Module 2: Recommended Exercises - Solution

TMA4268 Statistical Learning V2025

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Problem 1

a) Classification

Example 1: Diagnosing cancer. Response: cancer (yes/no). Predictors: smoking status, age, family history, gene expression etc. Goal: prediction.

Example 2: Understanding stock market price direction. Response: up/down. Predictors: yesterday's price movement change, two previous days price movement etc. Goal: inference.

Example 3: Flower species. Response: species. Predictors: color, height, leaves, etc. Goal: prediction.

b) Regression

Example 1: Life expectancy. Response: age of death. Predictors: current age, gender, resting heart rate, resting breath rate etc. Goal: prediction.

Example 2: Price of a house. Response: Price. Predictors: age of house, average price in neighborhood, crime rate, distance to city center, distance to school, etc. Goal: prediction.

Example 3: What affects O2-uptake. Response: O2-uptake. Predictors: gender, age, amount of weekly exercise, type of exercise, smoking, heart disease, etc. Goal: inference.

Problem 2

- a) Based on the three different models compared here, the rigid method has the highest test MSE. However, this does not always have to be the case. For instance, in figure 2.10, we see that the most flexible model has the highest test MSE. See also figure 2.12 that summarizes the last three figures and shows some of the variation. So in general we cannot say anything certain about how the test MSE will vary based on model flexibility, this will depend on how the training data compares to the test data, and other model characteristics. However (though the question does not ask this), the training MSE will always decrease as the flexibility increases.
- b) A small (test) variance implies an underfit to the data.
- c) See figure 2.12. Underfit low variance high bias. Overfit high variance low bias. We wish to find a model that lies somewhere in-between, with low variance and low bias.

Problem 3

```
#install.packages("ISLR")
library(ISLR)
data(Auto)
  a)
str(Auto)
## 'data.frame':
                    392 obs. of 9 variables:
                         18 15 18 16 17 15 14 14 14 15 ...
##
   $ mpg
                  : num
##
   $ cylinders
                         888888888...
                  : num
## $ displacement: num
                         307 350 318 304 302 429 454 440 455 390 ...
## $ horsepower : num
                         130 165 150 150 140 198 220 215 225 190 ...
##
   $ weight
                         3504 3693 3436 3433 3449 ...
                  : num
                        12 11.5 11 12 10.5 10 9 8.5 10 8.5 ...
##
   $ acceleration: num
##
                         70 70 70 70 70 70 70 70 70 70 ...
  $ vear
                  : num
                  : num 1 1 1 1 1 1 1 1 1 1 ...
##
   $ origin
   $ name
                  : Factor w/ 304 levels "amc ambassador brougham",..: 49 36 231 14 161 141 54 223 241
summary(Auto)
##
                      cylinders
                                      displacement
                                                       horsepower
                                                                          weight
         mpg
           : 9.00
##
                           :3.000
                                           : 68.0
                                                            : 46.0
                                                                     Min.
                                                                             :1613
   Min.
                    Min.
                                    Min.
                                                     Min.
##
   1st Qu.:17.00
                    1st Qu.:4.000
                                     1st Qu.:105.0
                                                     1st Qu.: 75.0
                                                                      1st Qu.:2225
##
   Median :22.75
                    Median :4.000
                                    Median :151.0
                                                     Median: 93.5
                                                                     Median:2804
##
   Mean
           :23.45
                    Mean
                           :5.472
                                    Mean
                                            :194.4
                                                     Mean
                                                           :104.5
                                                                     Mean
                                                                            :2978
##
   3rd Qu.:29.00
                    3rd Qu.:8.000
                                     3rd Qu.:275.8
                                                     3rd Qu.:126.0
                                                                      3rd Qu.:3615
##
   Max.
           :46.60
                    Max.
                           :8.000
                                    Max.
                                            :455.0
                                                     Max.
                                                            :230.0
                                                                     Max.
                                                                             :5140
##
##
     acceleration
                         year
                                         origin
                                                                      name
##
  Min.
          : 8.00
                           :70.00
                                            :1.000
                                                     amc matador
                                                                        :
                                                                           5
                                    Min.
                    Min.
   1st Qu.:13.78
                    1st Qu.:73.00
                                     1st Qu.:1.000
                                                                           5
##
                                                     ford pinto
##
  Median :15.50
                    Median :76.00
                                    Median :1.000
                                                     toyota corolla
                                                                           5
  Mean
           :15.54
                    Mean
                           :75.98
                                    Mean
                                            :1.577
                                                     amc gremlin
                                     3rd Qu.:2.000
##
   3rd Qu.:17.02
                    3rd Qu.:79.00
                                                     amc hornet
                                                                           4
##
   Max.
           :24.80
                    Max.
                            :82.00
                                     Max.
                                            :3.000
                                                     chevrolet chevette:
                                                                           4
##
                                                     (Other)
                                                                        :365
```

