Please answer to the point, and do not spend time/space giving irrelevant details. Please state any additional assumptions you make while answering the questions. For Questions 1 to 5, 6(b) and 6(c), you need to submit your answers in a single PDF file on autolab, either a scanned handwritten version or a \LaTeX pdf file. Please make sure you write legibly for grading. For Question 6(a), submit your m-files on autolab.

You can work in groups. However, no written notes can be shared, or taken during group discussions. You may ask clarifying questions on Piazza. However, under no circumstances should you reveal any part of the answer publicly on Piazza or any other public website. The intention of this policy is to facilitate learning, not circumvent it. Any incidents of plagiarism will be handled in accordance with CMU’s Policy on Academic Integrity.

*: Code of Conduct Declaration

- Did you receive any help whatsoever from anyone in solving this assignment? Yes / No.
- If you answered yes, give full details: ________________________________ (e.g. Jane explained to me what is asked in Question 3.4)
- Did you give any help whatsoever to anyone in solving this assignment? Yes / No.
- If you answered yes, give full details: ________________________________ (e.g. I pointed Joe to section 2.3 to help him with Question 2).
Let $X$ and $Y$ be two random variables, $\beta$ be a constant, and $\epsilon \sim \mathcal{N}(0, \sigma^2)$ be a Gaussian random variable with zero mean and variance $\sigma^2$. We assume $Y = \beta X + \epsilon$, and that $\epsilon$ is independent of $X$.

(a) Show that given $X = x$, the distribution of $Y$ is $\mathcal{N}(\beta x, \sigma^2)$

(b) Let $\{(X_i, Y_i), i = 1, \cdots, n\}$ be $n$ independent samples from the model above. Show that the maximum likelihood estimation of $\beta$, where the likelihood is with regard to the conditional distribution $Y|X$, is the least square solution

$$\hat{\beta} = \arg\min_{\beta} \sum_{i=1}^{n} (Y_i - \beta X_i)^2$$

Solution

1. Given $X = x$, $Y = \beta x + \epsilon$, since $\beta x$ is a constant and $\epsilon$ is a Gaussian random variable, $Y$ is also a Gaussian random variable. A Gaussian random variable only has two parameters, the mean $E(Y|X = x) = E(\beta x + \epsilon|X = x) = \beta x$, and the variance, $var(Y|X = x) = var(\beta x + \epsilon|X = x) = var(\epsilon) = \sigma^2$. Therefore $(Y|X = x) \sim \mathcal{N}(\beta x, \sigma^2)$.

2. The likelihood function conditioned on $X_i$'s

$$L((Y_1|X_1), \cdots, (Y_n|X_n)) = \prod_{i=1}^{n} \frac{1}{2\pi\sigma} \exp\left(-\frac{1}{2\sigma^2}(Y_i - \beta X_i)^2\right)$$

$$\log L((Y_1|X_1), \cdots, (Y_n|X_n)) \propto -\frac{1}{2\sigma^2} \sum_{i=1}^{n} (Y_i - \beta X_i)^2$$

$$\max \log L((Y_1|X_1), \cdots, (Y_n|X_n)) \Leftrightarrow \min \left(\sum_{i=1}^{n} (Y_i - \beta X_i)^2\right)$$
2: One-dimensional ridge regression (TA: Ying Yang)

Let $Y$ and $X$ be two random variables, and $Y = \beta X + \epsilon$ given $X$, where $\beta$ is a constant, and $\epsilon \sim \mathcal{N}(0, \sigma^2)$, independent of $X$. Given $n$ independent sample pairs, $(x_1, y_1), (x_2, y_2), \ldots, (x_n, y_n)$, instead of ordinary least square, here we estimate $\beta$ with “ridge regression”, by solving the following problem.

$$\hat{\beta} = \arg \min_{\beta} \frac{1}{2} \left( \sum_{i=1}^{n} (y_i - \beta x_i)^2 + \lambda \beta^2 \right)$$

where $\lambda \geq 0$ is a tuning parameter.

