# Statistical Learning Topic 1 Introduction - Answers to exercises

## Exercise 1: Inference vs. Prediction?

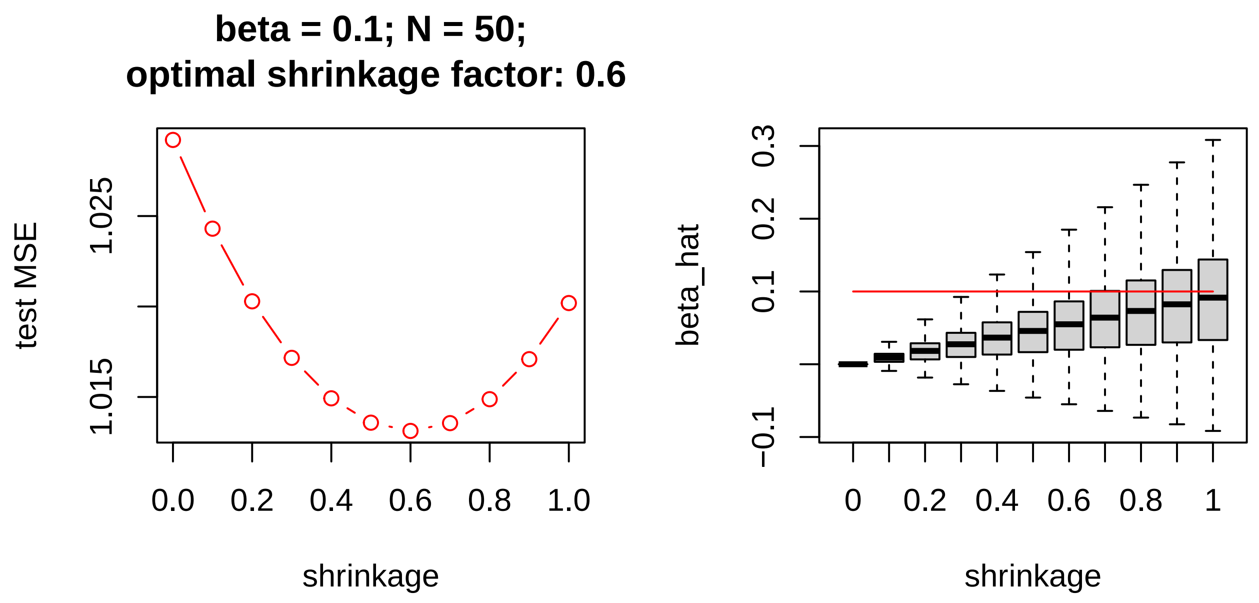
(a) The response is continuous, specifically the salary of a CEO. Hence, it is a regression problem. The goal is not to predict the salary of a CEO, but to understand the impact that certain predictors have on it. It is thus an inference task. The sample size for this problem is $n = 500$ and the predictors include profit, number of employees, and industry, thus, $p = 3$.

(b) In this case, the response is binary, specifically success or failure, and hence it is a classification problem. The aim here is to predict success or failure. $n = 20$ and $p = 13$.

(c) This problem involves a response that is continuous, specifically the % change in the USD/Euro exchange rate, and hence it is a regression problem. The goal is to predict the response, the % change in the USD/Euro exchange rate. $n = 52$ and $p = 3$

