# TMA4268 - Project 1

```
# Libraries used throughout the exercise
library(ggplot2)
library(palmerpenguins) # Contains the data set 'penguins'.
library(ggfortify)
library(tidyverse)
library(GGally)
library(MASS)
library(class)
library(base)
library(ROSE)
```

## Problem 1

a)

If we have that  $y_0 = f(x_0) + \epsilon$ , where  $\epsilon$  is a random error independent of x with 0 mean. And  $x_0$  is a unseen test observation we find,

$$E\left[\left(y_{0} - \hat{f}(x_{0})\right)^{2}\right] = E\left[\left(f(x_{0}) - \hat{f}(x_{0})\right)^{2}\right] + E\left[\epsilon^{2}\right] + 2E\left[\left(f(x_{0}) - \hat{f}(x_{0})\right) \cdot \epsilon\right]$$

$$= E\left[f(x_{0})^{2} - 2f(x_{0})\hat{f}(x_{0}) + \hat{f}(x_{0})^{2}\right] + E\left[\epsilon^{2}\right] + 2E\left[\left(f(x_{0}) - \hat{f}(x_{0})\right)\right] \cdot E[\epsilon]$$

$$= f(x_{0})^{2} - 2f(x_{0})E[\hat{f}(x_{0})] + E[\hat{f}(x_{0})^{2}] + Var\left[\epsilon\right]$$

$$= \left(f(x_{0}) - E[\hat{f}(x_{0})]\right)^{2} + Var[\hat{f}(x_{0})] + Var\left[\epsilon\right]$$

$$= \text{Bias}^{2} + \text{Variance} + \text{Irreducible error}$$

b)

The irreducible error is a term that can't be reduced by fitting the data well. The variance is a term describing how much uncertainty our statistical model  $\hat{f}$ , how much  $\hat{f}$  changes if we change the training data. The bias is the expected difference between the true model f and our statistical model  $\hat{f}$ .

**c**)

- i) True
- ii) False
- iii) True
- iv) False

d)

- i) False
- ii) False
- iii) True
- iv) False

**e**)

(iii) 0.76

$$\rho_{x_1, x_2} = \frac{\text{cov}(x_1, x_2)}{\sigma_{x_1} \sigma_{x_2}} = \frac{33}{\sqrt{50}\sqrt{38}} = 0.76$$

## Problem 2

a)

One error made is excluding sex because of a low p-value, the p-value is the probability to observe a result equal or more extreme than the one we did, given that the null hypothesis  $H_0: \beta = 0$ , so a lower p-value means the result is more statistically significant.

Another error made is deciding whether to reject the null hypothesis that the species coefficient overall is actually zero based on the p-values of the coefficients. Since the null hypothesis in this case is  $H_0$ :  $\beta_{Chinstrap} = \beta_{Gentoo} = 0$  at the same time. We need to do a F-test.

A third error made is claiming that chinstrap penguins are the largest since they have the largest coefficient. Having a large coefficient only means that for a given set of parameters a chinstrap penguin is going to be heavier than another type of penguin. And when we include interaction terms which changes the the slopes, a large coefficient only guarantees it is larger for a range of parameters near zero. And by looking at body mass of the penguins in the data set we find that in fact gentoo penguins have the highest mean body mass.