The dimensions are 392 observations (rows) of 9 variables (columns). See from looking at the structure (str()) and summary() origin (encoded by values 1, 2, 3) and name (name of the car) are qualitative predictors. The rest of the predictors are quantitative.

b)

To see the range of the quantitative predictors, either apply the range() function to each column with a quantitative predictor separately

```
range(Auto[, 1])
## [1] 9.0 46.6
range(Auto[, 3])
## [1] 68 455
range(Auto[, 4])
```

```
## [1] 46 230
range(Auto[, 5])
## [1] 1613 5140
range(Auto[, 6])
## [1] 8.0 24.8
range(Auto[, 7])
## [1] 70 82
or use the sapply() function to run the range() function on the specified columns with a single line of code:
quant <- 1:7
sapply(Auto[, quant], range)
         mpg cylinders displacement horsepower weight acceleration year
## [1,] 9.0
                                               46
                                                    1613
                                                                    8.0
                                                                          70
                                   68
                      3
## [2,] 46.6
                                  455
                      8
                                              230
                                                     5140
                                                                   24.8
                                                                          82
  c)
To get the sample mean and sample standard deviation of the quantitative predictors, we can again either use
the sapply() function in the same manner as above, or apply the mean() and sd() commands column-wise.
sapply(Auto[, quant], mean)
##
                    cylinders displacement
                                               horsepower
                                                                 weight acceleration
             mpg
##
      23.445918
                     5.471939
                                 194.411990
                                               104.469388 2977.584184
                                                                            15.541327
##
           year
      75.979592
##
#or
mean(Auto[, 1])
## [1] 23.44592
mean(Auto[, 2])
## [1] 5.471939
mean(Auto[, 3])
## [1] 194.412
mean(Auto[, 4])
## [1] 104.4694
mean(Auto[, 5])
## [1] 2977.584
mean(Auto[, 6])
## [1] 15.54133
mean(Auto[, 7])
## [1] 75.97959
```

```
colMeans(Auto[, quant])
##
                    cylinders displacement
                                                                weight acceleration
                                              horsepower
            mpg
                                194.411990
##
      23.445918
                     5.471939
                                               104.469388 2977.584184
                                                                           15.541327
##
           year
##
      75.979592
#sd
sapply(Auto[, quant], sd)
##
                    cylinders displacement
                                               horsepower
                                                                weight acceleration
            mpg
##
       7.805007
                     1.705783
                                 104.644004
                                               38.491160
                                                            849.402560
                                                                            2.758864
##
           year
##
       3.683737
#or
sd(Auto[, 1])
## [1] 7.805007
sd(Auto[, 2])
## [1] 1.705783
sd(Auto[, 3])
## [1] 104.644
sd(Auto[, 4])
## [1] 38.49116
sd(Auto[, 5])
## [1] 849.4026
sd(Auto[, 6])
## [1] 2.758864
sd(Auto[, 7])
## [1] 3.683737
  d)
Remove 10th to 85th observations and look at the range, mean and standard deviation of the reduced set.
We now only show the solutions using sapply() to save space.
#remove observations
ReducedAuto \leftarrow Auto[-c(10:85), ]
#range, mean and sd
sapply(ReducedAuto[, quant], range)
         mpg cylinders displacement horsepower weight acceleration year
##
## [1,] 11.0
                      3
                                   68
                                               46
                                                    1649
                                                                   8.5
                                                                         70
## [2,] 46.6
                                  455
                                             230
                                                    4997
                                                                  24.8
                                                                         82
sapply(ReducedAuto[, quant], mean)
##
                    cylinders displacement
                                              horsepower
                                                                weight acceleration
```

