Stat 441/505 Winter 2019
Due date: Mar 18, 2019

Q1. ##----------##

Here we explore the maximal margin classifier on a toy data set.

(a) We are given $n = 7$ observations in $p = 2$ dimensions. For each observation, there is an associated class label.

Obs.	X_1	X_2	Y
1	3	4	Red
2	2	2	Red
3	4	4	Red
4	1	4	Red
5	2	1	Blue
6	4	3	Blue
7	4	1	Blue

Sketch the observations.

(b) Sketch the optimal separating hyperplane, and provide the equation for this hyperplane

(c) Describe the classification rule for the maximal margin classifier. It should be something along the lines of "Classify to Red if $\beta_0 + \beta_1 X_1 + \beta_2 X_2 > 0$, and classify to Blue otherwise." Provide the values for β_0, β_1, and β_2.

(d) On your sketch, indicate the margin for the maximal margin hyperplane.

(e) Indicate the support vectors for the maximal margin classifier.

(f) Argue that a slight movement of the seventh observation would not affect the maximal margin hyperplane.

(g) Sketch a hyperplane that is *not* the optimal separating hyperplane, and provide the equation for this hyperplane.

(h) Draw an additional observation on the plot so that the two classes are no longer separable by a hyperplane.

Q2. ##----------##

This problem involves the `OJ` data set which is part of the `ISLR` package.

(a) Create a training set containing a random sample of 800 observations, and a test set containing the remaining observations.

(b) Fit a support vector classifier to the training data using `cost=0.01`, with `Purchase` as the response and the other variables as predictors. Use the `summary()` function to produce summary statistics, and describe the results obtained.

(c) What are the training and test error rates?

(d) Use the `tune()` function to select an optimal `cost`. Consider values in the range 0.01 to 10.

(e) Compute the training and test error rates using this new value for `cost`.

(f) Repeat parts (b) through (e) using a support vector machine with a radial kernel. Use the default value for `gamma`.

(g) Repeat parts (b) through (e) using a support vector machine with a polynomial kernel. Set `degree=2`.

(h) Overall, which approach seems to give the best results on this data?

Q3. ##----------##

It was mentioned in the chapter that a cubic regression spline with one knot at ξ can be obtained using a basis of the form x, x^2, x^3, $(x-\xi)^3_+$, where $(x-\xi)^3_+ = (x-\xi)^3$ if $x > \xi$ and equals 0 otherwise. We will now show that a function of the form

$$f(x) = \beta_0 + \beta_1 x + \beta_2 x^2 + \beta_3 x^3 + \beta_4 (x-\xi)^3_+$$

is indeed a cubic regression spline, regardless of the values of $\beta_0, \beta_1, \beta_2, \beta_3, \beta_4$.

(a) Find a cubic polynomial

$$f_1(x) = a_1 + b_1 x + c_1 x^2 + d_1 x^3$$

such that $f(x) = f_1(x)$ for all $x \leq \xi$. Express a_1, b_1, c_1, d_1 in terms of $\beta_0, \beta_1, \beta_2, \beta_3, \beta_4$.

(b) Find a cubic polynomial

$$f_2(x) = a_2 + b_2x + c_2x^2 + d_2x^3$$

such that $f(x) = f_2(x)$ for all $x > \xi$. Express a_2, b_2, c_2, d_2 in terms of $\beta_0, \beta_1, \beta_2, \beta_3, \beta_4$. We have now established that $f(x)$ is a piecewise polynomial.

(c) Show that $f_1(\xi) = f_2(\xi)$. That is, $f(x)$ is continuous at ξ.

(d) Show that $f_1'(\xi) = f_2'(\xi)$. That is, $f'(x)$ is continuous at ξ.

(e) Show that $f_1''(\xi) = f_2''(\xi)$. That is, $f''(x)$ is continuous at ξ.

Therefore, $f(x)$ is indeed a cubic spline.

Hint: Parts (d) and (e) of this problem require knowledge of single-variable calculus. As a reminder, given a cubic polynomial

$$f_1(x) = a_1 + b_1x + c_1x^2 + d_1x^3,$$

the first derivative takes the form

$$f_1'(x) = b_1 + 2c_1x + 3d_1x^2$$

and the second derivative takes the form

$$f_1''(x) = 2c_1 + 6d_1x.$$

Q4. ##----------##

This question uses the variables `dis` (the weighted mean of distances to five Boston employment centers) and `nox` (nitrogen oxides concentration in parts per 10 million) from the `Boston` data. We will treat `dis` as the predictor and `nox` as the response.