(a) Give a solution in explicit formula for $\hat{\beta}$. i.e. Compute $\hat{\beta}$ using only the training data and $\lambda$.

(b) When $\lambda$ goes from 0 to infinity, how does $\hat{\beta}$ change? Give a brief explanation of your answer.

Solution

1. Take the derivative of the objective function and set it to zero, we have

$$-\sum_{i=1}^{n} x_i (y_i - \beta x_i) + \lambda \beta = 0$$

$$\hat{\beta} = \frac{\sum_{i=1}^{n} x_i y_i}{\lambda + \sum_{i=1}^{n} x_i^2} \quad (1)$$

2. The close form of $\hat{\beta}$ (Equation 1) is a monotonic function. When $\lambda$ increases, the denominator gets larger, and the absolute value of $\hat{\beta}$ decreases, i.e. $\hat{\beta}$ shrinks to zero.
3: Least square (TA:- Ying Yang)

Suppose $X$ and $Y$ are random variables. Let $(x_1, y_1), \cdots, (x_n, y_n)$ be $n$ pairs of independent samples. Compute the least square solutions for the following models. $\epsilon \sim N(0, \sigma^2)$

1. $Y = \beta X + \epsilon$
2. $Y = \beta^2 X + \epsilon$

Which of the models above yields to a lower training error? (Hint: The answer may depend on the training samples. If so, please explain in what case one is better than the other.)

Solution:

1. The prediction error (training error) is $\sum_{i=1}^{n} (y_i - \beta x_i)^2$.
   Take the derivative and set it to zero, we have $-2 \sum_{i=1}^{n} x_i (y_i - x_i \hat{\beta}) = 0$, $\hat{\beta} = \frac{\sum_{i=1}^{n} x_i y_i}{\sum_{i=1}^{n} x_i^2}$.

2. The prediction error (training error) is $\sum_{i=1}^{n} (y_i - \beta^2 x_i)^2$.
   Take the derivative by $\beta$ and set it to zero, we have $-4 \sum_{i=1}^{n} x_i \beta (y_i - \beta^2 x_i) = 0$.
   Therefore $\beta = 0$ or $\beta^2 = \frac{\sum_{i=1}^{n} x_i y_i}{\sum_{i=1}^{n} x_i^2}$. Note that setting the gradient to 0 is only a necessary condition for the optimal $\beta$. So we need choose between the two equations for $\beta$ and find which minimizes the error. If $\sum_{i=1}^{n} x_i y_i \geq 0$, $|\hat{\beta}| = \sqrt{\frac{\sum_{i=1}^{n} x_i y_i}{\sum_{i=1}^{n} x_i^2}}$; if $\sum_{i=1}^{n} x_i y_i < 0$, $\hat{\beta} = 0$.

If $\sum_{i=1}^{n} x_i y_i \geq 0$, then two models are the same. If $\sum_{i=1}^{n} x_i y_i < 0$, the first model has a lower training error. Because $\beta^2 \geq 0$ in the (b), and optimal $\beta$ is zero.

The computation of the least square solution is worth 1 points each. If you did not show the derivations, we took 0.5 point for each off.
Suppose you know the number of keyboard and mice sold at various locations around the world and from that you want to estimate the number of computers sold using linear regression. Your model is \( Y = \beta_1 k + \beta_2 m \) where \( Y \) is the number of computers sold, \( k \) is the number of keyboards sold and \( m \) is the number of mice sold. You get 101 observations such that 100 of them have 1 keyboard, 1 mouse and 1 computer, but the 101st has 1 keyboard, 0 mouse, and 1 computer.

For (a) and (b), you can use \texttt{regress} in Matlab to compute the answers.