## Exercise 2: Bias can be beneficial

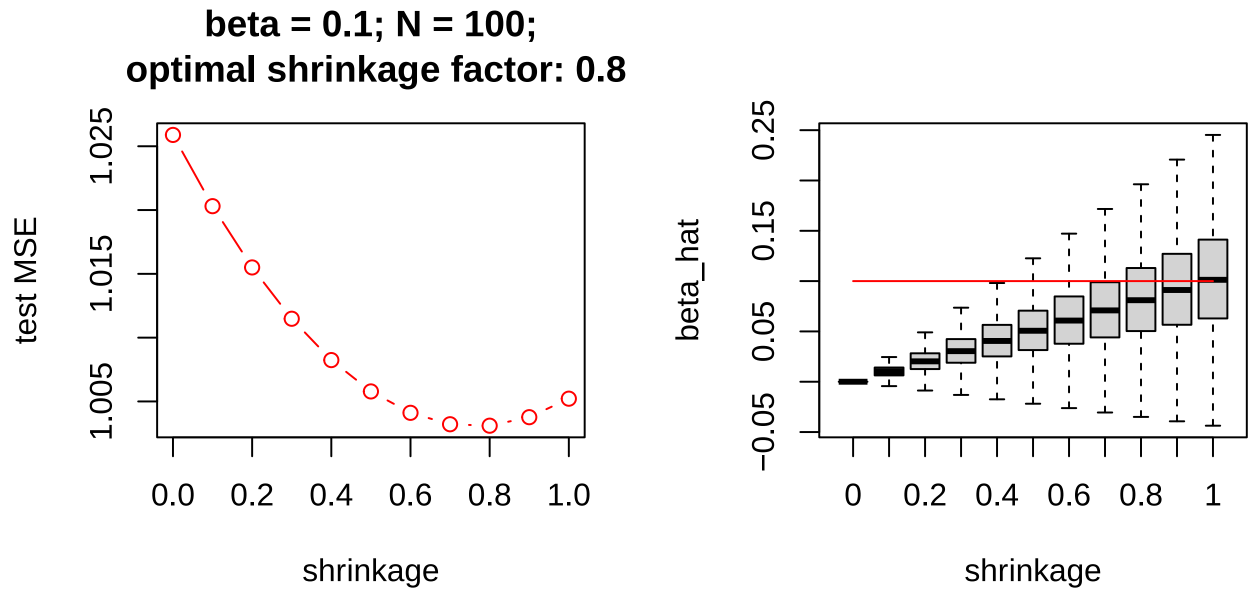
```r
source("functions.R")
part1 <- make_ex_1()
```



With shrinkage, we see that the estimated coefficient $\hat{\beta}$ becomes biased downwards (the red line in the middle plot indicates the true value $\beta$), but the variance of the estimate also gets (much) smaller. A shrinkage factor of 0.6 was optimal. The red line in the right plot indicates the irreducible error.

What if we increase training sample size?

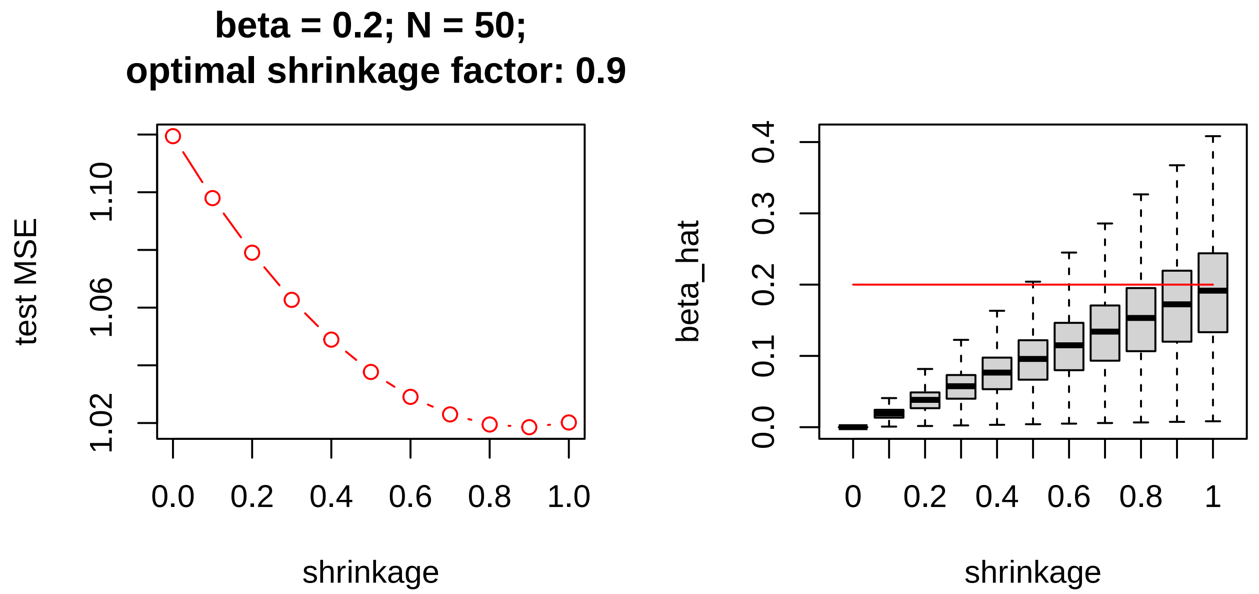
```
part2 <- make_ex_1(n_train = 100)
```



