Compulsory Exercise 1 - Solutions

TMA4268 Statistical Learning V2025

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R packages

You need to install the following packages in R to run the code in this file.

```
install.packages("knitr")
install.packages("rmarkdown")
install.packages("ggplot2")
install.packages("ggfortify")
install.packages("MASS")
install.packages("dplyr")
```

Problem 1 - 10P

We have a univariate continuous random variable Y and a covariate x. Further, we have observed a training set of independent observation pairs $\{x_i, y_i\}$ for $i = 1, \ldots, n$. Assume a regression model

$$Y_i = f(x_i) + \varepsilon_i \ ,$$

where f is the true regression function, and ε_i is an unobserved random variable with mean zero and constant variance σ^2 (not dependent on the covariate). Using the training set we can find an estimate of the regression function f, and we denote this estimate by $\hat{f}$. We want to use $\hat{f}$ to make a prediction for an independent new observation (not included in the training set) at a covariate value x_0. The predicted response value is then $\hat{f}(x_0)$. We are interested in the error associated with this prediction.

a) (1P)

Write down the definition of the expected test mean squared error (MSE) at x_0.

Solution:

The *expected test mean squared error (MSE) at* x_0 is defined as:

$$\mathrm{E}\left[Y - \hat{f}\left(x_0\right)\right]^2$$

b) (2P)

Derive the decomposition of the expected test MSE into three terms.

Solution:

Useful rule: $\mathrm{Var}[Y] = \mathrm{E}[Y^2] - \mathrm{E}[Y]^2$.

Use that $y_0 = f(x_0) + \varepsilon$:

$$\begin{aligned}\mathrm{E}[y_0 - \hat{f}(x_0)]^2 &= \mathrm{E}[f(x_0) + \varepsilon - \hat{f}(x_0)]^2 \\ &= \mathrm{E}[f(x_0)^2] + \mathrm{E}[\varepsilon^2] + \mathrm{E}[\hat{f}(x_0)^2] - 2\mathrm{E}[f(x_0)\hat{f}(x_0)] - \underbrace{2\mathrm{E}[\varepsilon \hat{f}(x_0)]}_{=0} + \underbrace{2\mathrm{E}[\varepsilon f(x_0)]}_{=0},\end{aligned}$$

where the last two terms are zero due to the independence of ϵ, and $\mathrm{E}[\varepsilon] = 0$. Using that $\mathrm{E}[\hat{f}(x_0)^2] = \mathrm{Var}[\hat{f}(x_0)^2] + \mathrm{E}[\hat{f}(x_0)]^2$, $\mathrm{E}[f(x_0)^2] = f(x_0)^2$ and $\mathrm{E}[\varepsilon^2] = \mathrm{Var}[\varepsilon]$, we get

$$\begin{aligned}&= f(x_0)^2 + \mathrm{Var}[\varepsilon] + \mathrm{Var}[\hat{f}(x_0)] + \mathrm{E}[\hat{f}(x_0)]^2 - 2f(x_0)\mathrm{E}[\hat{f}(x_0)] \\ &= \mathrm{Var}[\varepsilon] + \mathrm{Var}[\hat{f}(x_0)] + [\mathrm{Bias}(\hat{f}(x_0))]^2,\end{aligned}$$

where the last equation just rearranges the terms and uses the definition $[\mathrm{Bias}(\hat{f}(x_0))]^2 = (f(x_0) - \mathrm{E}[\hat{f}(x_0)])^2$.

c) (1P)

Explain with words how we can interpret the three terms.

Solution:

$$\mathrm{E}[(Y - \hat{f}(x_0))^2] = \mathrm{Var}(\varepsilon) + \mathrm{Var}[\hat{f}(x_0)] + [\mathrm{Bias}(\hat{f}(x_0))]^2$$

- First term: irreducible error, σ^2 and is always present unless we have measurements without error. This term cannot be reduced regardless how well our statistical model fits the data.

- Second term: variance of the prediction at x_0 or the expected deviation around the mean at x_0. If the variance is high, different training data sets would give very varying predictions at x_0.
- Third term: squared bias. The bias gives an estimate of how much the prediction differs from the true mean $f(x_0)$. If the bias is low at x_0 the model gives predictions which on average are close to the true value at x_0.

d) (2P) - Multiple choice

Which of the following statements are true and which are false? Say for **each** of them whether it is true or false.

(i) The bias-variance tradeoff is more relevant in inference than in prediction.
(ii) As the sample size n increases, the expected test MSE will approach zero.
(iii) Given two methods for estimating f, we get the best predictions from the one with the lowest squared bias.
(iv) If σ^2 is very large, we need a very flexible method to estimate f reliably.

List of answers:

Solution:

FALSE, FALSE, FALSE, FALSE

(i) FALSE: The bias-variance is more relevant in prediction - in inference we are interested in finding the true relationships between the response and the predictors, not minimizing test set MSE.
(ii) FALSE: The expected test MSE will not go to zero, as the irreducible error will not go down regardless of the sample size.
(iii) FALSE: This will depend on the variance of the two methods - a method with higher bias can potentially give better predictions if its variance is lower.
(iv) FALSE: How flexible the model should be depends on the bias and variance, not on the irreducible error.

e) (2P) - Multiple choice

Figure 1 shows an example of squared bias, variance, irreducible error and total error in a validation set for increasing values of K in a K nearest neighbor (KNN) regression prediction model. Which of the following statements are true and which are false? Say for **each** of them if it is true or false.

(i) As K decreases, the flexibility of the model increases.
(ii) The squared bias always contributes the most to the total error.
(iii) We have enough information to decide on a value of K to use in the KNN model.
(iv) For the plotted range of values of K, overfitting would be preferable to underfitting in this scenario, if we had to choose.

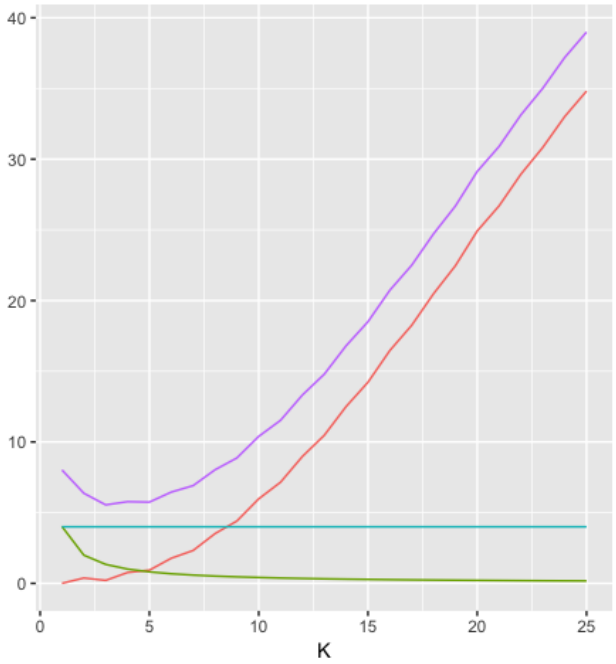


Figure 1: Squared bias (red), variance (green), irreducible error (light blue) and total error (lila) for increasing values of K in KNN.

