Data Mining and Machine Learning in Bioinformatics

Exercise Series 1

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a) Compute a 150 x 150 Euclidean distance matrix between flowers.

CODE

```
# Implemented in two ways - using dist(), and using self-created function
# function for calculating Euclidean Distance
euclidean_distance <- function(p, q) {
    ed = 0
    for (i in 1:4) {
        ed <- ed + (p[,i] - q[,i]) ^ 2
    }
    ed <- sqrt(ed)
    return(ed)
}

data(iris) #load iris data
iris2 <- iris[-5] # delete column 5 with string
# compute distances using dist() function
distances <- as.matrix(dist(head(iris2, size)))

# compute distances using self-created function
distances2 <- matrix(nrow=size, ncol=size)
for (p in 1:size) {
  for (q in 1:size) {
    row_p = iris2[p,]
    row_q = iris2[q,]
    distances2[p, q] <- euclidean_distance(row_p, row_q)
  }
}
```

b) Given that distance matrix calculate for each flower its so-called nearest neighbor (i.e. the one, which is most similar to it).

CODE

```
Flower = c()
Species = c()
Nearest.neighbor = c()
NN.species = c()

for (i in 1:size) {
    Flower[i] <- i
    Species[i] <- levels(iris$Species)[iris[i, 5]] # convert the factor to string

    # find the nearest neighbor using sort
    line = distances2[i,]
    nn = sort(line)[2] # first one is itself, so choose 2
    index_nn = which(line == nn)
    Nearest.neighbor[i] <- index_nn
    NN.species[i] <- levels(iris$Species)[iris[index_nn, 5]]
}

data_frame = data.frame(Flower, Species, Nearest.neighbor, NN.species)
#print(data_frame)
write.csv(data_frame, file = "EX_B_distance.csv")
```

c) Calculate the percentage of flowers of species X that has a nearest neighbor of species Y. The output should be a 3 x 3 matrix X (because there are 3 species).

CODE

```
cc = table ( data_frame$Species, data_frame$NN.species ) [,]
write.csv(cc, file = "EX_C_distance_3x3.csv")
```

RESULT

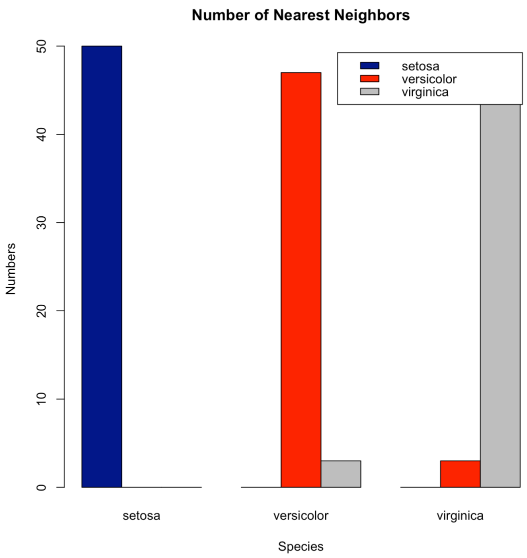
```
             setosa versicolor virginica
  setosa         50          0         0
  versicolor      0         47         3
  virginica       0          3        47
```

d) Generate three grouped barplots

CODE

```
barplot(cc, main="Number of Nearest Neighbors", xlab="Species", ylab="Numbers", co
l=c("darkblue", "red", "gray"), legend = rownames(cc), beside=TRUE)
```

