Data Mining and Machine Learning in Bioinformatics

Exercise Series 2

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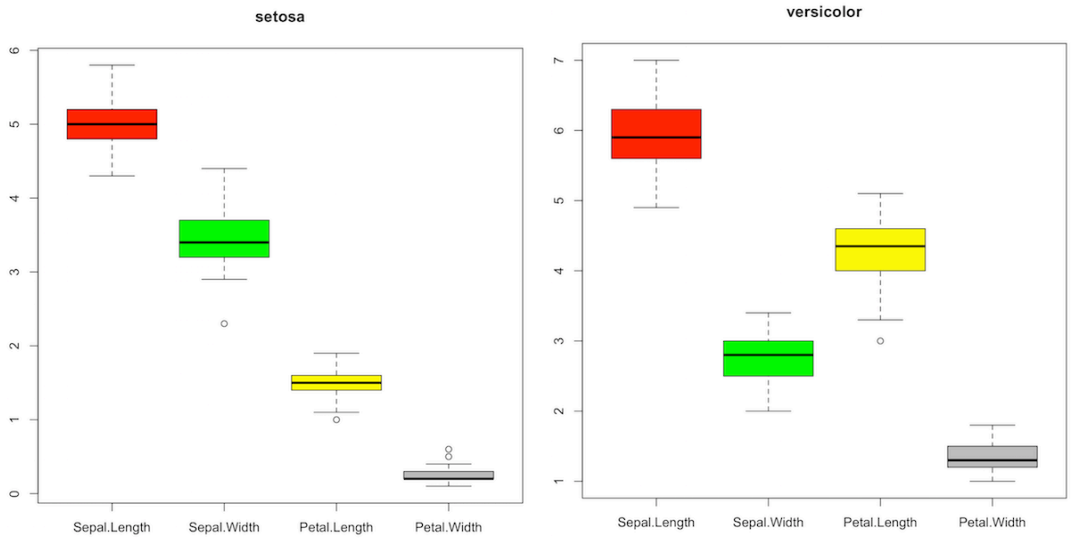
Task 1

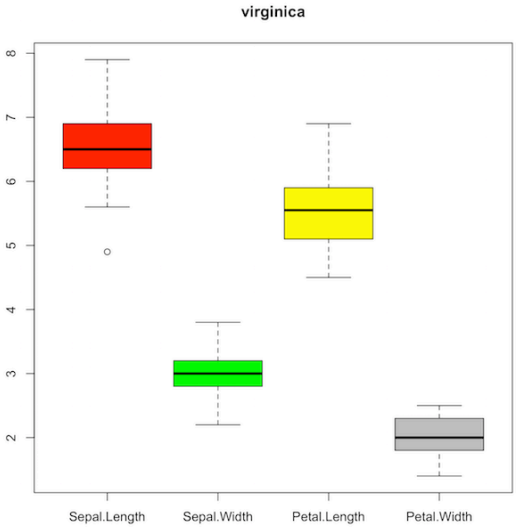
a) Generate boxplots visualizing the distribution of values for each of the variables sepal length, sepal width, petal length and petal height. The boxplots should be plotted separately for each of the 3 species classes.

CODE

```
setosa <- iris[iris$Species == 'setosa',]
versicolor <- iris[iris$Species == 'versicolor',]
virginica <- iris[iris$Species == 'virginica',]

boxplot(setosa[1:4], main="setosa", col=c("red","green","yellow","gray"),
    names=colnames(iris)[1:4])
boxplot(versicolor[1:4], main="versicolor", col=c("red","green","yellow","gray"),
    names=colnames(iris)[1:4])
boxplot(virginica[1:4], main="virginica", col=c("red","green","yellow","gray"),
    names=colnames(iris)[1:4])
```

RESULT





b) distribution skewness

EXPLANATION:

Distribution Skewness: is a measure of the asymmetry of the probability distribution of a real-valued random variable about its mean. The skewness value can be positive or negative, or even undefined.

Negative skew:
* Mean is greater than median.
* The left tail is longer; the mass of the distribution is concentrated on the right of the figure.

Positive skew:
* Mean is less than median.
* The right tail is longer; the mass of the distribution is concentrated on the left of the figure.