List of answers:

Solution:

TRUE, FALSE, TRUE, TRUE

Explanation: (i) TRUE: A low K means the model relies on a smaller set of points to make predictions, so the model is more flexible. (ii) FALSE: The squared bias (orange line) is not always higher than the variance (green line) and irreducible error (blue line), so this is not true in (iii) TRUE: We can see from the plot that the total error (purple line) is lowest for $K = 3$, so this is the best choice. (iv) TRUE: The total error (purple line) is lower for very low K (overfitting) than for very high K (underfitting), so in this scenario the overfitting is preferable to underfitting.

f) (1P) - Single choice

$\mathbf{X}$ is a 2-dimensional random vector with covariance matrix

$$\mathbf{\Sigma} = \begin{bmatrix} 9 & 0.3 \\ 0.3 & 4 \end{bmatrix}$$

The correlation between the two elements of $\mathbf{X}$ is: (i) 0.05 (ii) 0.15 (iii) 0.0083 (iv) 0.60 (v) 0.10

Answer:

Solution (i): $\frac{0.3}{\sqrt{9 \cdot 4}} = 0.05$

g) (1P) - Single choice

Which of the plots (A-D) in Figure 2 corresponds to the following covariance matrix?

$$\mathbf{\Sigma} = \begin{bmatrix} 1 & 0.2 \\ 0.2 & 4 \end{bmatrix}$$

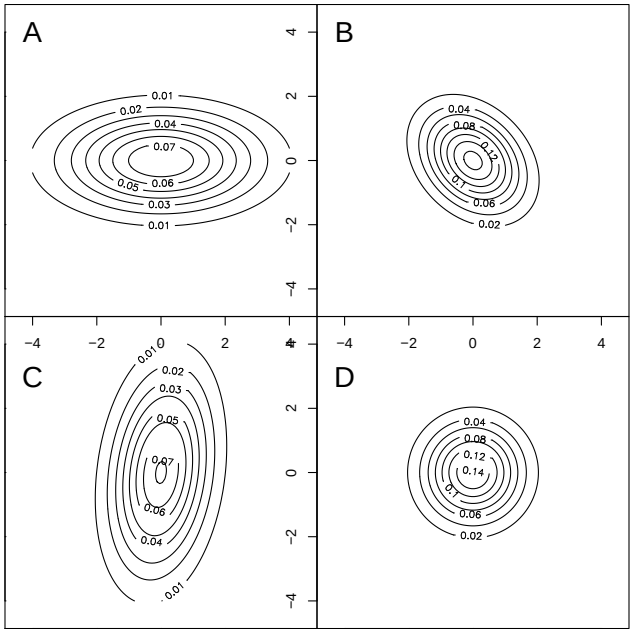


Figure 2: Contour plots

Solution: C

Problem 2 - 15P

We consider a linear regression problem. A group of biologists in Switzerland studied badgers, which mainly eat earthworms. In the badger's excrement one can find a non-digestible part of the earthworm (the muscular stomach). To find out how much energy a badger absorbed by eating earthworms, the biologists wanted to investigate the relationship between the circumference of the muscular stomach and the weight of the earthworm that the badger ate. Therefore, they collected a sample of earthworms, and for each worm the they measured its weight and the circumference of its muscular stomach.

The earthworm dataset can be loaded as follows:

```
id <- "1nLen1ckdnX4P9n8ShZeU7zbXpLc7qiwt"  # google file ID
d.worm <- read.csv(sprintf("https://docs.google.com/uc?id=%s&export=download", id))
```

Look at the data by using both `head(d.worm)` and `str(d.worm)`. The dataset contains the following variables:

- `Gattung`: The genus of the earthworm (L=Lumbricus; N=Nicodrilus; Oc=Octolasion)
- `Nummer`: A worm-specific ID

- `GEWICHT`: The weight of the earthworm
- `FANGDATUM`: The date when the sample was collected
- `MAGENUMF`: The circumference of the earthworm's muscular stomach

a) (2P)

What is the dimension of the dataset (number of rows and columns)? Which of the variables are qualitative, which are quantitative?

Solution:

```
id <- "1nLen1ckdnX4P9n8ShZeU7zbXpLc7qiwt"  # google file ID
d.worm <- read.csv(sprintf("https://docs.google.com/uc?id=%s&export=download", id))
head(d.worm)
```

```
##   Gattung Nummer GEWICHT FANGDATUM MAGENUMF
## 1      Oc     32    0.19  23.09.97     1.56
## 2      Oc     34    0.59  23.09.97     1.63
## 3      Oc     48    0.09  23.09.97     1.69
## 4      Oc     55    0.23  23.09.97     1.69
## 5      Oc     41    0.24  23.09.97     1.75
## 6      Oc     24    0.19  23.09.97     1.81
```

```
str(d.worm)
```

```
## 'data.frame':    143 obs. of  5 variables:
##  $ Gattung  : chr  "Oc" "Oc" "Oc" "Oc" ...
##  $ Nummer   : int  32 34 48 55 41 24 39 35 45 27 ...
##  $ GEWICHT  : num  0.19 0.59 0.09 0.23 0.24 0.19 0.26 0.19 0.15 0.34 ...
##  $ FANGDATUM: chr  "23.09.97" "23.09.97" "23.09.97" "23.09.97" ...
##  $ MAGENUMF : num  1.56 1.63 1.69 1.69 1.75 1.81 1.81 1.88 2 2.13 ...
```

The dimension of the dataset is 143 times 5. `Gattung` and `FANGDATUM` are encoded as factor variables, and these are categorical (qualitative). The `Nummer` (ID) is encoded as an integer, but it is actually also a qualitative variable. `Gewicht` and `Magenumf` are quantitative (one could argue that the date is also quantitative, so this is not counted as wrong here).

b) (2P)

An important step before fitting an exploratory model is to look at the data to understand if the modelling assumptions are reasonable. In a linear regression setup, it is for example recommended to look at the relation between the variables to see if the linearity assumption makes sense. If this is not the case, one can try to transform the variables.

Make a scatterplot of `GEWICHT` (weight) against `MAGENUMF` (circumference of stomach), where you color the points according to the three genus (variable `Gattung`).

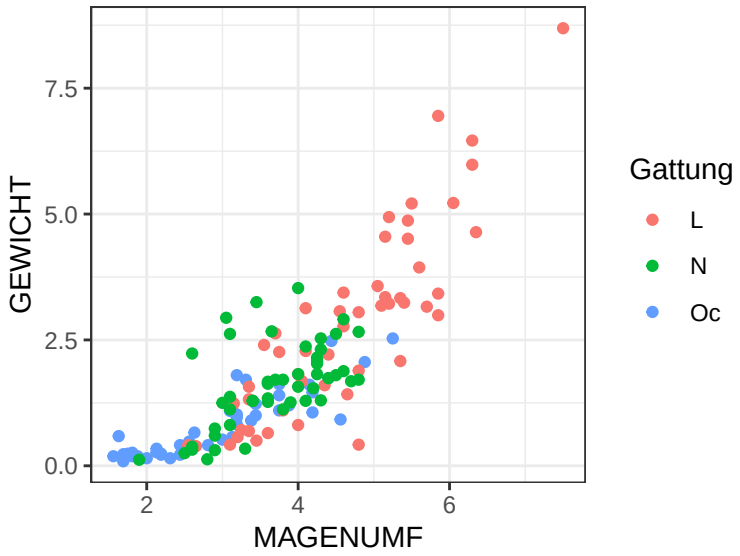
Does this relationship look linear? If not, try out some transformations of `GEWICHT` and `MAGENUMF` until you are happy.