RESULT

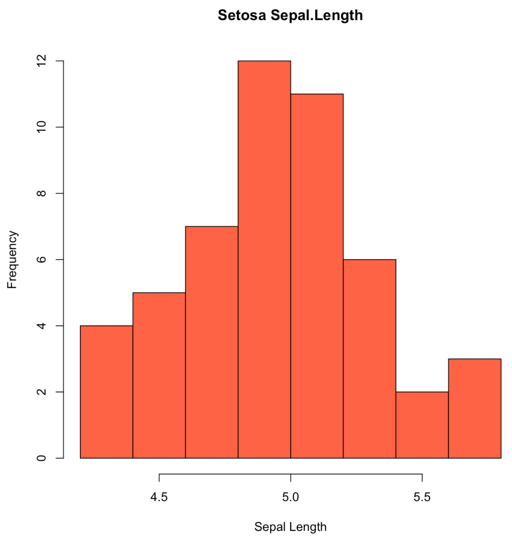


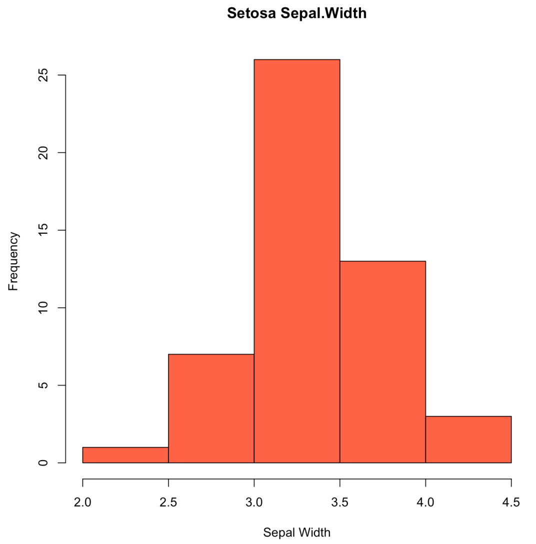
e) Generate histograms

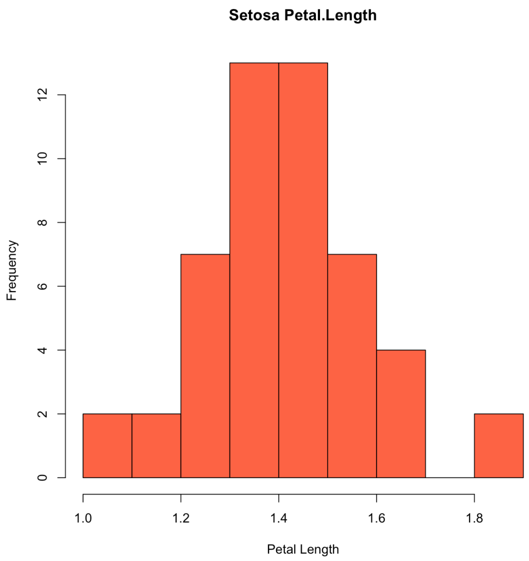
CODE

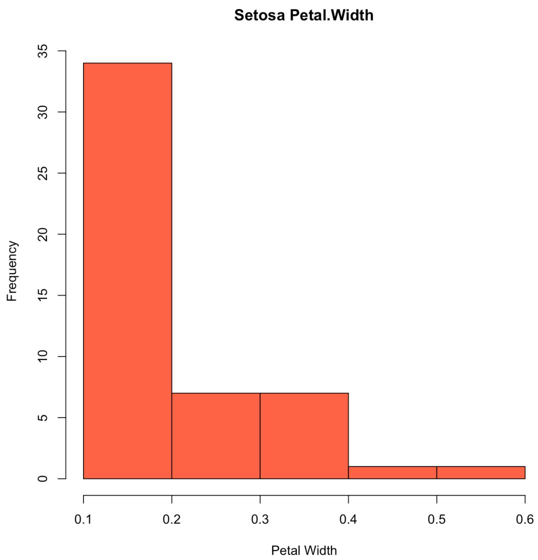
```
# setosa

setosa <- iris[iris$Species == 'setosa',]

hist(setosa$Sepal.Length, col="Tomato", main="Setosa Sepal.Length", xlab="Sepal Le
ngth")
hist(setosa$Sepal.Width, col="Tomato", main="Setosa Sepal.Width", xlab="Sepal Widt
h")
hist(setosa$Petal.Length, col="Tomato", main="Setosa Petal.Length", xlab="Petal Le
ngth")
hist(setosa$Petal.Width, col="Tomato", main="Setosa Petal.Width", xlab="Petal Widt
h")

# versicolor

versicolor <- iris[iris$Species == 'versicolor',]

hist(versicolor$Sepal.Length, col="Violet", main="Versicolor Sepal.Length", xlab="
Sepal Length")
hist(versicolor$Sepal.Width, col="Violet", main="Versicolor Sepal.Width", xlab="Se
pal Width")
hist(versicolor$Petal.Length, col="Violet", main="Versicolor Petal.Length", xlab="
Petal Length")
hist(versicolor$Petal.Width, col="Violet", main="Versicolor Petal.Width", xlab="Pe
tal Width")

# virginica

virginica <- iris[iris$Species == 'virginica',]

hist(virginica$Sepal.Length, col="Turquoise", main="Virginica Sepal.Length", xlab=
"Sepal Length")
hist(virginica$Sepal.Width, col="Turquoise", main="Virginica Sepal.Width", xlab="S
epal Width")
hist(virginica$Petal.Length, col="Turquoise", main="Virginica Petal.Length", xlab=
"Petal Length")
hist(virginica$Petal.Width, col="Turquoise", main="Virginica Petal.Width", xlab="P
etal Width")
```

