Prof. Dr. Steffen Wagner
Angewandte Statistik
Fachbereich II
Berliner Hochschule für Technik

Exercise 08: Classification with LDA/QDA

Machine Learning I – SoSe 24

This workshop covers hierarchical clustering and soft clustering. At the end of the worksheet there are a couple of written exercises for you to do at home, which should be good practice for the exam.

1 Preparations

1.1 RStudio Project

1. Open your Machine Learning 1 RStudio Project
2. Create an R Script file to perform this exercise

1.2 Required Packages

For this exercise you require the following additional R packages. Please make sure that you have installed them on your computer before coming to the workshop session for the case that Eduroam is not working.

```
# check if packages can be loaded, i.e. they are already installed
library(ggplot2)          # for visualisation
library(MASS)             # for LDA nd QDA
library(pROC)
```

If you get an error at this stage, you need to install the packages.

1.3 Required Data

In this Worksheet we will use again the data set `Diabetes.Rda` that is available via Moodle.

2 Bayes Classifier

2.1 Bayes Classifier by hand

Let Y be a random variable, which takes the values 0 or 1, dependent on a predictor variable x. Assume that, if $Y{=}0$ then $X|Y{=}0$ is $N(4,1)$ distributed, and if $Y{=}1$ then $X|Y{=}1$ is $N(5,1)$ distributed. The prior probabilities, when x is unknown, are $P(Y{=}0) = P(Y{=}1) = 0.5$

Tasks:

a) Write down the formula for $\phi_0(x)$, the density of $X|Y{=}0$ and for $\phi_1(x)$, the density of $X|Y{=}1$. Hint: The general formula for a normal distribution can be found here: https://en.wikipedia.org/wiki/Normal_distribution.

b) Write down the expression for the posterior probability $\pi_1(x) = P(Y{=}1|x)$ and simplify as much as possible.

c) Check that the Bayes classifier corresponds to:
classify Y equal to one if and only if $P(Y{=}1|x) > P(Y{=}0|x)$.

d) Use your answer from part (b) to write $P(Y{=}1|x) > P(Y{=}0|x)$ as an inequality in terms of x. Simplify to obtain the inequality

$$\exp\left\{-\frac{1}{2}(x-5)^2\right\} > \exp\left\{-\frac{1}{2}(x-4)^2\right\}.$$

e) Taking the logarithm of this inequality, show that the Bayes Classifier simplifies to: classify Y equal to one if and only if $x > 4.5$.

Solution:

a) $$\phi_0(x) = \frac{1}{\sqrt{2\pi}} \exp\left\{-\tfrac{1}{2}(x-4)^2\right\}$$
$$\phi_1(x) = \frac{1}{\sqrt{2\pi}} \exp\left\{-\tfrac{1}{2}(x-5)^2\right\}$$

b)
$$\pi_1(x) = P(Y{=}1|x) = \frac{\frac{1}{\sqrt{2\pi}} \exp\left\{-\frac{1}{2}(x-5)^2\right\} \cdot 0.5}{\frac{1}{\sqrt{2\pi}} \exp\left\{-\frac{1}{2}(x-5)^2\right\} \cdot 0.5 + \frac{1}{\sqrt{2\pi}} \exp\left\{-\frac{1}{2}(x-4)^2\right\} \cdot 0.5}$$
$$= \frac{\exp\left\{-\frac{1}{2}(x-5)^2\right\}}{\exp\left\{-\frac{1}{2}(x-5)^2\right\} + \exp\left\{-\frac{1}{2}(x-4)^2\right\}}$$

c) This follows directly from the definition of a Bayes classifier, “choose the class which maximises the posterior prob” $\Rightarrow$:

- Choose $Y = 1$ if $P(Y{=}1|x) > P(Y{=}0|x)$,
- choose $Y = 0$ if $P(Y{=}0|x) > P(Y{=}1|x)$

d)
$$P(Y{=}1|x) > P(Y{=}0|x)$$
$$\frac{\exp\left\{-\frac{1}{2}(x-5)^2\right\}}{\exp\left\{-\frac{1}{2}(x-5)^2\right\} + \exp\left\{-\frac{1}{2}(x-4)^2\right\}} > \frac{\exp\left\{-\frac{1}{2}(x-4)^2\right\}}{\exp\left\{-\frac{1}{2}(x-5)^2\right\} + \exp\left\{-\frac{1}{2}(x-4)^2\right\}}$$