R-hint:

```
# Replace the '...'
ggplot(d.worm, aes(x = ..., y = ..., colour = ...)) + geom_point() + theme_bw()
```

Solution:

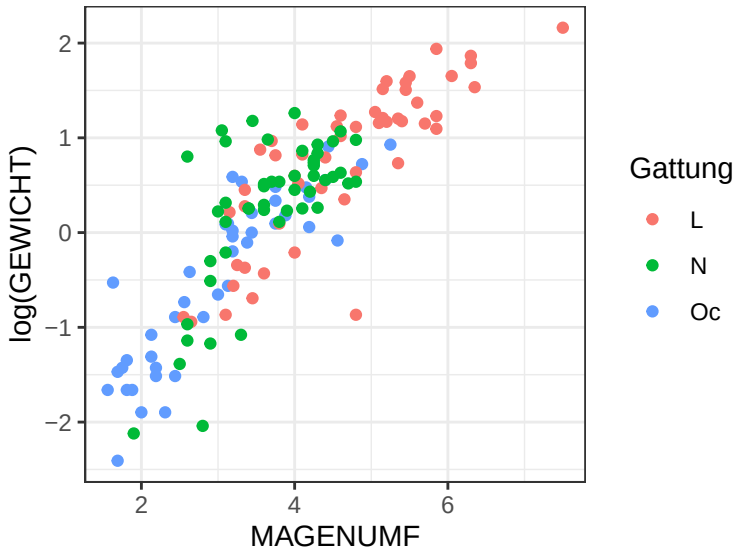
```
library(ggplot2)
ggplot(d.worm, aes(x = MAGENUMF, y = GEWICHT, colour = Gattung)) + geom_point() +
    theme_bw()
```



We see that the relation between weight and the stomach circumference is not linear. So it is a good idea to look for some transformations.

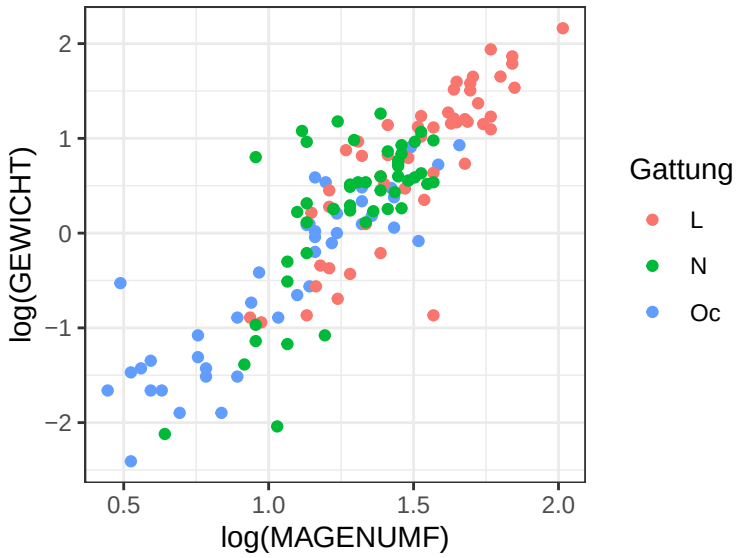
Given that the relation looks somewhat exponential, a reasonable starting point is to use a log-transformation for the response variable and then continue like this for the rest of the exercise:

```
ggplot(d.worm, aes(x = MAGENUMF, y = log(GEWICHT), colour = Gattung)) + geom_point() +
    theme_bw()
```



However, it seems also good (or even better?) to also use the log of `MAGENUMF`:

```
ggplot(d.worm, aes(x = log(MAGENUMF), y = log(GEWICHT), colour = Gattung)) + geom_point() +
    theme_bw()
```



Other solutions are possible. You can continue with the solution you find here, given that it in fact renders the relation (reasonably) linear.

c) (3P)

Fit a regression model for an earthworm's weight (`GEWICHT`) given the circumference of its muscular stomach (`MAGENUMF`) and the genus (`Gattung`). **Use the transformed version of the variable(s) from b)**. Use only linear terms that you combine with `+` (no interactions) (1P). After fitting the models, write down the model equations with the estimated parameters for the three genus as three separate equations (1P). Is `Gattung` a relevant predictor? (1P)

R-hints : `lm()`, `summary()`, `anova()`

Solution: (Students that use another transformation are given the full points here if they otherwise solve the question right.)

```
r.worm <- lm(log(GEWICHT) ~ MAGENUMF + Gattung, data = d.worm)
summary(r.worm)
```

```
##
## Call:
## lm(formula = log(GEWICHT) ~ MAGENUMF + Gattung, data = d.worm)
##
## Residuals:
##      Min       1Q   Median       3Q      Max
## -1.74894 -0.27575  0.02197  0.28513  1.30867
##
## Coefficients:
##             Estimate Std. Error t value Pr(>|t|)
## (Intercept) -2.53555    0.22147 -11.449   <2e-16 ***
## MAGENUMF     0.71187    0.04529  15.719   <2e-16 ***
## GattungN     0.17801    0.11009   1.617    0.108
## GattungOc   -0.09073    0.12791  -0.709    0.479
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 0.5059 on 139 degrees of freedom
```

```
## Multiple R-squared:  0.7367, Adjusted R-squared:  0.731
## F-statistic: 129.6 on 3 and 139 DF,  p-value: < 2.2e-16
```

```
anova(r.worm)
```

```
## Analysis of Variance Table
##
## Response: log(GEWICHT)
##            Df Sum Sq Mean Sq  F value  Pr(>F)
## MAGENUMF    1 97.802  97.802 382.0947 < 2e-16 ***
## Gattung     2  1.725   0.862   3.3691 0.03725 *
## Residuals 139 35.579   0.256
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

The anova table shows some evidence that `Gattung` could impact the weight, that is, the intercept is dependent on the genus ($p = 0.037$). Note, however, that other transformations may lead to somewhat different conclusions. The three separate models are given as

- Lumbricus: $\log(weight)_i$ = -2.54 + -0.09 ·MAGENUMF$_i + \varepsilon_i$
- Nicodrilus: $\log(weight)_i$ = -2.54 + 0.71 + -0.09 ·MAGENUMF$_i + \varepsilon_i$
- Octolasion: $\log(weight)_i$ = -2.54 + 0.18 + -0.09 ·MAGENUMF$_i + \varepsilon_i$

So the three models differ in their intercept value. However, we enforce the slope for `GEWICHT` (weight) to be the same for all three genus.

d) (2P)

In question c) it was assumed that there is no interaction between the genus and `MAGENUMF` to predict the weight of a worm. Test whether an interaction term would be relevant by fitting an appropriate model.

Solution:

```
r.worm2 <- lm(log(GEWICHT) ~ MAGENUMF * Gattung, data = d.worm)
anova(r.worm2)
```

```
## Analysis of Variance Table
##
## Response: log(GEWICHT)
##                    Df Sum Sq Mean Sq  F value  Pr(>F)
## MAGENUMF            1 97.802  97.802 386.5547 < 2e-16 ***
## Gattung             2  1.725   0.862   3.4084 0.03592 *
## MAGENUMF:Gattung    2  0.917   0.458   1.8112 0.16735
## Residuals         137 34.662   0.253
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

The p-value for the interaction term is not very small ($p = 0.167$), so there is no evidence that we need it. Although remember that a large p-value does not mean that the effect does not exist (we cannot prove the null hypothesis) - the only thing we can say is that we cannot reject it.

e) (2P)