mpg

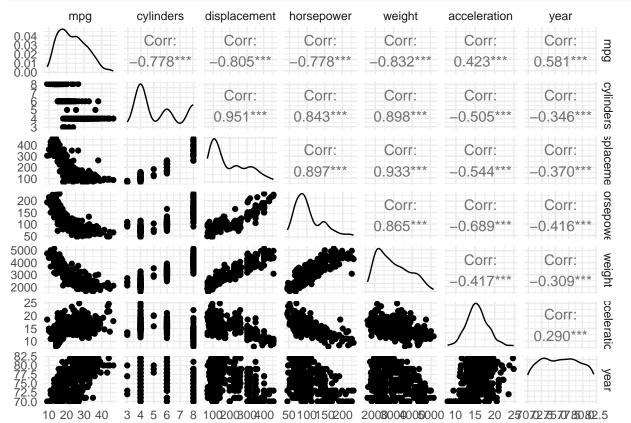
```
##
      24.404430
                     5.373418
                                 187.240506
                                               100.721519
                                                            2935.971519
                                                                            15.726899
##
           year
##
      77.145570
sapply(ReducedAuto[, quant], sd)
##
             mpg
                    cylinders displacement
                                               horsepower
                                                                  weight acceleration
##
       7.867283
                     1.654179
                                  99.678367
                                                35.708853
                                                             811.300208
                                                                              2.693721
##
           year
       3.106217
##
  e)
```

We make a scatter plot of the full dataset using the ggpairs() function.

library(GGally)

```
## Loading required package: ggplot2
## Registered S3 method overwritten by 'GGally':
## method from
## +.gg ggplot2
```

ggpairs(Auto[, quant]) + theme_minimal()

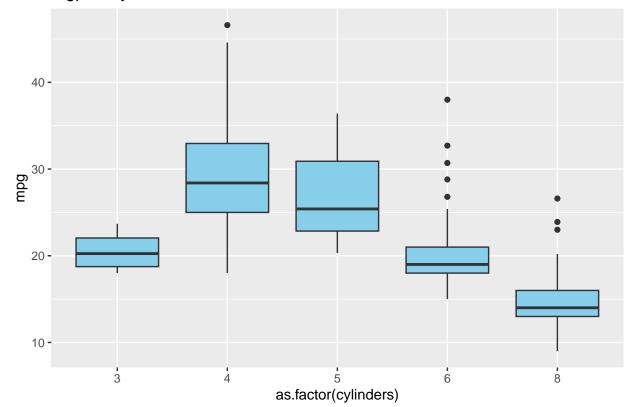


We see that there seems to be strong relationships (based on curve trends and correlation) between the pairs: mpg and displacement, mpg and horsepower, mpg and weight, displacement and horsepower, displacement and weight, horsepower and weight, and horsepower and acceleration.

f) Wish to predict gas mileage based on the other variables. From the scatter plot we see that displacement, horsepower and weight could be good choices for prediction of mpg. Check if the qualitative predictors could also be good choices by plotting them against mpg.

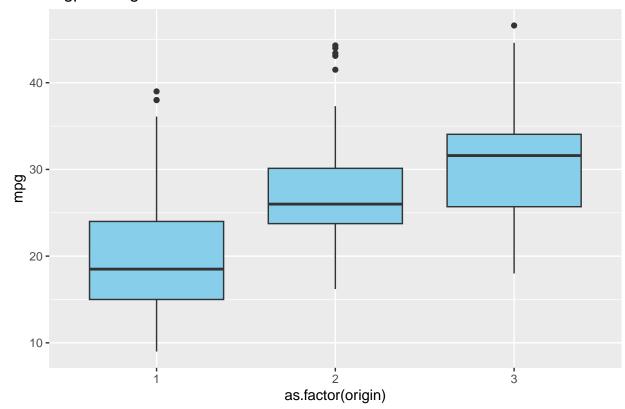
```
ggplot(Auto, aes(as.factor(cylinders), mpg)) +
geom_boxplot(fill = "skyblue") +
labs(title = "mgp vs cylinders")
```

mgp vs cylinders



```
ggplot(Auto, aes(as.factor(origin), mpg)) +
geom_boxplot(fill = "skyblue") +
labs(title = "mgp vs origin")
```

mgp vs origin



From these plots we see that both cylinders and origin could be good choices for prediction of mgp, because the miles per gallon (mpg) seems to depend on these two variables.