Sepal Length and Width has positive skew.
from the below density plot, we can see that the right tail is slightly longer than left tail on Sepal Length and Width.

Petal Length and Width has negative skew.
from the below density plot of the petal length and width, we can see two hump but the most dense part is on the right side (slightly).

We also can say, the absolute of the skewness is bigger, the data is more concentrated on one-side.

CODE

```
(mean(iris$Sepal.Length) - median(iris$Sepal.Length)) / sd(iris$Sepal.Length)
(mean(iris$Sepal.Width) - median(iris$Sepal.Width)) / sd(iris$Sepal.Width)
(mean(iris$Petal.Length) - median(iris$Petal.Length)) / sd(iris$Petal.Length)
(mean(iris$Petal.Width) - median(iris$Petal.Width)) / sd(iris$Petal.Width)

d <- density(iris$Sepal.Length) # returns the density data
plot(d) # plots the results
d <- density(iris$Sepal.Width) # returns the density data
plot(d) # plots the results
d <- density(iris$Petal.Length) # returns the density data
plot(d) # plots the results
d <- density(iris$Petal.Width) # returns the density data
plot(d) # plots the results
```

RESULT

`Sepal.Length: 0.05233076`
`Sepal.Width: 0.1315388`
`Petal.Length: -0.3353541`
`Petal.Width: -0.1320673`

c) Calculate Pearson and Spearman rank correlations

EXPLANATION

Pearson's Correlation

+1: Perfect direct linear relationship (correlation)
-1: Perfect decreasing linear relationship (anti-correlation)
0: uncorrelated

One can observe that when considering the whole Iris data set, there is a decreasing linear relationship between the variables

Petal.Width/Lenght and Sepal.Width, on the contrary there is an increasing correlation between the variables Sepal.Length and Petal.Width/Length.

In contrast when every group of species is analyzed individually one can observe that there is only an

increasing correlation. In the case of species type Setosa the correlation between Sepal.Length and Petal.Width/Length reduces considerably.

One possible explanation for these discrepancies between correlations is the existence/addition of "outliers" affecting the measure when the data is correlated all together and individually.

CODE

```
co <- cor(iris[1:4])
corsp <- cor(iris[1:4], method="spearman")

coSetosa <- cor(setosa[1:4])
corspSetosa <- cor(setosa[1:4], method="spearman")

coVersicolor <- cor(versicolor[1:4])
corspVersicolor <- cor(versicolor[1:4], method="spearman")

coVirginica <- cor(virginica[1:4])
corspVirginica <- cor(virginica[1:4], method="spearman")
```