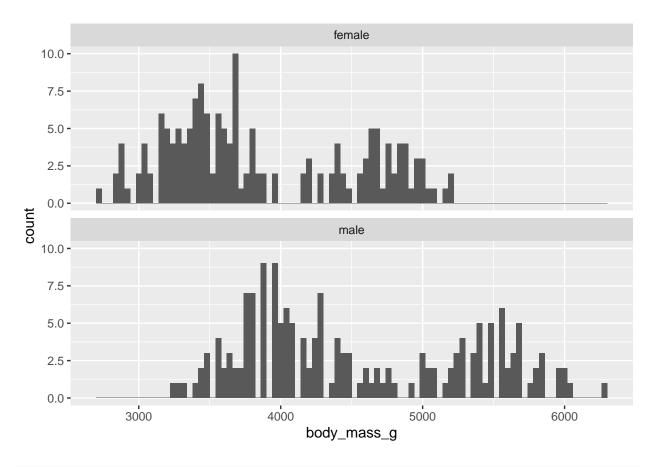
b)

```
data(penguins)

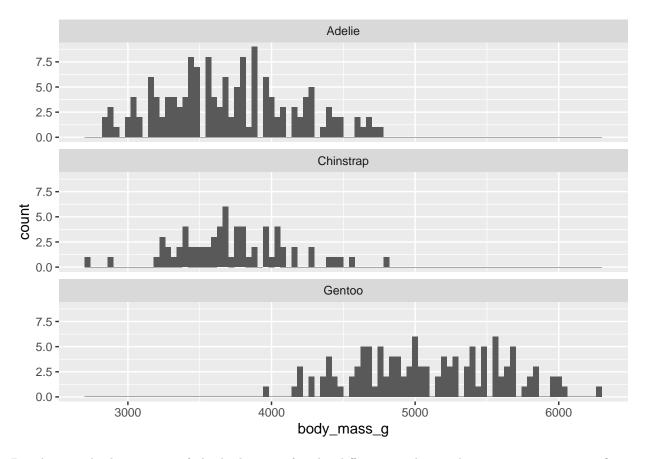
Penguins <- subset(penguins, select = -c(island, year))

Penguins <- na.omit(Penguins)

ggplot(data = Penguins) +
   geom_histogram(binwidth = 40, mapping = aes(x = body_mass_g)) +
   facet_wrap(~ sex, nrow = 2)</pre>
```



```
ggplot(data = Penguins) +
geom_histogram(binwidth = 40, mapping = aes(x = body_mass_g)) +
facet_wrap(~ species, nrow = 3)
```



By plotting the histograms of the body mass for the different genders and species, we see a significant correlation between sex and body mass. And we also see that gentoo penguins have the largest mean body mass of the species, not chinstrap as concluded in the report.

**c**)

```
Penguins <- subset(penguins, select = -c(island, year))</pre>
penguin.model <- lm(body_mass_g ~ flipper_length_mm + sex + bill_depth_mm * species,</pre>
                     data = Penguins)
summary(penguin.model)
##
## Call:
## lm(formula = body_mass_g ~ flipper_length_mm + sex + bill_depth_mm *
##
       species, data = Penguins)
##
## Residuals:
##
      Min
              1Q Median
                             3Q
                                   Max
  -751.2 -183.8
                    -9.8 191.1
                                 906.9
##
##
## Coefficients:
##
                                   Estimate Std. Error t value Pr(>|t|)
## (Intercept)
                                                 646.92 -2.066 0.039615 *
                                   -1336.58
```

```
## flipper_length_mm
                                     17.38
                                                 2.91
                                                        5.971 6.17e-09 ***
## sexmale
                                    432.90
                                                44.63
                                                        9.699 < 2e-16 ***
                                                        3.717 0.000237 ***
## bill depth mm
                                     82.98
                                                22.32
## speciesChinstrap
                                               680.39
                                                        2.146 0.032610 *
                                   1460.15
## speciesGentoo
                                    644.88
                                               542.57
                                                        1.189 0.235481
## bill depth mm:speciesChinstrap
                                                37.01
                                    -83.53
                                                       -2.257 0.024666 *
## bill depth mm:speciesGentoo
                                                        1.049 0.294955
                                     36.17
                                                34.48
## ---
## Signif. codes: 0 '***' 0.001 '**' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 286.8 on 325 degrees of freedom
     (11 observations deleted due to missingness)
## Multiple R-squared: 0.8758, Adjusted R-squared: 0.8732
## F-statistic: 327.5 on 7 and 325 DF, p-value: < 2.2e-16
```

We see that the p-value of the F-test is very small (2.2e-16), so we know almost for certain that at least one coefficient is not zero. Looking at the summary we see that all the coefficients have p-values small enough to be statistically significant, except the coefficients for spesiesGentoo and its interaction term. However these are categorical covariates so the null hypothesis we need to test is different.

To test the null hypothesis  $H_0: \beta_{Chinstrap} = \beta_{Gentoo} = 0$ , we do a F-test. We do the same for the interaction term.