(a) Use the `poly()` function to fit a cubic polynomial regression to predict `nox` using `dis`. Report the regression output, and plot the resulting data and polynomial fits.

(b) Plot the polynomial fits for a range of different polynomial degrees (say, from 1 to 10), and report the associated residual sum of squares.

(c) Perform cross-validation or another approach to select the optimal degree for the polynomial, and explain your results.

(d) Use the `bs()` function to fit a regression spline to predict `nox` using `dis`. Report the output for the fit using four degrees of freedom. How did you choose the knots? Plot the resulting fit.

(e) Now fit a regression spline for a range of degrees of freedom, and plot the resulting fits and report the resulting RSS. Describe the results obtained.

(f) Perform cross-validation or another approach in order to select the best degrees of freedom for a regression spline on this data. Describe your results.

Q5. ##----------##

This question uses the variables `dis` (the weighted mean of distances to five Boston employment centers) and `nox` (nitrogen oxides concentration in parts per 10 million) from the `Boston` data. We will treat `dis` as the predictor and `nox` as the response.

(a) Plot the kernel smoothing fits using the box kernel for a range of bandwidths (say, from 0.1 to 5), and report the associated residual sum of squares.
(b) Perform cross-validation or another approach to select the optimal bandwidth for the polynomial, and explain your results.
(c) Plot the kernel smoothing fits using the Gaussian kernel for a range of bandwidths (say, from 0.11 to 5), and report the associated residual sum of squares.
(d) Perform cross-validation or another approach to select the optimal bandwidth for the polynomial, and explain your results.
(e) Plot the loess fits for a range of spans (say, from 0.1 to 5), and report the associated residual sum of squares.
(f) Perform cross-validation or another approach to select the optimal span for the polynomial, and explain your results.

Q6. ##----------##

We now review k-fold cross-validation.

(a) Explain how k-fold cross-validation is implemented.

(b) What are the advantages and disadvantages of k-fold cross-validation relative to:

i. The validation set approach?
ii. LOOCV?

Q7. ##----------##

We will now perform cross-validation on a simulated data set.

(a) Generate a simulated data set as follows:

```
> set.seed(1)
> y=rnorm(100)
> x=rnorm(100)
> y=x-2*x^2+rnorm(100)
```

In this data set, what is n and what is p? Write out the model used to generate the data in equation form.

(b) Create a scatterplot of X against Y. Comment on what you find.

(c) Set a random seed, and then compute the LOOCV errors that result from fitting the following four models using least squares:

i. $Y = \beta_0 + \beta_1 X + \epsilon$
ii. $Y = \beta_0 + \beta_1 X + \beta_2 X^2 + \epsilon$
iii. $Y = \beta_0 + \beta_1 X + \beta_2 X^2 + \beta_3 X^3 + \epsilon$
iv. $Y = \beta_0 + \beta_1 X + \beta_2 X^2 + \beta_3 X^3 + \beta_4 X^4 + \epsilon.$

Note you may find it helpful to use the `data.frame()` function to create a single data set containing both X and Y.

(d) Repeat (c) using another random seed, and report your results. Are your results the same as what you got in (c)? Why?

(e) Which of the models in (c) had the smallest LOOCV error? Is this what you expected? Explain your answer.

(f) Comment on the statistical significance of the coefficient estimates that results from fitting each of the models in (c) using least squares. Do these results agree with the conclusions drawn based on the cross-validation results?

Q8. ##----------##

We will now consider the `Boston` housing data set, from the `MASS` library.

(a) Based on this data set, provide an estimate for the population mean of `medv`. Call this estimate $\hat{\mu}$.

(b) Provide an estimate of the standard error of $\hat{\mu}$. Interpret this result.
Hint: We can compute the standard error of the sample mean by dividing the sample standard deviation by the square root of the number of observations.

(c) Now estimate the standard error of $\hat{\mu}$ using the bootstrap. How does this compare to your answer from (b)?

(d) Based on your bootstrap estimate from (c), provide a 95 % confidence interval for the mean of `medv`. Compare it to the results obtained using `t.test(Boston$medv)`.
Hint: You can approximate a 95 % confidence interval using the formula $[\hat{\mu} - 2SE(\hat{\mu}), \hat{\mu} + 2SE(\hat{\mu})]$.