(a) What are the optimal values of \( \beta_1, \beta_2 \) in the scenario above.

\[ 3 \text{ points} \]

(b) Now suppose you get two additional observations, both with 0 keyboard, 1 mouse, and 1 computer. What are the optimal \( \beta \) values now?

\[ 3 \text{ points} \]

(c) As you should notice, the optimal values for \( \beta \) fluctuate wildly with the addition of even very few observations. This is a problem as then it’s hard to converge on a set of values for \( \beta \). Why is this behavior happening? Given an arbitrary dataset \( X, Y \), how can we test whether such behavior might occur?

\[ 3 \text{ points} \]

Solution

1. 1, 0
2. 1/3, 2/3
3. A small number of additional observations cause a huge fluctuation in the parameter coefficients. If our parameters supposedly represent some real world hidden parameter, then this is not good behavior. This is happening because the parameters are highly correlated.

We can compute the correlation for \( X \) to check is something like this may be a problem.

Other answers from students: The training sample is not distributed. Most of them are one point.
Let $Y \in \{0, 1\}$ be class labels, and let $X \in \mathbb{R}^p$ denote a $p$-dimensional feature.

(a) In a Gaussian naive Bayes model, where the conditional distribution of each feature is a one-dimensional Gaussian. Given $n$ independent training data points, $\{(X_1, Y_1), \cdots, (X_n, Y_n)\}$, give a maximum-likelihood estimate (MLE) of the conditional distribution of feature $X^{(j)}$, $j = 1, \cdots, p$, $(X^{(j)}|Y \sim N(\mu^{(j)}_Y, (\sigma^{(j)}_Y)^2))$.

(b) In a full Gaussian Bayes model, we assume that the conditional distribution $\text{Pr}(X|Y)$ is a multidimensional Gaussian, $X|Y \sim \mathcal{N}(\mu_Y, \Sigma_Y)$, where $\mu$ is the mean vector and $\Sigma \in \mathbb{R}^{p \times p}$ is the covariance matrix. Suppose the prior of $Y$ is already given. How many parameters do you need to estimate in Gaussian naive Bayes model? How many in a full Gaussian Bayes model?

(c) In a two dimensional case, we can visualize how Naive Bayes behaves when input features are correlated. A data set shown in Figure 1 (A), where red points are in Class 0, blue points are in Class 1. The conditional distributions are two-dimensional Gaussians. In (B) (C) and (D), the ellipses represent conditional distributions for each class. The centers of ellipses show the mean and the contours show the boundary of two standard deviations. Which of them is most likely to be the true conditional distribution? Which of them is most likely to be estimates by a Gaussian naive Bayes model? If we assume the prior probabilities for both classes are equal, which model will achieve a higher accuracy on the training data?

Solution:

1. Let $X^{(j)}_{i,0}$ denote the $j$th feature of the $i$th sample in Class 0 ($Y = 0$), $X^{(j)}_{i,1}$ in Class 1. Suppose there $n_0$ samples in Class 0, and $n_1$ samples in Class 1, the MLE of the parameters are just the sample mean and sample variance in each class.

$$\hat{\mu}^{(j)}_0 = \frac{1}{n_0} \sum_i X^{(j)}_{i,0}$$
$$\left(\hat{\sigma}^{(j)}_0\right)^2 = \frac{1}{n_0} \sum_i (X^{(j)}_{i,0} - \hat{\mu}^{(j)}_0)^2$$
$$\hat{\mu}^{(j)}_1 = \frac{1}{n_1} \sum_i X^{(j)}_{i,1}$$
$$\left(\hat{\sigma}^{(j)}_1\right)^2 = \frac{1}{n_1} \sum_i (X^{(j)}_{i,1} - \hat{\mu}^{(j)}_1)^2$$
Let’s write out the MLE derivation for one class. The likelihood of the samples in Class 0 is

\[ L(X_{i,0}^{(j)} | \mu_0^{(j)}, (\sigma_0^{(j)})^2) = \prod_{i=1}^{n_0} \frac{1}{2\pi\sigma_0^{(j)}} \exp\left(-\frac{(X_{i,0}^{(j)} - \mu_0^{(j)})^2}{2(\sigma_0^{(j)})^2}\right) \]

and the log-likelihood is

\[ \log L = -n_0 \log \sigma_0^{(j)} - \frac{1}{2(\sigma_0^{(j)})^2} \sum_{i=1}^{n_0} (X_{i,0}^{(j)} - \mu_0^{(j)})^2 + \text{constant} \]