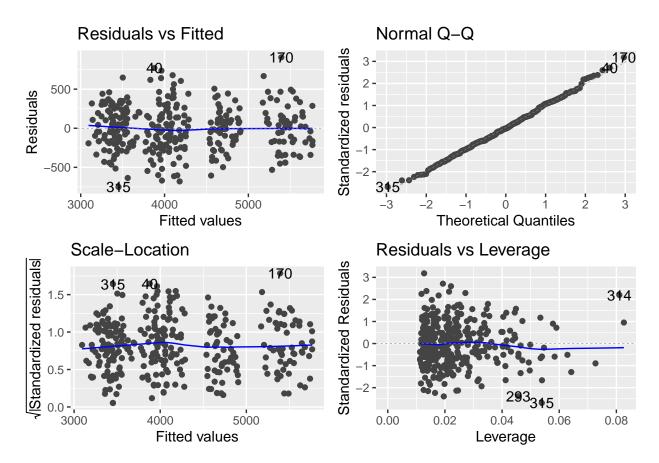
#### anova(penguin.model)

```
## Analysis of Variance Table
##
## Response: body mass g
##
                                                    F value
                                                               Pr(>F)
                          Df
                                Sum Sq
                                         Mean Sq
## flipper length mm
                           1 164047703 164047703 1994.7424 < 2.2e-16 ***
                               9416589
                                          9416589
                                                   114.5013 < 2.2e-16 ***
## sex
                           1
## bill_depth_mm
                           1
                                3667377
                                          3667377
                                                    44.5936 1.051e-10 ***
                                                    64.8743 < 2.2e-16 ***
## species
                              10670525
                                          5335262
                           2
## bill depth mm:species
                           2
                                                     4.4349
                                                              0.01258 *
                                729458
                                           364729
## Residuals
                         325
                              26728014
                                            82240
## Signif. codes: 0 '*** 0.001 '** 0.01 '* 0.05 '.' 0.1 ' 1
```

We see that the p-value for species is very low, so we do reject the null hypothesis. We find that the interaction term is also statistically significant however the p-value is not as small.

We now now evaluate the fit of the model with some graphical tools.

```
autoplot(penguin.model)
```



Looking at the Tukey-Anscombe diagram we see that the residuals are centered around zero, and that they are not increasing or decreasing. This indicates a good fit since it shows us that the residuals have zero mean and constant variance.

Looking at the QQ-diagram we see that it is very close to a straight line, which indicates that the residuals are normal distributed as we have asumed.

The scale-location diagram is also not increasing or decreasing, indicating a constant variance.

And finally looking at the leverage plot we see that there are not any worrying points or groups of points with very high leverage and residuals compared to the rest of the points, except maybe the point in the top right of the diagram.

From looking at the diagrams we conclude that the fit of the model is good.

## Problem 3

Now, the main idea is to classify the species of the penguins for a given body mass and flipper length. The dataset contains 3 type of penguin species, yet, classifying 3 penguin species is not straightforward. So, for simplicity, we define our goal to classify a penguin belonging to the species - Adelie, or not Adelie. This will give us two-class classification problem instead of three.

Since, we will use only three parameters from the dataset, it is wise to create a small dataset, and work with it. First, the variables should be converted to numeric (because knn function cannot handle the int class, and generates errors) and removes any missing observations.

```
penguins$adelie <- ifelse(penguins$species == "Adelie", 1, 0)</pre>
```

Now, we need two datasets: the one to train the model, then to test the model. It is common to divide 70% of dataset as a training dataset, and the rest will be a test dataset.

```
set.seed(4268)

# 70% of the sample size for training set
training_set_size <- floor(0.7 * nrow(Penguins_reduced))
train_ind <- sample(seq_len(nrow(Penguins_reduced)), size = training_set_size)
train <- Penguins_reduced[train_ind, ]
test <- Penguins_reduced[-train_ind, ]</pre>
```

a)

