Module 2: Recommended Exercises - Solution

TMA4268 Statistical Learning V2024

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Problem 1

a) Classification

Example 1: Cancer diagnostics. Response: cancer (yes/no). Predictors: smoking, age, family history, gene expression ect. Goal: prediction.

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

Example 3: Flower species. Response: species. Predictors: color, height, leafes ect. Goal: prediction

b) Regression

Example 1: Illness classification. Response: age of death. Predictors: current age, gender, resting heart rate, resting breath rate ect. Goal: prediction

Example 2: House price. Response: Price. Predictors: age of house, price of neighbourhood, crime rate, distance to town, distance to school, ect. Goal: prediction

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

Problem 2

- a) Based on the three different models compared here, a rigid method will have 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 inbetween, with low variance and low bias.

Problem 3

##

##

##

##

##

##

Min.

Mean

Max.

: 8.00

:15.54

:24.80

1st Qu.:13.78

3rd Qu.:17.02

Median :15.50

:70.00

:75.98

:82.00

1st Qu.:73.00

Median :76.00

3rd Qu.:79.00

Min.

Mean

Max.

Min.

Mean

Max.

```
#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
                         130 165 150 150 140 198 220 215 225 190 ...
                 : num
##
   $ 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 ...
   $ year
                  : 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
```

The dimensions are 392 observations (rows) of 9 variables (columns). See from looking at the structure (str()) and summary() that cylinders (taking values 3,4,5,6,8), origin (taking values 1,2,3) and name (name of the cars) are qualitative predictors. The rest of the predictors are quantitative.

:1.000

:1.577

:3.000

1st Qu.:1.000

Median :1.000

3rd Qu.:2.000

amc matador

ford pinto

amc gremlin

amc hornet

(Other)

toyota corolla

chevrolet chevette:

:

5

4

4

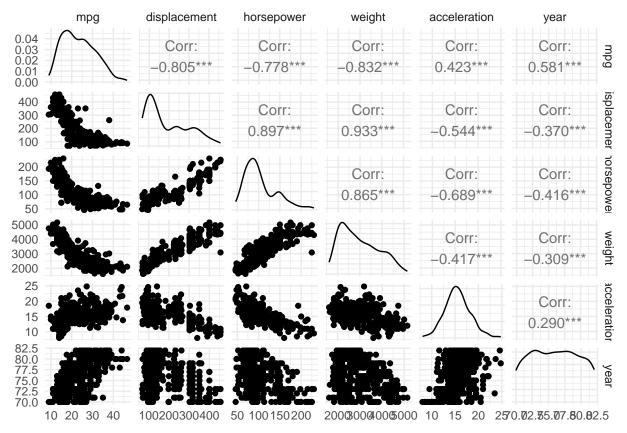
:365

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 \leftarrow c(1, 3, 4, 5, 6, 7)
sapply(Auto[, quant], range)
         mpg displacement horsepower weight acceleration year
## [1,] 9.0
                         68
                                     46
                                          1613
                                                         8.0
                                                                70
## [2,] 46.6
                        455
                                    230
                                          5140
                                                        24.8
                                                                82
  c) To get the and 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 columnwise.
#mean
sapply(Auto[, quant], mean)
##
             mpg displacement
                                  horsepower
                                                    weight acceleration
                                                                                   year
                    194.41199
                                                                              75.97959
##
       23.44592
                                  104.46939
                                                2977.58418
                                                                15.54133
#or
mean(Auto[, 1])
## [1] 23.44592
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
#or
colMeans(Auto[, quant])
##
             mpg displacement
                                 horsepower
                                                    weight acceleration
                                                                                   year
##
       23.44592
                    194.41199
                                  104.46939
                                                2977.58418
                                                                15.54133
                                                                              75.97959
#sd
sapply(Auto[, quant], sd)
```