With larger sample size (i.e., more information in the sample), shrinkage is still beneficial. However, with larger sample size, variance of $\hat{\beta}$ is smaller, so we need less shrinkage (bias) to optimize prediction error. Now, a shrinkage factor of 0.6 was optimal.

What if we increase the effect of $X$?

```
part3 <- make_ex_1(beta = .2)
```

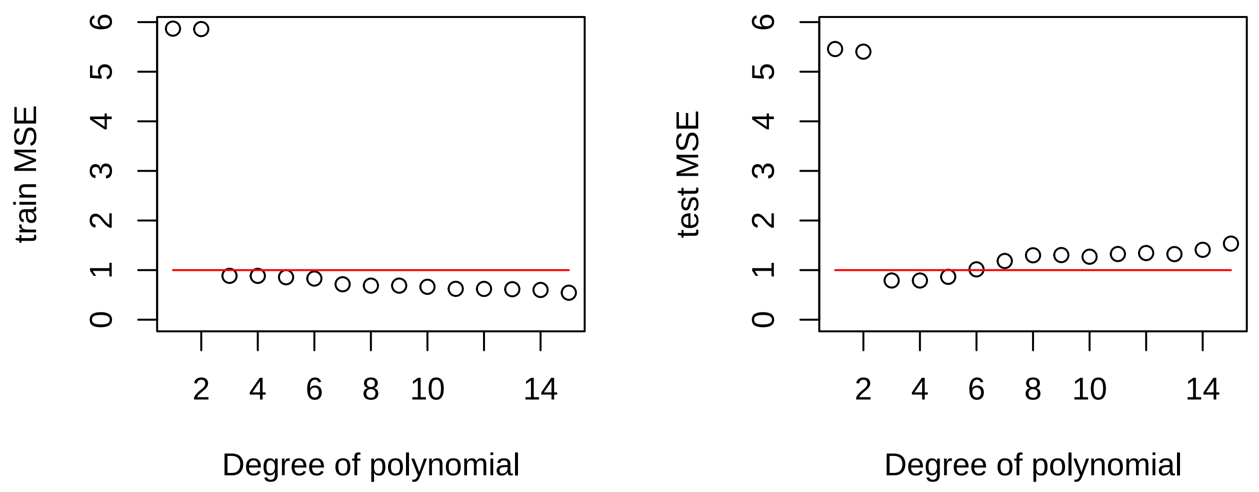


With larger effect size (i.e., larger $\beta$, so higher signal-to-noise ratio), shrinkage is still beneficial. Note that the variance of $\hat{\beta}$ does not change as a function of effect size. However, the shrinkage factor $c$ has a stronger effect on larger coefficients, so we need less shrinkage (bias) to optimize prediction error. A shrinkage factor of 0.9 was optimal.

Conclusion: Shrinkage is beneficial for prediction. With higher signal-to-noise ratio and/or larger training sample size (i.e., there is more information in the training data), a lower amount of shrinkage is optimal.

