Machine Learning Lab1

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

Q1

See appendix.

Q2

```
## Confusion matrix for the training data:
```

```
##           train_predict
## train_true   0   1   2   3   4   5   6   7   8   9
##          0 202   0   0   0   0   0   0   0   0   0
##          1   0 179  11   0   0   0   0   1   1   3
##          2   0   1 190   0   0   0   0   1   0   0
##          3   0   0   0 185   0   1   0   1   0   1
##          4   1   3   0   0 159   0   0   7   1   4
##          5   0   0   0   1   0 171   0   1   0   8
##          6   0   2   0   0   0   0 190   0   0   0
##          7   0   3   0   0   0   0   0 178   1   0
##          8   0  10   0   2   0   0   2   0 188   2
##          9   1   3   0   5   2   0   0   3   3 183
```

```
## Confusion matrix for the test data:
```

```
##          test_predict
## test_true  0  1  2  3  4  5  6  7  8  9
##         0 82  0  0  0  1  0  1  0  0  0
##         1  0 90  2  0  0  0  0  0  0  3
##         2  0  1 92  0  0  0  0  1  1  1
##         3  0  0  0 85  0  2  0  3  1  1
##         4  0  1  0  0 89  0  1  6  0  5
##         5  0  1  0  1  0 97  1  1  0  7
##         6  0  0  0  0  0  0 97  0  0  0
##         7  0  1  0  1  0  0  0 99  0  0
##         8  0  7  0  0  0  0  0  0 84  0
##         9  0  2  0  0  0  0  0  2  1 86
```

```
## Misclassification error for the training data: 0.045
```

```
## Misclassification error for the test data: 0.05852
```

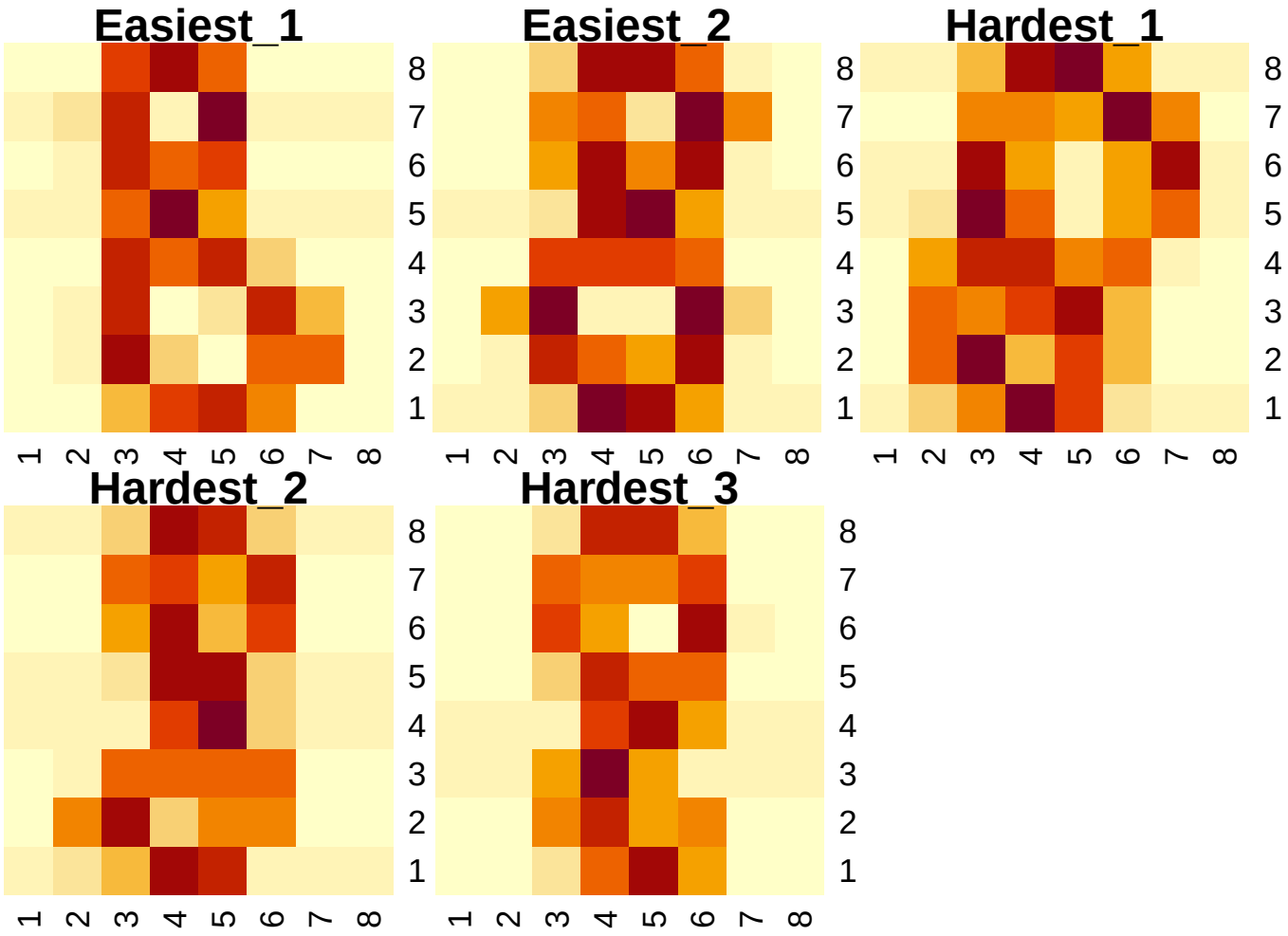
```
## Misclassification error for each digit in the test data:
```

```
##    digit error_rate
## 5      4 0.12745098
## 6      5 0.10185185
## 9      8 0.07692308
## 4      3 0.07608696
## 10     9 0.05494505
## 2      1 0.05263158
## 3      2 0.04166667
## 1      0 0.02380952
## 8      7 0.01980198
## 7      6 0.00000000
```