RESULT

```
> co
             Sepal.Length Sepal.Width Petal.Length Petal.Width
Sepal.Length    1.0000000  -0.1175698    0.8717538   0.8179411
Sepal.Width    -0.1175698   1.0000000   -0.4284401  -0.3661259
Petal.Length    0.8717538  -0.4284401    1.0000000   0.9628654
Petal.Width     0.8179411  -0.3661259    0.9628654   1.0000000
> corsp
             Sepal.Length Sepal.Width Petal.Length Petal.Width
Sepal.Length    1.0000000  -0.1667777    0.8818981   0.8342888
Sepal.Width    -0.1667777   1.0000000   -0.3096351  -0.2890317
Petal.Length    0.8818981  -0.3096351    1.0000000   0.9376668
Petal.Width     0.8342888  -0.2890317    0.9376668   1.0000000
> coSetosa
             Sepal.Length Sepal.Width Petal.Length Petal.Width
Sepal.Length    1.0000000   0.7425467    0.2671758   0.2780984
Sepal.Width     0.7425467   1.0000000    0.1777000   0.2327520
Petal.Length    0.2671758   0.1777000    1.0000000   0.3316300
Petal.Width     0.2780984   0.2327520    0.3316300   1.0000000
> corspSetosa
             Sepal.Length Sepal.Width Petal.Length Petal.Width
Sepal.Length    1.0000000   0.7553375    0.2788849   0.2994989
Sepal.Width     0.7553375   1.0000000    0.1799110   0.2865359
Petal.Length    0.2788849   0.1799110    1.0000000   0.2711414
Petal.Width     0.2994989   0.2865359    0.2711414   1.0000000
> coVersicolor
             Sepal.Length Sepal.Width Petal.Length Petal.Width
Sepal.Length    1.0000000   0.5259107    0.7540490   0.5464611
Sepal.Width     0.5259107   1.0000000    0.5605221   0.6639987
Petal.Length    0.7540490   0.5605221    1.0000000   0.7866681
Petal.Width     0.5464611   0.6639987    0.7866681   1.0000000
> corspVersicolor
             Sepal.Length Sepal.Width Petal.Length Petal.Width
Sepal.Length    1.0000000   0.5176060    0.7366251   0.5486791
Sepal.Width     0.5176060   1.0000000    0.5747272   0.6599826
Petal.Length    0.7366251   0.5747272    1.0000000   0.7870096
Petal.Width     0.5486791   0.6599826    0.7870096   1.0000000
> coVirginica
             Sepal.Length Sepal.Width Petal.Length Petal.Width
Sepal.Length    1.0000000   0.4572278    0.8642247   0.2811077
Sepal.Width     0.4572278   1.0000000    0.4010446   0.5377280
Petal.Length    0.8642247   0.4010446    1.0000000   0.3221082
Petal.Width     0.2811077   0.5377280    0.3221082   1.0000000
> corspVirginica
             Sepal.Length Sepal.Width Petal.Length Petal.Width
Sepal.Length    1.0000000   0.4265165    0.8243234   0.3157721
Sepal.Width     0.4265165   1.0000000    0.3873587   0.5443098
Petal.Length    0.8243234   0.3873587    1.0000000   0.3629133
Petal.Width     0.3157721   0.5443098    0.3629133   1.0000000
```

d) visualize the correlation matrices calculated in c) via heatmaps.

EXPLANATION

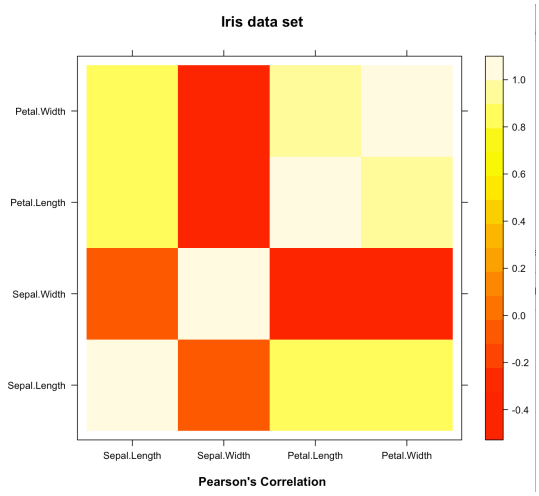
using the heat.colors color scheme, heat map displays correlation matrix values as color.
the map is symmetric.
color is bright yellow if the value is close to 1.
color is red if the value is close to lowest value of the map.

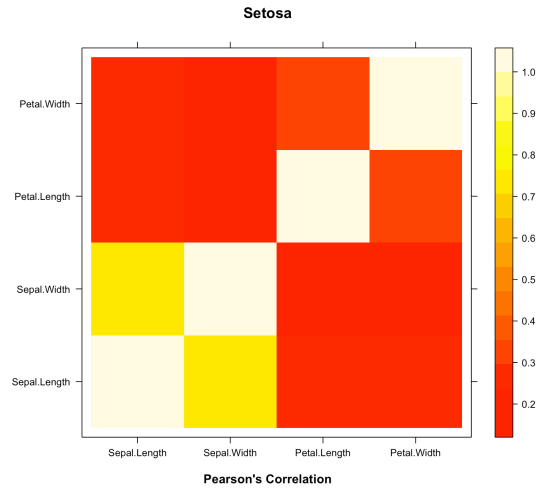
Bacause each matrix has different range of correlation, each map shows relative difference of correlation in the matrix.