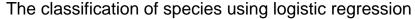
## i) Logistic regression

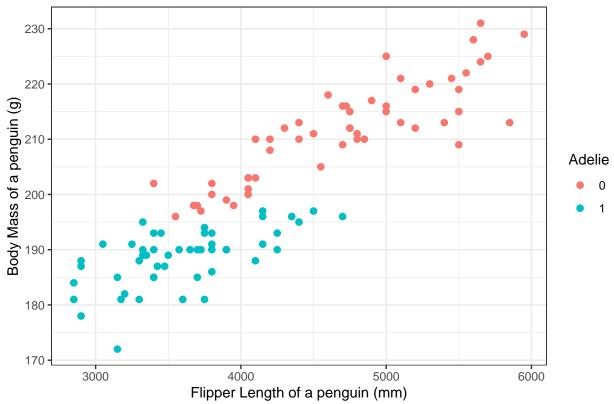
```
## Estimate Std. Error z value Pr(>|z|)
## (Intercept) 37.7618776 5.1761640773 7.295340 2.979055e-13
## body_mass_g 0.0007120 0.0004619996 1.541127 1.232859e-01
## flipper_length_mm -0.2055804 0.0324291723 -6.339367 2.307116e-10
```

Here, we train the model using train dataset, and the result is available above.

```
prob_test_lr <- predict(log_reg, newdata = test, type = "response")
pred_test_lr <- ifelse(prob_test_lr > 0.5, 1, 0)
```

predict() gives the probabilities of the species = Adelie (class = 1). Then, we apply a cutoff value of 0.5 to those probabilities, to get predicted classes.





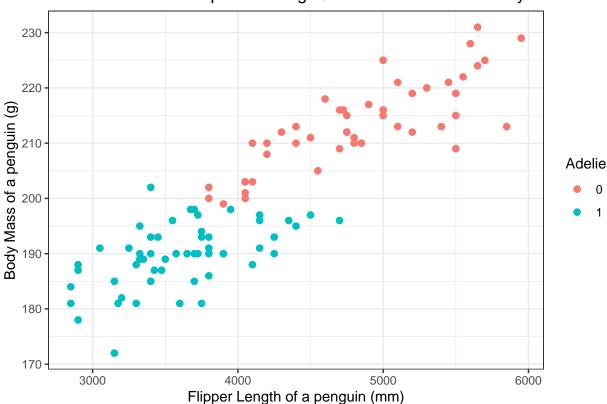
Then, we use test dataset for testing the model. The plot illustrates the testing result.

ii) Quadratic Discriminant Analysis We do the same for classification using Quadratic Discriminant Analysis

```
qda_reg = qda(adelie ~ body_mass_g + flipper_length_mm, data = train)
prob_test_qda <- predict(qda_reg, newdata = test, type = "response")$posterior
pred_test_qda <- predict(qda_reg, newdata = test, type = "response")$class</pre>
```

Because QDA identifies the probabilities of having species = Adelie (class = 1), and having species = not Adelie (class = 0), predict() function will give both probabilities and already cut-off value (0.5) applied predictions. So, \$posteriors will give the probabilities, \$class will give 0.5 cut-off value applied corresponding classes.





Again, this plot illustrates the testing result.

```
knnMod = knn(train = train, test = test, cl = train$adelie, k = 25, prob = T)
knn_r <- data.frame(data.matrix(knnMod), attributes(knnMod)$prob)</pre>
```

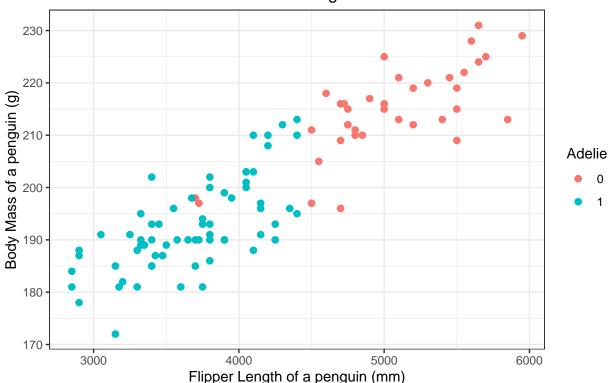
iii) K-nearest Neighbors After having the model, we put the result in matrix form for better usage.

```
probKNN = ifelse(knnMod == 0, 1 - attributes(knnMod)$prob, attributes(knnMod)$prob)
predKNN = ifelse(probKNN > 0.5, 1, 0)
```