The model predicts 4 worst with 12.7 % error rate and predicts 6 best with 100 % accuracy. Both error rates for 4 and 5 are over 10 %, and error rates for 8, 3, 9, 1 are over 5 %. While, error rates for 2, 0, 7, 6 are below 5 %. Note that these error rates are computed based on the predictions on the test data.

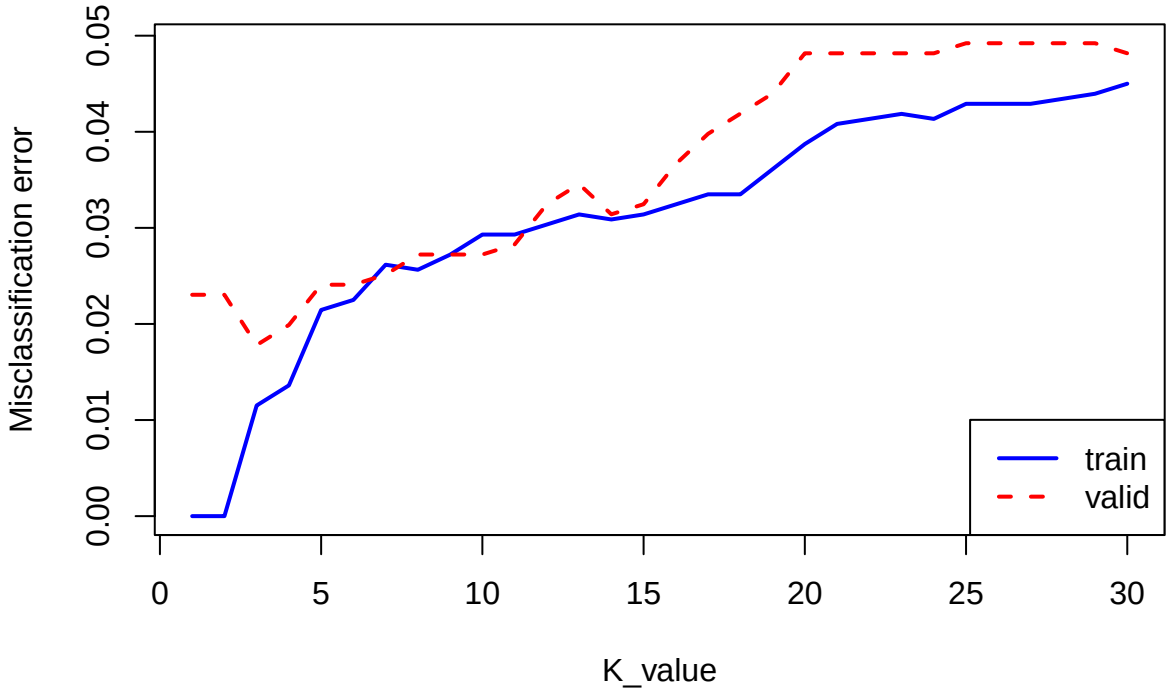
Besides, misclassification error for the test data is 5.852 %. It is not bad but still has improvement room.