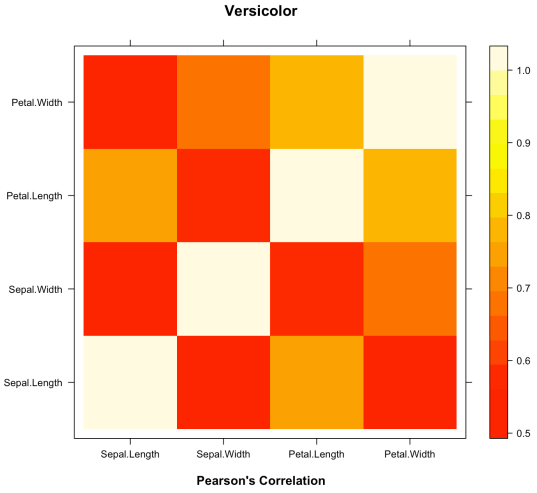
CODE

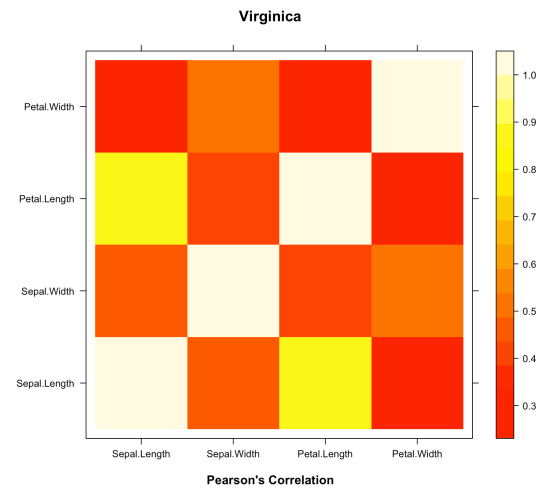
```
pdf('my_test.pdf',width=8,height=8,paper='special')
library("lattice")
# displays Pearson's Correlation
levelplot(co, colorkey = T, region = T, main="Iris data set", sub="Pearson's Corre
lation",
          col.regions=heat.colors, xlab="", ylab="")
levelplot(coSetosa, colorkey = T, region = T, main="Setosa", sub="Pearson's Correl
ation",
          col.regions=heat.colors, xlab="", ylab="")
levelplot(coVersicolor, colorkey = T, region = T, main="Versicolor", sub="Pearson'
s Correlation",
          col.regions=heat.colors, xlab="", ylab="")
levelplot(coVirginica, colorkey = T, region = T, main="Virginica", sub="Pearson's
Correlation",
          col.regions=heat.colors, xlab="", ylab="")

# displays spearman's Correlation
levelplot(corsp, colorkey = T, region = T, main="Iris data set", sub="Spearman's C
orrelation",
          col.regions=heat.colors, xlab="", ylab="")
levelplot(corspSetosa, colorkey = T, region = T, main="Setosa", sub="Spearman's Co
rrelation",
          col.regions=heat.colors, xlab="", ylab="")
levelplot(corspVersicolor, colorkey = T, region = T, main="Versicolor", sub="Spear
man's Correlation",
          col.regions=heat.colors, xlab="", ylab="")
levelplot(corspVirginica, colorkey = T, region = T, main="Virginica", sub="Spearma
n's Correlation",
          col.regions=heat.colors, xlab="", ylab="")

dev.off()
```