## Exercise 3: Under- and overfitting with polynomial regression

```r
set.seed(42)
n <- 50

## generate training data
x <- runif(n, min = -5, max = 5)
y <- x + 8*sin(x/2) + rnorm(n)
train <- data.frame(x, y)

## generate test data:
xtest <- runif(n, min = -5, max = 5)
ytest <- xtest + 8*sin(xtest/2) + rnorm(n)
test <- data.frame(x = xtest, y = ytest)

degrees <- 1:15
train_err <- test_err <- rep(NA, length(degrees))
train_pred <- matrix(NA, nrow = length(degrees), ncol = n)

for (d in 1:15) {
  fit <- lm(y ~ poly(x, degree = d), data = train)
  train_pred[d,] <- predict(fit, newdata = train)
  test_pred <- predict(fit, newdata = test)
  test_err[d] <- mean((test$y - test_pred)^2)
  train_err[d] <- mean((train$y - train_pred[d,])^2)
}

par(mfrow = c(1, 2))
plot(1:15, train_err, xlab = "Degree of polynomial",
     ylab = "train MSE", ylim = c(0, max(c(train_err, test_err))))
lines(c(1, 15), c(1, 1), col = "red")
plot(1:15, test_err, xlab = "Degree of polynomial",
     ylab = "test MSE", ylim = c(0, max(c(train_err, test_err))))
lines(c(1, 15), c(1, 1), col = "red")
```

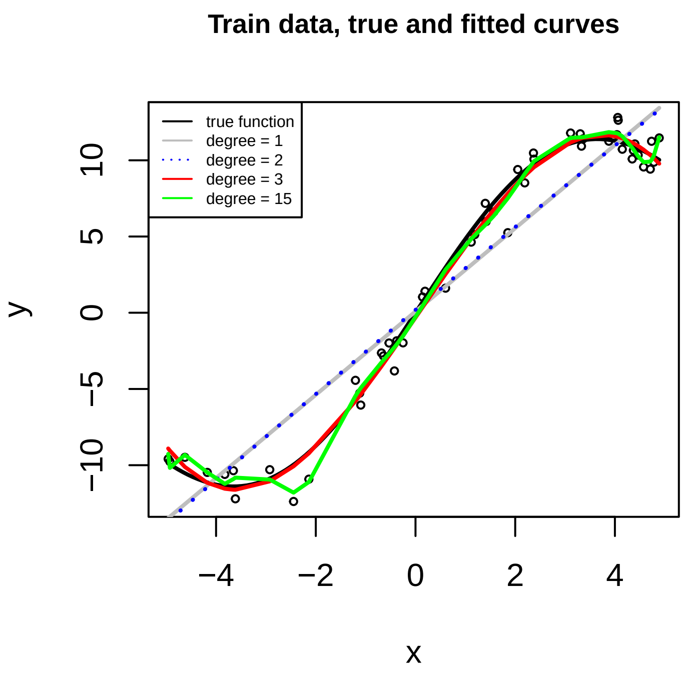


The MSE is depicted against the degree of the polynomial. The red curve represents irreducible error. We see rather high train and test MSE for polynomials of degree 1 and 2, and then a sharp decrease afterwards.

After degree 6, the overfitting begins and test MSE starts to increase, while train MSE continues decreasing. The cubic (degree 3) seems to provide a good bias-variance trade-off: complex enough to capture the true function, not too flexible so it does not adjust to the sample at hand too much.

We plot the fitted curves against the training observations:

```r
plot(x, y, main = "Train data, true and fitted curves", cex = .5, cex.main = .8)
curve(x + 8*sin(x/2), add = TRUE, lwd = 2)
lines(sort(x), train_pred[1, order(x)], col = "grey", lwd = 2)
lines(sort(x), train_pred[2, order(x)], col = "blue", lwd = 2, lty = 3)
lines(sort(x), train_pred[3, order(x)], col = "red", lwd = 2)
lines(sort(x), train_pred[15, order(x)], col = "green", lwd = 2)
legend("topleft", legend = c("true function", paste("degree =", c(1, 2, 3, 15))),
       lty = c(1, 1, 3, 1, 1), col = c("black", "grey", "blue", "red", "green"),
       cex = .5)
```