g) To find the correlation of the given variables, we need the covariance of these variable as well as the standard deviations, which are both available in the covariance matrix. Remember the the variance of each variable is given in the diagonal of the covariance matrix.

```
covMat <- cov(Auto[, quant])</pre>
covMat[1, 2] / (sqrt(covMat[1, 1]) * sqrt(covMat[2, 2]))
## [1] -0.7776175
covMat[1, 3] / (sqrt(covMat[1, 1]) * sqrt(covMat[3, 3]))
## [1] -0.8051269
covMat[1, 4] / (sqrt(covMat[1, 1]) * sqrt(covMat[4, 4]))
## [1] -0.7784268
cor(Auto[, quant])
                      mpg cylinders displacement horsepower
##
                                                               weight
## mpg
                1.0000000 -0.7776175
                                      -0.8051269 -0.7784268 -0.8322442
## cylinders
               -0.7776175 1.0000000
                                       ## displacement -0.8051269 0.9508233
                                       1.0000000 0.8972570 0.9329944
## horsepower
               -0.7784268 0.8429834
                                       0.8972570 1.0000000 0.8645377
## weight
               -0.8322442 0.8975273
                                       0.9329944 0.8645377 1.0000000
## acceleration 0.4233285 -0.5046834
                                      -0.5438005 -0.6891955 -0.4168392
                                      -0.3698552 -0.4163615 -0.3091199
## year
                0.5805410 -0.3456474
```

```
##
               acceleration
                                  year
                  0.4233285 0.5805410
## mpg
## cylinders
                 -0.5046834 -0.3456474
## displacement -0.5438005 -0.3698552
## horsepower
                 -0.6891955 -0.4163615
## weight
                 -0.4168392 -0.3091199
## acceleration
                  1.0000000 0.2903161
                  0.2903161 1.0000000
## year
```

We see that the obtained correlations coincide with the given elements in the correlation matrix.

Problem 4

a) Simulate values from the four multivariate distributions using mvnorm().

```
# Simulate 1000 values from the multivariate normal distribution 4 times, with
# 4 different covariance matrices
library(MASS)
n <- 1000
mu <- c(2, 3)
set1 <- data.frame(mvrnorm(n, mu, Sigma = matrix(c(1, 0, 0, 1), ncol = 2)))
colnames(set1) <- c("x1", "x2")

set2 <- data.frame(mvrnorm(n, mu, Sigma = matrix(c(1, 0, 0, 5), ncol = 2)))
colnames(set2) <- c("x1", "x2")

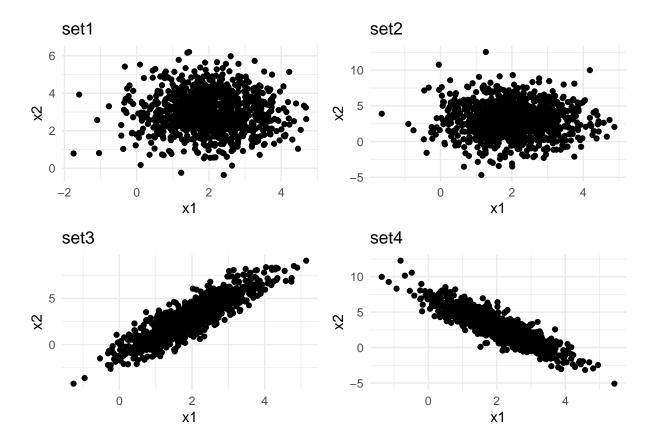
set3 <- data.frame(mvrnorm(n, mu, Sigma = matrix(c(1, 2, 2, 5), ncol = 2)))
colnames(set3) <- c("x1", "x2")

set4 <- data.frame(mvrnorm(n, mu, Sigma = matrix(c(1, -2, -2, 5), ncol = 2)))
colnames(set4) <- c("x1", "x2")</pre>
```