This is the way to get the probabilities of species = Adelie (class = 1). Then, again we apply 0.5 cut-off value to get the predictions.

```
colour=predKNN), data=adelie_knn_df, size=2) +
    xlab("Flipper Length of a penguin (mm)") + ylab("Body Mass of a penguin (g)") +
    labs(shape = "Adelie", color = "Adelie") +
    ggtitle("The classification of species using \n K-nearest Neighbors") +
    theme_bw() + theme(plot.title = element_text(hjust = 0.5))
gg_knn
```

# The classification of species using K–nearest Neighbors



# iv) Sensitivity & specificity For Logistic regression

```
Estim. prob. of Y=1 Predicted class True class
##
## 1
               0.9616473
                                        1
## 2
               0.9028693
                                        1
                                                    1
               0.6321050
## 3
                                        1
                                                    1
## 4
               0.7859021
                                        1
                                                    1
                                        1
## 5
               0.9324308
                                                    1
               0.7688126
                                        1
                                                    1
## 6
```

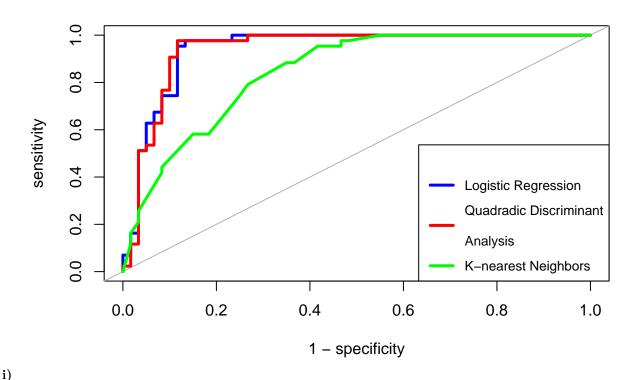
```
conf_mat_log_r = table(predicted = predictions_log_reg["Predicted class"][,1], true =
        predictions_log_reg["True class"][,1] )
print("The confusion matrix is:")
## [1] "The confusion matrix is:"
conf_mat_log_r
##
            true
## predicted 0 1
##
           0 52 1
##
           1 8 42
test_error_rate_lr = (conf_mat_log_r[1, 2] + conf_mat_log_r[2, 1])/sum(conf_mat_log_r)
print(paste( "The test error for Logistic regression -", signif(test_error_rate_lr, digits = 4)))
## [1] "The test error for Logistic regression - 0.08738"
sensitivity_lr = conf_mat_log_r[2, 2]/(conf_mat_log_r[1, 2]+conf_mat_log_r[2, 2])
specificity_lr = conf_mat_log_r[1, 1]/(conf_mat_log_r[2, 1]+conf_mat_log_r[1, 1])
print(paste( "The sensitivity - ", signif(sensitivity_lr, digits=4)))
## [1] "The sensitivity - 0.9767"
print(paste( "The specificity - ", signif(specificity_lr, digits=4)))
## [1] "The specificity - 0.8667"
For Quadratic Discriminant Analysis
predictions_qda = data.frame(pred_test_qda, test[, "adelie"])
colnames(predictions_qda) = c("Predicted class", "True class")
head(predictions_qda)
    Predicted class True class
##
## 1
                   1
## 2
                   1
                              1
## 3
                   1
## 4
                   1
                              1
## 5
## 6
                   1
                              1
conf_mat_qda = table(predicted = predictions_qda["Predicted class"][,1], true =
        predictions_qda["True class"][,1] )
print("The confusion matrix is:")
```