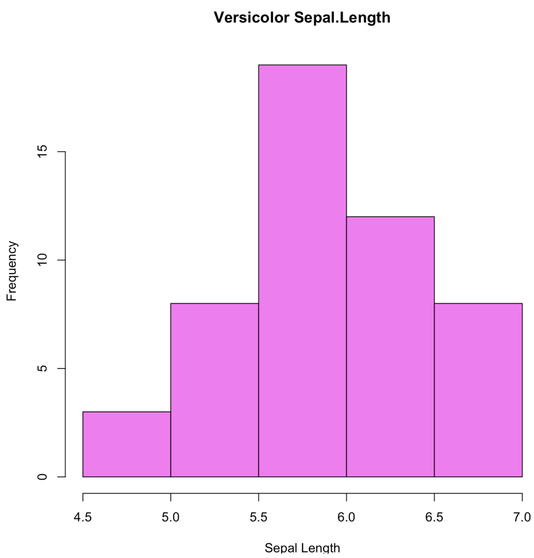
RESULT

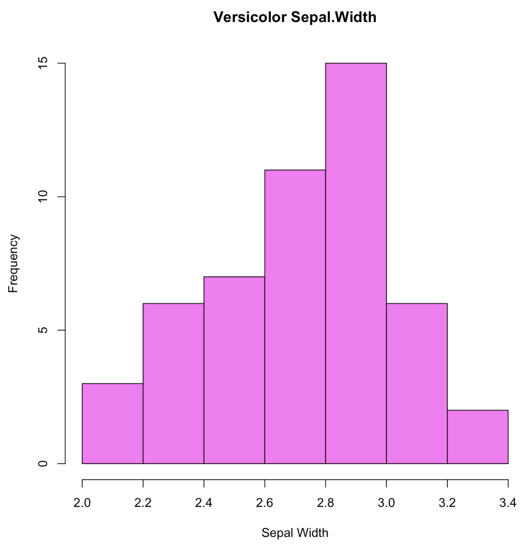

Setosa Sepal.Length
Frequency
0
2
4
6
8
10
12
4.5
5.0
5.5
Sepal Length

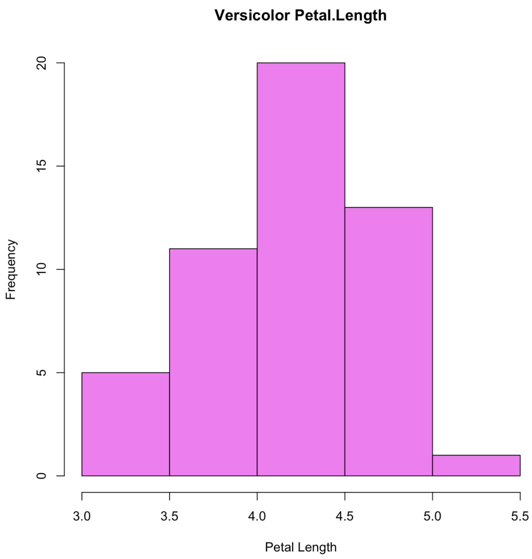

Setosa Sepal.Width
Frequency
0
5
10
15
20
25
2.0
2.5
3.0
3.5
4.0
4.5
Sepal Width

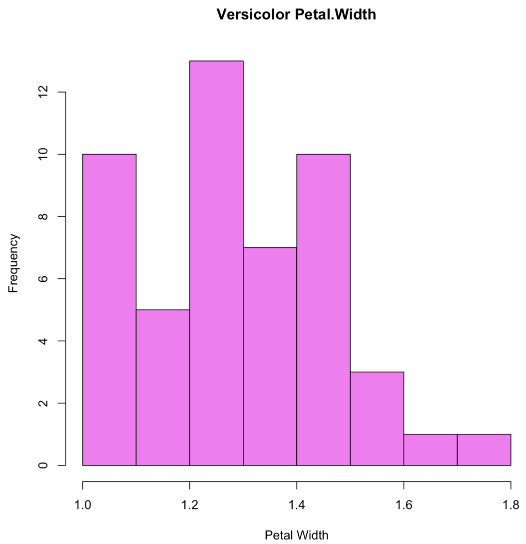

Setosa Petal.Length
Frequency
0
2
4
6
8
10
12
1.0
1.2
1.4
1.6
1.8
