Lab 1: Bias-Var Tradeoff & Poly Regression

Parijat Dube

2/4/2023

Please submit your finished lab on Canvas as a knitted pdf or html document. The lab is due on Feb 20, 2023.

Section I: Goal

The learning objective of this lab is to investigate the important bias-variance tradeoff in a linear regression setting under squared loss. This will be accomplished by running a small simulation study. The required tasks are stated in Section V.

Section II: Bias-Variance Tradeoff

Let $(x_1, y_1), \ldots, (x_n, y_n)$ be the training data and denote the trained model by $\hat{f}(x)$. Consider a single test case (x_0, y_0), which was not used to train $\hat{f}(x)$. The mean square error at test case (x_0, y_0) can be decomposed into three parts; i) variance of $\hat{f}(x_0)$, ii) squared bias of $\hat{f}(x_0)$, and iii) irreducible error variance $\text{Var}(\epsilon_0)$. The decomposition is stated below:

$$\begin{aligned} MSE(x_0) &= MSE\hat{f}(x_0) \\ &= E[(y_0 - \hat{f}(x_0))^2] \\ &= \text{Var}(\hat{f}(x_0)) + (E\hat{f}(x_0) - f(x_0))^2 + \text{Var}(\epsilon_0) \end{aligned}$$

Section III: True Model and Simulated Data

Assume X is not random taking on values in the interval $[4, 20]$ and the true relationship between fixed X and response Y is:

$$y = f(x) + \epsilon = (x - 5)(x - 12) + \epsilon,$$

where ϵ is normally distributed with $E(\epsilon) = 0$ and $\text{Var}(\epsilon_0) = 20^2$. Note that for test case (x_0, y_0), the statistical relation between x_0 and y_0 is

$$y_0 = f(x_0) + \epsilon.$$

The function **true.f()** defined in the code chunk below defines $f(x)$ and is evaluated at $x = 16$.

```
true.f <- function(x) {
  f.out <- (x-5)*(x-12)
  return(f.out)
}
true.f(16)
```

```
## [1] 44
```

The function **sim.training()** simulates a training dataset of size $n = 20$ based on our regression model. The training feature x is hard-coded and takes on equally spaced values over the interval $[4, 20]$. The only input of **sim.training()** is the feature test case x_0. The function returns the simulated dataset and the response for test case(s) x_0.

```
sim.training <- function(x.test=c(16)
                         ) {
  # Hard-coded sample size and standard deviation
  n <- 20
  sd.error <- 20

  # Training x vector
  x <- seq(4,20,length=n)

  # Simulate training Y based on f(x) and normal error
  y <- true.f(x)+rnorm(n,sd=sd.error)

  # Simulate test case
  y.test <- true.f(x.test)+rnorm(length(x.test),sd=sd.error)

  # Return a list of two entries:
    # 1) the dataframe data.train
    # 2) test respone vector y_0
  return(list(data.train=data.frame(x=x,y=y),
              y.test=y.test))
}
```

To illustrate **sim.training()**, we simulate a training dataset using **set.seed(1)**. Two test cases are chosen at $x_0 = 10, 16$. The following code chunk also plots the simulated data with the true relationship $f(x)$ and chosen test cases. Make sure to run the entire code chunk at once.

```
# Simulate data
set.seed(1)
x.test <- c(10, 16)
sim.data.train <- sim.training(x.test = x.test)
head(sim.data.train$data.train, 4)
```

