Laboration report in Machine Learning

Computer lab 1 block 1

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Contents

1 Assignment 1. Handwritten digit recognition with K-nearest neighbors.

The data in this task is from the file optdigits.csv. Data consists of 3822 handwritten digits from 0 to 9 and are stored as images of size 8x8.

1.1 1.1

Question: Import the data into R and divide it into training, validation and test sets (50%/25%/25%) by using the partitioning principle specified in the lecture slides.

Answer: The code used is presented as follows:

```
# Read in data
data <- read.csv("optdigits.csv")

# Renaming the response variable and changing it to a factor variable
data <- rename(data, y=X0.26)
data$y <- as.factor(data$y)

# Partitioning training data (50%)
n=dim(data)[1]
set.seed(12345)
id=sample(1:n, floor(n*0.5))
train=data[id,]

# Partitioning validation data (25%)
id1=setdiff(1:n, id)
set.seed(12345)
id2=sample(id1, floor(n*0.25))
valid=data[id2,]

# Partitioning test data (25%)
id3=setdiff(id1,id2)
test=data[id3,]
```

1.2 1.2

Question: Use training data to fit 30-nearest neighbor classifier with function kknn() and kernel=”rectangular” from package kknn and estimate

- Confusion matrices for the training and test data (use table())
- Misclassification errors for the training and test data

Comment on the quality of predictions for different digits and on the overall prediction quality.

Answer: The confusion matrix for the model trained on training data with k=30 and evaluated on training data is presented in table 1.

```
# kknn on training data and evaluation on training data
model_kknn_train <- kknn(formula=y~.,
                         train=train,
```

```
                         test=train,
                         kernel="rectangular",
                         k=30)
conf_mat_train <- table(train$y, model_kknn_train$fitted.values)
acc_train <- sum(diag(conf_mat_train)) / sum(conf_mat_train)
miss_train <- 1-acc_train

# kknn on training data and evaluation on test data
model_kknn_test <- kknn(formula=y~.,
                         train=train,
                         test=test,
                         kernel="rectangular",
                         k=30)
conf_mat_test <- table(test$y, model_kknn_test$fitted.values)
acc_test <- sum(diag(conf_mat_test)) / sum(conf_mat_test)
miss_test <- 1-acc_test

# Rows are true values, columns are model prediction
kable(conf_mat_train, caption = "Confusion matrix for training data, model
      predictions by columns and true value by rows.")
```

Table 1: Confusion matrix for training data, model predictions by columns and true value by rows.

	0	1	2	3	4	5	6	7	8	9
0	177	0	0	0	1	0	0	0	0	0
1	0	174	9	0	0	0	1	0	1	3
2	0	0	170	0	0	0	0	1	2	0
3	0	0	0	197	0	2	0	1	0	0
4	0	1	0	0	166	0	2	6	2	2
5	0	0	0	0	0	183	1	2	0	11
6	0	0	0	0	0	0	200	0	0	0
7	0	1	0	1	0	1	0	192	0	0
8	0	10	0	1	0	0	2	0	190	2
9	0	3	0	4	2	0	0	2	4	181

```
miss_train
```

```
## [1] 0.04238619
```

The misclassification error on training data from table 1 is around 4.24%. The two number with the highest number of wrong predictions are 8 and 9, with 15 wrong predictions each. The model also struggles to predict number 1 and 5 where both had 14 wrong predictions. Examining the most common misclassification, the number 5 was predicted as 9 a total of eleven times and the number 8 was predicted as 1 a total of ten times.

The easiest numbers to predict are 0 and 6. For 0 the model correctly predicted 177 out of 178 numbers and did not predict the number 0 for any other number. For the number 6, the model correctly predicted all 200 numbers, but it did however predict six other numbers as 6 incorrectly.

The confusion matrix for the model trained on training data with k=30 and evaluated on test data is presented

in table 2.

```
kable(conf_mat_test, caption = "Confusion matrix for test data, model
      predictions by columns and true value by rows.")
```

Table 2: Confusion matrix for test data, model predictions by columns and true value by rows.

	0	1	2	3	4	5	6	7	8	9
0	97	0	0	0	0	0	1	0	0	0
1	0	91	3	0	0	0	0	0	0	3
2	0	0	93	1	0	0	0	0	1	0
3	0	0	0	95	0	0	0	2	1	0
4	1	0	0	0	89	0	1	5	1	3
5	0	1	0	1	0	79	1	0	0	5
6	0	0	0	0	0	0	94	0	0	0
7	0	2	0	0	0	1	0	91	1	0
8	0	3	0	1	0	0	1	0	86	0
9	0	0	0	4	0	0	0	2	1	94

```
miss_test
```

```
## [1] 0.04916318
```

The misclassification error on test data from table 2 is around 4.92%. The two number with the highest number of wrong predictions are 4 and 5. The number 4 had ten wrong predictions and the number 5 had eight wrong predictions.

The easiest numbers to predict are 0 and 6. For 0 the model correctly predicted 97 out of 98 number and the misclassification was as number 6.
For the number 6, the model correctly predicted all 94 numbers, but it did however predict four times for other numbers as 6 incorrectly.

The overall prediction quality from the model is good, especially for the numbers 0 and 6.

1.3 1.3

Question: Find any 2 cases of digit "8" in the training data which were easiest to classify and 3 cases that were hardest to classify (i.e. having highest and lowest probabilities of the correct class). Reshape features for each of these cases as matrix 8x8 and visualize the corresponding digits (by using e.g. heatmap() function with parameters Colv=NA and Rowv=NA) and comment on whether these cases seem to be hard or easy to recognize visually.

Answer: The code used to find the 2 digits that are hardest to classify were found with the code as follows

```
y <- train$y
fit_y <- model_kknn_train$fitted.values
# probabilities given from number 0 to 9, index 9 = number 8.
prob_8 <- model_kknn_train$prob[, 9]

# Data frame consisting of true value of y, model prediction and the models
# probability that the number is 8.
```

```
data_8 <- data.frame(y = y, fit_y = fit_y, prob = prob_8)
data_8$observation_id <- rownames(data_8)

# Only observations with the label 8 is kept.
data_8 <- data_8[data_8$y == "8", ]
head(arrange(data_8, prob), 2)
```

```
##   y fit_y      prob observation_id
## 1 8     6 0.1000000           1624
## 2 8     1 0.1666667           1663
```

From the output, observation 1624 and 1663 were hardest to classify as 8 from the model. The three observations that were easiest to identify as 8 were found with the code as follows

```
tail(arrange(data_8, prob), 3)
```

```
##     y fit_y prob observation_id
## 203 8     8    1           1810
## 204 8     8    1           1811
## 205 8     8    1           1864
```

From the output observation 1810, 1811, and 1864 were three observations that were easiest to identify as 8 with a probability from the model as 100% (in total there were 49 observations that had 100% probability).

A function that reshapes each observation to a 8x8 cases and then visualizing the result in a heatmap was done with the code as follows

```
# Change colour palette to black and white
colfunc <- colorRampPalette(c("white", "black"))

plot_8 <- function(index){
  title <- paste0("Obs: ", index)
  # Reshapes the observations to a 8x8
  plot <- as.matrix(train[index, -65]) # Remove response variable
  plot <- matrix(plot, nrow=8, byrow=TRUE)
  heatmap(plot, col=colfunc(16), Colv=NA, Rowv=NA, main=title, margins=c(2,2))
}
```

The heatmaps for observations 1624 and 1663 are presented in figure 1.

```
plot_8(1624)
plot_8(1663)
```

Figure 1: Heatmap for two observations that were hard to classify: 1624 and 1663.

In figure 1, it is hard to visually recognize what number the observations 1624 and 1663 are.