## [1] "The confusion matrix is:"

```
conf_mat_qda
##
            true
## predicted 0 1
           0 46 1
##
##
           1 14 42
test_error_rate_qda = (conf_mat_qda[1, 2] + conf_mat_qda[2, 1])/sum(conf_mat_qda)
print(paste( "The test error for Quadratic Discriminant Analysis -",
             signif(test error rate qda, digits = 4)))
## [1] "The test error for Quadratic Discriminant Analysis - 0.1456"
sensitivity_qda = conf_mat_qda[2, 2]/(conf_mat_qda[1, 2]+conf_mat_qda[2, 2])
specificity_qda = conf_mat_qda[1, 1]/(conf_mat_qda[2, 1]+conf_mat_qda[1, 1])
print(paste( "The sensitivity - ", signif(sensitivity_qda, digits=4)))
## [1] "The sensitivity - 0.9767"
print(paste( "The specificity - ", signif(specificity_qda, digits=4)))
## [1] "The specificity - 0.7667"
For K-nearest Neighbors
predictions_knn = data.frame(knn_r[, 2], knn_r[, 1], test[, "adelie"])
colnames(predictions_knn) = c("Estim. prob. of Y=1", "Predicted class", "True class")
head(predictions_knn)
    Estim. prob. of Y=1 Predicted class True class
               0.6000000
## 1
                                       1
## 2
               0.6666667
                                       1
                                                  1
## 3
               0.6800000
                                       1
                                                  1
               0.6400000
                                       1
                                                  1
               0.6800000
## 5
                                       1
                                                  1
               0.6400000
                                                  1
## 6
                                       1
conf_mat_knn = table(predicted = predictions_knn["Predicted class"][,1], true =
        predictions_knn["True class"][,1] )
print("The confusion matrix is:")
## [1] "The confusion matrix is:"
conf_mat_knn
##
            true
## predicted 0 1
##
           0 35 2
##
           1 25 41
```

```
test_error_rate_knn = (conf_mat_knn[1, 2] + conf_mat_knn[2, 1])/sum(conf_mat_knn)
print(paste( "The test error for K-nearest Neighbors -", signif(test_error_rate_knn, digits = 4)))
## [1] "The test error for K-nearest Neighbors - 0.2621"
sensitivity_knn = conf_mat_knn[2, 2]/(conf_mat_knn[1, 2]+conf_mat_knn[2, 2])
specificity_knn = conf_mat_knn[1, 1]/(conf_mat_knn[2, 1]+conf_mat_knn[1, 1])
print(paste( "The sensitivity - ", signif(sensitivity_knn, digits=4)))
## [1] "The sensitivity - 0.9535"
print(paste( "The specificity - ", signif(specificity_knn, digits=4)))
## [1] "The specificity - 0.5833"
b)
lr_roc = roc.curve(test$adelie, prob_test_lr, col = "blue", lwd=3,
                   xlab = "1 - specificity", ylab = "sensitivity")
qda_roc = roc.curve(test$adelie, prob_test_qda[,2], col = "red", lwd=3, add = T)
probKNN = ifelse(knnMod == 0, 1 - attributes(knnMod)$prob, attributes(knnMod)$prob)
knn_roc = roc.curve(test$adelie, probKNN, col = "green", lwd=3, add = T)
legend("bottomright", legend = c("Logistic Regression", "Quadradic Discriminant
       \nAnalysis", "K-nearest Neighbors"), cex=0.8, lwd = 3,
       col = c("blue", "red", "green"))
```

# **ROC** curve



Areas Under Curves:

```
print(paste( "AUC of Logistic Regression ", signif(lr_roc$auc, digits = 4)))
```

## [1] "AUC of Logistic Regression 0.9391"

```
print(paste( "AUC of Quadradic Discriminant Analysis ", signif(qda_roc$auc, digits = 4)))
```

## [1] "AUC of Quadradic Discriminant Analysis 0.938"

```
print(paste( "AUC of K-nearest Neighbors ", signif(knn_roc$auc, digits = 4)))
```

## [1] "AUC of K-nearest Neighbors 0.8417"

ii) ROC curve - Receiver operating characteristics curve displays the relation between False Positive rate and True Positive rate for all possible threshold values (0 to 1). Since True Positive rate is  $\frac{True\ Positives}{All\ Positives}$ , it is expressed as sensitivity, and False Positive rate as 1 - Specificity. If the model is ideal model, the sensitivity = 1, and specificity = 1, so, the curve will be on the top left. While a straight line will represent a model with random guesses on the outcome.

In order to check the overall performance of the model, AUC (Area Under Curve) values are compared, meaning that if AUC value is high, that means the curve is closer to the ideal situation.

The comparison of the models we have: Logistic regression, Quadratic Discriminant Analysis, K-nearest Neighbors

When we look at the ROC Curves, we clearly see that the model that performs worse than others is K-nearest Neighbors. This is proved by AUC area. (AUC area of KNN = 0.8417).