(e) Based on this data set, provide an estimate, $\hat{\mu}_{med}$, for the median value of `medv` in the population.

(f) We now would like to estimate the standard error of $\hat{\mu}_{med}$. Unfortunately, there is no simple formula for computing the standard error of the median. Instead, estimate the standard error of the median using the bootstrap. Comment on your findings.

(g) Based on this data set, provide an estimate for the tenth percentile of `medv` in Boston suburbs. Call this quantity $\hat{\mu}_{0.1}$. (You can use the `quantile()` function.)

(h) Use the bootstrap to estimate the standard error of $\hat{\mu}_{0.1}$. Comment on your findings.

Q9. ##----------##

Suppose we produce ten bootstrapped samples from a data set containing red and green classes. We then apply a classification tree to each bootstrapped sample and, for a specific value of X, produce 10 estimates of $P(\text{Class is Red}|X)$:

$$0.1, 0.15, 0.2, 0.2, 0.55, 0.6, 0.6, 0.65, 0.7, \text{ and } 0.75.$$

There are two common ways to combine these results together into a single class prediction. One is the majority vote approach discussed in this chapter. The second approach is to classify based on the average probability. In this example, what is the final classification under each of these two approaches?

Q10. ##----------##

In the lab, a classification tree was applied to the `Carseats` data set after converting `Sales` into a qualitative response variable. Now we will seek to predict `Sales` using regression trees and related approaches, treating the response as a quantitative variable.

(a) Split the data set into a training set and a test set.

(b) Fit a regression tree to the training set. Plot the tree, and interpret the results. What test MSE do you obtain?

(c) Use cross-validation in order to determine the optimal level of tree complexity. Does pruning the tree improve the test MSE?

(d) Use the bagging approach in order to analyze this data. What test MSE do you obtain? Use the `importance()` function to determine which variables are most important.

(e) Use random forests to analyze this data. What test MSE do you obtain? Use the `importance()` function to determine which variables are most important. Describe the effect of m, the number of variables considered at each split, on the error rate obtained.

Q11. ##----------##

This problem involves the `OJ` data set which is part of the `ISLR` package.

(a) Create a training set containing a random sample of 800 observations, and a test set containing the remaining observations.

(b) Fit a tree to the training data, with `Purchase` as the response and the other variables except for `Buy` as predictors. Use the `summary()` function to produce summary statistics about the tree, and describe the results obtained. What is the training error rate? How many terminal nodes does the tree have?

(c) Type in the name of the tree object in order to get a detailed text output. Pick one of the terminal nodes, and interpret the information displayed.

(d) Create a plot of the tree, and interpret the results.

(e) Predict the response on the test data, and produce a confusion matrix comparing the test labels to the predicted test labels. What is the test error rate?

(f) Apply the `cv.tree()` function to the training set in order to determine the optimal tree size.

(g) Produce a plot with tree size on the x-axis and cross-validated classification error rate on the y-axis.

(h) Which tree size corresponds to the lowest cross-validated classification error rate?

(i) Produce a pruned tree corresponding to the optimal tree size obtained using cross-validation. If cross-validation does not lead to selection of a pruned tree, then create a pruned tree with five terminal nodes.

(j) Compare the training error rates between the pruned and unpruned trees. Which is higher?

(k) Compare the test error rates between the pruned and unpruned trees. Which is higher?

Q12. ##----------##

We now use boosting to predict `Salary` in the `Hitters` data set.

(a) Remove the observations for whom the salary information is unknown, and then log-transform the salaries.

(b) Create a training set consisting of the first 200 observations, and a test set consisting of the remaining observations.

(c) Perform boosting on the training set with 1,000 trees for a range of values of the shrinkage parameter λ. Produce a plot with different shrinkage values on the x-axis and the corresponding training set MSE on the y-axis.

(d) Produce a plot with different shrinkage values on the x-axis and the corresponding test set MSE on the y-axis.

(e) Compare the test MSE of boosting to the test MSE that results from applying two of the regression approaches seen in regular linear regression and shrinkage linear regression (say, ridge or lasso).

(f) Which variables appear to be the most important predictors in the boosted model?

(g) Now apply bagging to the training set. What is the test set MSE for this approach?