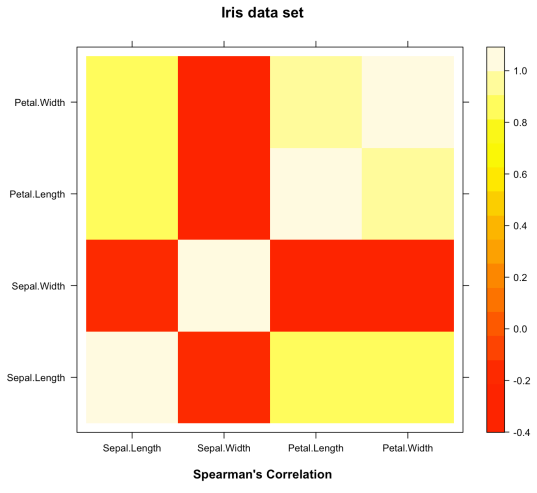
RESULT

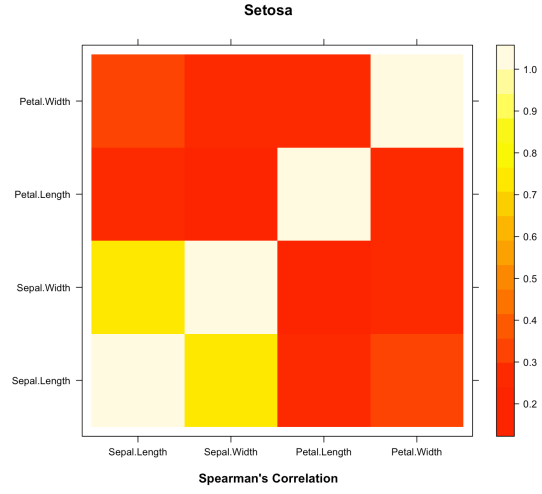

Iris data set
Petal.Width
Petal.Length
Sepal.Width
Sepal.Length
Sepal.Length
Sepal.Width
Petal.Length
Petal.Width
1.0
0.8
0.6
0.4
0.2
0.0
-0.2
-0.4
Pearson's Correlation

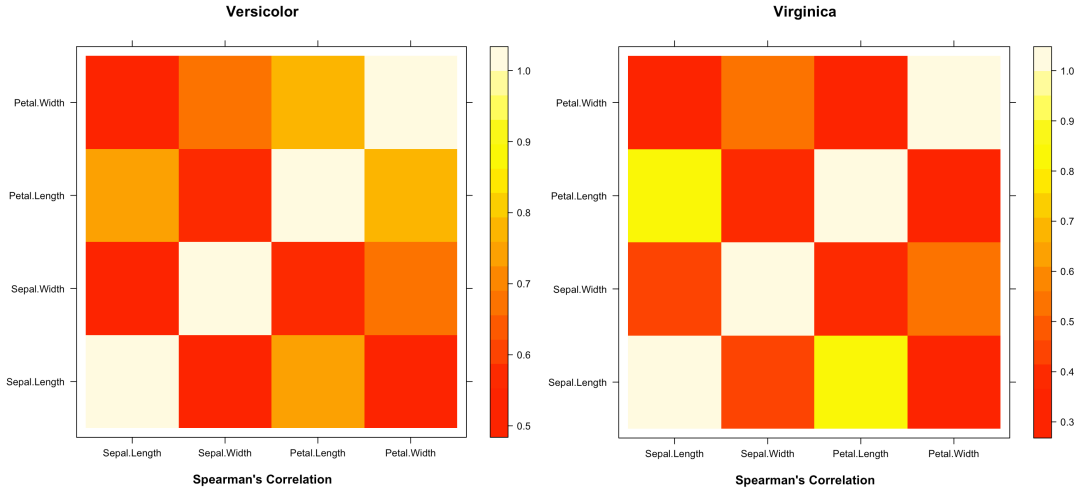

Setosa
Petal.Width
Petal.Length
Sepal.Width
Sepal.Length
Sepal.Length
Sepal.Width
Petal.Length
Petal.Width
1.0
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
Pearson's Correlation


Versicolor
Petal.Width
Petal.Length
Sepal.Width
Sepal.Length
Sepal.Length
Sepal.Width
Petal.Length
Petal.Width
1.0
0.9
0.8
0.7
0.6
0.5
Pearson's Correlation


Virginica
Petal.Width
Petal.Length
Sepal.Width
Sepal.Length
Sepal.Length
Sepal.Width
Petal.Length
Petal.Width
1.0
0.9
0.8
0.7
0.6
0.5
0.4
0.3
Pearson's Correlation


Iris data set
Petal.Width
Petal.Length
Sepal.Width
Sepal.Length
Sepal.Length
Sepal.Width
Petal.Length
Petal.Width
1.0
0.8
0.6
0.4
0.2
0.0
-0.2
-0.4
Spearman's Correlation


Setosa
Petal.Width
Petal.Length
Sepal.Width
Sepal.Length
Sepal.Length
Sepal.Width
Petal.Length
Petal.Width
1.0
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
Spearman's Correlation