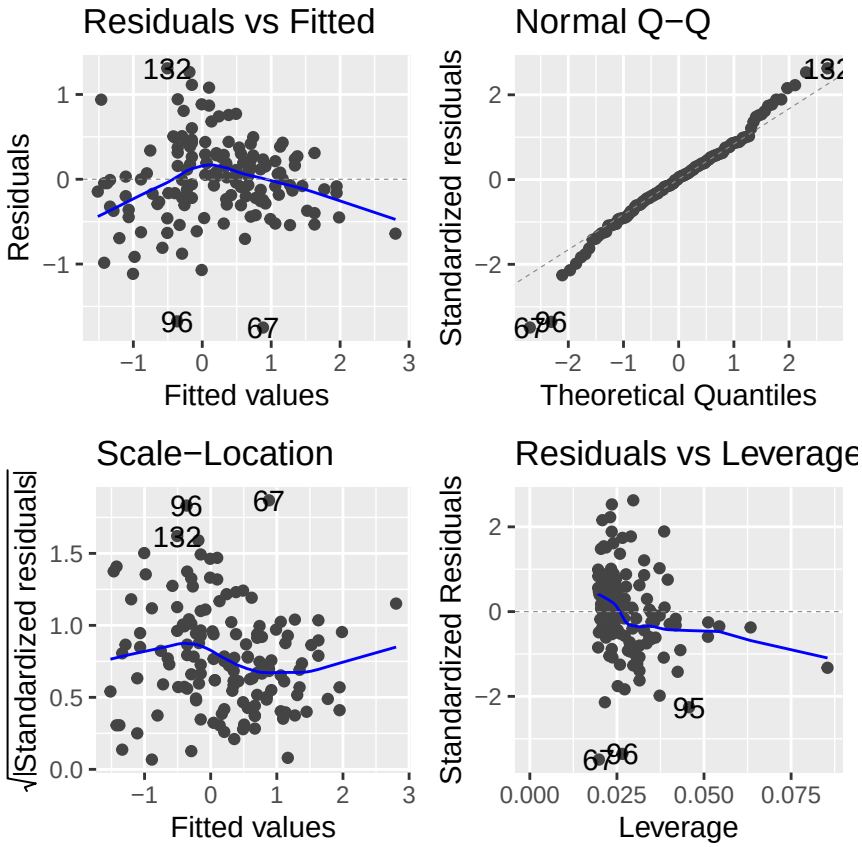
Perform a residual analysis using the `autoplot()` function from the `ggfortify` package. Use the model without interaction term.

- Do you think the assumptions are fulfilled? Explain why or why not.

- Compare to the residual plot that you would obtain when you would not use any variable transformations to fit the regression model.

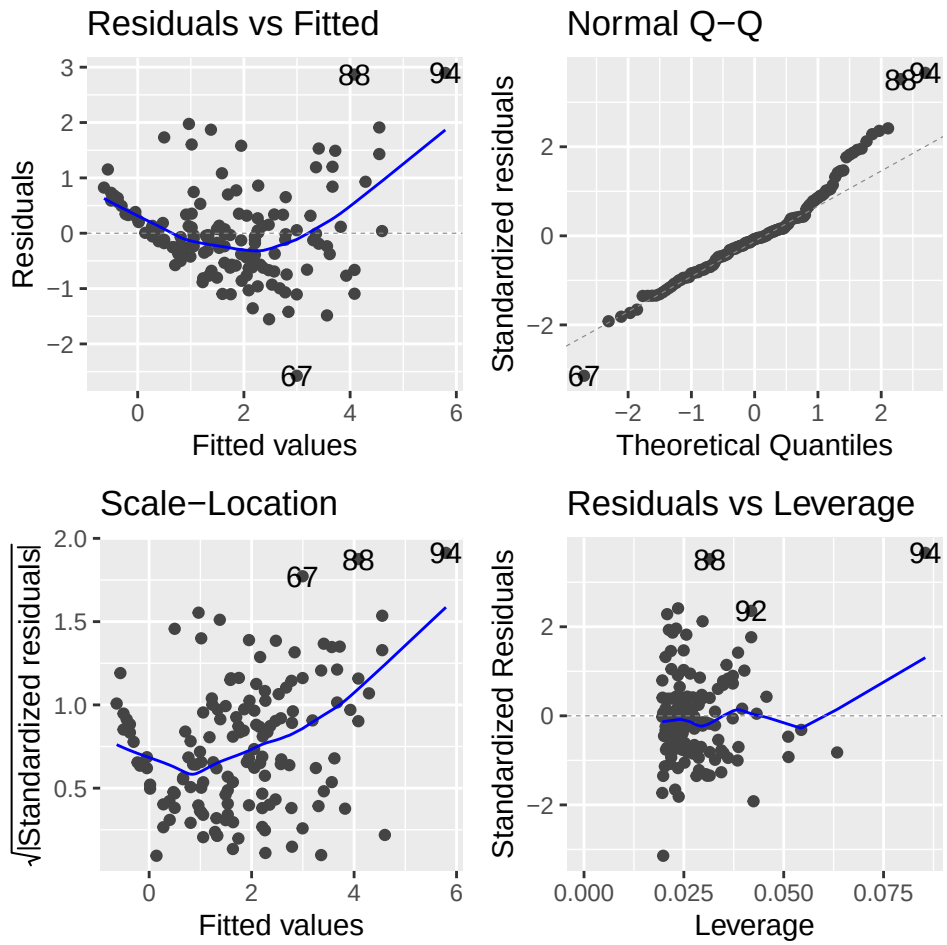
Solution: In the residual plot below we see that the assumptions seem more or less OK, although there is some kind of pattern in the Tukey-Anscombe plot (upper left). Perhaps it would be wise to continue looking for better transformations.

```
library(ggfortify)
autoplot(r.worm)
```



If we would use untransformed variables, we would see some pattern in the residuals. In particular the Tukey-Anscombe plot shows a clear curvature:

```
r.worm3 <- lm(GEWICHT ~ Gattung + MAGENUMF, data = d.worm)
autoplot(r.worm3)
```



f) (2P)

- Why is it important that we carry out a residual analysis, i.e., what happens if our assumptions are not fulfilled?
- Mention at least one thing that you could do with your data / model in case of violated assumptions.

Solution:

- To check assumptions that we put into the model. If these are violated, we may draw invalid conclusions. This is particularly problematic if we want to do inference.
- Ideas are: Use another model, transform variables, be careful with your conclusions, check if there are outliers, ...

g) (2P) - Multiple choice

Given a null hypothesis (H_0), an alternative hypothesis (H_1) and an observed result with an associated p-value (think, for example, of the case where H_0 is that a slope parameter in a regression model is $\beta = 0$), which of the following statements are true and which are false? Say for **each** of them if it is true or false.

(i) The $1 - p$ is the probability that H_0 is true.
(ii) If the p-value is higher than 0.05, then H_1 is not true.
(iii) p is the probability to observe a data summary under the null hypothesis (H_0) that is at least as extreme as the one observed.
(iv) The p-value tells you the probability that the results happened by random chance.

List of answers:

Solution:

FALSE - FALSE - TRUE - FALSE

Problem 3 - 16P

In this problem, we will use a dataset from the Wimbledon tennis tournament for Women in 2013. We will predict the result for player 1 (coded as win=1 or lose=0), based on the number of aces won by each player and the number of unforced errors committed by each player. The data set is a subset of a data set from https://archive.ics.uci.edu/ml/datasets/Tennis+Major+Tournament+Match+Statistics, see that page for information of the source of the data.

The files can be read using the following code.

```
# read file
id <- "1GNbIhjdhuwPOBr0Qz82JMkdjUVBuSoZd"
tennis <- read.csv(sprintf("https://docs.google.com/uc?id=%s&export=download", id),
    header = TRUE)
```

We will first create a logistic regression model where the probability to win for player 1 has the form

$$P(Y_i = 1|\mathbf{X} = \boldsymbol{x}_i) = p_i = \frac{e^{\beta_0+\beta_1 x_{i1}+\beta_2 x_{i2}+\beta_3 x_{i3}+\beta_4 x_{i4}}}{1 + e^{\beta_0+\beta_1 x_{i1}+\beta_2 x_{i2}+\beta_3 x_{i3}+\beta_4 x_{i4}}} ,$$

where x_{i1} is the number of aces for player 1 in match i, x_{i2} is the number of aces for player 2 in match i, and x_{i3} and x_{i4} are the number of unforced errors commited by player 1 and 2 in match i.

a) (1P)

Use the above expression to show that $\text{logit}(p_i) = \log(\frac{p_i}{1-p_i})$ is a linear function of the covariates.

b) (1P)