Multiply both sides by the common denominator, which is positive, to give:

$$\exp\left\{-\frac{1}{2}(x-5)^2\right\} > \exp\left\{-\frac{1}{2}(x-4)^2\right\}$$

e) Taking logs:

$$-\frac{1}{2}(x-5)^2 > -\frac{1}{2}(x-4)^2$$

Multiplying by $-\frac{1}{2}$ means the inequality flips direction:

$$(x-5)^2 < (x-4)^2$$
$$x^2 - 10x + 25 < x^2 - 8x + 16$$
$$9 < 2x$$
$$x > 4.5$$

2.2 Posterior function in R

Use your answer from Exercise 1 Part (b) to write an R function called `posterior` to compute the posterior probability of $P(Y=1|x)$.

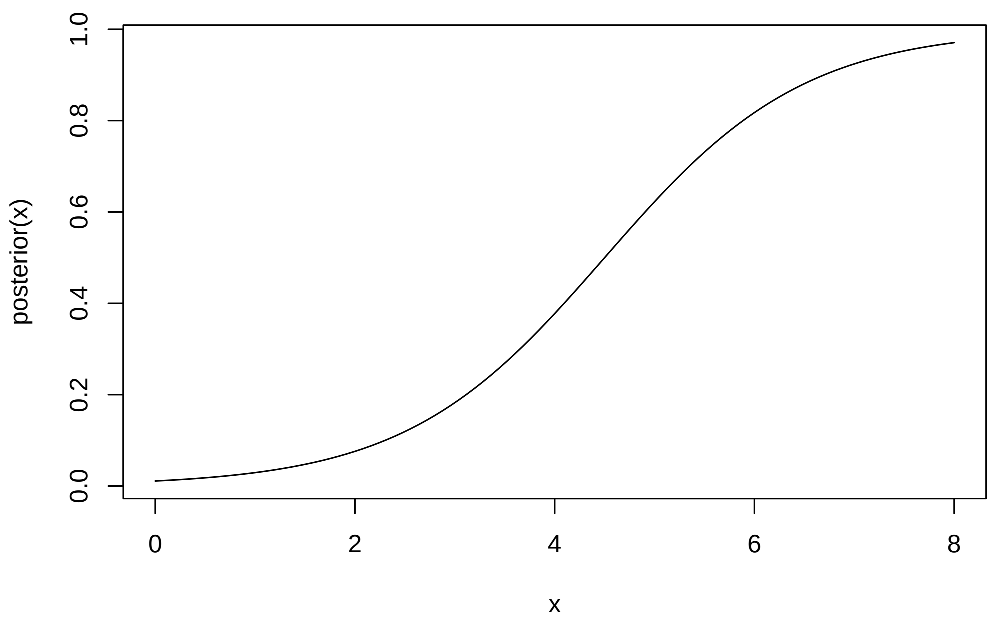
You will start by assuming the same model as in Ex 1, and then generalise it to general π_0, μ_0, μ_1 and σ.

a) You can use the function `dnorm(x, mean =, sd = )` to compute the density of a normal distribution. `x` should be an argument to the function `posterior` so your function should use the following template:

```
posterior <- function(x, pi0 = 0.5, mu0 = 4, mu1 = 5,  sigma = 1){
  (dnorm(x, mean = mu1, sd = sigma)) * (1 - pi0) /
    (dnorm(x, mean = mu1, sd = sigma) * (1 - pi0) +
       dnorm(x, mean = mu0, sd = sigma) * pi0)
}
```

b) Plot the function using the R function `curve()` for x values from 0 to 8 so that you obtain

```
curve(posterior, from = 0, to = 8)
```



In Exercise 1 you showed that the most-likely-outcome changes at the point $x=4.5$.

c) Use `posterior(4.5)` to find the posterior probability at $x=4.5$. Why is this result "obvious"?

