1:5"
##  $ equidist: logi TRUE
##  - attr(*, "class")= chr "histogram"
```

```
object.size(hist) # How much memory the object consumes
```

```
## 832 bytes
```

Objects – fix

We can easily modify values of object's **atributes**:

```
attributes(his)
```

```
## $names
## [1] "breaks"   "counts"   "density"  "mids"     "xname"
##
## $class
## [1] "histogram"
```

```
attr(his, "names")
```

```
## [1] "breaks"   "counts"   "density"  "mids"     "xname"
```

```
#fix(his) # Opens an object editor
```

Lists as S3 classes

A list that has been named, becomes an S3 class:

```
my.list <- list(numbers = c(1:5),
                letters = letters[1:5])
class(my.list)
```

```
## [1] "list"
```

```
class(my.list) <- 'my.list.class'
class(my.list) # Now the list is of S3 class
```

```
## [1] "my.list.class"
```

However, that was it. We cannot enforce that *numbers* will contain numeric values and that *letters* will contain only characters. S3 is a very primitive class.

S3 classes

For an S3 class we can define a *generic function* applicable to all objects of this class.

```
print.my.list.class <- function(x) {
  cat('Numbers:', x$numbers, '\n')
  cat('Letters:', x$letters)
}
print(my.list)
```

```
## Numbers: 1 2 3 4 5
## Letters: a b c d e
```

But here, we have no error-proofing. If the object will lack *numbers*, the function will still be called:

```
class(his) <- 'my.list.class' # alter class
print(his) # Gibberish but no error...
```

S3 classes – still useful?

Well, S3 class mechanism is still in use, esp. when writing **generic** functions, most common examples being *print* and *plot*. For example, if you plot an object of a Manhattan.plot class, you write *plot(gwas.result)* but the true call is: *plot.manhattan(gwas.result)*. This makes life easier as it requires less writing, but it is up to the function developers to make sure everything works!

S4 class mechanism

S4 classes are more advanced as you actually define the structure of the data within the object of your particular class:

```
setClass('gene',
         representation(name='character',
                        coords='numeric')
         )
my.gene <- new('gene', name='ANK3',
               coords=c(1.4e6, 1.412e6))
```

S4 class – slots

The variables within an S4 class are stored in the so-called **slots**. In the above example, we have 2 such slots: *name* and *coords*. Here is how to access them:

```
my.gene@name # access using @ operator
```

```
## [1] "ANK3"
```

```
my.gene@coords[2] # access the 2nd element in slot coords
```

```
## [1] 1412000
```

S4 class – methods

The power of classes lies in the fact that they define both the data types in particular slots and operations (functions) we can perform on them. Let us define a *generic print function* for an S4 class:

```
setMethod('print', 'gene',
          function(x) {
              cat('GENE: ', x@name, ' --> ')
              cat('[', x@coords, ']')
          })
```

```
## Creating a generic function for 'print' from package 'ba
```

```
## [1] "print"
```

```
print(my.gene) # and we use the newly defined print
```

```
## GENE:  ANK3  --> [ 1400000 1412000 ]
```