Q3



The two cases in the easiest group are easy to recognize as 8 visually. While, for the first two cases in the hardest group, they can recognize 8 roughly. But for the third one, it is quite hard to tell what digit it is.

Q4



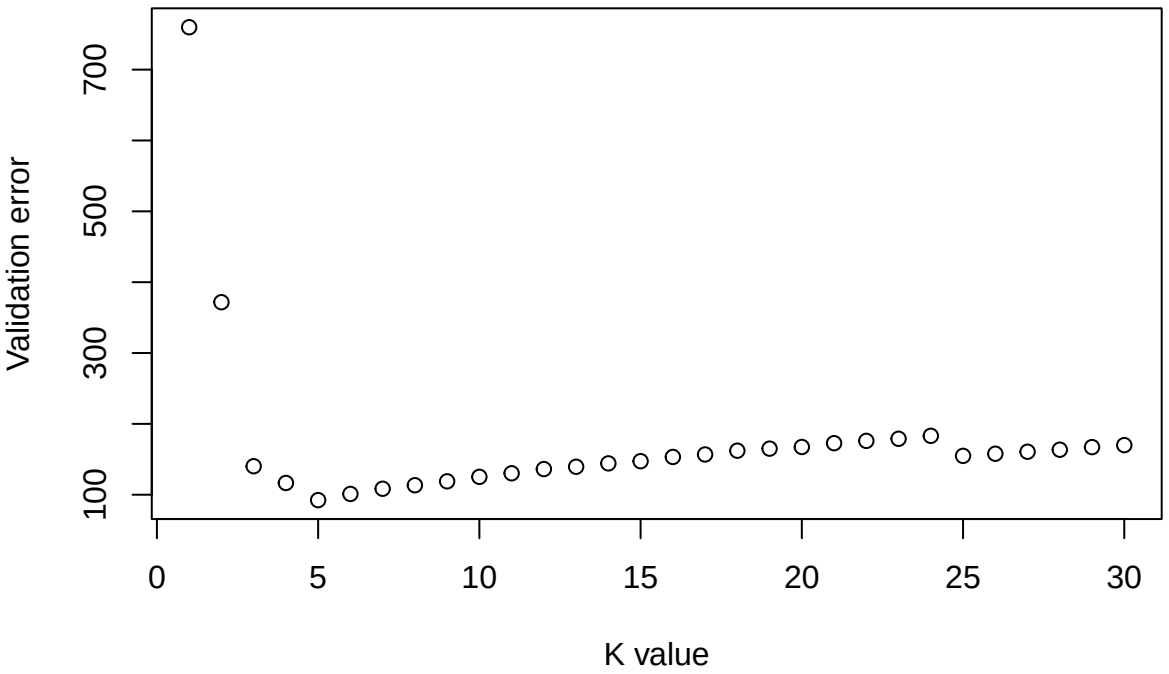
When K increases, the model becomes less complex, as the predictions are based on a majority vote from more neighbors.
In general, the training error increases with the increase of K after $K = 2$, while the rate of increase gradually decreases. For validation error, it decreases at first and reaches the minimum at $K = 3$ and then increases with the increase of K. These relationships indirectly indicate that larger K leads to simpler model.
According to this plot, the optimal $K = 3$.

```
## Misclassification error for the test data: 0.0313479623824452
```

```
##   K train_error valid_error test_error
## 3 3   0.0115123  0.01780105 0.03134796
```

It can be computed that test_error is 1.76 times of valid_error and 2.72 times of train_error. In other words, test_error is quite larger than the other two errors. Nonetheless, the absolute value of test_error is small. Therefore, this model has a good prediction quality.