The model above has been fitted and gives the following output. Interpret the effect of β_1, i.e. how will one more ace for player 1 affect the result of the tennis match?

```
r.tennis <- glm(Result ~ ACE.1 + ACE.2 + UFE.1 + UFE.2, data = tennis, family = "binomial")
summary(r.tennis)
```

```
##
## Call:
## glm(formula = Result ~ ACE.1 + ACE.2 + UFE.1 + UFE.2, family = "binomial",
##     data = tennis)
##
## Coefficients:
##             Estimate Std. Error z value Pr(>|z|)
## (Intercept) -0.02438    0.59302  -0.041 0.967211
## ACE.1        0.36338    0.10136   3.585 0.000337 ***
## ACE.2       -0.22388    0.07369  -3.038 0.002381 **
## UFE.1       -0.09847    0.02840  -3.467 0.000527 ***
## UFE.2        0.09010    0.02479   3.635 0.000278 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## (Dispersion parameter for binomial family taken to be 1)
##
```

```
##     Null deviance: 163.04  on 117  degrees of freedom
## Residual deviance: 124.96  on 113  degrees of freedom
## AIC: 134.96
##
## Number of Fisher Scoring iterations: 4
```

Solution: a-b

- Let us write $\eta = \beta_0 + \boldsymbol{x_i}^\top \boldsymbol{\beta}$

$$\begin{aligned}\text{logit}(p_i) &= \log(\frac{p_i}{1-p_i}) = \log(\frac{\frac{\exp(\eta)}{1+\exp(\eta)}}{1-\frac{\exp(\eta)}{1+\exp(\eta)}}) = \log(\frac{\frac{\exp(\eta)}{1+\exp(\eta)}}{\frac{1+\exp(\eta)-\exp(\eta)}{1+\exp(\eta)}}) \\ &= \log(\frac{\exp(\eta)}{1}) = \eta \\ &= \eta\end{aligned}$$

- The logit function is the log odds, that is, the log of the probability of success divided by probability of failure. So increasing the number of aces by 1, we see that the odds will increase by

$$\frac{odds(x_1+1)}{odds(x_1)} = \frac{\exp(\beta_0+\beta_1(x_1+1)+\beta_2x_2+\beta_3x_3+\beta_4x_4)}{\exp(\beta_0+\beta_1x_1+\beta_2x_2+\beta_3x_3+\beta_4x_4)} = \exp(\beta_1) = \exp(0.36) = 1.43.$$

This means that for each ace player 1 manages, they will multiplicatively increase their predicted odds of winning by 1.43.

The same interpretation goes for the other coefficients, where the negative coefficients (`ACE.2` and `UFE.1`) gives a reduced odds for player 1 winning, while the positive coefficients gives an increased odds.

c) (4P)

We will now reduce the number of covariates in our model by looking at the difference between aces performed by player 1 and 2 and the difference in unforced errors made by the players. Use the following code to create these variables, and divide the data into a training set and a test set.

```r
# make variables for difference
tennis$ACEdiff <- tennis$ACE.1 - tennis$ACE.2
tennis$UFEdiff <- tennis$UFE.1 - tennis$UFE.2

# divide into test and train set
n <- nrow(tennis)
set.seed(1234)  # to reproduce the same test and train sets each time you run the code
train <- sort(sample(n, size = n/2, replace = FALSE))
tennisTest <- tennis[-train, ]
tennisTrain <- tennis[train, ]
```

- Use these variables to fit a logistic regression model for `Result` with two covariates `ACEdiff` and `UFEdiff`, on your training set.
- Using a 0.5 cutoff as decision rule, we classify an observation with covariates $\boldsymbol{x}$ as "Player 1 wins" if $\hat{P}(Y=1|\boldsymbol{x}) > 0.5$. Write down the formula for the class boundary between the classes (results) using this decision rule. The boundary should be of the form $x_2 = bx_1 + a$.
- Make a plot with the training observations, then add a line that represents the class boundary. Hint: in `ggplot` points are added with `geom_point` and a line with `geom_abline(slope=b, intercept=a)`, where a and b comes from your class boundary.
- Use your fitted model to predict the results for the data in the test set. Make a confusion table using a 0.5 cutoff and calculate the sensitivity and specificity.

Solution:

```
# fit model
r.tennis2 <- glm(Result ~ ACEdiff + UFEdiff, data = tennisTrain, family = "binomial")
summary(r.tennis2)
```

```
##
## Call:
## glm(formula = Result ~ ACEdiff + UFEdiff, family = "binomial",
##     data = tennisTrain)
##
## Coefficients:
##             Estimate Std. Error z value Pr(>|z|)
## (Intercept)  0.28272    0.31175   0.907  0.36447
## ACEdiff      0.22355    0.07959   2.809  0.00497 **
## UFEdiff     -0.08607    0.02832  -3.039  0.00237 **
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## (Dispersion parameter for binomial family taken to be 1)
##
##     Null deviance: 80.959  on 58  degrees of freedom
## Residual deviance: 63.476  on 56  degrees of freedom
## AIC: 69.476
##
## Number of Fisher Scoring iterations: 4
```

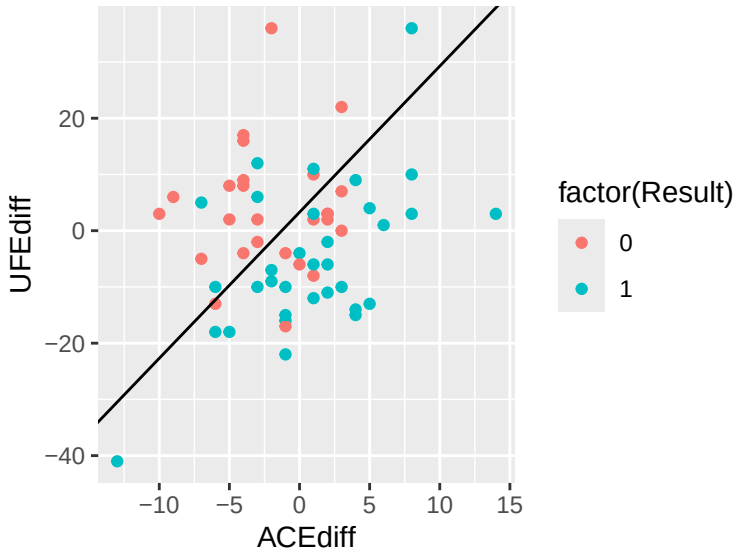
- The decision boundary with decision rule 0.5 are found using the following

$$
\begin{aligned}
\hat{P}(Y=1|X) &= \frac{\exp(\hat{\beta}_0+\hat{\beta}_1x_1+\hat{\beta}_2x_2)}{1+\exp(\hat{\beta}_0+\hat{\beta}_1x_1+\hat{\beta}_2x_2)} = 0.5 \\
\exp(\hat{\beta}_0+\hat{\beta}_1x_1+\hat{\beta}_2x_2) &= 0.5+0.5\exp(\hat{\beta}_0+\hat{\beta}_1x_1+\hat{\beta}_2x_2) \\
(1-0.5)\exp(\hat{\beta}_0+\hat{\beta}_1x_1+\hat{\beta}_2x_2) &= 0.5 \\
\exp(\hat{\beta}_0+\hat{\beta}_1x_1+\hat{\beta}_2x_2) &= 1 \\
\hat{\beta}_0+\hat{\beta}_1x_1+\hat{\beta}_2x_2 &= \log(1) = 0 \\
x_2 &= \frac{-\hat{\beta}_0-\hat{\beta}_1x_1}{\hat{\beta}_2} = \frac{-0.28272-0.22355x_1}{-0.08607} \approx 3.3+2.6x_1
\end{aligned}
$$