The performances of Logistic regression and Quadratic Discriminant Analysis are almost the same. Yet, there is a slight difference in AUC areas. Based on AUC areas, Logistic regression performs a bit better than Quadratic Discriminant Analysis (AUC area of LogReg = 0.9391, AUC area of QDA = 0.938). However, the overall conclusion is Logistic Regression and Quadratic Discriminant Analysis are similarly good models for interpreting the data.

iii) If the task is to create an interpretable model, the model that has to be chosen is Logistic Regression. The reason is Logistic Regression outputs a table that contains all the necessary information to analyze the relation between two variable. The features like Intercept, p-value, t-value have key roles in interpretation.

**c**)

$$odds = \frac{p_i}{1 - p_i} = \frac{P(Y_i = 1 \mid X = x)}{P(Y_i = 0 \mid X = x)} = exp(\beta_0) \cdot exp(\beta_1 x_1) \cdot exp(\beta_2 x_2)$$

$$odds \ ratio = \frac{odds[Y_i = 1 \mid X = x_1 + 1000]}{odds[Y_i = 1 \mid X = x_1]} = \frac{exp(\beta_0) \cdot exp(\beta_1(x_1 + 1000)) \cdot exp(\beta_2x_2)}{exp(\beta_0) \cdot exp(\beta_1x_1) \cdot exp(\beta_2x_2)} = exp(\beta_1 * 1000)$$

We find  $\beta_1$  from coefficient table of Logistic regression

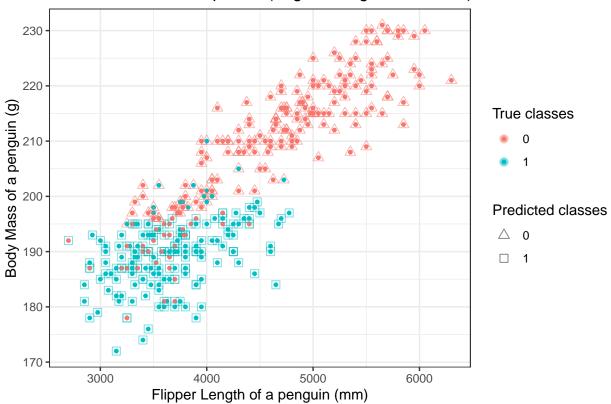
#### summary(log\_reg)\$coef

```
## (Intercept) 37.7618776 5.1761640773 7.295340 2.979055e-13 ## body_mass_g 0.0007120 0.0004619996 1.541127 1.232859e-01 ## flipper_length_mm -0.2055804 0.0324291723 -6.339367 2.307116e-10 So, \beta_1 = 0.000712 print(paste( "The odds will be multiplied by ", signif(exp(coef(log_reg)[2]*1000), digits = 4))) ## [1] "The odds will be multiplied by 2.038"
```

d)

```
prob_whole_lr <- predict(log_reg, newdata = Penguins_reduced, type = "response")
pred_whole_lr <- ifelse(prob_whole_lr > 0.5, 1, 0)
pred_whole_lr_sh = pred_whole_lr
whole_lr_df = bind_rows(mutate(Penguins_reduced, pred_whole_lr, pred_whole_lr_sh))
whole_lr_df$pred_whole_lr = as.factor(whole_lr_df$pred_whole_lr)
```

# The classification of species (Logistic Regression used)



#### Problem 4

**a**)

Answers for the questions are as follows: (i) True; (ii) False; (iii) True; (iv) False;

b)

The given data for the problem was loaded into R firstly. The heart disease (chd) predicting function was created using global linear function and three variables sex, systolic blood pressure (sbp) and if a person smokes or not. The data-frame representing a non-smoking male with sbp 150 was insterted into the predicting function.

```
#Accessing the data
id<-"1chRpybM5cJn4Eow3-_xwDKPKyddL9M2N"
d.chd<-read.csv(sprintf("https://docs.google.com/uc?id=%s&export=download",id))

#Creating a predicting model
glm_fit = glm(chd~sex+sbp+smoking, data = d.chd, family = binomial)

#Predicting the disease probability

temp_d <- data.frame(sex=1, sbp=150, smoking=0)
predict(glm_fit,temp_d,type = 'response')</pre>
```

## 0.10096

The chd probability for a non-smoking male with sbp 150 equals to 0.10096 according to our predicting function.