The heatmaps for observations 1810, 1811, and 1864 are presented in figure 2.

```
plot_8(1810)
plot_8(1811)
plot_8(1864)
```

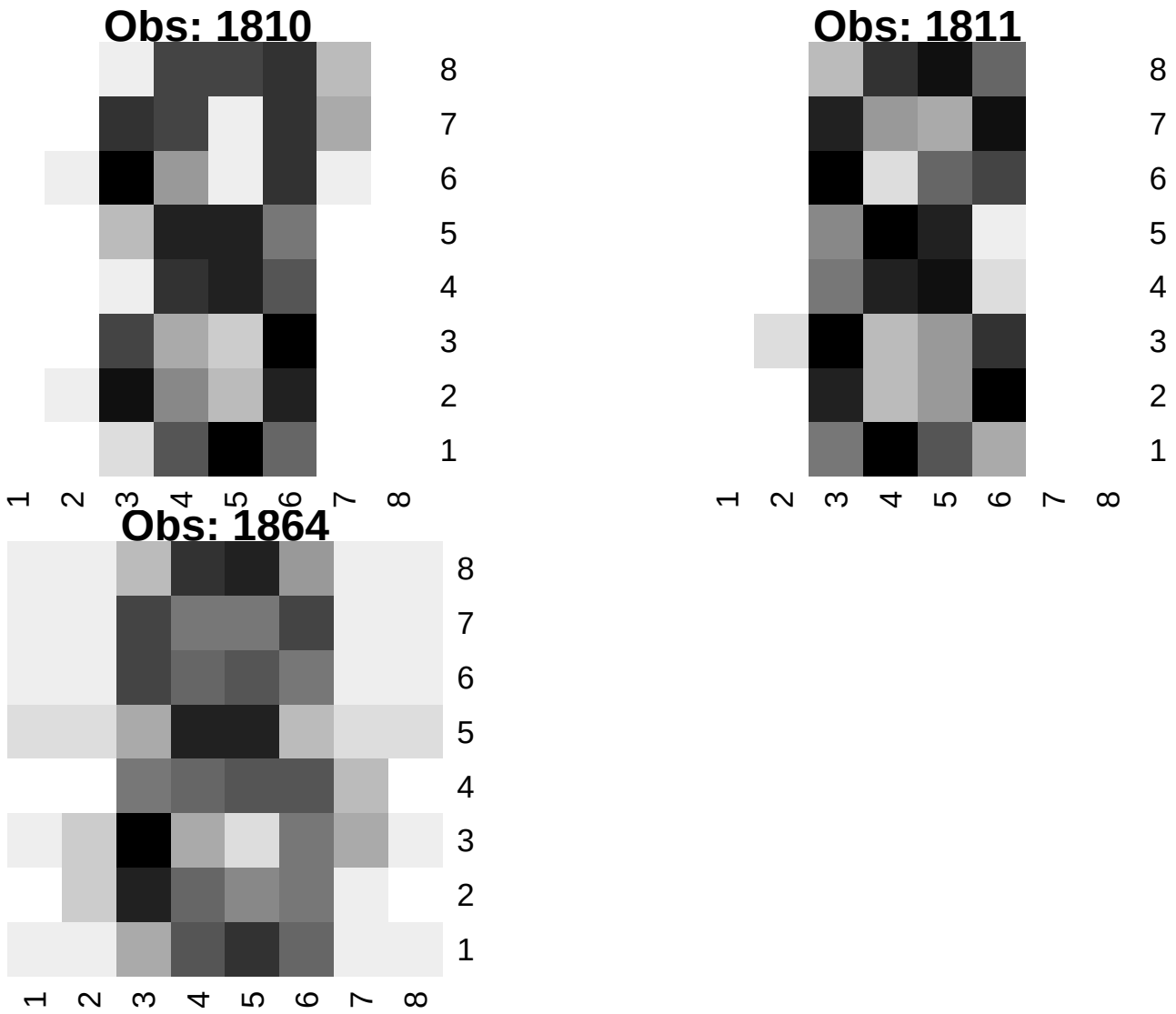


Figure 2: Heatmap for three observations that were easy to classify: 1810, 1811, and 1864.

In figure 2, is is easy to visually recognize that observations 1810, 1811, and 1864 are of the number 8.

1.4 1.4

Question: Fit a K-nearest neighbor classifiers to the training data for different values of $K = 1, 2, ..., 30$ and plot the dependence of the training and validation misclassification errors on the value of K (in the same plot). How does the model complexity change when K increases and how does it affect the training and validation errors? Report the optimal k according to this plot. Finally, estimate the test error for the model having the

optimal K, compare it with the training and validation errors and make necessary conclusions about the model quality.

Answer: The code to create K-nearest neighbor clasifiers for different k and the misclassification error on training and validation is as follows

```
fit_kknn <- function(k){
  model_kknn_train <- kknn(formula=y~., train=train, test=train, kernel="rectangular", k=k)
  # Confusion matrix for train data
  conf_mat_train <- table(model_kknn_train$fitted.values, train$y)
  acc_train <- sum(diag(conf_mat_train)) / sum(conf_mat_train)
  # Missclassification for training data
  miss_train <- 1-acc_train

  model_kknn_valid <- kknn(formula=y~., train=train, test=valid, kernel="rectangular", k=k)
  # Confusion matrix for validation data
  conf_mat_valid <- table(model_kknn_valid$fitted.values, valid$y)
  acc_valid <- sum(diag(conf_mat_valid)) / sum(conf_mat_valid)
  # Missclassification for validation data
  miss_valid <- 1-acc_valid

  result <- c(miss_train, miss_valid)
  return(result)
}

# Missclassification for k=1,...,30 for training and validation data
result <- data.frame(train = 0, valid = 0)
for(i in 1:30){
  model <- fit_kknn(i)
  result[i,1] <- model[1]
  result[i,2] <- model[2]
}
result$index <- 1:30
```

The plot showing the dependence of misclassification error for training and validation data is presented in figure 3.

```
ggplot(result, aes(x=index)) +
  geom_line(aes(y=train, colour="train")) +
  geom_point(aes(y=train, colour="train")) +
  geom_line(aes(y=valid, colour="valid")) +
  geom_point(aes(y=valid, colour="valid")) +
  scale_color_manual(name = "Data",
                     values = c("train" = "steelblue", "valid" = "indianred")) +
  scale_x_continuous(breaks = c(seq(from=0, to=30, by=5))) +
  scale_y_continuous(limits = c(0, 0.06)) +
  theme_bw() +
  labs(x = "k",
       y = "Missclassification rate")
```

In figure 3, the model complexity is highest when k = 1 and decreases with larger k. With k = 1, the prediction

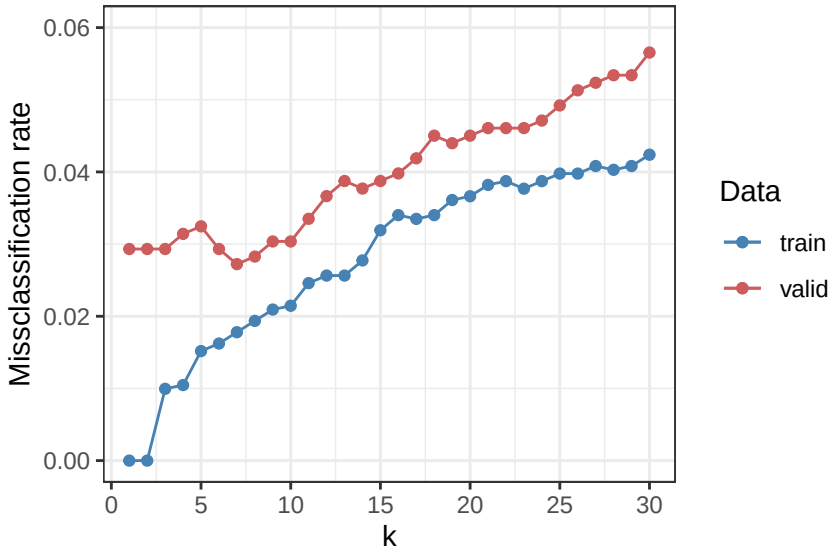


Figure 3: Misclassification errors for training and validation data for k=1,...,30 on model trained on training data.

in the model is by the observation in training data closest to the value we want to predict and when k is equal to the number of observations, the model will always predict the same value (except situations with ties). The training error increases when the model complexity decreases, this is because the model will be less overfitted on the training data with larger k and after some k, the model will be underfitted. Validation error also generally increased when the model complexity decreased, however at some k, the model will be between overfitted and underfitted which will give lowest validation error. This happened at k=7, which is considered to be the optimal k.

```
which(result$valid == min(result$valid))
```

```
## [1] 7
```

With k=7, the error for the test data is calculated. The errors for training, validation, and test data are compared in table 3.

```
model_test_7 <- kknn(formula = y~., train = train, test = test, kernel = "rectangular", k=7)

conf_mat_test <- table(model_test_7$fitted.values, test$y)
acc_test <- sum(diag(conf_mat_test)) / sum(conf_mat_test)
miss_test <- 1-acc_test

table_data <- cbind(training=result[7, 1], validation=result[7, 2], test=miss_test)
kable(table_data, digits=3, caption="Misclassification error k=7 for different data.")
```

Table 3: Misclassification error k=7 for different data.

training	validation	test
0.018	0.027	0.039

In table 3, the error for training is the lowest, followed by validation, and then test. Since the error for training is decently lower the model is a bit overfitted on training data. The difference between validation and test can be interpreted that for k=7 the error is smallest for the validation data, but it might not be the best since there is a bias when picking k from validation data.

1.5 1.5

Question: Fit K-nearest neighbor classifiers to the training data for different values of $K = 1, 2, ..., 30$, compute the error for the validation data as cross-entropy (when computing log of probabilities add a small constant within log, e.g. 1e-15, to avoid numerical problems) and plot the dependence of the validation error on the value of K. What is the optimal K value here? Assuming that response has multinomial distribution, why might the cross-entropy be a more suitable choice of the error function than the misclassification error for this problem?