b) Plot the simulated distribtions

```
#install.packages("patchwork")
library(patchwork)
##
```

```
## Attaching package: 'patchwork'
## The following object is masked from 'package:MASS':
##
## area
p1 <- ggplot(set1, aes(x = x1, y = x2)) + geom_point() + labs(title = "set1") + theme_minimal()
p2 <- ggplot(set2, aes(x = x1, y = x2)) + geom_point() + labs(title = "set2") + theme_minimal()
p3 <- ggplot(set3, aes(x = x1, y = x2)) + geom_point() + labs(title = "set3") + theme_minimal()
p4 <- ggplot(set4, aes(x = x1, y = x2)) + geom_point() + labs(title = "set4") + theme_minimal()
(p1 + p2) / (p3 + p4)</pre>
```

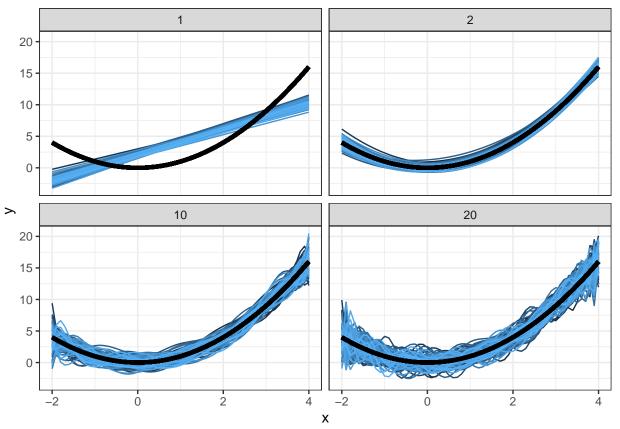


Problem 5

a) We sample from the model $y = x^2 + \epsilon$ where $\epsilon \sim \mathcal{N}(0, 2^2)$ and $x \in \{-2, -1.9, -1.8, ..., 3.8, 3.9, 4\}$. This means that $y \sim \mathcal{N}(x^2, 2^2)$. A total of 100 samples from this model are generated for each of the 61 x's. See comments in code for further explanations.

```
byrow = TRUE)
# The 100 samples or the observations are stored in this matrix. Each row is a simulation.
ymat <- matrix(rep(true_y, M), byrow = TRUE, nrow = M) + error</pre>
#----
# Based on the response y_i and the x_i's, we fit a polynomial model of degree
# 1, ..., 20. This means that we assume y i~Normal(x i^j,0).
predictions_list <- lapply(1:nord, matrix, data = NA, nrow = M, ncol = ncol(ymat))</pre>
for (i in 1:nord) {
 for (j in 1:M) {
    predictions_list[[i]][j, ] <- predict(lm(ymat[j, ] ~ poly(x, i, raw = TRUE)))</pre>
}
# Plotting -----
library(tidyverse) # The tidyverse contains ggplot2, as well as tidyr and dplyr,
# which we can use for dataframe manipulation.
list_of_matrices_with_deg_id <-</pre>
  lapply(1:nord,
         function(poly_degree) {
           cbind(predictions_list[[poly_degree]],
                 simulation_num = 1:M, poly_degree)
         }
  )
# Now predictions_list is a list with 20 entries, where each entry is a matrix
# with 100 rows, where each row is the predicted polynomial of that degree.
# We also have a column for the simulation number, and a column for polynomial degree.
# Extract each matrix and bind them to one large matrix
stacked_matrices <- NULL</pre>
for (i in 1:nord) {
  stacked_matrices <-
    rbind(stacked_matrices, list_of_matrices_with_deg_id[[i]])
stacked_matrices_df <- as.data.frame(stacked_matrices)</pre>
# Convert from wide to long (because that is the best format for ggplot2)
long_predictions_df <- pivot_longer(stacked_matrices_df,</pre>
                                     !c(simulation_num, poly_degree),
                                     values to = "y")
# Now we can use ggplot2!
# We just want to plot for degrees 1, 2, 10 and 20.
# Add x-vector to dataframe:
plotting_df <- cbind(long_predictions_df, x = x) %>%
  filter(poly_degree %in% c(1, 2, 10, 20)) # Keep only the predictions for some degrees
ggplot(plotting_df, aes(x = x, y = y, group = simulation_num)) +
  geom_line(aes(color = simulation_num)) +
  geom_line(aes(x = x, y = x^2), size = 1.5) +
```

```
facet_wrap(~ poly_degree) +
theme_bw() +
theme(legend.position = "none")
```