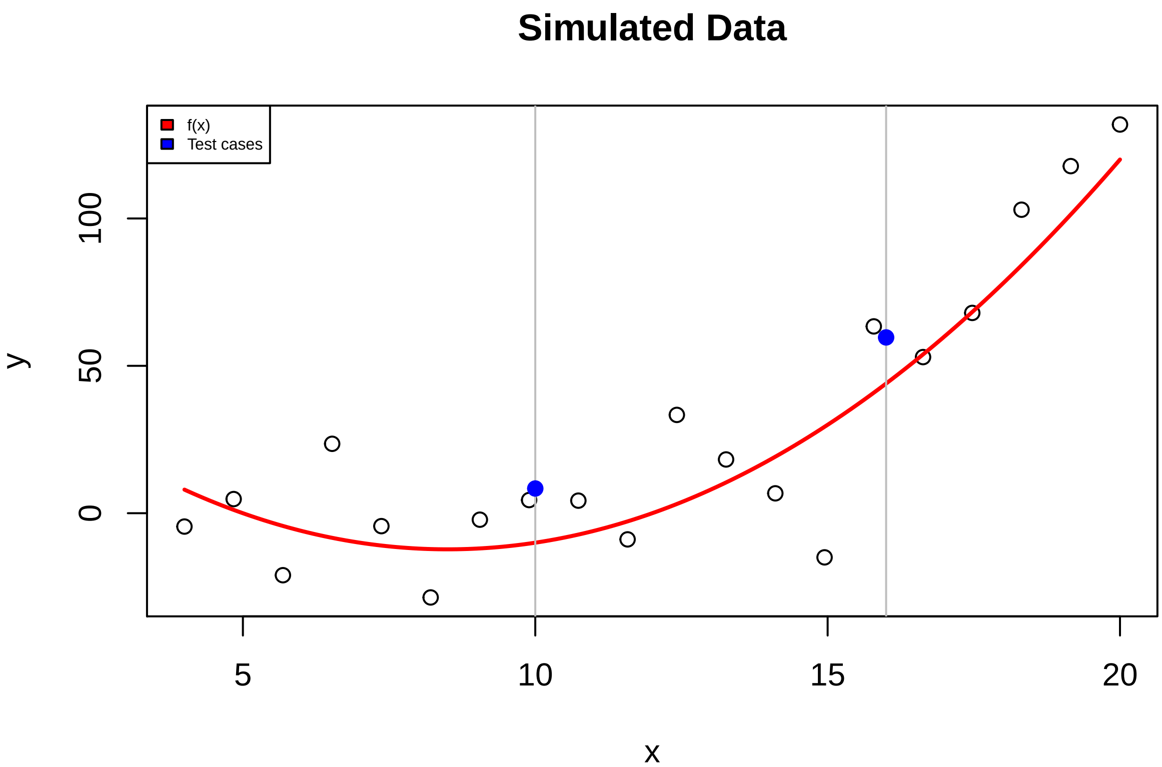
```
##          x          y
## 1 4.000000  -4.529076
## 2 4.842105   4.803060
## 3 5.684211 -21.033902
## 4 6.526316  23.551045
```

```
sim.data.train$y.test
```

```
## [1]  8.379547 59.642726
```

```
# Plot simulated data
x.plot <- seq(4, 20, by = 0.01)
x <- sim.data.train$data.train$x
y <- sim.data.train$data.train$y
plot(x, y, main = "Simulated Data")

# Plot f(x)
lines(x.plot, true.f(x.plot), lwd = 2, col = "red")

# Plot test cases
y.test <- sim.data.train$y.test
abline(v = x.test, col = "grey")
```

```
points(x.test, y.test, pch = 20, cex = 1.5, col = "blue")

# Legend
legend("topleft", legend = c("f(x)", "Test cases"), fill = c("red", "blue"), cex = 0.5)
```



Section IV: Polynomial Regression and Tuning Parameter

Recall form lecture, the number of features (p) in a multiple linear regression model is a tuning parameter. This naturally extends to polynomial regression as stated in the below model:

$$y = \beta_0 + \beta_1 x + \beta_2 x^2 + \cdots + \beta_p x^p + \epsilon$$

In this case, the tuning parameter is the degree of our polynomial p. High degree polynomials can approximate any continuous differentiable function. However, too high of a degree can lead to overfitting and poor generalization.

To fit this model, use the the **lm()** function in conjunction with **poly()**. Technically we will utilize orthogonal polynomials which is not exactly the same as the polynomial regression model above. The function **predict.test.case()** defined in the code chunk below estimates y_0 based on the p^{th} degree trained polynomial, i.e., $\hat{f}_p(x_0)$. The inputs are; i) the degree of the polynomial **degree**, ii) the training data **data**, and iii) a vector test cases **x.test**.