Answer: The code used to compute cross-entropy for validation data

```
cross_entropy <- function(k){
  model_kknn_valid <-
    kknn(formula = y~.,
         train = train,
         test = valid,
         kernel = "rectangular",
         k=k)

  y <- as.integer(valid$y)

  prob <- c()
  for(i in 1:length(y)){
    prob[i] <- model_kknn_valid$prob[i, y[i]]
  }

  value <- -sum(log(prob + 1e-15))
  return(value)
}

result <- c()
for(i in 1:30){
  model <- cross_entropy(i)
  result[i] <- model
}
```

The cross-entropy for different k is presented in figure 4.

```
plot_data <- data.frame(index=1:30, result)
ggplot(plot_data, aes(x=index, y=result)) +
  geom_point(color="forestgreen") +
  geom_line(color="forestgreen") +
  scale_x_continuous(breaks = c(seq(from=0, to=30, by=5))) +
  theme_bw() +
  labs(x="K",
       y="Cross-entropy")
```

```
which(min(result) == result)
```

```
## [1] 8
```

From figure 4, the model with k=8 has the lowest value for cross-entropy and is considered to be the best k.

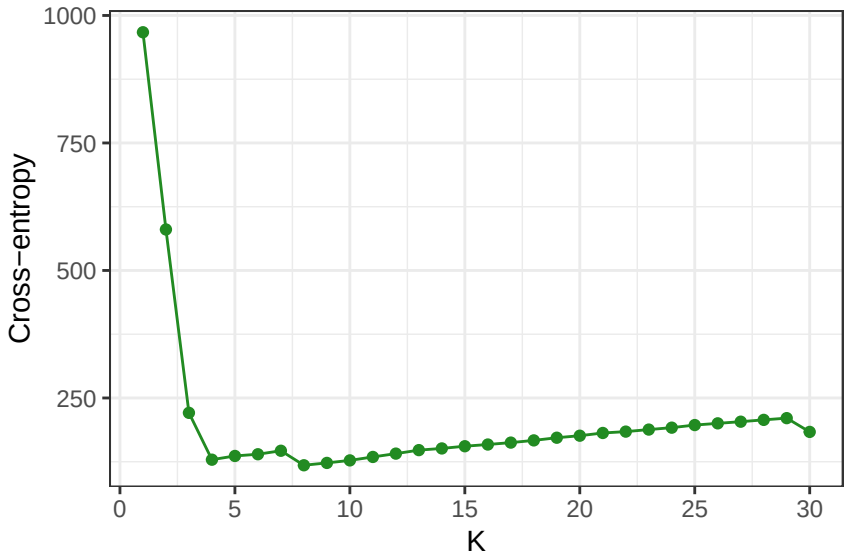


Figure 4: Cross-entropy error for validation data for different values of k for kknn models.

If the response has multinomial distribution, the maximum likelihood estimation is:

$$L(Y_i = C_1, Y_i = C_2, ..., Y_i = C_m|\theta) = \prod_{i=1}^{N} p_\theta(Y_i = C_m) \tag{1}$$

where Y_i is observation i, N is number of observations, and C_m is class m.

The log-likelihood of equation 1 is:

$$logL(Y_i = C_1, Y_i = C_2, ..., Y_i = C_m) = \sum_{i=1}^{N} logp_\theta(Y_i = C_m) \tag{2}$$

2 Assignment 2

```
df2 <- read.csv("parkinsons.csv")

# Shuffle the data
set.seed(123)
df2 <- df2[sample(nrow(df2)), ]
```

2.1 Question 1,2)

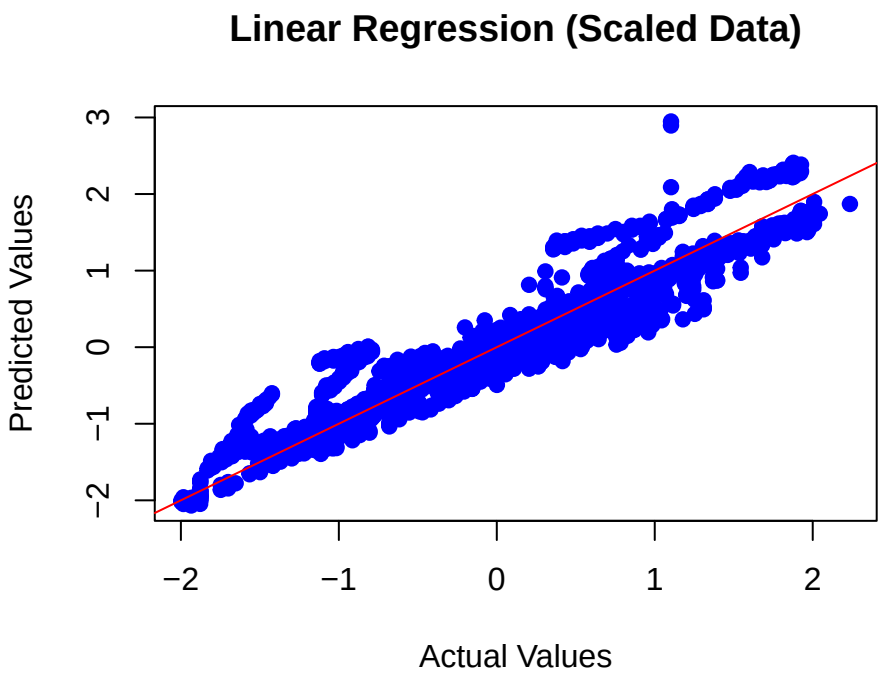
```
set.seed(123)
# Split train and test
train_indices <- createDataPartition(df2$motor_UPDRS, p = 0.6, list = FALSE)
train_data <- df2[train_indices, ]
test_data <- df2[-train_indices, ]

predictor_cols <- setdiff(names(train_data), "motor_UPDRS")
scaler <- preProcess(train_data)
trainS <- predict(scaler, train_data)
testS <- predict(scaler, test_data)

#train_sd <- apply(train_data, 2, sd)

# Linear regression model
lm_model <- lm(motor_UPDRS ~ ., data = trainS)

# Predictions on the test data
trainS_x <- trainS[, predictor_cols]
testS_x <- testS[, predictor_cols]

predS_train <- predict(lm_model, newdata = trainS_x)
predS_test <- predict(lm_model, newdata = testS_x)

mse_train <- mean((trainS$motor_UPDRS - predS_train)^2)
mse_test <- mean((testS$motor_UPDRS - predS_test)^2)

cat("Mean Squared Error (MSE) on the training data:", mse_train, "\n")
```

```
## Mean Squared Error (MSE) on the training data: 0.09478013
```

```
cat("Mean Squared Error (MSE) on the test data:", mse_test, "\n")
```

```
## Mean Squared Error (MSE) on the test data: 0.09364679
```

```
plot(testS$motor_UPDRS, predS_test, main = "Linear Regression (Scaled Data)",
     xlab = "Actual Values", ylab = "Predicted Values", pch = 19, col = "blue")
abline(a = 0, b = 1, col = "red")
```



2.2 Question 3)

```r
# Define the functions
Loglikelihood <- function(theta, std){
  n <- nrow(trainS_x)
  prediction <- as.matrix(trainS_x) %*% as.matrix(theta)
  actual <- trainS$motor_UPDRS
  res <- actual-prediction
  likelihood <- (-(n/2) * log(2*pi*std^2) - (1/(2*std^2)) * sum(res^2))
  return(likelihood)
}

Ridge <- function(theta, std, lambda){
  likelihood_ridge <- -Loglikelihood(theta, std) + (lambda/2)*sum(theta^2)
  return(likelihood_ridge)
}

#optim() function minimizes
RidgeOpt <- function(lambda){
  # Define a new function to optimize
  my_fnc <- function(parameters){
    theta <- parameters[1:(length(parameters)-1)]
    std <- parameters[length(parameters)]
    return(Ridge(theta, std, lambda))
  }
  initial_values <- c(rep(0, ncol(trainS_x)), 1)
```

```
  optimal_values <- optim(par = initial_values, fn = my_fnc, method = "BFGS")$par
  optimal_theta <- optimal_values[1:length(predictor_cols)]
  optimal_std <- optimal_values[length(predictor_cols) + 1]
  optimal_lambda <- optimal_values[length(optimal_values)]

  result_list <- list(theta = optimal_theta, std = optimal_std, lambda = optimal_lambda)
  return(result_list)
}
```

Formula for the degree of freedom in ridge regression is as follows:

$$df(\lambda) = trace(X(X^T X + \lambda I)^{-1} X^T)$$

```
library(psych)
DF <- function(lambda){
  X <- as.matrix(trainS_x)
  dof <- tr(X %*% (solve(t(X) %*% X + lambda*diag(ncol(trainS_x)))) %*% t(X))
  return(dof)
}
```