The upper left plot shows 100 predictions when we assume that y is a linear function of x, the upper right plot hows 100 predictions when we assume that y is function of polynomials up to x^2 , the lower left plot shows 100 predictions when we assume y is a function of polynomials up to x^{10} and the lower right plot shows 100 predictions when assuming y is a function of polynomials up to x^{20} .

b) Run the code attached and consider the following plots:

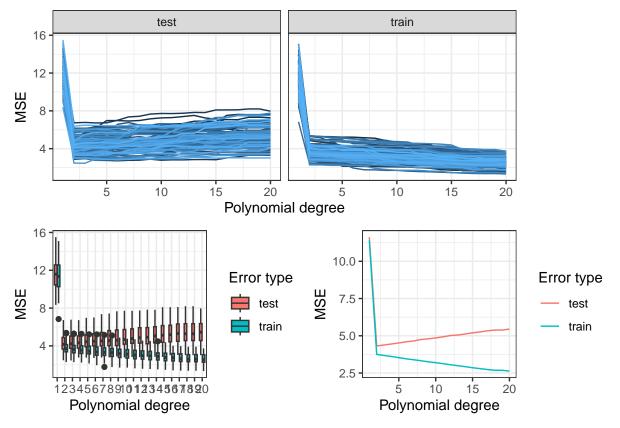
```
set.seed(2) # to reproduce
M <- 100 # repeated samplings,x fixed but new errors
nord <- 20

x <- seq(from = -2, to = 4, by = 0.1)
truefunc <- function(x) {
   return(x^2)
}
true_y <- truefunc(x)
error <- matrix(rnorm(length(x) * M, mean = 0, sd = 2), nrow = M, byrow = TRUE)
testerror <- matrix(rnorm(length(x) * M, mean = 0, sd = 2), nrow = M, byrow = TRUE)
ymat <- matrix(rep(true_y, M), byrow = TRUE, nrow = M) + error
testymat <- matrix(rep(true_y, M), byrow = TRUE, nrow = M) + testerror

predictions_list <- lapply(1:nord, matrix, data = NA, nrow = M, ncol = ncol(ymat))
for (i in 1:nord) {
   for (j in 1:M) {</pre>
```

```
predictions_list[[i]][j, ] <- predict(lm(ymat[j, ] ~ poly(x, i, raw = TRUE)))</pre>
 }
}
trainMSE <- lapply(1:nord,</pre>
                    function(poly_degree) {
                      rowMeans((predictions_list[[poly_degree]] - ymat)^2)
)
testMSE <- lapply(1:nord,</pre>
                  function(poly_degree) {
                     rowMeans((predictions_list[[poly_degree]] - testymat)^2)
                  }
)
# Plotting -----
library(tidyverse) # The tidyverse contains ggplot2, as well as tidyr and dplyr,
# which we can use for dataframe manipulation.
# Convert each matrix in the list form wide to long
# (because that is the best format for ggplot2)
list_train_MSE <- lapply(1:nord, function(poly_degree) {</pre>
  cbind(error = trainMSE[[poly_degree]],
        poly_degree,
        error_type = "train",
        simulation num = 1:M)
})
list_test_MSE <- lapply(1:nord, function(poly_degree) {</pre>
  cbind(error = testMSE[[poly_degree]],
        poly_degree,
        error_type = "test",
        simulation_num = 1:M)
})
# Now predictions_list is a list with 20 entries, where each entry is a matrix
# with 100 rows, where each row is the predicted polynomial of that degree.
stacked_train <- NULL</pre>
for (i in 1:nord) {
  stacked_train <-
    rbind(stacked_train, list_train_MSE[[i]])
stacked test <- NULL
for (i in 1:nord) {
  stacked test <-
    rbind(stacked_test, list_test_MSE[[i]])
}
stacked_errors_df <- as.data.frame(rbind(stacked_train, stacked_test))</pre>
# This is already on long format.
stacked_errors_df$error <- as.numeric(stacked_errors_df$error)</pre>
stacked_errors_df$simulation_num <- as.integer(stacked_errors_df$simulation_num)
stacked_errors_df$poly_degree <- as.integer(stacked_errors_df$poly_degree)
```

```
p.all_lines <- ggplot(data = stacked_errors_df,</pre>
                      aes(x = poly_degree, y = error, group = simulation_num)) +
  geom_line(aes(color = simulation_num)) +
  facet wrap(~ error type) +
  xlab("Polynomial degree") +
  ylab("MSE") +
  theme_bw() +
  theme(legend.position = "none")
p.bars <- ggplot(stacked_errors_df, aes(x = as.factor(poly_degree), y = error)) +</pre>
  geom_boxplot(aes(fill = error_type)) +
  scale_fill_discrete(name = "Error type") +
  xlab("Polynomial degree") +
  ylab("MSE") +
  theme_bw()
# Here we find the average test error and training error across the repeated simulations.
# The symbol "\%" is called a pipe, and comes from the tidyverse packages,
# which provide convenient functions for working with data frames.
means_across_simulations <- stacked_errors_df %>%
  group_by(error_type, poly_degree) %>%
summarise(mean = mean(error))
## `summarise()` has grouped output by 'error_type'. You can override using the
## `.groups` argument.
p.means <- ggplot(means_across_simulations, aes(x = poly_degree, y = mean)) +</pre>
  geom_line(aes(color = error_type)) +
  scale_color_discrete(name = "Error type") +
  xlab("Polynomial degree") +
 ylab("MSE") +
  theme bw()
library(patchwork) # The library patchwork is the best way of combining applot2 objects.
# You could also use the function ggarrange from the ggpubr package.
p.all_lines / (p.bars + p.means)
```



