Homework 1

Due: noon, Friday, January 20

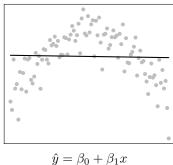
Submission instructions:

- Submit *only* one write-up per group on Gradescope. Suggested group size is 3 people. You can work by yourself on the homework.
- [IMPORTANT] Make sure to add all group members on Gradescope. https://help.gradescope.com/article/m5qz2xsnjy-student-add-group-members
- Additionally, write names of everyone that worked on the assignment on the submission.

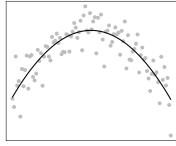
1 Question 1

For each one the ten statements below say whether they are true or not and explain why.

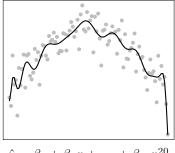
- 1. As one increases k, the number of nearest neighbor, in a kNN classifier,
 - (a) the bias of the classifier will increase;
 - (b) the variance of the classifier will increase;
 - (c) the misclassification rate on the training dataset will increase;
 - (d) the misclassification rate on a test dataset will increase.
- 2. Consider the three line regression fits to the gray points plotted below.







$$\hat{y} = \beta_0 + \beta_1 x + \beta_2 x^2 \tag{2}$$



$$\hat{y} = \beta_0 + \beta_1 x + \dots + \beta_{20} x^{20}$$
(3)

- (a) The estimate in (2) has a higher variance than the estimate in (1).
- (b) The estimate in (2) has a higher bias than the estimate in (3).
- (c) The estimate in (3) has the smallest training error.
- (d) The estimate in (1) has the smallest test error.
- 3. Misclassification rate of a classifier evaluated on a validation set will never be smaller than the one evaluated on the training set that is used to build the classifier.
- 4. *k*-fold cross-validation provides an unbiased estimate of the predictive error of the models.

2 Question 2

In this question, you will run a simulation study to explore the bias-variance trade-off in more depth. The exercise will walk you through prediction using linear regression versus k-NN. You will discover under what circumstances one outperforms the other (in terms of the test error). In the end you will reproduce something similar to what you see in figures 3.17 through 3.20 in Section 3.6 of *Introduction to Statistical Learning*.

1. You will start by exploring a scenario where the true relationship between x and y is linear. You will generate data from the linear model

$$y = f(x) + \epsilon$$

where f(x)=1.8x+2. To create a synthetic training set, make 100 independent draws of x from a uniform distribution on [-1,1] to form $\{x_1,\cdots,x_{100}\}$. Similarly draw random noise ϵ from a Normal distribution with mean zero and standard deviation 0.1 to have $\{\epsilon_1,\cdots,\epsilon_{100}\}$. For each $i\in\{1,\cdots,100\}$, generate y_i from the linear model where $y_i=1.8x_i+2+\epsilon_i$. Now, repeat the above process and generate additional 10,000 observations that will form the test set. Note that we are constructing a huge test set in order to have an accurate out-of-sample MSE estimate. You will use this simulated dataset to try out and compare different models.

- 2. Create a scatter plot of y vs x. In the same figure, draw the true relationship in black solid line.
- 3. Using ordinary linear regression, find a relationship between y and x of the form

$$y = b_0 + b_1 \times x + e$$

using the training data you simulated. On the same plot from the last question, draw a blue dashed line that is the least squares fit to the data.

- 4. You may find that the linear regression line provides a very good estimate of f(X). Now, use k-NN to find the relationship between y and x. You should experiment with $k=2,3,\cdots,15$ to see how model complexity affects prediction accuracy. On one plot, redraw the scatter plot and the true relationship, but this time overlay it with predicted fit using k-NN with k=2. On a juxtaposed graph, do the same for k=12.
- 5. Plot the test set mean squared error using k-NN against $\log(1/k)$ for $k=2,3,\cdots,15$. On the same graph, draw a horizontal dashed line that represents the test set mean squared error using linear regression. Which model performs the best? Comment on the relative performance of linear regression and k-NN with different values of k.
- 6. Redo 1-5, but consider a different data generating process where the true relationship between x and y is near, but not perfectly linear. Precisely, simulate data from the following model

$$y_i = \tanh(1.1 \times x_i) + 2 + \epsilon_i.$$

How does your conclusion in 5 change?

7. Consider yet another data generating process where the true relationship is strongly non-linear. Simulate data from the following model

$$y_i = \sin(2x_i) + 2 + \epsilon_i.$$

What can you say about the relative performance of the two methods now?

8. You might suspect, from your previous results, that in real world when none of the relationship could be linear, it would always pay off using k-NN over linear regression. Examine this hypothesis in the situation with more than 1 variable. Stay with the same true relationship from the model in 7, add additional noise variables that are not predictors of *y*. In particular, consider the model

$$y_i = \sin(2 \times x_{i1}) + 2 + 0 \times x_{i2} + \dots + 0 \times x_{ip} + \epsilon_i$$

where p is 2, 5, 10, or 20. Additional, noisy x_{i2}, \ldots, x_{ip} variables are drawn from a uniform distribution on [-1,1]. Create a plot for every p taking values in 1,2,5,10,20. Each plot should have the test set MSE against model complexity $\log(1/K)$ and a dashed horizontal line showing test set MSE for best linear fit. Briefly explain the result of the simulation.

9. Suppose that instead of 100 training samples, you had 1,000 training samples. Would that change conclusions you made above? Think about how the range of values of k for which k-NN does better that linear regression would change. What does having a large training set allow you to do?

3 Question 3

In this question, you will explore prices of used cars as a function of different input variables. Download the file UsedCars.csv from Canvas.

- 1. Take a look at the data-set and describe for what kind of business related problems you could use this data. That is, why would anyone care to collect this data?
- 2. Using ordinary linear regression, find a relationship between price and mileage of the form

$$price = b_0 + b_1 \times mileage + e$$

using the training data. Create a scatter plot of price vs mileage. Include the best linear regression fit onto the plot.

3. You might notice that the linear fit does not capture the true relationship well. Use k-NN and regression trees to find the relationship between price and mileage. Use cross-validation to find the optimal tuning parameters for these two procedures: k for k-NN and the number of leaves for decision trees. Create plots showing the cross-validation estimate of the mean-squared error as a function of tuning parameters. Create a scatter plot of price vs mileage that shows the best k-NN and regression tree fits. Which fit would you use and why? Report the estimate of the test error for the model you select.

Hint: You should not try every value of k here as this would take too long.

- 4. Now try using mileage and year to predict price using k-NN and regression trees. Remember to rescale data when using k-NN. As before, use cross-validation to pick optimal tuning parameters and plot the cross-validation error curves. How does the optimal k change as compared to when you were using only mileage? How about the size of the optimal tree? Does your model perform better when including year as an additional variable?
- 5. Finally, run a regression tree using all the variables to predict price. Report the estimate of the test error for the chosen tree.
- 6. We can use cross-validation to select relevant variables for predicting the price of a used car. Try finding out whether all variables are predictive using regression trees and cross-validation. Think about and describe how would you try to find a simpler model, that is, one that does not include all the variables.