- Plot decision boundary and predict test set

```
slopeGLM <- -summary(r.tennis2)$coefficients[2, 1]/summary(r.tennis2)$coefficients[3,
    1]
interceptGLM <- -summary(r.tennis2)$coefficients[1, 1]/summary(r.tennis2)$coefficients[3,
    1]

ggplot(tennisTrain, aes(x = ACEdiff, y = UFEdiff, color = factor(Result))) + geom_point() +
    geom_abline(intercept = interceptGLM, slope = slopeGLM)
```




```
# predict
pred <- predict(r.tennis2, newdata = tennisTest, type = "response")

# confusion table - columns represents predictions
tab <- table(tennisTest$Result, round(pred))
tab
```

```
##
##      0  1
##   0 22  7
##   1  6 24
```

```
# Sens and spes
sens <- tab[2, 2]/(tab[2, 1] + tab[2, 2])
spes <- tab[1, 1]/(tab[1, 1] + tab[1, 2])

c(sens, spes)
```

```
## [1] 0.8000000 0.7586207
```

d) (1P)

Next, we will use LDA and QDA to classify the result using the same covariates (`ACEdiff` and `UFEdiff`) from the tennis data. In linear discriminant analysis with K classes, we assign a class to a new observation based on the posterior probability

$$P(Y = k|\mathbf{X} = \boldsymbol{x}) = \frac{\pi_k f_k(\boldsymbol{x})}{\sum_{l=1}^{K} \pi_l f_l(\boldsymbol{x})},$$

where

$$f_k(\boldsymbol{x}) = \frac{1}{(2\pi)^{p/2}|\boldsymbol{\Sigma}|^{1/2}} e^{-\frac{1}{2}(\boldsymbol{x}-\boldsymbol{\mu_k})^\top \boldsymbol{\Sigma}^{-1}(\boldsymbol{x}-\boldsymbol{\mu_k})}.$$

- Explain what π_k, $\boldsymbol{\mu}_k$, $\boldsymbol{\Sigma}$ and $f_k(x)$ are in a problem with two covariates (no calculations, only explanations).

e) (3P)

In a two class problem ($K = 2$) the decision boundary for LDA between class 0 and class 1 is where x satisfies

$$P(Y = 0|\mathbf{X} = \boldsymbol{x}) = P(Y = 1|\mathbf{X} = \boldsymbol{x}).$$

- (1P) Show that we can express this as
$$\delta_0(\boldsymbol{x}) = \delta_1(\boldsymbol{x}),$$
where
$$\delta_k(\boldsymbol{x}) = \boldsymbol{x}^\top \boldsymbol{\Sigma}^{-1}\boldsymbol{\mu}_k - \frac{1}{2}\boldsymbol{\mu}_k^\top \boldsymbol{\Sigma}^{-1}\boldsymbol{\mu}_k + \log \pi_k; \quad k \in \{0, 1\}.$$
- (1P) We use the rule to classify an observation with covariates $\boldsymbol{x}$ to class 1 if $\hat{P}(Y = 1 \mid \boldsymbol{x}) > 0.5$. Write down the formula for the class boundary. Hint: formulate it as $ax_1 + bx_2 + c = 0$ and solve for x_2. Use `R` for the calculations.
- (1P) Make a plot with the training observations and the class boundary. Add the test observations to the plot (different markings). Hint: in `ggplot` points are added with `geom_points` and a line with `geom_abline(slope=b, intercept=a)` where a and b comes from your class boundary.

f) (3P)

- (1P) Perform LDA on the training data (using the `lda()` function in `R`).
- (1P) Use your model to classify the results of the test set. Make the confusion table for the test set when using 0.5 as cut-off.
- (1P) Calculate the sensitivity and specificity on the test set.

Solution: d-f

- Here π_k is the prior probability that a randomly chosen observation comes from the kth class. We assume that the observations of class k comes from a multivariate normal distribution $f_k(x)$, where μ_k is the mean for the kth class and $\boldsymbol{\Sigma}$ is the variance.
- Showing that $P(Y = 0|\mathbf{X} = \mathbf{x}) = P(Y = 1|\mathbf{X} = \mathbf{x})$ can be expressed as $\delta_0(\boldsymbol{x}) = \delta_1(\boldsymbol{x})$.

$$\begin{aligned}
\frac{\pi_0 f_0(x)}{\pi_0 f_0(x) + \pi_1 f_1(x)} &= \frac{\pi_1 f_1(x)}{\pi_0 f_0(x) + \pi_1 f_1(x)} \\
\pi_0 f_0(x) &= p_1 f_1(x) \\
\pi_0 \frac{1}{(2\pi)^{p/2}|\boldsymbol{\Sigma}|^{1/2}} \exp(-\frac{1}{2}(\boldsymbol{x} - \boldsymbol{\mu_0})^\top \boldsymbol{\Sigma}^{-1}(\boldsymbol{x} - \boldsymbol{\mu_0})) &= \pi_1 \frac{1}{(2\pi)^{p/2}|\boldsymbol{\Sigma}|^{1/2}} \exp(-\frac{1}{2}(\boldsymbol{x} - \boldsymbol{\mu_1})^\top \boldsymbol{\Sigma}^{-1}(\boldsymbol{x} - \boldsymbol{\mu_1})) \\
\log(\pi_0) - \frac{1}{2}(\boldsymbol{x} - \boldsymbol{\mu_0})^\top \boldsymbol{\Sigma}^{-1}(\boldsymbol{x} - \boldsymbol{\mu_0}) &= \log(\pi_1) - \frac{1}{2}(\boldsymbol{x} - \boldsymbol{\mu_1})^\top \boldsymbol{\Sigma}^{-1}(\boldsymbol{x} - \boldsymbol{\mu_1}) \\
\log(\pi_0) - \frac{1}{2}\boldsymbol{x}^\top \boldsymbol{\Sigma}^{-1}\boldsymbol{x} + \boldsymbol{x}^\top \boldsymbol{\Sigma}^{-1}\boldsymbol{\mu_0} - \frac{1}{2}\boldsymbol{\mu_0}^\top \boldsymbol{\Sigma}^{-1}\boldsymbol{\mu_0} &= \log(\pi_1) - \frac{1}{2}\boldsymbol{x}^\top \boldsymbol{\Sigma}^{-1}\boldsymbol{x} + \boldsymbol{x}^\top \boldsymbol{\Sigma}^{-1}\boldsymbol{\mu_1} - \frac{1}{2}\boldsymbol{\mu_1}^\top \boldsymbol{\Sigma}^{-1}\boldsymbol{\mu_1} \\
\delta_0(\boldsymbol{x}) &= \delta_1(\boldsymbol{x})
\end{aligned}$$

- LDA on training set

```
library(MASS)
ldaMod <- lda(Result ~ ACEdiff + UFEdiff, data = tennisTrain)
```

- Class boundary and plot

$$\delta_0(\boldsymbol{x}) - \delta_1(\boldsymbol{x}) = 0$$
$$\log(\pi_0) - \frac{1}{2}\boldsymbol{x}^\top\boldsymbol{\Sigma}^{-1}\boldsymbol{x} + \boldsymbol{x}^\top\boldsymbol{\Sigma}^{-1}\boldsymbol{\mu_0} - \frac{1}{2}\boldsymbol{\mu_0}^\top\boldsymbol{\Sigma}^{-1}\boldsymbol{\mu_0} - \log(\pi_1) + \frac{1}{2}\boldsymbol{x}^\top\boldsymbol{\Sigma}^{-1}\boldsymbol{x} - \boldsymbol{x}^\top\boldsymbol{\Sigma}^{-1}\boldsymbol{\mu_1} + \frac{1}{2}\boldsymbol{\mu_1}^\top\boldsymbol{\Sigma}^{-1}\boldsymbol{\mu_1} = 0$$
$$\log(\pi_0) + \boldsymbol{x}^\top\boldsymbol{\Sigma}^{-1}\boldsymbol{\mu_0} - \frac{1}{2}\boldsymbol{\mu_0}^\top\boldsymbol{\Sigma}^{-1}\boldsymbol{\mu_0} - \log(\pi_1) - \boldsymbol{x}^\top\boldsymbol{\Sigma}^{-1}\boldsymbol{\mu_1} + \frac{1}{2}\boldsymbol{\mu_1}^\top\boldsymbol{\Sigma}^{-1}\boldsymbol{\mu_1} = 0$$
$$\boldsymbol{x}^\top\boldsymbol{\Sigma}^{-1}(\boldsymbol{\mu_0} - \boldsymbol{\mu_1}) - \frac{1}{2}\boldsymbol{\mu_0}^\top\boldsymbol{\Sigma}^{-1}\boldsymbol{\mu_0} + \frac{1}{2}\boldsymbol{\mu_1}^\top\boldsymbol{\Sigma}^{-1}\boldsymbol{\mu_1} + \log(\frac{\pi_0}{\pi_1}) = 0$$
$$ax_1 + bx_2 + c = 0$$
$$x_2 = -c/b - a/bx_1$$