```
mpg displacement
##
                                                   weight acceleration
                                 horsepower
                                                                                  year
##
       7.805007
                   104.644004
                                  38.491160
                                               849.402560
                                                               2.758864
                                                                             3.683737
#or
sd(Auto[, 1])
## [1] 7.805007
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 displacement horsepower weight acceleration year
## [1,] 11.0
                        68
                                    46
                                          1649
                                                         8.5
                                                               70
                                   230
## [2,] 46.6
                       455
                                          4997
                                                        24.8
                                                               82
sapply(ReducedAuto[, quant], mean)
##
            mpg displacement
                                 horsepower
                                                   weight acceleration
                                                                                  year
##
                    187.24051
                                  100.72152
                                                                             77.14557
       24.40443
                                               2935.97152
                                                               15.72690
sapply(ReducedAuto[, quant], sd)
##
            mpg displacement
                                 horsepower
                                                   weight acceleration
                                                                                  year
                    99.678367
##
       7.867283
                                  35.708853
                                               811.300208
                                                               2.693721
                                                                             3.106217
  e) Make a scatterplot 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()
```

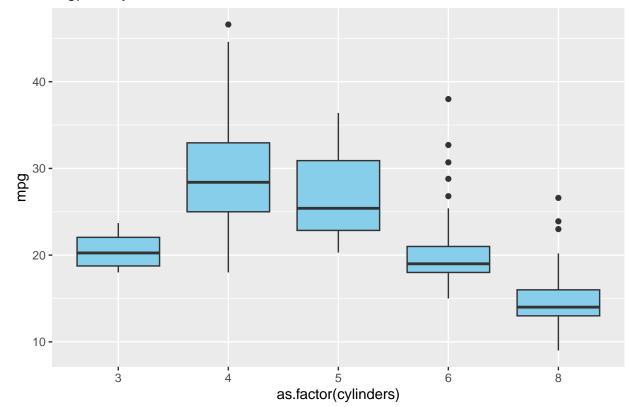


We see that there seems to be strong relationships (based on curve trends and correlation) between the pairs: mpg and displacement, mpg and horsepower, mpg and weight, displacement and horsepower, displacement and weight, horsepower and weight, and horsepower and acceleration.

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

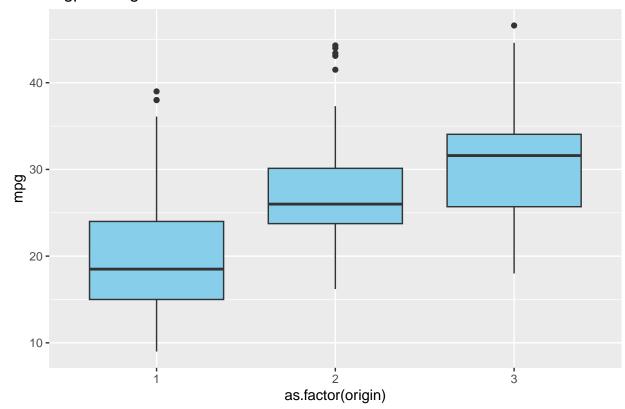
```
ggplot(Auto, aes(as.factor(cylinders), mpg)) +
geom_boxplot(fill = "skyblue") +
labs(title = "mgp vs cylinders")
```

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] -0.8051269
covMat[1, 3] / (sqrt(covMat[1, 1]) * sqrt(covMat[3, 3]))
## [1] -0.7784268
covMat[1, 4] / (sqrt(covMat[1, 1]) * sqrt(covMat[4, 4]))
## [1] -0.8322442
cor(Auto[, quant])
##
                       mpg displacement horsepower
                                                        weight acceleration
## mpg
                 1.0000000
                             -0.8051269 -0.7784268 -0.8322442
                                                                  0.4233285
## displacement -0.8051269
                              1.0000000 0.8972570 0.9329944
                                                                 -0.5438005
## horsepower
                -0.7784268
                              0.8972570 1.0000000 0.8645377
                                                                 -0.6891955
## weight
                -0.8322442
                              0.9329944 0.8645377 1.0000000
                                                                 -0.4168392
## acceleration 0.4233285
                             -0.5438005 -0.6891955 -0.4168392
                                                                  1.0000000
## year
                 0.5805410
                             -0.3698552 -0.4163615 -0.3091199
                                                                  0.2903161
##
                      year
```

```
## mpg 0.5805410

## displacement -0.3698552

## horsepower -0.4163615

## weight -0.3091199

## acceleration 0.2903161

## year 1.0000000
```

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

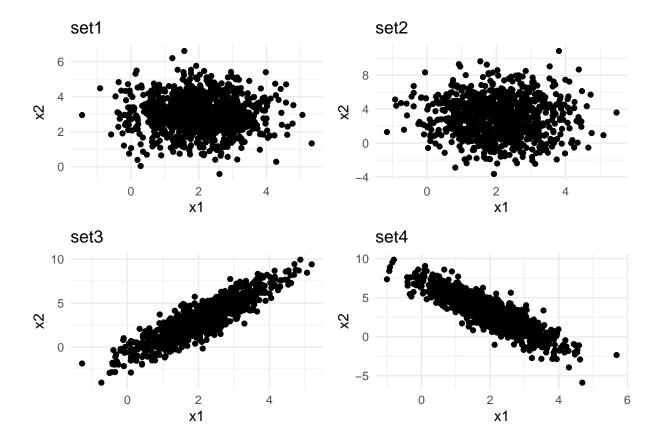
p1 <- ggplot(set1, aes(x1, x2)) + geom_point() + labs(title = "set1") + theme_minimal()

p2 <- ggplot(set2, aes(x1, x2)) + geom_point() + labs(title = "set2") + theme_minimal()

p3 <- ggplot(set3, aes(x1, x2)) + geom_point() + labs(title = "set3") + theme_minimal()

p4 <- ggplot(set4, aes(x1, x2)) + geom_point() + labs(title = "set4") + theme_minimal()