Taking the derivative of the log-likelihood, we have

\[
\frac{\partial \log L}{\partial \mu_0^{(j)}} = - \sum_{i=1}^{n_0} (X_{i,0}^{(j)} - \mu_0^{(j)}) = 0 \Rightarrow \mu_0^{(j)} = \frac{1}{n_0} \sum_{i}^{n_0} X_{i,0}^{(j)} \\
\frac{\partial \log L}{\partial \sigma_0^{(j)}} = - \frac{n_0}{\sigma_0^{(j)}} + \frac{\sum_{i=1}^{n_0} (X_{i,0}^{(j)} - \mu_0^{(j)})^2}{(\sigma_0^{(j)})^3} = 0 \Rightarrow (\sigma_0^{(j)})^2 = \frac{1}{n_0} \sum_{i=1}^{n_0} (X_{i,0}^{(j)} - \mu_0^{(j)})^2 
\]

Similarly, one can derive the MLE for the parameters in Class 1.

2. Gaussian Naive Bayes: For each class, there are 2 parameters (the mean and variance) for each feature, therefore there are \(2 \times 2p = 4p\) parameters for all features in the two classes. A full Gaussian Bayesian model: For each class, there are \(p\) parameters for the mean, \(p(p+1)/2\) parameters for the covariance. Because the covariance matrix is symmetric. So the number of parameters is \(2 \times (p + p(p+1)/2) = p^2 + 3p\) in total for the two classes.

Grading note: If you only got the order correct, like \(p\) and \(p^2\), you get 2 points out of 3.

3. (C) is the truth. (B) are the Gaussian naive Bayes estimates. Because the Gaussian naive Bayes model assume independence of the two features conditioned on the class label. So the estimated model should be aligned with the axies. Both (B) and (D) satisfy this, but only in (B), the width and hight of the oval, which are proportional to the standard error of each axis matched the data. (C) gives the lowest training error.
Figure 1: Figure of Q5 (c)
6: Text classification using Naive Bayes. (TA:- Siddhartha Jain& Ying Yang)

In this assignment, you are going to program a naive Bayes classifier to classify documents from a serious European magazine “economist” (Class 1) and a not-so-serious American magazine “the onion” (Class 0).

1. Data description
   If you load the `handout.mat` into Octave (or Matlab) with `load handout.mat`, you will see the following matrices, Xtrain, Ytrain, Xtest, Ytest. We also provided a dictionary of V tokens (or words) in dictionary.mat, and denote the tokens in the dictionary by indices, \{1, 2, \cdots, V\}. There are n training documents and m testing documents. For each document, we counted the number of occurrence of each token, resulting in a vector \( (c_1, c_2, \cdots, c_V) \). Each row in Xtrain and Xtest is such a vector for one document. Ytrain and Ytest are \( n \times 1 \) and \( m \times 1 \) binary class labels.

2. Model description (multinomial model)
   We view a document as an ordered sequence of word events. Suppose we have a document with label \( Y = y \in \{0, 1\} \), which contains \( q \) words in total, we use \( W_i = j \) to denote the event that the \( i \)th word is the \( j \)th token in the dictionary, \( j \in \{1, 2, \cdots, V\} \). With a naive Bayes model, we assume that the \( q \) word events in one class are independent, and have an identical multinomial distribution with \( V \) outcomes.

   **Learning the conditional probability**
   Given one training document in Class \( y \), if we do not use smoothing (or pseudocounts), we estimate the conditional probability for a word event \( W \) in the following way,

   \[
   \Pr(W = j | Y = y) = \frac{\text{number of occurrence of token } j}{\text{total number of words}} = \frac{\text{number of occurrence of token } j}{\text{total number of occurrence of all } V \text{ tokens}}
   \]

   In Xtrain, you are given multiple training documents in one class, you should think in a way as concatenating them all into a large document. You need to use additive smoothing (or pseudocount) http://en.wikipedia.org/wiki/Additive_smoothing in your implementation, setting \( \alpha = 1 \).