Q5



The optimal $K = 5$ since validation error reaches minimum here.

In a multinomial classification task, misclassification error cannot reflect the extent of mistakes. Specifically, when an observation is misclassified, the number of misclassified cases, which is used to compute the misclassification error, will always add 1 no matter how large the probability that the model calculates about this observation is.

However, cross-entropy can reflect the extent of mistakes by function $-log(probability)$. For example, two observations are mislassified with probabilities of 0.1 and 0.2, repectively. Their contributions to the whole cross-entropy are different. And this difference provides a better capability of measuring the quality of the model.

Assignment 2. Linear regression and ridge regression

Q1

See appendix.

```
## Loading required package: ggplot2
```

```
## Loading required package: lattice
```

```
##
## Attaching package: 'caret'
```

```
## The following object is masked from 'package:kknn':
##
##     contr.dummy
```

```
##
## Attaching package: 'dplyr'
```

```
## The following objects are masked from 'package:stats':
##
##     filter, lag
```

```
## The following objects are masked from 'package:base':
##
##     intersect, setdiff, setequal, union
```

Q2

```
## Training MSE is: 0.878543102826276.
```

```
## Test MSE is: 0.935447712156708.
```

```
##
## Call:
## lm(formula = motor_UPDRS ~ ., data = train_scaled)
##
## Residuals:
##     Min      1Q  Median      3Q     Max
## -3.0255 -0.7363 -0.1087  0.7333  2.1960
##
## Coefficients:
##                  Estimate Std. Error t value Pr(>|t|)
## (Intercept)    6.575e-15  1.583e-02   0.000 1.000000
## Jitter...      1.869e-01  1.496e-01   1.250 0.211496
## Jitter.Abs.   -1.696e-01  4.081e-02  -4.156 3.32e-05 ***
## Jitter.RAP    -5.270e+00  1.884e+01  -0.280 0.779688
## Jitter.PPQ5   -7.457e-02  8.778e-02  -0.850 0.395659
## Jitter.DDP     5.250e+00  1.884e+01   0.279 0.780541
## Shimmer        5.924e-01  2.060e-01   2.876 0.004055 **
## Shimmer.dB.   -1.727e-01  1.393e-01  -1.239 0.215380
## Shimmer.APQ3   3.207e+01  7.717e+01   0.416 0.677738
## Shimmer.APQ5  -3.875e-01  1.138e-01  -3.405 0.000669 ***
## Shimmer.APQ11  3.055e-01  6.124e-02   4.989 6.37e-07 ***
## Shimmer.DDA   -3.239e+01  7.717e+01  -0.420 0.674739
## NHR           -1.854e-01  4.557e-02  -4.068 4.85e-05 ***
## HNR           -2.385e-01  3.640e-02  -6.553 6.45e-11 ***
## RPDE           4.068e-03  2.267e-02   0.179 0.857576
## DFA           -2.803e-01  2.014e-02 -13.919  < 2e-16 ***
## PPE            2.265e-01  3.289e-02   6.886 6.75e-12 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 0.9396 on 3508 degrees of freedom
## Multiple R-squared:  0.1212, Adjusted R-squared:  0.1172
## F-statistic: 30.24 on 16 and 3508 DF,  p-value: < 2.2e-16
```

The significant contributors are Jitter.Abs., Shimmer.APQ5, Shimmer.APQ11, NHR, HNR, DFA, and PPE, which are marked $***$ in summary output.

Q3

See appendix.

Q4

```
##   lambda train_MSE  test_MSE       DoF     sigma
## 1      1 0.8786272 0.9350013 13.860736 0.9373538
## 2    100 0.8844134 0.9323346  9.924887 0.9404627
```

```
## 3   1000 0.9211180 0.9539465  5.643925 0.9597496
```

As the table shown, train_MSE increases slightly as λ increases, while test_MSE reaches minimum at $\lambda = 100$, which is regarded as the optimal penalty parameter among these three.
Larger λ results to smaller DoF. As λ increases, the parameters are heavily constrained and the degrees of freedom will effectively be lower, tending to 0 as $\lambda \to \infty$. In summary, λ controls the complexity of the model, when it increases (DoF decreases), model becomes simpler; when it decreases (DoF increases), model becomes more complex. Since there is a trade-off of model complexity for the best model, there exists optimal values of λ and DoF.