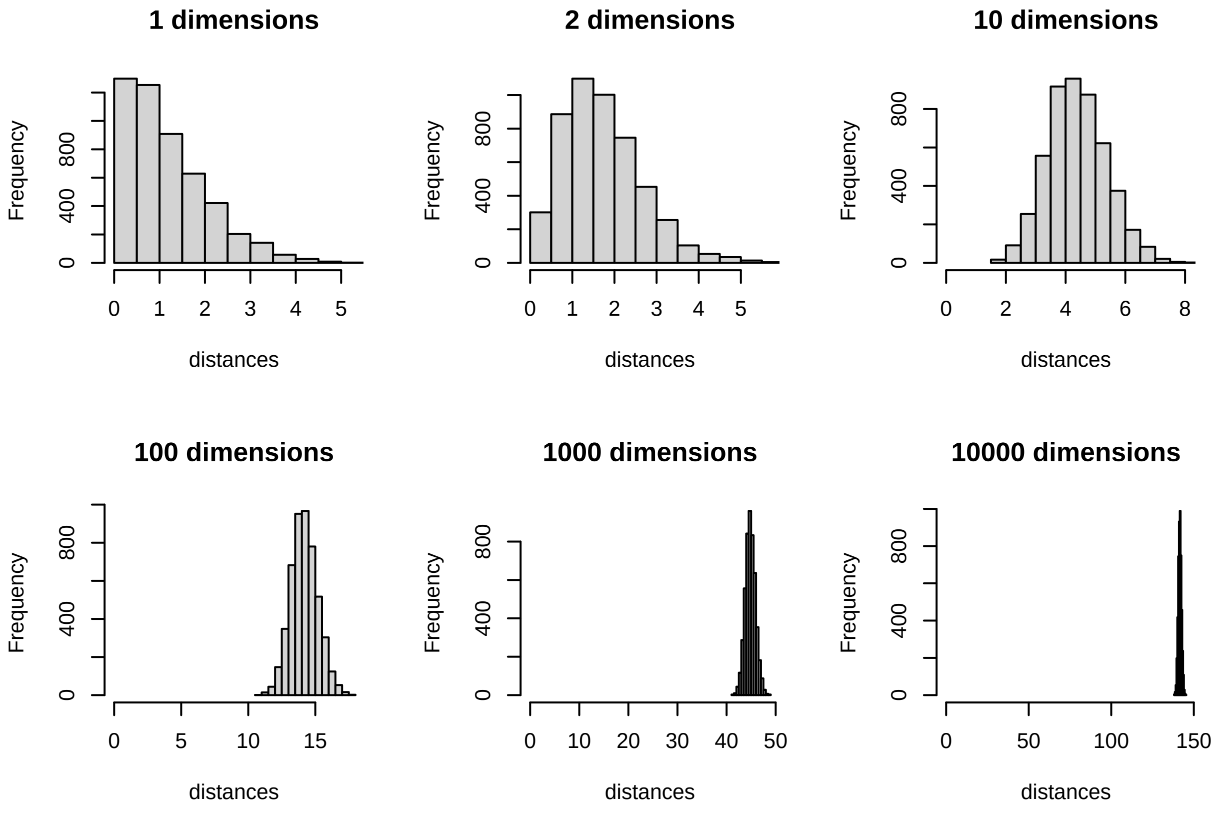


The linear and quadratic clearly stand out, failing to capture non-linearities. The other curves follow closely the true relationship, although the higher-order polynomials show aberrant behaviour at the boundaries and may adjust to the training data too much. Note that for these data, the erratic behavior near the boundaries might not affect test MSE too much, because observations near the boundary are relatively rare in a single dimension. In increasingly higher dimension, observations will be increasingly closer to the boundaries of the predictor variable space.

## Exercise 4: Curse of dimensionality

```r
p <- 10000
N <- 100
set.seed(42)
X <- matrix(rnorm(p*N), ncol = p, nrow = N)
par(mfrow = c(2, 3))
## L_2
for (p in c(1, 2, 10, 100, 1000, 10000)) {
  distances <- dist(X[ , 1:p])
  if (p == 1) print(head(distances))
  hist(distances, main = paste(p, "dimensions"), xlim = c(0, max(distances)))
}
```

```
## [1] 1.9356566 1.0078300 0.7380958 0.9666901 1.4770830 0.1405636
```



$k$ nearest neighbours assumes that nearness is meaningful: that observations that are closer by are more similar than observations further apart.

In low dimensions, the Euclidian distances between observations indeed seem meaningful: Distances show quite some variability, there are many observation pairs very near (almost zero distance), and many observation pairs are further away (not neighbours).