Petal Length

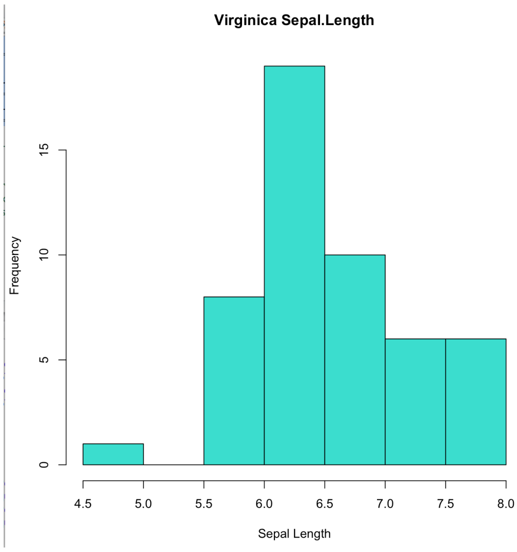

Setosa Petal.Width
Frequency
0
5
10
15
20
25
30
35
0.1
0.2
0.3
0.4
0.5
0.6
Petal Width

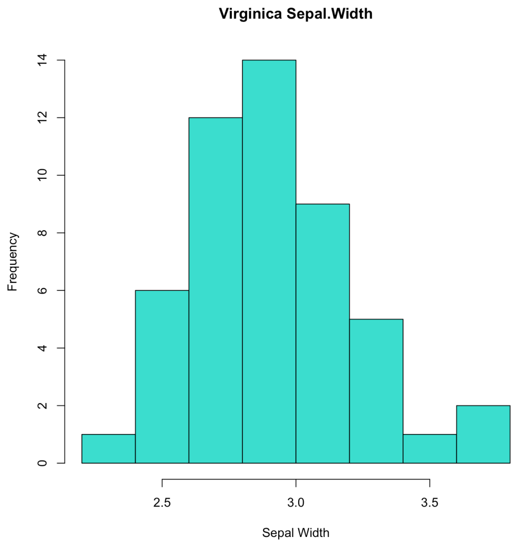

Versicolor Sepal.Length
Frequency
0
5
10
15
4.5
5.0
5.5
6.0
6.5
7.0
Sepal Length

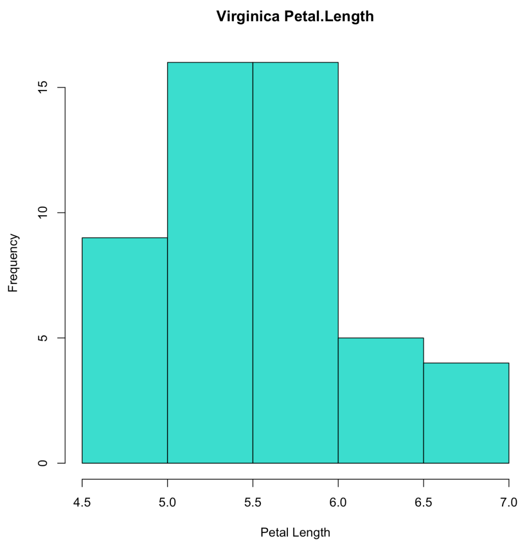

Versicolor Sepal.Width
Frequency
0
5
10
15
2.0
2.2
2.4
2.6
2.8
3.0
3.2
3.4
Sepal Width