Task 2

a-i) Calculate the mean and variance for x and y

CODE

```
dat = read.csv("exercise2-2.csv")

# Here we calculate the mean and the variance for each colum in the dat dataset
meanByCol = apply(dat, 2, mean)
varByCol = apply(dat, 2, var)
sdByCol = apply(dat, 2, sd)

meanByCol
varByCol
sdByCol
```

RESULT

```
> meanByCol
      x1       y1       x2       y2       x3       y3       x4       y4
9.000000 7.500909 9.000000 7.500909 9.000000 7.500000 9.000000 7.500909
> varByCol
       x1        y1        x2        y2        x3        y3        x4        y4
11.000000  4.127269 11.000000  4.127629 11.000000  4.122620 11.000000  4.123249
> sdByCol
      x1       y1       x2       y2       x3       y3       x4       y4
3.316625 2.031568 3.316625 2.031657 3.316625 2.030424 3.316625 2.030579
```

a-ii) Calculate the correlation between x and y

CODE

```
# A-ii
# calculate correlation between X and Y.
c1 = cor(dat$x1, dat$y1)
c2 = cor(dat$x2, dat$y2)
c3 = cor(dat$x3, dat$y3)
c4 = cor(dat$x4, dat$y4)
```

RESULT

```
> c1
[1] 0.8164205
> c2
[1] 0.8162365
> c3
[1] 0.8162867
> c4
[1] 0.8165214
```

a-iii) Linear regression

CODE

```
# A-iii
# Here calculate the values for a and b, that will be used later to draw the regre
ssion line
b1 <- c1 * sdByCol[1] / sdByCol[2]
#b1 <- 0.5
a1 <- meanByCol[2] - (b1 * meanByCol[1])

b2 <- c2 * sqrt(varByCol[3]) / sqrt(varByCol[4])
#b2 = 0.5
a2 <- meanByCol[4] - (b1 * meanByCol[3])

b3 <- c3 * sqrt(varByCol[5]) / sqrt(varByCol[6])
#b3 <- 0.5
a3 <- meanByCol[6] - (b1 * meanByCol[5])

b4 <- c4 * sqrt(varByCol[7]) / sqrt(varByCol[8])
#b4 <- 0.5
a4 <- meanByCol[8] - (b1 * meanByCol[7])
```

RESULT

```
> b1
1.332843
> b2
1.332484
> b3
1.333375
> b4
1.333657
```

b) For each data set plot the data in a scatter plot and add the regression line to the scatter plot.

CODE

```
plot(dat$x1, dat$y1, xlim=c(0, 20), ylim=c(-5,15), xlab="X1", ylab="Y1", main="X1-
Y1 scatterplot")
abline(a=a1, b=b1, col="red")
#abline(lm(dat$y1~dat$x1), col="blue")

plot(dat$x2, dat$y2, xlim=c(0, 20), ylim=c(-5,15), xlab="X2", ylab="Y2", main="X2-
Y2 scatterplot")
abline(a=a2, b=b2, col="red")
#abline(lm(dat$y2~dat$x2), col="blue")

plot(dat$x3, dat$y3, xlim=c(0, 20), ylim=c(-5,15), xlab="X3", ylab="Y3", main="X3-
Y3 scatterplot")
abline(a=a3, b=b3, col="red")
#abline(lm(dat$y3~dat$x3), col="blue")

plot(dat$x4, dat$y4, xlim=c(0, 20), ylim=c(-5,15), xlab="X4", ylab="Y4", main="X4-
Y4 scatterplot")
abline(a=a4, b=b4, col="red")
#abline(lm(dat$y4~dat$x4), col="blue")
```

EXPLANATION

```
# With color red we draw a line using the equation line.
# With color blue we draw a line using the `lm` function provide by R.

# We can see that the case 3 is the data which better fits the regression line. Al
most perfect. But it does exist an outlier value.

# If we compare the scatterplots and the correlation value that we calculated befo
re we can check that...
# 1. we have a very well distributed data, and a normal distribution.
# 2. we can see a relationship between X and Y, this one is a functional relations
hip.
# 3. we have a linear relationship between X and Y.
# 4. we can see that is not a linear relationship, the outlier modifies markedly t
he regression line.
```

RESULT