The plots show that the test MSE in general is larger than the train MSE. This is makes sense, since the model is fitted based on the training set. Thus, the error will be smaller for the train data than for the test data. Furthermore, the plots show that the difference between the MSE for the test set and the training set increases when the degree of the polynomial increases. When the degree of the polynomial increases, we get a more flexible model. The fitted curve will try to pass through the training data if possible, which typically leads to an overfitted model that performs bad for test data.

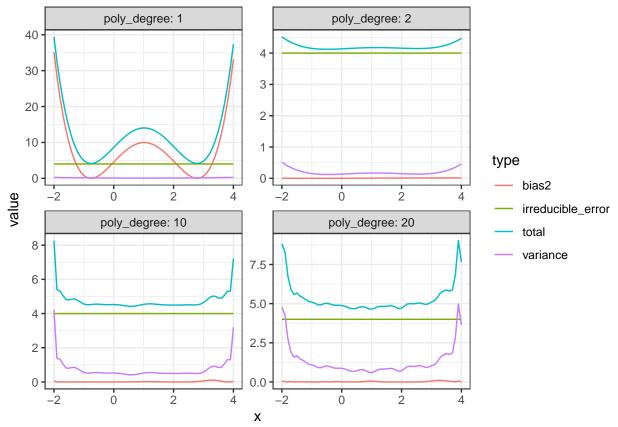
- We observe that poly 2 gives the smallest mean testMSE, while poly 20 gives the smallest trainMSE. Based on these plots, we would choose poly 2 for prediction of a new value of y, as the testMSE tells us how the model performs on new data, which was not used to train the model.
- c) Run the code and consider the following plots:

```
df$total <- df$bias2 + df$variance + df$irreducible_error

df_long <- pivot_longer(df, cols = !c(x, poly_degree), names_to = "type")

df_select_poly <- filter(df_long, poly_degree %in% c(1, 2, 10, 20))

ggplot(df_select_poly, aes(x = x, y = value, group = type)) +
    geom_line(aes(color = type)) +
    facet_wrap(~poly_degree, scales = "free", labeller = label_both) +
    theme_bw()</pre>
```