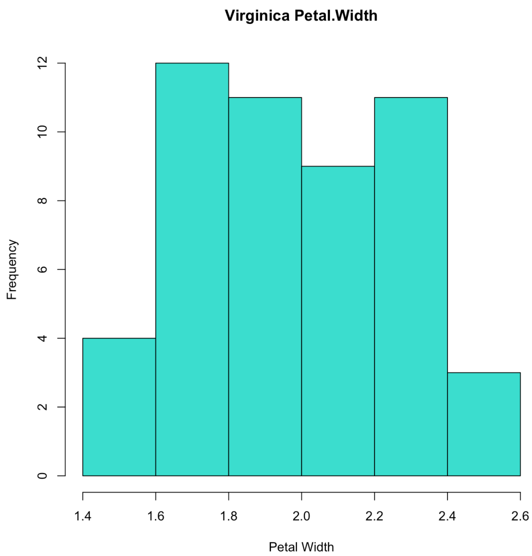












f) Explain in your own words what a histogram visualizes and how you have to interpret the figure.

A histogram visualizes a distribution of numerical data. The y-axis shows how frequently the values on the x-axis occur in the data, the bars represent ranges of values on the x-axis.

Figures description

#Setosa Sepal.Length

It is observed that the higher frequencies are defined between the range of 4.5 - 5.5, having a maximum frequency approximately of 15 units.

#Versicolor Sepal.Length

This figure shows a maximum frequency of approximately 20 units for Sepal lengths between the range 5.5. and 6.0.

#Virginica Sepal.Length

Higher frequencies are defined between the range of 6.0 - 6.5, with a frequency of approximately of 20 units. There is an evenly distribution for values between the range of 7.0 - 8.0, furthermore there are no Sepals with lengths in a range of 5.0 - 5.5.

#Setosa Sepal.Width

The frequency reach its maximum of approximately 25 units for values defined between the range 3.0 - 3.5 and its minimum between 2.0 - 2.5.

#Versicolor Sepal.Width

Increasing distribution of frequencies is observed between the range 2.0 - 3.0, reaching a maximum of approximately 15 units between the range 2.8 - 3.0.

#Virginica Sepal.Width

This figure shows a maximum frequencies of approximately 15 units for widths between 2.5 and 3.0.

#Setosa Petal.Length

An evenly minimal distribution of frequencies is observed for lengths between the range 1.0 - 1.2 and greater than 1.8, the frequencies reach its maximum at a length of around 1.4 with approximately 15 units.

#Versicolor Petal.Length

It is observed that the maximum frequency is reached between the range of 4.0 - 4.5 with a frequency of a approximately 20 units, whereas the minimum length is between 5.0 - 5.5 with a a frequency of 1 unit.

#Virginica Petal.Length

One can observe that the maximum frequency is evenly distributed for ranges 5.0 - 5.5 and 5.5 - 6.0 with a maximum frequency of approximately 15 units.

#Setosa Petal.Width

Most of the values of petal width are defined at its very minimum between the range 0.1 - 0.2 with a frequency of approximately 35 units, the minimum is defined between the range 0.4 - 0.6.

#Versicolor Petal.Width

The minimum frequency is defined between the range 1.6 - 1.8, whereas the maximum is defined for widths of 1.2 or 1.3 with a frequency of approximately 15 units.

#Virginica Petal.Width

Most of the frequencies are almost evenly distributed between the range 1.6 - 2.4, reaching their maximum between the range 1.6 - 1.8.

#General Comparison

Among the three groups of species, Virginica has the higher Sepal lengths frequency for values between 6.0 ??? 6.5 and Satosa has the maximum Sepal widths for values between 3.0 and 3.5.

On the other side, Setosa specie presents the minimum Petal lengths with values between 1.0 - 1.8, on the contrary, Virginica has the maximum petal lengths between the range 5.0 - 6.0. It is clear to notice that species of type Setosa have the minimum widths of Petals.