Appendix

Code for Assignment 1

Q1

```
rawdata <- read.csv("optdigits.csv", header = F)
n <- nrow(rawdata)
set.seed(12345)
id <- sample(1:n,floor(n*0.5))
id1 <- setdiff(1:n,id)
id2 <- sample(id1,floor(n*0.25))
id3 <- setdiff(id1,id2)

train <- rawdata[id,]
valid <- rawdata[id2,]
test <- rawdata[id3,]
```

Q2

```
suppressWarnings({
  library(kknn)
})
m1 <- kknn(as.factor(train$V65)~.,train,train,k=30,kernel="rectangular")
train_true <- train$V65
train_predict <- m1$fitted.values
train_table <- table(train_true, train_predict)
cat("Confusion matrix for the training data:\n")
print(train_table)

m2 <- kknn(as.factor(train$V65)~.,train,test,k=30,kernel="rectangular")
test_true <- test$V65
test_predict <- m2$fitted.values
test_table <- table(test_true, test_predict)
cat("Confusion matrix for the test data:\n")
print(test_table)

train_mis <- 1-sum(diag(train_table))/sum(train_table)
cat(paste0("Misclassification error for the training data: ",round(train_mis,5),"\n"))

test_mis <- 1-sum(diag(test_table))/sum(test_table)
cat(paste0("Misclassification error for the test data: ",round(test_mis,5),"\n"))

error_list <- list()
```

```
for (i in 1:10){
  error_Rate <- 1-test_table[i,i]/sum(test_table[i,])
  error_list$digit[i] <- i-1
  error_list$error_rate[i] <- error_Rate
}
error_df <- as.data.frame(error_list)
error_df <- error_df[order(error_df$error,decreasing = T),]
cat("Misclassification error for each digit in the test data:\n")
print(error_df)
```

Q3

```
correct_index <- which(train_predict==8 & train_true==8)

correst_prob <- m1$prob[correct_index,9]

easy_index <- order(correst_prob, decreasing = TRUE)[1:2]
hard_index <- order(correst_prob)[1:3]

for (i in 1:length(easy_index)){
  df <- train[correct_index[easy_index[i]],-ncol(train)]
  mat <- matrix(as.numeric(df),8,byrow = T)
  heatmap(mat, Colv=NA, Rowv=NA, main=paste0("Easiest_", i))
}

for (i in 1:length(hard_index)){
  df <- train[correct_index[hard_index[i]],-ncol(train)]
  mat <- matrix(as.numeric(df),8,byrow = T)
  heatmap(mat, Colv=NA, Rowv=NA, main=paste0("Hardest_", i))
}
```

Q4

```
store_list <- list()
for (i in 1:30){
  store_list$K[i] <- i
  train_model <- kknn(as.factor(train$V65)~.,train,train,k=i,kernel="rectangular")
  train_table <- table(train$V65,train_model$fitted.values)
  store_list$train_error[i] <- 1-sum(diag(train_table))/sum(train_table)

  valid_model <- kknn(as.factor(train$V65)~.,train,valid,k=i,kernel="rectangular")
  valid_table <- table(valid$V65,valid_model$fitted.values)
  store_list$valid_error[i] <- 1-sum(diag(valid_table))/sum(valid_table)
}
store_df <- as.data.frame(store_list)

plot(store_df$K, store_df$train_error, type = "l", col = "blue", lty = 1, lwd = 2, ylim = range(c(store
lines(store_df$K, store_df$valid_error, col = "red", lty = 2, lwd = 2)
legend("bottomright", legend = c("train", "valid"), col = c("blue", "red"), lty = 1:2, lwd = 2)

m3 <- kknn(as.factor(train$V65)~.,train,test,k=3,kernel="rectangular")
test_true <- test$V65
test_predict <- m3$fitted.values
```

```r
test_table <- table(test_true, test_predict)
test_error <- 1-sum(diag(test_table))/sum(test_table)
cat(paste0("Misclassification error for the test data: ",test_error))

errors <- cbind(store_df[3,],test_error)
print(errors)
```