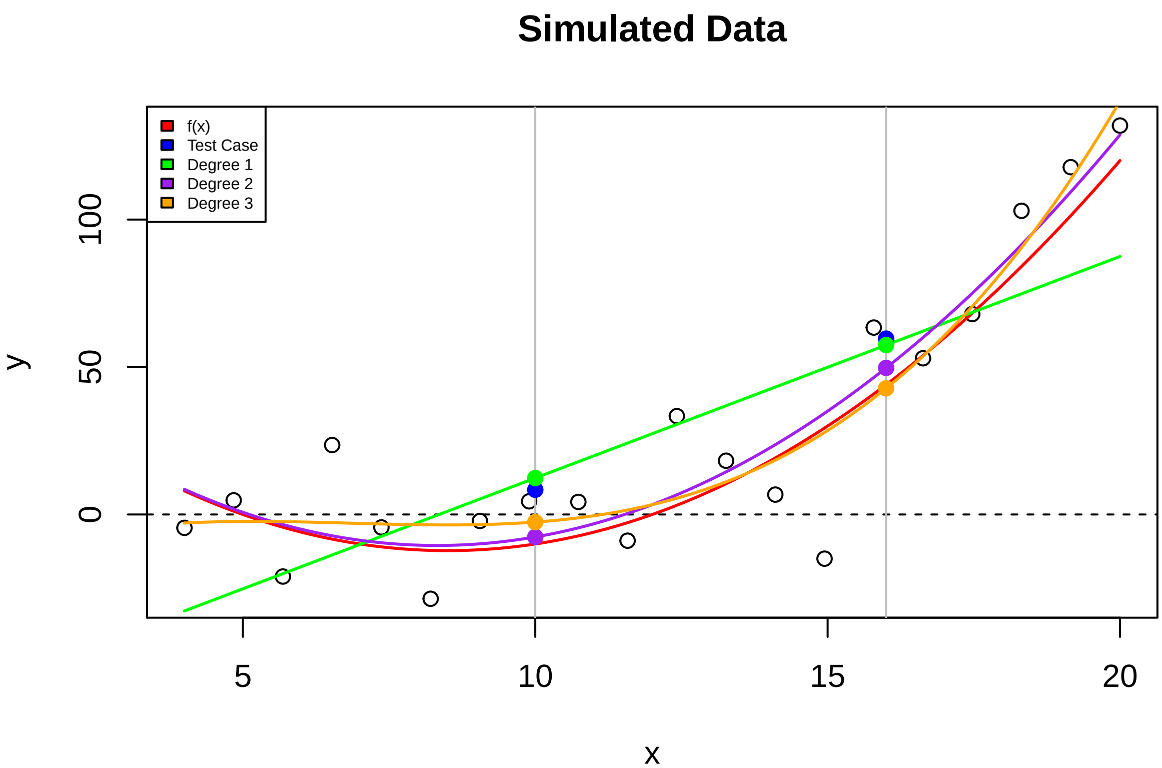
```
predict.test.case <- function(degree,
                              data,
                              x.test) {

  # Train model
  model <- lm(y~poly(x,degree=degree),data=data)
  # Predict test cases
  y.test.hat <- predict(model,newdata=data.frame(x=x.test))
```

```
  # Return y test case
  return(y.test.hat)
}
```

To illustrate **predict.test.case()**, consider estimating y_0 for inputs $x_0 = 10, 16$, where the polynomial is trained using our simulated data **sim.data.train**. Notice that **predict.test.case()** can also be used for plotting.

```
x.plot <- seq(4,20,by=.01)
x.test <- c(10,16)
# Predict for degree=1
y.pred.1 <- predict.test.case(degree=1,
                              data=sim.data.train$data.train,
                              x.test=x.test)
y.plot.1 <- predict.test.case(degree=1,
                              data=sim.data.train$data.train,
                              x.test=x.plot)
# Predict for degree=2
y.pred.2 <- predict.test.case(degree=2,
                              data=sim.data.train$data.train,
                              x.test=x.test)
y.plot.2 <- predict.test.case(degree=2,
                              data=sim.data.train$data.train,
                              x.test=x.plot)
# Predict for degree=3
y.pred.3 <- predict.test.case(degree=3,
                              data=sim.data.train$data.train,
                              x.test=x.test)
y.plot.3 <- predict.test.case(degree=3,
                              data=sim.data.train$data.train,
                              x.test=x.plot)

# Plot simulated data
x <- sim.data.train$data.train$x
y <- sim.data.train$data.train$y
plot(x,y,main="Simulated Data")
abline(h=0,lty=2)

# Plot f(x)
lines(x.plot,true.f(x.plot),lwd=1.5,col="red")

# Plot the estimated curves
lines(x.plot,y.plot.1,lwd=1.5,col="green")
lines(x.plot,y.plot.2,lwd=1.5,col="purple")
lines(x.plot,y.plot.3,lwd=1.5,col="orange")

# Plot test cases
y.test <- sim.data.train$y.test
abline(v=x.test,col="grey")
points(x.test,y.test,pch=20,cex=1.5,col="blue")

# Plot estimated test cases
points(x.test,y.pred.1,pch=20,cex=1.5,col="green")
points(x.test,y.pred.2,pch=20,cex=1.5,col="purple")
```

```r
points(x.test,y.pred.3,pch=20,cex=1.5,col="orange")

# Legend
legend("topleft",
       legend=c("f(x)","Test Case","Degree 1","Degree 2","Degree 3"),
       fill=c("red","blue","green","purple","orange"),
       cex=.5)
```