2.3 Question 4)

```
lambda <- 1
result_ridge_1 <- RidgeOpt(lambda)

optimal_theta_1 <- result_ridge_1$theta
optimal_std_1 <- result_ridge_1$std
optimal_lambda_1 <- result_ridge_1$lambda

ridge_pred_train_1 <- as.matrix(trainS_x) %*% as.matrix(optimal_theta_1)
ridge_pred_test_1 <- as.matrix(testS_x) %*% as.matrix(optimal_theta_1)

mse_ridge_train_1 <- mean((trainS$motor_UPDRS - ridge_pred_train_1)^2)
mse_ridge_test_1 <- mean((testS$motor_UPDRS - ridge_pred_test_1)^2)

cat("Lambda:", lambda, "\n")
```

```
## Lambda: 1
```

```
cat("Mean Squared Error (MSE) ridge regression on training data:", mse_ridge_train_1, "\n")
```

```
## Mean Squared Error (MSE) ridge regression on training data: 0.09481838
```

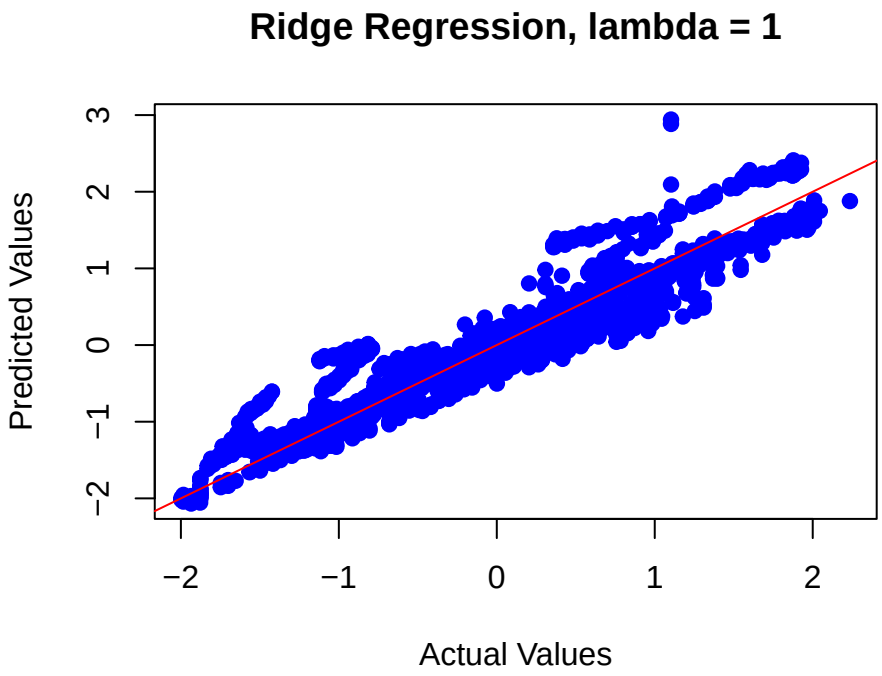
```
cat("Mean Squared Error (MSE) ridge regression on test data:", mse_ridge_test_1, "\n")
```

```
## Mean Squared Error (MSE) ridge regression on test data: 0.09360224
```

```
cat("Degree of freedom:", DF(lambda), "\n")
```

```
## Degree of freedom: 18.84537
```

```
plot(testS$motor_UPDRS, ridge_pred_test_1, main = "Ridge Regression, lambda = 1",
     xlab = "Actual Values", ylab = "Predicted Values", pch = 19, col = "blue")
abline(a = 0, b = 1, col = "red")
```




```
lambda <- 100
result_ridge_100 <- RidgeOpt(lambda)

optimal_theta_100 <- result_ridge_100$theta
optimal_std_100 <- result_ridge_100$std
optimal_lambda_100 <- result_ridge_100$lambda

ridge_pred_train_100 <- as.matrix(trainS_x) %*% as.matrix(optimal_theta_100)
ridge_pred_test_100 <- as.matrix(testS_x) %*% as.matrix(optimal_theta_100)

mse_ridge_train_100 <- mean((trainS$motor_UPDRS - ridge_pred_train_100)^2)
mse_ridge_test_100 <- mean((testS$motor_UPDRS - ridge_pred_test_100)^2)

cat("Lambda:", lambda, "\n")
```

```
## Lambda: 100
```

```
cat("Mean Squared Error (MSE) ridge regression on training data:", mse_ridge_train_100, "\n")
```

```
## Mean Squared Error (MSE) ridge regression on training data: 0.09487141
```

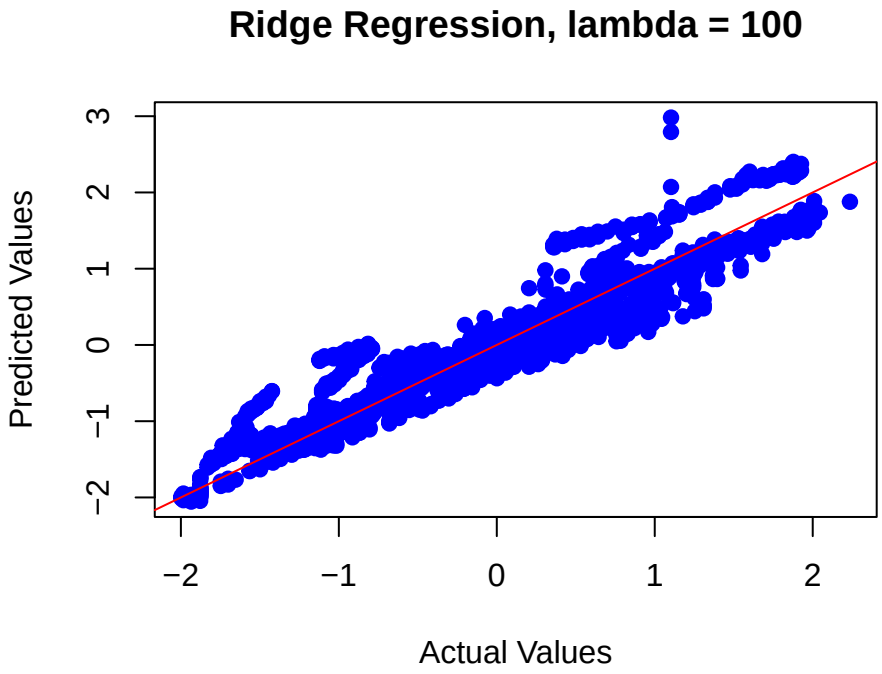
```
cat("Mean Squared Error (MSE) ridge regression on test data:", mse_ridge_test_100, "\n")
```

```
## Mean Squared Error (MSE) ridge regression on test data: 0.09361211
```

```r
cat("Degree of freedom:", DF(lambda), "\n")
```

```
## Degree of freedom: 14.61243
```

```r
plot(testS$motor_UPDRS, ridge_pred_test_100, main = "Ridge Regression, lambda = 100",
     xlab = "Actual Values", ylab = "Predicted Values", pch = 19, col = "blue")
abline(a = 0, b = 1, col = "red")
```




```r
lambda <- 1000
result_ridge_1000 <- RidgeOpt(lambda)

optimal_theta_1000 <- result_ridge_1000$theta
optimal_std_1000 <- result_ridge_1000$std
optimal_lambda_1000 <- result_ridge_1000$lambda

ridge_pred_train_1000 <- as.matrix(trainS_x) %*% as.matrix(optimal_theta_1000)
ridge_pred_test_1000 <- as.matrix(testS_x) %*% as.matrix(optimal_theta_1000)

mse_ridge_train_1000 <- mean((trainS$motor_UPDRS - ridge_pred_train_1000)^2)
mse_ridge_test_1000 <- mean((testS$motor_UPDRS - ridge_pred_test_1000)^2)

cat("Lambda:", lambda, "\n")
```

```
## Lambda: 1000
```

```r
cat("Mean Squared Error (MSE) ridge regression on training data:", mse_ridge_train_1000, "\n")
```

```
## Mean Squared Error (MSE) ridge regression on training data: 0.09621063
```

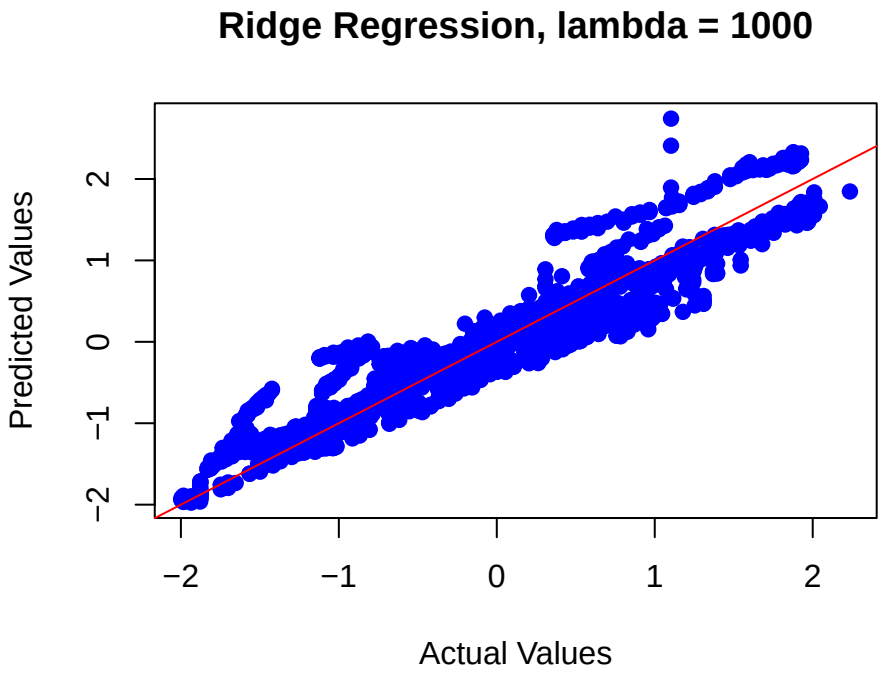
```
cat("Mean Squared Error (MSE) ridge regression on test data:", mse_ridge_test_1000, "\n")
```

```
## Mean Squared Error (MSE) ridge regression on test data: 0.09423032
```

```
cat("Degree of freedom:", DF(lambda), "\n")
```

```
## Degree of freedom: 9.222909
```

```
plot(testS$motor_UPDRS, ridge_pred_test_1000, main = "Ridge Regression, lambda = 1000",
     xlab = "Actual Values", ylab = "Predicted Values", pch = 19, col = "blue")
abline(a = 0, b = 1, col = "red")
```