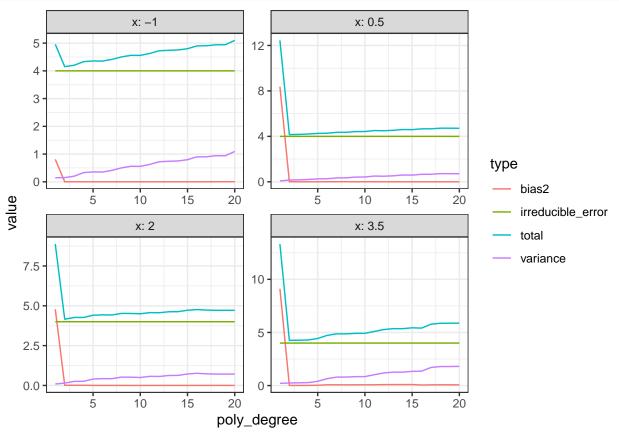
We see that the irriducible error remains constant with the complexity (flexibility) of the model and the variance (purple) increases with the complexity. A linear model gives variance close to zero, while a polynomial of degree 20 gives variance close to 1 (larger at the borders). A more complex model is more flexible as it can turn up and down and change direction fast. This leads to larger variance. (Look at the plot in 2a, there is a larger variety of curves you can make when the degree is 20 compared to if the degree is 1.).

Furthermore, we see that the bias is large for poly1, the linear model. The linear model is quite rigid, so if the true underlying model is non-linear, we typically get large deviations between the fitted line and the training data. If we study the first plot, it seems like the fitted line goes through the training data in x = -1 and x = 3 as the bias is close to zero here (this is confirmed by looking at the upper left plot in 2a).

The polynomial models with degree larger than one lead to lower bias. Recall that this is the training bias: The polynomial models will try to pass through the training points if possible, and when the degree of the polynomial is large they are able to do so because they have large flexibility compared to a linear model.

```
df_select_x <- filter(df_long, x %in% c(-1, 0.5, 2, 3.5))
```

```
ggplot(df_select_x, aes(x = poly_degree, y = value, group = type)) +
geom_line(aes(color = type)) +
facet_wrap(~x, scales = "free", labeller = label_both) +
theme_bw()
```



Compare to Figures in 2.12 on page 36 in ISL (our textbook).

d) To change f(x), replace

```
truefunc <- function(x) return(x^2)</pre>
```

by for example

```
truefunc <- function(x) return(x^4)</pre>
```

or

```
truefunc <- function(x) return(exp(2 * x))</pre>
```

and rerun the code. Study the results.

If you want to set the variance to 1 for example, set sd = 1 in these parts of the code in 2a and 2b:

```
{r rnorm(length(x)*M, mean=0, sd=1)
```

Also change the following part in 2c:

to get correct plots of the irreducible error. Here, rep(4,prod(dim(varmat))) is replaced by rep(1,prod(dim(varmat))).

R packages

If you want to look at the .Rmd file and knit it, you need to first install the following packages (only once).

```
install.packages("ggplot2")
install.packages("gamlss.data")
install.packages("tidyverse")
install.packages("GGally")
install.packages("Matrix")
install.packages("patchwork")
```

installed.packages()[names(sessionInfo()\$otherPkgs), "Version"]

##	lubridate	forcats	stringr	dplyr	purrr	readr
##	"1.9.3"	"1.0.0"	"1.5.1"	"1.1.4"	"1.0.2"	"2.1.5"
##	tidyr	tibble	tidyverse	patchwork	MASS	GGally
##	"1.3.1"	"3.2.1"	"2.0.0"	"1.2.0"	"7.3-60.0.1"	"2.2.1"
##	ggplot2	ISLR				
##	"3.5.0"	"1.4"				