The above code is clunky and can easily be refined. To clean up this process, the function **poly.predict()** defined below trains several polynomial models based on a vector of degrees and outputs the predicted response simultaneously. This function vectorizes **predict.test.case()**. The inputs are; i) a vector of degrees **degree.vec**, ii) a vector of x test points **x.test**, iii) a training dataset **data**. The output of **poly.predict()** is a matrix where the row corresponds to the respective test cases. To see this function in action, the below code also evaluates $\hat{f}_p(x_0)$ at inputs $x_0 = 10, 16$ using polynomial degrees 1,2,3,4.

```r
poly.predict <- function(degree.vec,
                         data,
                         x.test) {

  # Vectorize predict.test.case()
  pred <- sapply(degree.vec,
                 predict.test.case,
                 data=data,
                 x.test=x.test)

  # Name rows and columns
  rownames(pred)  <- paste("TestCase",1:length(x.test),sep="")
  colnames(pred)  <- paste("D",degree.vec,sep="")
  # Return
  return(pred)
```

```
}

# Test function poly.predict()
x.test <- c(10,16)
poly.predict(degree.vec=1:4,
             data=sim.data.train$data.train,
             x.test=x.test)
```

```
##                 D1       D2        D3        D4
## TestCase1 12.36425 -7.61066 -2.568078 -2.819858
## TestCase2 57.43977 49.70754 42.782198 43.149616
```

Section V: Student Tasks: (1) - (3)

Students will solve three major tasks in this lab. The first task is described below.

Task 1

Simulate **R=1000** training datasets and for each iteration (or each simulated dataset), store the predicted test cases corresponding to inputs $x_0 = 10, 16$. For each simulated dataset, you must predict y_0 using polynomial regression having degrees $p = 1, 2, 3, 4, 5$. You can easily solve this problem using a loop and calling on the two functions **sim.training()** and **poly.predict()**.

Your final result will be three matrices. The first matrix **mat.pred.1** is the collection of predicted test cases for each degree corresponding to input $x_0 = 10$. Similarly, the matrix **mat.pred.2** corresponds to $x_0 = 16$. The first two matrices are dimension (5×1000). The third matrix **y.test.mat** is the collection of all test cases y_0 for each simulated dataset. This matrix is dimension (2×1000). After completing this problem, display the first three columns of each matrix.

```
# Solution goes here -----------
```

Task 2

The second task is to estimate three different quantities based on the simulation from Task (1). For each polynomial degree ($p = 1, 2, 3, 4, 5$), use the matrices **mat.pred.1**, **mat.pred.2** and **y.test.mat** to estimate:

1. The mean square error $MSE(x_0)$
2. The variance $\text{Var}(\hat{f}(x_0))$
3. The squared bias $(E\hat{f}(x_0) - f(x_0))^2$

After solving this problem, display the 6 vectors of interest.

Notes:

1) When estimating the squared bias, students will use **y.test.mat** to estimate $E\hat{f}(x_0)$ but will also call the function **true.f()** for computing $f(x_0)$. Obviously in practice we never know the true relation $f(x)$.
2) To estimate $MSE(x_0)$, you can slightly modify your loop from Task (1) or write a new program that computes $(y_0 - \hat{f}(x_0))^2$ for all $R = 1000$ iterations. Then take the average of the resulting vectors.

```
# Solution goes here -----------
```

Task 3

The third task requires students to construct a plots showing $MSE(x_0)$, $\text{Var}(\hat{f}(x_0))$ and $\text{Bias}^2(\hat{f}(x_0))$ as a function of the polynomial degree. There should be two graphics corresponding to the two test cases $x_0 = 10$

and $x_0 = 16$.

```
# Solution goes here -----------
```