As lambda increases, the degrees of freedom decreases and the MSE increases

3 Assignment 3. Logistic regression and basis function expansion

3.1 Data

The data contains information about the onset of diabetes within 5 years in Pima Indians given medical details. The variables are:

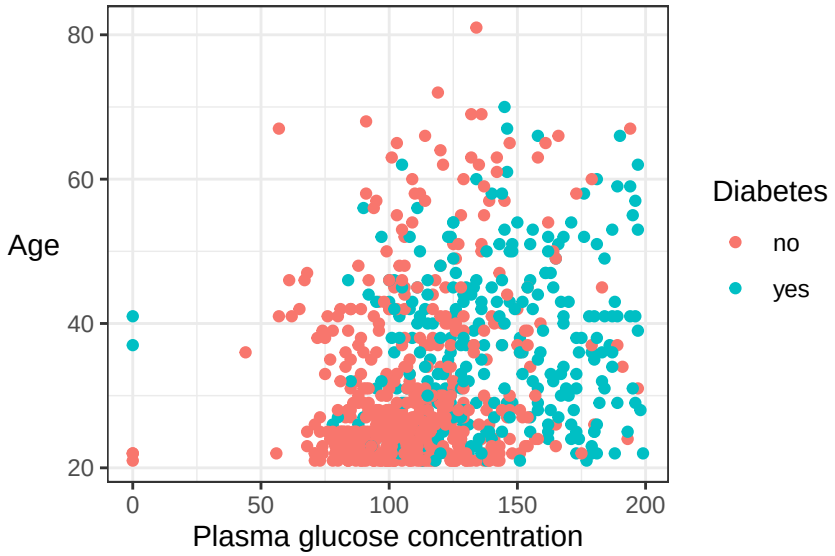
- Number of times pregnant
- Plasma glucose concentration a 2 hours in an oral glucose tolerance test.
- Diastolic blood pressure (mm Hg).
- Triceps skinfold thickness (mm).
- 2-Hour serum insulin (mu U/ml).
- Body mass index (weight in kg/(height in m)^2).
- Diabetes pedigree function.
- Age (years).
- Diabetes (0=no or 1=yes).

```
diabetes_df <- read.csv("pima-indians-diabetes.csv", header=FALSE)

colnames(diabetes_df) <- c("times_pregnant", "plasma_glucose_conc",
                           "diastolic_blood_pressure", "triceps_skinfold_thickness",
                           "serum_insulin","body_mass_index", "diabetes_pedigree",
                           "age", "diabetes")

diabetes_df$diabetes <- ifelse(diabetes_df$diabetes == 0, "no", "yes")
diabetes_df$diabetes <- as.factor(diabetes_df$diabetes)
```

3.2 3.1

Question: Make a scatterplot showing a Plasma glucose concentration on Age where observations are colored by Diabetes levels.

```
library(ggplot2)

ggplot(diabetes_df, aes(x = plasma_glucose_conc, y = age, color = diabetes)) +
  geom_point() +
  theme_bw() +
  theme(axis.title.y = element_text(angle = 0,vjust = 0.5)) +
  labs(colour = "Diabetes",
       x = "Plasma glucose concentration",
       y = "Age")
```



Question: Do you think that Diabetes is easy to classify by a standard logistic regression model that uses these two variables as features? Motivate your answer.

We don't think these two variables are good variables to classify Diabetes because there is no clear relationship between age, plasma glucose concentration with Diabetes.

3.3 3.2

Question:

Train a logistic regression model with y = Diabetes as target x_1 = Plasma glucose concentration and x_2 = Age as features and make a prediction for all observations by using $r = 0.5$ as the classification threshold. Report the probabilistic equation of the estimated model and compute also the training misclassification error.

The probabilistic equation:

$$$$

```
model <- glm(diabetes ~ plasma_glucose_conc + age, data = diabetes_df,
             family =  "binomial")

pred <- predict(model, newdata = diabetes_df, type = "response")

# Using 0.5 as the classification threshold
pred <- ifelse(pred > 0.5, "yes", "no")

confusion <- table(diabetes_df$diabetes, pred)
misclass_rate <- (confusion[1,2] + confusion[2,1]) / sum(confusion)


knitr::kable(as.data.frame(round(misclass_rate,2)), col.names = "Misclassification error",
             caption = "Misclassification error")
```

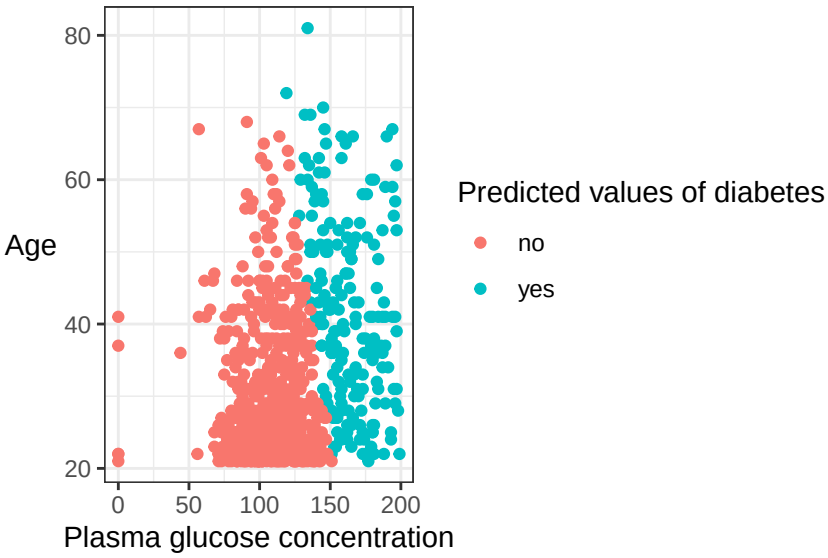
Table 4: Misclassification error

Misclassification error
0.26

Question:

Make a scatter plot of the same kind as in step 1 but showing the predicted values of Diabetes as a color instead.

```
diabetes_df_pred <- diabetes_df
diabetes_df_pred$pred <- pred

ggplot(diabetes_df_pred, aes(x = plasma_glucose_conc, y = age, color = pred)) +
  geom_point() +
  theme_bw() +
  theme(axis.title.y = element_text(angle = 0,vjust = 0.5)) +
  labs(colour = "Predicted values of diabetes",
       x = "Plasma glucose concentration",
       y = "Age")
```



Question:

Comment on the quality of the classification by using these results.

3.4 3.3

Question:

Use the model estimated in step 2 to a) report the equation of the decision boundary between the two classes b) add a curve showing this boundary to the scatter plot in step 2.