Q5

```r
compute_cross_entropy <- function(true_labels, predicted_probs) {
  -sum(log(predicted_probs[cbind(1:length(true_labels), true_labels + 1)] + 1e-15))
}

store_list <- list()
for (i in 1:30){
  store_list$K[i] <- i
  valid_model <- kknn(as.factor(train$V65)~.,train,valid,k=i,kernel="rectangular")
  store_list$valid_error[i] <- compute_cross_entropy(valid$V65,valid_model$prob)
}

store_df <- as.data.frame(store_list)
plot(store_df$K, store_df$valid_error, xlab = "K value", ylab = "Validation error")
```

Code for Assignment 2

Q1

```r
# load necessary package
library(caret)
library(dplyr)
# import data
rawdata <- read.csv("parkinsons.csv")

rawdata <- rawdata %>% select(-c(1:4,6))
n <- nrow(rawdata)
set.seed(12345)
id <- sample(1:n,floor(n*0.6))
train <- rawdata[id,]
test <- rawdata[-id,]

# scale data
param <- preProcess(train)
train_scaled <- predict(param,train)
test_scaled <- predict(param,test)
```

Q2

```r
# calculate mse
mse <- function(true_value, predict_value){
  mean((true_value - predict_value)^2)
}
```

```r
# linear regression model
model <- lm(motor_UPDRS ~ ., data = train_scaled)

# Training and test MSE
train_mse <- mse(train_scaled$motor_UPDRS, predict(model, train_scaled))
cat(paste0("Training MSE is: ",train_mse,".\n"))

test_mse <- mse(test_scaled$motor_UPDRS, predict(model, test_scaled))
cat(paste0("Test MSE is: ",test_mse,".\n"))

# Significant variables
summary(model)
```

Q3

```r
# Log-likelihood function
Loglikelihood <- function(theta_vec, sigma){
  y <- train_scaled[,1]
  x <- as.matrix(train_scaled[,-1])
  n <- nrow(train_scaled)
  value <- -(n/2*log(sigma^2*2*pi)+sum((y-x%*%theta_vec)^2)/(2*sigma^2))
  return(value)
}
# Ridge log-likelihood function
Ridge <- function(theta_vec, sigma, lambda){
  -Loglikelihood(theta_vec, sigma)+lambda*sum(theta_vec^2)
}
# Ridge log-likelihood optimization function
RidgeOpt <- function(lambda){
  init_theta <- rep(0, ncol(train_scaled)-1)
  init_sigma <- 0.9

  objective_function <- function(params) {
    theta_vec <- params[-length(params)]
    sigma <- params[length(params)]
    return(Ridge(theta_vec, sigma, lambda))
  }

  rlt <- optim(c(init_theta, init_sigma), fn = objective_function, method = "BFGS")

  optimal_theta_vec <- rlt$par[-length(rlt$par)]
  optimal_sigma <- rlt$par[length(rlt$par)]

  return(list(theta_vec = optimal_theta_vec, sigma = optimal_sigma))
}
# Degrees of freedom function
DF <- function(lambda){
  x <- as.matrix(train_scaled[,-1])
  df <- sum(diag(x%*%solve(t(x)%*%x+lambda*diag(ncol(x)))%*%t(x)))
  return(df)
}
```

Q4

```
train_x <- as.matrix(train_scaled[,-1])
train_y <- train_scaled[,1]
test_x <- as.matrix(test_scaled[,-1])
test_y <- test_scaled[,1]

# Ridge optimization for different lambdas
Lambda <- c(1,100,1000)
store_list <- list()

for (i in 1:length(Lambda)){
  store_list$lambda[i] <- Lambda[i]
  optimal_theta_vec <- RidgeOpt(Lambda[i])$theta_vec
  store_list$train_MSE[i] <- mse(train_y, train_x%*%optimal_theta_vec)
  store_list$test_MSE[i] <- mse(test_y, test_x%*%optimal_theta_vec)
  store_list$DoF[i] <- DF(Lambda[i])
  store_list$sigma[i] <- RidgeOpt(Lambda[i])$sigma
}
store_df <- as.data.frame(store_list)
print(store_df)
```