where c is all terms not involving $\boldsymbol{x}$, and a and b are found from solving $\boldsymbol{x}^\top\boldsymbol{\Sigma}^{-1}(\boldsymbol{\mu_0} - \boldsymbol{\mu_1})$.

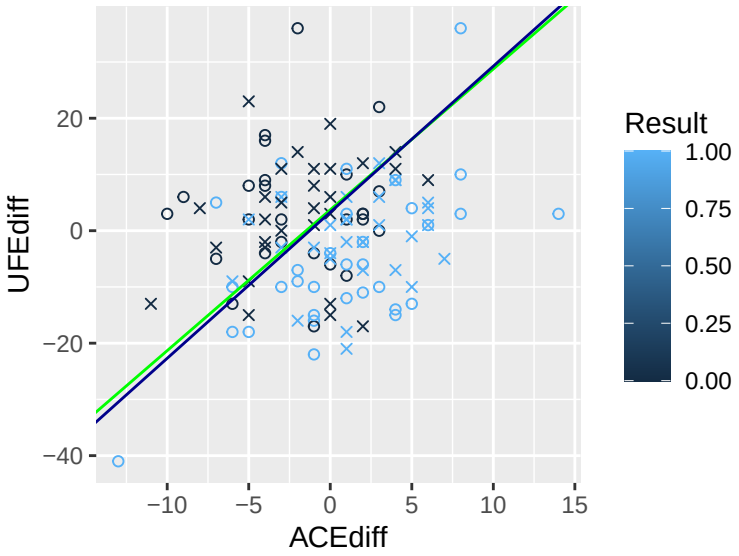
```
pi0 <- ldaMod$prior[1]
pi1 <- ldaMod$prior[2]
mu0 <- ldaMod$means[1, ]
mu1 <- ldaMod$means[2, ]
sigma0 <- cov(tennisTrain[which(tennisTrain$Result == 0), c(8, 9)])
sigma1 <- cov(tennisTrain[which(tennisTrain$Result == 1), c(8, 9)])
n0 <- dim(tennisTrain[which(tennisTrain$Result == 0), ])[1]
n1 <- dim(tennisTrain[which(tennisTrain$Result == 1), ])[1]
sigma <- ((n0 - 1) * sigma0 + (n1 - 1) * sigma1)/(n0 + n1 - 2)

ab <- solve(sigma) %*% (mu0 - mu1)
a <- ab[1]
b <- ab[2]
c <- -0.5 * t(mu0) %*% solve(sigma) %*% mu0 + 0.5 * t(mu1) %*% solve(sigma) %*% mu1 +
    log(pi0/pi1)

slopeLDA <- -a/b
interceptLDA <- -c/b

# make plot - add glm-boundary to compare. Not required by the students.
LDAplot <- ggplot(data = tennisTrain, aes(x = ACEdiff, y = UFEdiff, colour = Result)) +
    geom_point(pch = 1)

LDAplot + geom_point(data = tennisTest, pch = 4) + geom_abline(slope = slopeLDA,
    intercept = interceptLDA, colour = "green") + geom_abline(slope = slopeGLM, intercept = interceptGL
    colour = "darkblue")
```



The green line shows the decision boundary for LDA while the dark blue line shows the decision boundary for the GLM. They are very similar. Circles represents the training observations while crosses represents the test observations. We see that the lines separates well for both train and test set.

- Predicting classes of test set and make confusion table with sensitivity and specificity. Columns shows predictions.

```
LDApred <- predict(ldaMod, newdata = tennisTest)$class
tLDA <- table(tennisTest$Result, LDApred)
tLDA
```

```
##    LDApred
##       0  1
##   0 20  9
##   1  5 25
```

```
sensLDA <- tLDA[2, 2]/(tLDA[2, 1] + tLDA[2, 2])
spesLDA <- tLDA[1, 1]/(tLDA[1, 1] + tLDA[1, 2])
c(sensLDA, spesLDA)
```

```
## [1] 0.8333333 0.6896552
```

Both sensitivity and specificity are high and we see from the confusion table that most observations are classified correctly. The confusion table with our data is exactly the same, which makes sense since the decision boundary is so similar for logistic regression and LDA.

g) (2P)

- Perform QDA on the training set. What is the difference between LDA and QDA?
- Make the confusion table for the test set when using 0.5 as cut-off. Calculate the sensitivity and specificity on the test set.

Solution:

QDA assumes that the classes have different covariance matrices and gives a quadratic decision boundary (as we see below).

```
qdaMod <- qda(Result ~ ACEdiff + UFEdiff, data = tennisTrain)
QDApred <- predict(qdaMod, newdata = tennisTest)$class
```

```
tQDA <- table(tennisTest$Result, QDApred)
tQDA
```

```
##    QDApred
##       0  1
##   0 20  9
##   1  6 24
```

```
sensQDA <- tQDA[2, 2]/(tQDA[2, 1] + tQDA[2, 2])
spesQDA <- tQDA[1, 1]/(tQDA[1, 1] + tQDA[1, 2])
c(sensQDA, spesQDA)
```

```
## [1] 0.8000000 0.6896552
```

h) (1P)

Figure 3 shows the decision boundary for QDA, where observations falling into the red area will be classified as 0 (lose), and observations in the blue area will be classified as 1 (win). Circles represents observations from the train set, while crosses represents observations from the test set.

- Compare this plot with your corresponding plots for the logistic regression and LDA. Would you prefer logistic regression, LDA or QDA for these data? Justify your answer this based on the results from the confusion matrices and in light of the decision boundaries meaning for your tennis-covariates.

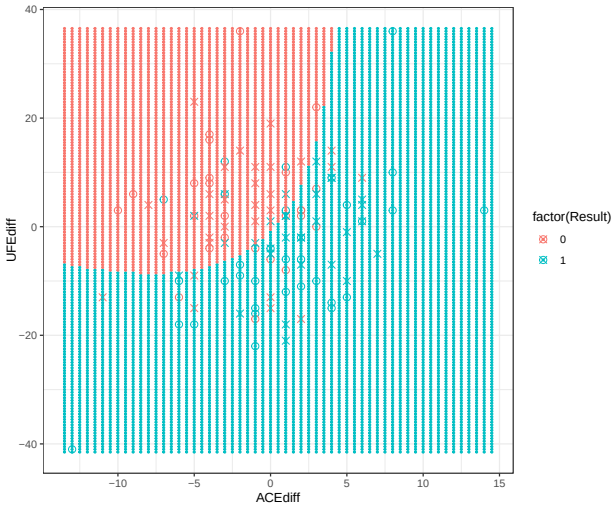


Figure 3: QDA decision boundary

Solutions

From the confusion table with corresponding sensitivity and specificity, we see that also QDA performs very similar to the methods above. It has only one more false prediction for the true 0 results, giving it a slightly poorer specificity. The decision boundary shows that only observations in the upper left half are classified as 0, which could make much sense since this corresponds to player 1 having many unforced errors and few aces and is hence loosing. However, the lower left corner and upper right corner will always be classified as a win for player 1 with QDA, but these regions corresponds to player 1 having few aces and less unforced errors than player 2 and vise verca. One could argue that these regions are problematic for both players, and the result will vary. For this reason, perhaps LDA and logistic regression are better models, as they have linear decision boundaries in these regions.