With increasing dimension $p$, it is increasingly the case that all observations are far apart. With very high dimensions, distances between observations seem not so meaningful anymore: All observations are far apart, none are near. One could argue, among observations that are all at a large distance, there are no real neighbours. Being nearer by 1 or 2 is likely to reflect only chance fluctuation. It seems a bit like living in Leiden and that you would call anyone from the eastern part of New York would be your neighbour, but anyone from the western part of New York would not be your neighbour.

## Exercise 5: Classifying digits

This exercise is about zipcode data; the aim is to recognize handwritten numbers 0 through 9. The observations are images of handwritten digits, automatically scanned from envelopes by the U.S. Postal Service. The images have been deslanted and size normalized, resulting in 16 x 16 grayscale images (Le Cun et al., 1990), yielding 256 predictor variables, reflecting the grayscale value for each pixel.

```
## Prepare training data
train <- read.table("zip.train", sep = " ")
dim(train)
```

```
## [1] 7291  258
```

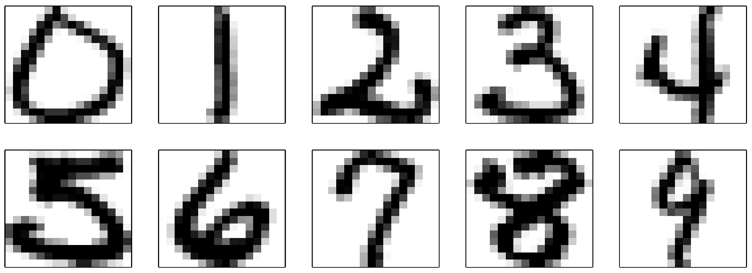
```
#head(train[1:10]) ## not run for space considerations
#colSums(is.na(train)) # last columns has only missings
train <- train[ , -258]

## Prepare test data
test <- read.table("zip.test", sep = " ")
#colSums(is.na(test)) ## not run for space considerations
dim(test)
```

```
## [1] 2007  257
```

```
#head(test[1:10]) ## not run for space considerations
```

This is what some of the images look like:

```
par(mfrow = c(2, 5), par(mar = c(1, 1, 0.1, 0.1))) # set graphical parameters
for (i in 0:9) {
  im <- matrix(as.numeric(train[train$V1 == i, 2:257][1, ]), nrow = 16, ncol = 16)
  image(t(apply(-im, 1, rev)), col = gray((0:63)/63), yaxt = "n", xaxt = "n")
  ## 63 is the minimum number of unique grayscale values observed for any variable
}
```



Select only 2s and 3s (V1 is an indicator for digit):

```
train <- train[train$V1 %in% 2:3, ]
train$V1 <- train$V1 - 2
dim(train)
```

```
## [1] 1389  257
```

```r
test <- test[test$V1 %in% 2:3, ]
test$V1 <- test$V1 - 2
dim(test)
```

```
## [1] 364 257
```

```r
table(train$V1)
```

```
##
##   0   1
## 731 658
```

```r
table(test$V1)
```

```
##
##   0   1
## 198 166
```

Fit a GLM and generate predictions:

```r
lmod <- glm(V1 ~ ., data = train, family = "binomial")
```

```
## Warning: glm.fit: algorithm did not converge
```

```
## Warning: glm.fit: fitted probabilities numerically 0 or 1 occurred
```

```r
#summary(lmod) ## not run for space considerations
y_hat_train <- predict(lmod, newdata = train, type = "response") > 0.5
y_hat_test <- predict(lmod, newdata = test, type = "response") > 0.5
train_mcr_lm <- mean((train$V1 != y_hat_train))
test_mcr_lm <- mean((test$V1 != y_hat_test))
train_mcr_lm
```

```
## [1] 0
```

```r
test_mcr_lm
```

```
## [1] 0.05494505
```