The decision boundary equation:

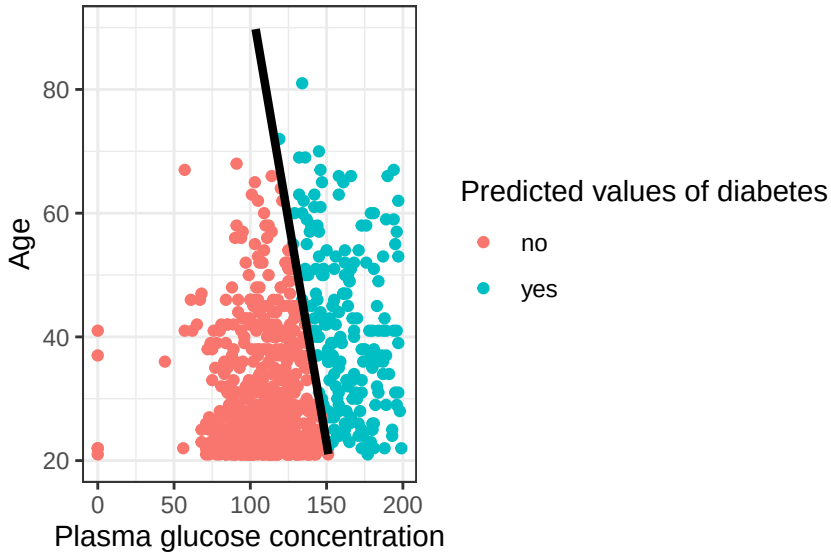
$\beta_0 + \beta_1 \cdot$ plasma glucos econc

```
summary(model)
```

```
##
## Call:
## glm(formula = diabetes ~ plasma_glucose_conc + age, family = "binomial",
##     data = diabetes_df)
##
## Deviance Residuals:
##     Min       1Q   Median       3Q      Max
## -2.3367  -0.7775  -0.5087   0.8367   3.1630
##
## Coefficients:
##                       Estimate Std. Error z value Pr(>|z|)
## (Intercept)         -5.912449   0.462620  -12.78  < 2e-16 ***
## plasma_glucose_conc  0.035644   0.003290   10.83  < 2e-16 ***
## age                  0.024778   0.007374    3.36 0.000778 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## (Dispersion parameter for binomial family taken to be 1)
##
##     Null deviance: 993.48  on 767  degrees of freedom
## Residual deviance: 797.36  on 765  degrees of freedom
## AIC: 803.36
##
## Number of Fisher Scoring iterations: 4
```

```
slope <- coef(model)[2]/(-coef(model)[3])
intercept <- coef(model)[1]/(-coef(model)[3])


# diabetes_df < commented this, do we need it?


 #coef(model)[1] + t(as.matrix(coef(model)[2:3])) %*% as.matrix(diabetes_df[,c("plasma_glucose_conc","ag

ggplot(diabetes_df_pred, aes(x = plasma_glucose_conc, y = age, color = pred)) +
  geom_point() +
  theme_bw() +
 stat_function(fun = ({function(x) (-coef(model)[1] - coef(model)[2]*x)/ coef(model)[3] }),
               size=1.5, color = "black") +
  ylim(20,90) +
  labs(colour = "Predicted values of diabetes",
       x = "Plasma glucose concentration",
       y = "Age")
```

```
## Warning: Removed 76 row(s) containing missing values (geom_path).
```



Question:

Comment whether the decision boundary seems to catch the data distribution well.

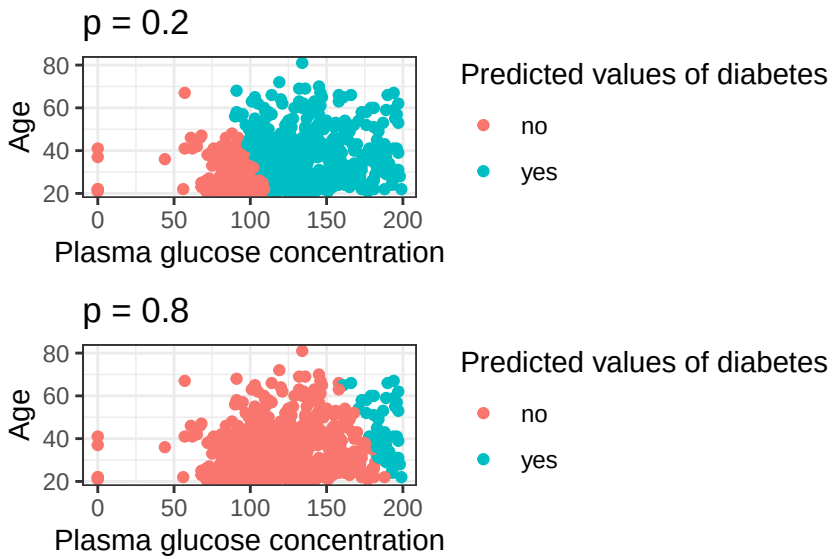
3.5 3.4

Question:

Make same kind of plots as in step 2 but use thresholds $r = 0.2$ and $r = 0.8$. By using these plots

```
library("ggpubr")

# Using 0.2 as the classification threshold
pred <- predict(model, newdata = diabetes_df, type = "response")
pred <- ifelse(pred > 0.2, "yes", "no")
diabetes_df_pred$pred <- pred


p1 <- ggplot(diabetes_df_pred, aes(x = plasma_glucose_conc, y = age, color = pred)) +
      geom_point() +
      theme_bw() +
      labs(colour = "Predicted values of diabetes",
           x = "Plasma glucose concentration",
           y = "Age") +
      ggtitle("p = 0.2")


# Using 0.8 as the classification threshold
pred <- predict(model, newdata = diabetes_df, type = "response")
pred <- ifelse(pred > 0.8, "yes", "no")
diabetes_df_pred$pred <- pred
```

```
p2 <- ggplot(diabetes_df_pred, aes(x = plasma_glucose_conc, y = age, color = pred)) +
      geom_point() +
      theme_bw() +
      labs(colour = "Predicted values of diabetes",
           x = "Plasma glucose concentration",
           y = "Age") +
  ggtitle("p = 0.8")


ggarrange(p1, p2,  ncol = 1, nrow = 2)
```



Question:

Comment on what happens with the prediction when r value changes.

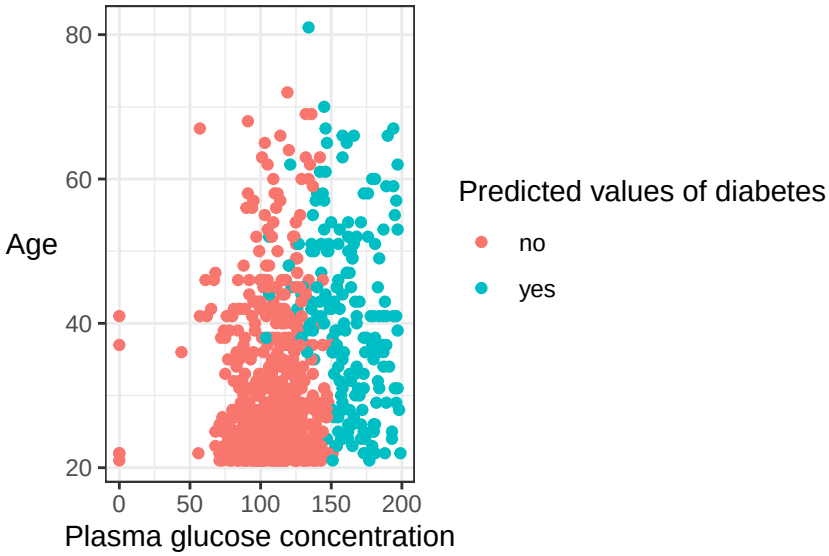
3.6 3.5

Question:

Perform a basis function expansion trick by computing new features $z_1 = x_1^4$, $z_2 = x_1^3 x^2$, $z_3 = x_1^2 x_2^2$, $z_4 = x_1 x_2^3$, $z_5 = x_2^4$, adding them to the data set and then computing a logistic regression model with y as target and $x_1, x_2, z_1, ..., z_5$ as features. Create a scatterplot of the same kind as in step 2 for this model.

```
diabetes_df$z1  <- diabetes_df$times_pregnant^4
diabetes_df$z2  <- diabetes_df$times_pregnant^3 * diabetes_df$plasma_glucose_conc^2
diabetes_df$z3  <- diabetes_df$times_pregnant^2 * diabetes_df$plasma_glucose_conc^2
diabetes_df$z4  <- diabetes_df$times_pregnant * diabetes_df$plasma_glucose_conc^3
diabetes_df$z5  <- diabetes_df$plasma_glucose_conc^4


model <- glm(diabetes ~ plasma_glucose_conc + age + z1 + z2 + z3 + z4 + z5, data = diabetes_df,
             family =  "binomial")
```

```r
pred <- predict(model, newdata = diabetes_df, type = "response")

# Using 0.5 as the classification threshold
pred <- ifelse(pred > 0.5, "yes", "no")

diabetes_df_pred <- diabetes_df
diabetes_df_pred$pred <- pred

ggplot(diabetes_df_pred, aes(x = plasma_glucose_conc, y = age, color = pred)) +
  geom_point() +
  theme_bw() +
  theme(axis.title.y = element_text(angle = 0,vjust = 0.5)) +
  labs(colour = "Predicted values of diabetes",
       x = "Plasma glucose concentration",
       y = "Age")
```



Question:

Compute the training misclassification rate. What can you say about the quality of this model compared to the previous logistic regression model? How have the basis expansion trick affected the shape of the decision boundary and the prediction accuracy?

4 Statement of Contribution

We worked on the assignment individually for the computer labs (to be more efficient when asking questions), Duc on task 1, Sigme on task 2, and William on task 3. We later solved all assignment individually and compared and discussed our solutions before dividing the task of writing the laboration report.

4.1 Question 1

Text written by Duc.

4.2 Question 2

Text written by Sigme.

4.3 Question 3

Text written by William.