**c**)

##

1

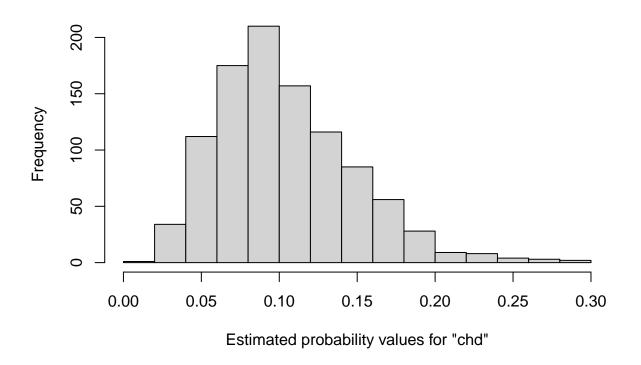
The function of the interest (which is chd predicting function for the male above) was created for bootstrapping. The bootstrapping was performed on function of the interest by replacing a row in the supplied data by another row in this data 1000 times. Each iteration result was saved in variable "A" and they were plotted as a histogram.

```
#Create function of interest
func_interest <- function(used_data){
   glm_fit = glm(chd~sex+sbp+smoking, data = used_data, family = binomial)
   predict(glm_fit,data.frame(sex=1, sbp=150, smoking=0),type = 'response')
}

#Implement bootstrap for 1000 iterations and save the results in A
B = 1000
A = replicate(B,0)
for (i in 1:B){
    A[i]=func_interest(d.chd[sample(1:nrow(d.chd), 500, replace = T),])
}

hist(A, main = 'Estimated probability for "chd"', xlab = 'Estimated probability values for "chd"')</pre>
```

# Estimated probability for "chd"



As one can see most of the prediction values are between 0.05 and 0.15.

We created the function that takes prediction values above for calculating the standard error.

```
#Calculating standard error
std_error_func <- function(x) sd(x) / sqrt(length(x))
Std_error <- std_error_func(A)
print(Std_error)</pre>
```

## [1] 0.001387751

The standard error derived from predictions above equals to 0.00134.

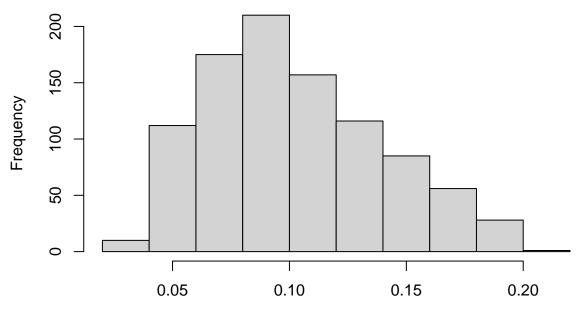
2.5~% and 97.5~% quantile values of the predictions were defined using "quantile" function. The values below and above these quantile values were deleted from the predictions data and plotted as a histogram.

```
#Deriving quantiles and sorting bootstrap results within them
q = quantile(A,probs = c(0.025, 0.975))

After_q <-A[A<q[2]]
After_q <-After_q[After_q>q[1]]

hist(After_q, main = 'Quantile of estimated probability of "chd"', xlab = 'Quatiled estimated probability
```

# Quantile of estimated probability of "chd"



Quatiled estimated probability values of "chd"

The remaining 95 % quantile interval for the bootstrap samples lies between 0.03915905 and 0.20153356. One can see how they distributed in the histogram above.

```
#Calculating values probabilities and expected probability value

EP = 0
for(i in 1:length(After_q)){
   EP = EP+After_q[i]*((1/950))
}
print(EP)
```

# ## [1] 0.1025979

The expected probability value is 0.1036039. In my opinion the range of plausible values are from 0.06 to 0.12.

# d)

The answers for the questions in problem d) are as follows. (i) True, (ii) Fal- se, (iii) True, (iv) False.