Fit $k$NN and generate predictions:

```r
library("class")
ks <- 1:15
train_knn <- matrix(NA, nrow = nrow(train), ncol = length(ks))
test_knn <- matrix(NA, nrow = nrow(test), ncol = length(ks))
colnames(test_knn) <- colnames(train_knn) <- ks
for (i in 1:length(ks)) {
  train_knn[ , i] <- knn(train = train[ , -1], test = train[ , -1], cl = train$V1, k = i)
  test_knn[ , i] <- knn(train = train[ , -1], test = test[ , -1], cl = train$V1, k = i)
}
head(train_knn[ , 1]) ## predictions are generated as 1 and 2, need to subtract 1
```

```
## [1] 2 2 2 2 2 1
```

```
train_mcr_knn <- apply(train$V1 != train_knn-1, 2, mean)
test_mcr_knn <- apply(test$V1 != test_knn-1, 2, mean)
## Print train and test misclassification rates for each value of k
round(train_mcr_knn, digits = 4L)
```

```
##      1      2      3      4      5      6      7      8      9     10     11
## 0.0000 0.0065 0.0050 0.0065 0.0058 0.0072 0.0065 0.0086 0.0094 0.0094 0.0086
##     12     13     14     15
## 0.0079 0.0086 0.0094 0.0094
```

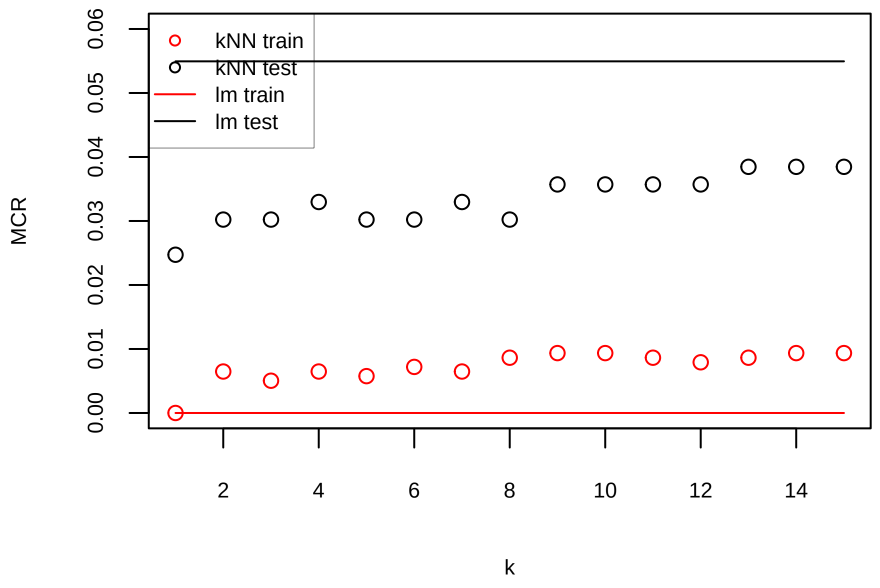
```
round(test_mcr_knn, digits = 4L)
```

```
##      1      2      3      4      5      6      7      8      9     10     11
## 0.0247 0.0302 0.0302 0.0330 0.0302 0.0302 0.0330 0.0302 0.0357 0.0357 0.0357
##     12     13     14     15
## 0.0357 0.0385 0.0385 0.0385
```

$k$NN outperforms logistic regression for all values of $k$ on the test data.

Plot performance:

```
## Plot results
plot(ks, test_mcr_knn, ylim = c(0, 0.06), ylab = "MCR", xlab = "k", cex.lab = .7,
     cex.axis=.7)
legend("topleft", legend = c("kNN train", "kNN test", "lm train", "lm test"),
       col = c("red", "black", "red", "black"), cex = .7,
       pch = c(1, 1, NA, NA), lty = c(NA, NA, 1, 1), box.lwd = 0)
points(ks, train_mcr_knn, col = "red")
lines(x = ks, y = rep(test_mcr_lm, times = length(ks)))
lines(x = ks, y = rep(train_mcr_lm, times = length(ks)), col = "red")
```



The dots are for $k$NN, the lines are for the logistic regression. The training error (red) indicates logistic regression did better than $k$NN on training data, but it overfits: The difference in training (red) and test error (black) is largest for the logistic regression, and the test error (black) indicates $k$NN in fact generalizes better. For these data, the lowest test error is obtained for $k = 1$.