(p1 + p2) / (p3 + p4)</pre>
```

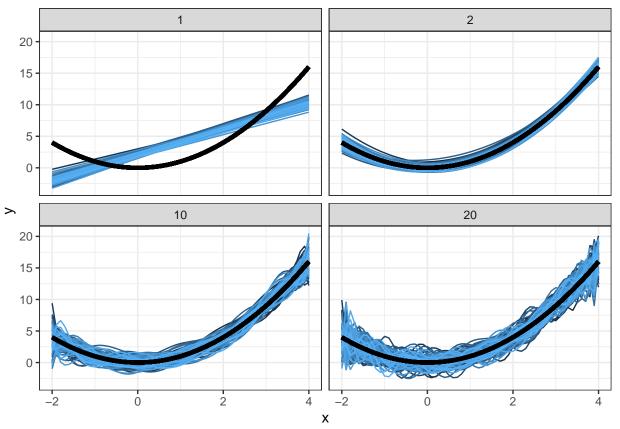


Problem 5

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:

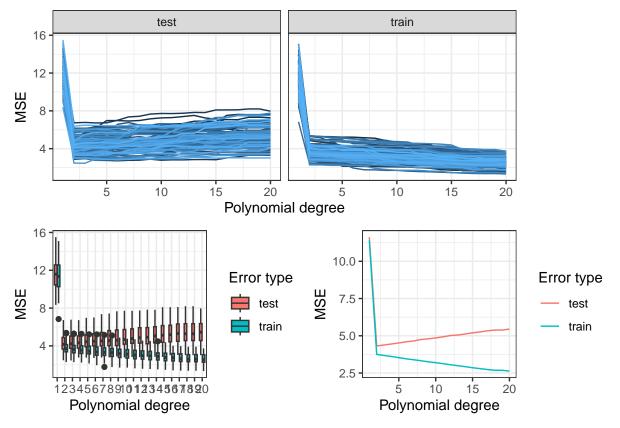
```
set.seed(2) # to reproduce
M <- 100 # repeated samplings,x fixed but new errors
nord <- 20

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 reasonable. The fitted 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.

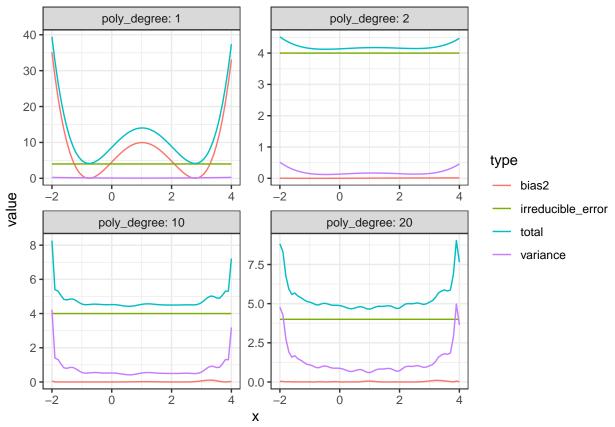
- We observe that poly 2 gives the smallest mean testMSE, while poly 20 gives the smallest trainMSE. Based on these plots, we would choose poly 2 for prediction of a new value of y, as the testMSE tells us more about how the model performs on data not used to train the model.
- c) Run the code and consider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



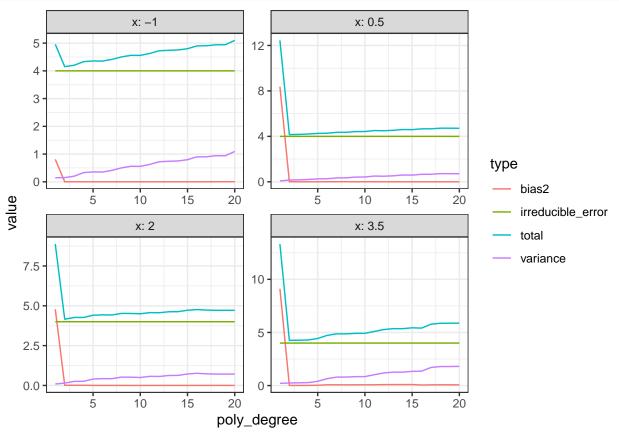
We see that the irriducible error remains constant with the complexity of the model and the variance (purple) increases with the complexity. A linear model gives variance close to zero, while a polynomial of degree 20 gives variance close to 1 (larger at the borders). A more complex model is more flexible 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.).

Further, 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"]
##
      forcats
                                                                 tidyr
                 stringr
                               dplyr
                                          purrr
                                                     readr
                                                                           tibble
##
      "0.5.2"
                 "1.5.0"
                             "1.1.2"
                                        "1.0.1"
                                                   "2.1.3"
                                                               "1.3.0"
                                                                          "3.2.1"
##
    tidyverse patchwork
                                MASS
                                         GGally
                                                                  ISLR
                                                   ggplot2
                 "1.1.2" "7.3-58.2"
##
      "1.3.2"
                                        "2.1.2"
                                                    "3.4.2"
                                                                 "1.4"
```