5 Appendix

The code used in this laboration report are summarised in the code as follows:

```
library(ggplot2)
library(kknn)
library(dplyr)
library(knitr)
library(caret)
library(psych)
knitr::opts_chunk$set(
  echo = TRUE,
  fig.width = 4.5,
  fig.height = 3)
# Read in data
data <- read.csv("optdigits.csv")

# Renaming the response variable and changing it to a factor variable
data <- rename(data, y=X0.26)
data$y <- as.factor(data$y)

# Partitioning training data (50%)
n=dim(data)[1]
set.seed(12345)
id=sample(1:n, floor(n*0.5))
train=data[id,]

# Partitioning validation data (25%)
id1=setdiff(1:n, id)
set.seed(12345)
id2=sample(id1, floor(n*0.25))
valid=data[id2,]
```

```
# Partitioning test data (25%)
id3=setdiff(id1,id2)
test=data[id3,]
# kknn on training data and evaluation on training data
model_kknn_train <- kknn(formula=y~.,
                         train=train,
                         test=train,
                         kernel="rectangular",
                         k=30)
conf_mat_train <- table(train$y, model_kknn_train$fitted.values)
acc_train <- sum(diag(conf_mat_train)) / sum(conf_mat_train)
miss_train <- 1-acc_train

# kknn on training data and evaluation on test data
model_kknn_test <- kknn(formula=y~.,
                        train=train,
                        test=test,
                        kernel="rectangular",
                        k=30)
conf_mat_test <- table(test$y, model_kknn_test$fitted.values)
acc_test <- sum(diag(conf_mat_test)) / sum(conf_mat_test)
miss_test <- 1-acc_test

# Rows are true values, columns are model prediction
kable(conf_mat_train, caption = "Confusion matrix for training data, model
      predictions by columns and true value by rows.")
miss_train
kable(conf_mat_test, caption = "Confusion matrix for test data, model
      predictions by columns and true value by rows.")
miss_test
y <- train$y
fit_y <- model_kknn_train$fitted.values
# probabilities given from number 0 to 9, index 9 = number 8.
prob_8 <- model_kknn_train$prob[, 9]

# Data frame consisting of true value of y, model prediction and the models
# probability that the number is 8.
data_8 <- data.frame(y = y, fit_y = fit_y, prob = prob_8)
data_8$observation_id <- rownames(data_8)

# Only observations with the label 8 is kept.
data_8 <- data_8[data_8$y == "8", ]
head(arrange(data_8, prob), 2)
tail(arrange(data_8, prob), 3)
# Change colour palette to black and white
colfunc <- colorRampPalette(c("white", "black"))

plot_8 <- function(index){
```

```
  title <- paste0("Obs: ", index)
  # Reshapes the observations to a 8x8
  plot <- as.matrix(train[index, -65]) # Remove response variable
  plot <- matrix(plot, nrow=8, byrow=TRUE)
  heatmap(plot, col=colfunc(16), Colv=NA, Rowv=NA, main=title, margins=c(2,2))
}
plot_8(1624)
plot_8(1663)
plot_8(1810)
plot_8(1811)
plot_8(1864)
fit_kknn <- function(k){
  model_kknn_train <- kknn(formula=y~., train=train, test=train, kernel="rectangular", k=k)
  # Confusion matrix for train data
  conf_mat_train <- table(model_kknn_train$fitted.values, train$y)
  acc_train <- sum(diag(conf_mat_train)) / sum(conf_mat_train)
  # Missclassification for training data
  miss_train <- 1-acc_train

  model_kknn_valid <- kknn(formula=y~., train=train, test=valid, kernel="rectangular", k=k)
  # Confusion matrix for validation data
  conf_mat_valid <- table(model_kknn_valid$fitted.values, valid$y)
  acc_valid <- sum(diag(conf_mat_valid)) / sum(conf_mat_valid)
  # Missclassification for validation data
  miss_valid <- 1-acc_valid

  result <- c(miss_train, miss_valid)
  return(result)
}

# Missclassification for k=1,...,30 for training and validation data
result <- data.frame(train = 0, valid = 0)
for(i in 1:30){
  model <- fit_kknn(i)
  result[i,1] <- model[1]
  result[i,2] <- model[2]
}
result$index <- 1:30
ggplot(result, aes(x=index)) +
  geom_line(aes(y=train, colour="train")) +
  geom_point(aes(y=train, colour="train")) +
  geom_line(aes(y=valid, colour="valid")) +
  geom_point(aes(y=valid, colour="valid")) +
  scale_color_manual(name = "Data",
                     values = c("train" = "steelblue", "valid" = "indianred")) +
  scale_x_continuous(breaks = c(seq(from=0, to=30, by=5))) +
  scale_y_continuous(limits = c(0, 0.06)) +
  theme_bw() +
  labs(x = "k",
```

```
       y = "Missclassification rate")
which(result$valid == min(result$valid))
model_test_7 <- kknn(formula = y~., train = train, test = test, kernel = "rectangular", k=7)

conf_mat_test <- table(model_test_7$fitted.values, test$y)
acc_test <- sum(diag(conf_mat_test)) / sum(conf_mat_test)
miss_test <- 1-acc_test

table_data <- cbind(training=result[7, 1], validation=result[7, 2], test=miss_test)
kable(table_data, digits=3, caption="Misclassification error k=7 for different data.")
cross_entropy <- function(k){
  model_kknn_valid <-
    kknn(formula = y~.,
         train = train,
         test = valid,
         kernel = "rectangular",
         k=k)

  y <- as.integer(valid$y)

  prob <- c()
  for(i in 1:length(y)){
    prob[i] <- model_kknn_valid$prob[i, y[i]]
  }

  value <- -sum(log(prob + 1e-15))
  return(value)
}

result <- c()
for(i in 1:30){
  model <- cross_entropy(i)
  result[i] <- model
}
plot_data <- data.frame(index=1:30, result)
ggplot(plot_data, aes(x=index, y=result)) +
  geom_point(color="forestgreen") +
  geom_line(color="forestgreen") +
  scale_x_continuous(breaks = c(seq(from=0, to=30, by=5))) +
  theme_bw() +
  labs(x="K",
       y="Cross-entropy")
which(min(result) == result)
df2 <- read.csv("parkinsons.csv")

# Shuffle the data
set.seed(123)
df2 <- df2[sample(nrow(df2)), ]
set.seed(123)
```

```r
# Split train and test
train_indices <- createDataPartition(df2$motor_UPDRS, p = 0.6, list = FALSE)
train_data <- df2[train_indices, ]
test_data <- df2[-train_indices, ]

predictor_cols <- setdiff(names(train_data), "motor_UPDRS")
scaler <- preProcess(train_data)
trainS <- predict(scaler, train_data)
testS <- predict(scaler, test_data)

#train_sd <- apply(train_data, 2, sd)

# Linear regression model
lm_model <- lm(motor_UPDRS ~ ., data = trainS)

# Predictions on the test data
trainS_x <- trainS[, predictor_cols]
testS_x <- testS[, predictor_cols]

predS_train <- predict(lm_model, newdata = trainS_x)
predS_test <- predict(lm_model, newdata = testS_x)

mse_train <- mean((trainS$motor_UPDRS - predS_train)^2)
mse_test <- mean((testS$motor_UPDRS - predS_test)^2)

cat("Mean Squared Error (MSE) on the training data:", mse_train, "\n")
cat("Mean Squared Error (MSE) on the test data:", mse_test, "\n")
plot(testS$motor_UPDRS, predS_test, main = "Linear Regression (Scaled Data)",
     xlab = "Actual Values", ylab = "Predicted Values", pch = 19, col = "blue")
abline(a = 0, b = 1, col = "red")
# Define the functions
Loglikelihood <- function(theta, std){
  n <- nrow(trainS_x)
  prediction <- as.matrix(trainS_x) %*% as.matrix(theta)
  actual <- trainS$motor_UPDRS
  res <- actual-prediction
  likelihood <- (-(n/2) * log(2*pi*std^2) - (1/(2*std^2)) * sum(res^2))
  return(likelihood)
}

Ridge <- function(theta, std, lambda){
  likelihood_ridge <- -Loglikelihood(theta, std) + (lambda/2)*sum(theta^2)
  return(likelihood_ridge)
}

#optim() function minimizes
RidgeOpt <- function(lambda){
  # Define a new function to optimize
  my_fnc <- function(parameters){
```

```
    theta <- parameters[1:(length(parameters)-1)]
    std <- parameters[length(parameters)]
    return(Ridge(theta, std, lambda))
  }
  initial_values <- c(rep(0, ncol(trainS_x)), 1)

  optimal_values <- optim(par = initial_values, fn = my_fnc, method = "BFGS")$par