Problem 4 (9P)

a) (2P)

Recall the formula for the K-nearest neighbor regression curve to predict at a covariate value x_0,

$$\hat{f}(x_0) = \frac{1}{K} \sum_{i \in \mathcal{N}_0} y_i \ ,$$

where for a given integer K, the KNN regression first identifies the K points in the training data that are closest (in Euclidean distance) to x_0, represented by the set $\mathcal{N}_0$. It then estimates the regression curve at x_0 as the average of the response values for the training observations in $\mathcal{N}_0$.

Given the set of possible values for K in the KNN regression problem specified in a), explain how 10-fold cross validation is performed, and specify which error measure you would use. Your answer should include a formula to specify how the validation error is calculated.

Solution:

We look at a set of possible values for K in the KNN, for example $K = (1, 2, 3, 5, 7, 9, 15, 25, 50, 100)$. First we divide the N data into a training set of n elements and a test set of $N - n$ elements- and lock away the test set for model evaluation.

We work now with the training set.

10-fold CV: we divide the training data randomly into 10 folds of size $n/10$ each and call the folds $j = 1$, to $j = 10$.

For each value of K we do the following.

For $j = 1, \ldots, 10$:

- use the 9/10 observations from the folds except fold j to define the K-neighborhood $\mathcal{N}_0$ for each of the observations in the jth fold
- the observations in the jth fold are left out as the validation set. There are $n/10$ observations in the validation set - and we denote them (x_{0jl}, y_{0jl}),
- we then estimate $\hat{f}(x_{0jl}) = \frac{1}{K} \sum_{i \in \mathcal{N}_0} y_i$.
- We calculate the error in the jth fold of the validation set as $\sum_l (y_{0jl} - \hat{f}(x_{0jl}))^2$ where the j is for the validation fold

The total error on the validation set is thus the validation MSE$= \frac{1}{n} \sum_{j=1}^{10} \sum_l (y_{0jl} - \hat{f}(x_{0jl}))^2$.

So, for each value of K we get an estimate of the validation MSE. Finally, we choose the value of K that gives the lowest validation MSE.

b) (2P) - Multiple choice

Which statements about validation set approach, k-fold cross-validation (CV) and leave-one-out cross validation (LOOCV) are true and which are false? Say for *each* of them if it is true or false.

(i) 5-fold CV will generally lead to an estimate of the prediction error with less bias, but more variance, than LOOCV.
(ii) 10-fold CV is computationally cheaper than LOOCV.
(iii) The validation set-approach is the same as 2-fold CV.
(iv) LOOCV is a form of bootstrapping.

Solution:

FALSE, TRUE, FALSE, FALSE

c) (1P)

We now consider an example of bootstrapping. Assume you want to fit a model that predicts the probability for coronary heart disease (`chd`) from systolic blood pressure (`sbp`) and sex (female coded as 0, male coded as 1). Load the data in `R` as follows

```
id <- "1I6dk1fA4ujBjZPo3Xj8pIfnzIa94WKcy"  # google file ID
d.chd <- read.csv(sprintf("https://docs.google.com/uc?id=%s&export=download", id))
```

and perform a logistic regression with `chd` as outcome and `sbp` and `sex` as covariates. What is the estimated probability of coronary heart disease for a male with a systolic blood pressure of 140?

Solution: Doing the regression

```
id <- "1I6dk1fA4ujBjZPo3Xj8pIfnzIa94WKcy"  # google file ID
d.chd <- read.csv(sprintf("https://docs.google.com/uc?id=%s&export=download", id))
r.glm <- glm(chd ~ sbp + sex, d.chd, family = "binomial")
summary(r.glm)
```

```
##
## Call:
## glm(formula = chd ~ sbp + sex, family = "binomial", data = d.chd)
##
## Coefficients:
##             Estimate Std. Error z value Pr(>|z|)
## (Intercept) -2.386252   0.790657  -3.018  0.00254 **
## sbp          0.011337   0.006273   1.807  0.07075 .
## sex          0.322764   0.235786   1.369  0.17103
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## (Dispersion parameter for binomial family taken to be 1)
##
##     Null deviance: 427.61  on 349  degrees of freedom
## Residual deviance: 422.63  on 347  degrees of freedom
## AIC: 428.63
##
## Number of Fisher Scoring iterations: 4
```

Deriving the probability:

To get the probability you can now either plug in the estimates and calculate $\hat{p} = 1/(1 + \exp(-\hat{\eta}))$ with $\hat{\eta} = \hat{\beta}_0 + \hat{\beta}_1 \cdot 140 + \hat{\beta}_2 \cdot 1$, or directly use the predict function in R:

```
newdata <- data.frame(sbp = 140, sex = 1)
(pred.p <- predict(r.glm, newdata, type = "response"))
```

```
##         1
## 0.3831131
```

d) (4P)

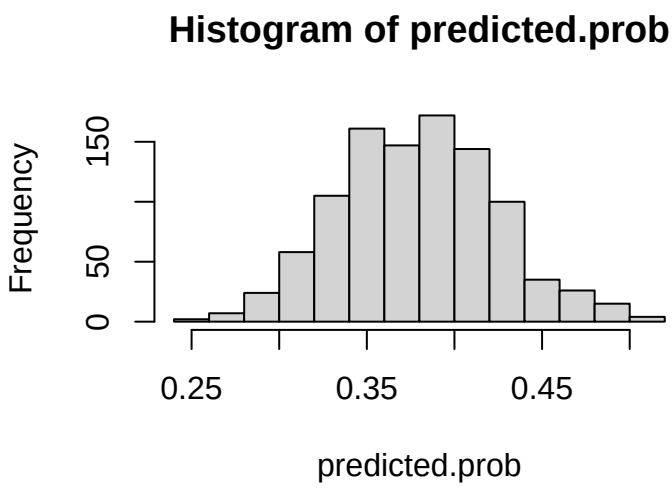
We now use the bootstrap to estimate the uncertainty of the probability derived in c). Proceed as follows:

- Use $B = 1000$ bootstrap samples.
- In each iteration, derive and store the estimated probability for `chd`, given that `sbp` equals 140 and `sex` is male.
- From the set of estimated probabilities, derive the standard error.
- Also derive 95% confidence interval for the estimates, using the bootstrap samples.

- Interpret what you see.

Solution:

```
B <- 1000
predicted.prob <- rep(NA, B)
for (ii in seq_len(B)) {
    d.boot <- d.chd[sample(nrow(d.chd), replace = TRUE), ]
    r.glm.boot <- glm(chd ~ sbp + sex, data = d.boot)
    newdata <- data.frame(sbp = 140, sex = 1)
    predicted.prob[ii] <- predict(r.glm.boot, newdata, type = "response")
}
hist(predicted.prob)
```



The standard error is just the bootstrap sample standard deviation. The 95% CI can be obtained by using the interval ranging from the 2.5% to the 97.5% quantile of the samples.

```
sd(predicted.prob)
```

```
## [1] 0.04492226
```

```
quantile(predicted.prob, probs = c(0.025, 0.975))
```

```
##      2.5%     97.5%
## 0.2947033 0.4713837
```

Interpretation: The predicted probability for coronary heart disease for a male with systolic blood pressure of 140 is 0.383, the respective standard error is 0.045 and the 95% CI ranges from 0.295 to 0.471