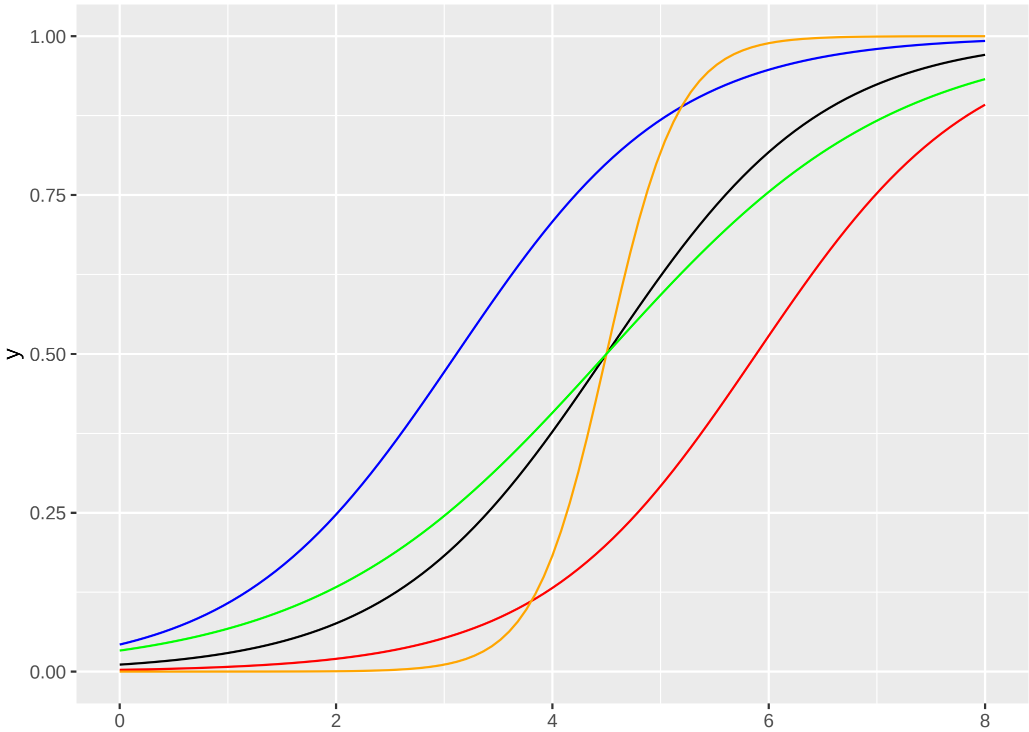
```
posterior(4.5)  # 4.5 is exactly in the middle of the two expection values
```

d) Now adapt you function `posterior` to accept the following *function arguments* with the given default values.

- `pi0` is the prior probability $P(Y=1)$ with default value 0.5
- `mu0` and `mu1` are the respective means for class 0 and class 1 with default values 4 and 5.
- `sigma` the variance (in both classes) with default value 1.

e) Check that your function gives sensible results by plotting the function with different argument values. If you want to use `ggplot2::ggplot()` instead of base R graphics use the following code:

```r
library(ggplot2)
ggplot() +
  geom_function(fun = posterior, col = "black") +
  geom_function(fun = posterior,
                args = list(pi0 = 0.8), col = "red") +
  geom_function(fun = posterior,
                args = list(pi0 = 0.2), col = "blue") +
  geom_function(fun = posterior,
                args = list(mu0 = 3, mu1 = 6), col = "orange") +
  geom_function(fun = posterior,
                args = list(mu0 = 3, mu1 = 6, sigma = 2), col = "green") +
  scale_x_continuous(limits = c(0, 8))
```



2.3 LDA and QDA with the Diabetes Data

In this exercise we will work again with the `Diabetes` data set applied to classification by logistic regression. This week you will use linear and quadratic discriminant analysis. You will use the functions `lda` and `qda` from the `MASS` package.

a) Preparations:

- Download the `Diabetes` dataset from Moodle and the R code template `Classification_Diabetes.R` you used last week.
- Use the template to split the data into the *exactly same* training and test data sets as last time.
- Delete all the code beginning with section `# 03b: model training ----` and save the R file with a new file name, e.g. `Classification_Diabetes_LDA_QDA.R`.

b) Instead of applying logistic regression to classify the data you will use LDA and QDA. For using an LDA model with only one variable, e.g. `Age` use the following code:

```
library(MASS)
lda.fit1 <- lda(YN ~ Age, data = train)
```

To assess the classification quality use

```
library(pROC)
pr1test <- predict(lda.fit1, newdata=test)
roc.obj1 <- roc(test$YN, pr1test$posterior[, 2])
ggroc(roc.obj1)
auc(roc.obj1)
```

c) Adapt the code to fit the following discriminant models, each time plotting the ROC curve and the obtaining the AUC.

- LDA model using `BMI`
- LDA model using `Age` and `BMI`
- QDA model using `Age` and `BMI`

d) Which model gives the best AUC on the test data? Compare the LDA/QDA model results also with last weeks logistic regression model using `Age` and `BMI`.

The given code in this exercise should be enough for you to fit the LDA and QDA models, but further help can be found in Labs 4.7.3 & 4.7.4 in James et. al.