  optimal_theta <- optimal_values[1:length(predictor_cols)]
  optimal_std <- optimal_values[length(predictor_cols) + 1]
  optimal_lambda <- optimal_values[length(optimal_values)]

  result_list <- list(theta = optimal_theta, std = optimal_std, lambda = optimal_lambda)
  return(result_list)
}
library(psych)
DF <- function(lambda){
  X <- as.matrix(trainS_x)
  dof <- tr(X %*% (solve(t(X) %*% X + lambda*diag(ncol(trainS_x)))) %*% t(X))
  return(dof)
}
lambda <- 1
result_ridge_1 <- RidgeOpt(lambda)

optimal_theta_1 <- result_ridge_1$theta
optimal_std_1 <- result_ridge_1$std
optimal_lambda_1 <- result_ridge_1$lambda

ridge_pred_train_1 <- as.matrix(trainS_x) %*% as.matrix(optimal_theta_1)
ridge_pred_test_1 <- as.matrix(testS_x) %*% as.matrix(optimal_theta_1)

mse_ridge_train_1 <- mean((trainS$motor_UPDRS - ridge_pred_train_1)^2)
mse_ridge_test_1 <- mean((testS$motor_UPDRS - ridge_pred_test_1)^2)

cat("Lambda:", lambda, "\n")
cat("Mean Squared Error (MSE) ridge regression on training data:", mse_ridge_train_1, "\n")
cat("Mean Squared Error (MSE) ridge regression on test data:", mse_ridge_test_1, "\n")
cat("Degree of freedom:", DF(lambda), "\n")
plot(testS$motor_UPDRS, ridge_pred_test_1, main = "Ridge Regression, lambda = 1",
     xlab = "Actual Values", ylab = "Predicted Values", pch = 19, col = "blue")
abline(a = 0, b = 1, col = "red")
lambda <- 100
result_ridge_100 <- RidgeOpt(lambda)

optimal_theta_100 <- result_ridge_100$theta
optimal_std_100 <- result_ridge_100$std
optimal_lambda_100 <- result_ridge_100$lambda

ridge_pred_train_100 <- as.matrix(trainS_x) %*% as.matrix(optimal_theta_100)
ridge_pred_test_100 <- as.matrix(testS_x) %*% as.matrix(optimal_theta_100)
```

```
mse_ridge_train_100 <- mean((trainS$motor_UPDRS - ridge_pred_train_100)^2)
mse_ridge_test_100 <- mean((testS$motor_UPDRS - ridge_pred_test_100)^2)

cat("Lambda:", lambda, "\n")
cat("Mean Squared Error (MSE) ridge regression on training data:", mse_ridge_train_100, "\n")
cat("Mean Squared Error (MSE) ridge regression on test data:", mse_ridge_test_100, "\n")
cat("Degree of freedom:", DF(lambda), "\n")
plot(testS$motor_UPDRS, ridge_pred_test_100, main = "Ridge Regression, lambda = 100",
     xlab = "Actual Values", ylab = "Predicted Values", pch = 19, col = "blue")
abline(a = 0, b = 1, col = "red")
lambda <- 1000
result_ridge_1000 <- RidgeOpt(lambda)

optimal_theta_1000 <- result_ridge_1000$theta
optimal_std_1000 <- result_ridge_1000$std
optimal_lambda_1000 <- result_ridge_1000$lambda

ridge_pred_train_1000 <- as.matrix(trainS_x) %*% as.matrix(optimal_theta_1000)
ridge_pred_test_1000 <- as.matrix(testS_x) %*% as.matrix(optimal_theta_1000)

mse_ridge_train_1000 <- mean((trainS$motor_UPDRS - ridge_pred_train_1000)^2)
mse_ridge_test_1000 <- mean((testS$motor_UPDRS - ridge_pred_test_1000)^2)

cat("Lambda:", lambda, "\n")
cat("Mean Squared Error (MSE) ridge regression on training data:", mse_ridge_train_1000, "\n")
cat("Mean Squared Error (MSE) ridge regression on test data:", mse_ridge_test_1000, "\n")
cat("Degree of freedom:", DF(lambda), "\n")
plot(testS$motor_UPDRS, ridge_pred_test_1000, main = "Ridge Regression, lambda = 1000",
     xlab = "Actual Values", ylab = "Predicted Values", pch = 19, col = "blue")
abline(a = 0, b = 1, col = "red")

diabetes_df <- read.csv("pima-indians-diabetes.csv", header=FALSE)

colnames(diabetes_df) <- c("times_pregnant", "plasma_glucose_conc",
                           "diastolic_blood_pressure", "triceps_skinfold_thickness",
                           "serum_insulin","body_mass_index", "diabetes_pedigree",
                           "age", "diabetes")

diabetes_df$diabetes <- ifelse(diabetes_df$diabetes == 0, "no", "yes")
diabetes_df$diabetes <- as.factor(diabetes_df$diabetes)



library(ggplot2)

ggplot(diabetes_df, aes(x = plasma_glucose_conc, y = age, color = diabetes)) +
  geom_point() +
  theme_bw() +
```

```
  theme(axis.title.y = element_text(angle = 0,vjust = 0.5)) +
  labs(colour = "Diabetes",
       x = "Plasma glucose concentration",
       y = "Age")


model <- glm(diabetes ~ plasma_glucose_conc + age, data = diabetes_df,
             family =  "binomial")

pred <- predict(model, newdata = diabetes_df, type = "response")

# Using 0.5 as the classification threshold
pred <- ifelse(pred > 0.5, "yes", "no")

confusion <- table(diabetes_df$diabetes, pred)
misclass_rate <- (confusion[1,2] + confusion[2,1]) / sum(confusion)


knitr::kable(as.data.frame(round(misclass_rate,2)), col.names = "Misclassification error",
             caption = "Misclassification error")


diabetes_df_pred <- diabetes_df
diabetes_df_pred$pred <- pred

ggplot(diabetes_df_pred, aes(x = plasma_glucose_conc, y = age, color = pred)) +
  geom_point() +
  theme_bw() +
  theme(axis.title.y = element_text(angle = 0,vjust = 0.5)) +
  labs(colour = "Predicted values of diabetes",
       x = "Plasma glucose concentration",
       y = "Age")



summary(model)

slope <- coef(model)[2]/(-coef(model)[3])
intercept <- coef(model)[1]/(-coef(model)[3])


# diabetes_df < commented this, do we need it?


 #coef(model)[1] + t(as.matrix(coef(model)[2:3])) %*% as.matrix(diabetes_df[,c("plasma_glucose_conc","ag

ggplot(diabetes_df_pred, aes(x = plasma_glucose_conc, y = age, color = pred)) +
  geom_point() +
  theme_bw() +
```

```
 stat_function(fun = ({function(x) (-coef(model)[1] - coef(model)[2]*x)/ coef(model)[3] }),
               size=1.5, color = "black") +
  ylim(20,90) +
  labs(colour = "Predicted values of diabetes",
       x = "Plasma glucose concentration",
       y = "Age")


library("ggpubr")

# Using 0.2 as the classification threshold
pred <- predict(model, newdata = diabetes_df, type = "response")
pred <- ifelse(pred > 0.2, "yes", "no")
diabetes_df_pred$pred <- pred


p1 <- ggplot(diabetes_df_pred, aes(x = plasma_glucose_conc, y = age, color = pred)) +
      geom_point() +
      theme_bw() +
      labs(colour = "Predicted values of diabetes",
           x = "Plasma glucose concentration",
           y = "Age") +
      ggtitle("p = 0.2")


# Using 0.8 as the classification threshold
pred <- predict(model, newdata = diabetes_df, type = "response")
pred <- ifelse(pred > 0.8, "yes", "no")
diabetes_df_pred$pred <- pred


p2 <- ggplot(diabetes_df_pred, aes(x = plasma_glucose_conc, y = age, color = pred)) +
      geom_point() +
      theme_bw() +
      labs(colour = "Predicted values of diabetes",
           x = "Plasma glucose concentration",
           y = "Age") +
  ggtitle("p = 0.8")


ggarrange(p1, p2,  ncol = 1, nrow = 2)


diabetes_df$z1  <- diabetes_df$times_pregnant^4
diabetes_df$z2  <- diabetes_df$times_pregnant^3 * diabetes_df$plasma_glucose_conc^2
diabetes_df$z3  <- diabetes_df$times_pregnant^2 * diabetes_df$plasma_glucose_conc^2
diabetes_df$z4  <- diabetes_df$times_pregnant * diabetes_df$plasma_glucose_conc^3
diabetes_df$z5  <- diabetes_df$plasma_glucose_conc^4
```

```r
model <- glm(diabetes ~ plasma_glucose_conc + age + z1 + z2 + z3 + z4 + z5, data = diabetes_df,
             family =  "binomial")

pred <- predict(model, newdata = diabetes_df, type = "response")

# Using 0.5 as the classification threshold
pred <- ifelse(pred > 0.5, "yes", "no")

diabetes_df_pred <- diabetes_df
diabetes_df_pred$pred <- pred

ggplot(diabetes_df_pred, aes(x = plasma_glucose_conc, y = age, color = pred)) +
  geom_point() +
  theme_bw() +
  theme(axis.title.y = element_text(angle = 0,vjust = 0.5)) +
  labs(colour = "Predicted values of diabetes",
       x = "Plasma glucose concentration",
       y = "Age")
```