   **Learning the prior**
   Assume the prior distribution of label \( Y \) is binomial, without smoothing, it is estimated as

   \[
   \Pr(Y = y) = \frac{\text{number of documents in Class } y}{\text{total number of documents}}
   \]

   **Making prediction**
   Now given the test document of length \( q \),

   \[
   y^\ast = \arg \max_y \Pr(Y = y | W_1, \cdots, W_q) = \arg \max_y \frac{\prod_{i=1}^{q} \Pr(W_i | Y = y) \Pr(Y = y)}{\Pr(W_1, \cdots, W_q)}
   \]

   \[
   = \arg \max_y \left( \prod_{i=1}^{q} \Pr(W_i | Y = y) \Pr(Y = y) \right)
   \]
However, we are only given the word counts of the document, \((c_1, c_2, \cdots, c_V)\), and we can only compute the multinomial probability.

\[
y^* = \arg \max_y \left( q! \prod_{j=1}^V \frac{\Pr(W = j | Y = y)^{c_j}}{c_j!} \Pr(Y = y) \right) \tag{2}
\]

\[
= \arg \max_y \left( \sum_{j=1}^V c_j \log \Pr(W = j | Y = y) + \log \Pr(Y = y) + \log(q!) - \sum_{j=1}^V \log(c_j!) \right) \tag{3}
\]

\[
= \arg \max_y \left( \sum_{j=1}^V c_j \log \Pr(W = j | Y = y) + \log \Pr(Y = y) + \text{constant} \right) \tag{4}
\]

\[
= \arg \max_y \left( \sum_{j=1}^V c_j \log \Pr(W = j | Y = y) + \log \Pr(Y = y) \right) \tag{5}
\]

In your implementation, to avoid multiplying very small probabilities and underflow, you should use the logarithmic transformation as in Equation 5.

(a) Create following three octave functions and save them in three files, `nb_train.m`, `nb_test.m` and `nb_run.m`.

\[
\text{model} = \text{nb}\_\text{train}(X\text{train}, Y\text{\_train})
\]

\[
\text{Pred\_nb} = \text{nb}\_\text{test}(\text{model}, X\text{test})
\]

\[
\text{accuracy} = \text{nb}\_\text{run}(X\text{train}, Y\text{train}, X\text{test}, Y\text{test})
\]

`model` is a structure that describes the model you learned. `Pred\_nb` is a \(m \times 1\) binary vector, which denotes your prediction for the testing documents. In `nb_run`, return the prediction accuracy computed by `accuracy = \text{mean}(\text{Pred\_nb}==\text{Y\text{\_test}})` , and use `\text{save('Pred\_nb.mat', 'Pred\_nb')}` to save your prediction into a mat file.

Note: Your score will be determined by your classification accuracy on the test dataset you’ve been given as well as the held-out dataset that has not been released.

[15 points]

(b) For the \(j\)th token in the dictionary, we can compute the following log-ratio,

\[
\left| \log \frac{\Pr(W = j | Y = 1)}{\Pr(W = j | Y = 0)} \right|
\]

Use this log-ratio as a measure, find the top five words that are most discriminative of the classes, report them in your pdf.

Solution:

Here are the top 10 words we got: percet, monday, yankees, sox, schmuck, u, favre, sen, lieberman, franks.

If your results are different from ours, we will look them up and see whether they make sense.
(c) State the Naive Bayes assumption. Are there any pairs of words that violate the Naive Bayes assumption? If so, give 1 example of such pairs and explain why they might be violating the Naive Bayes assumption.

Solution:

The Naive Bayes assumption is that the values of any two features are independent of each other. "White House" is a pair of words that violates the Naive Bayes assumption as white house refers to the US president’s house and frequently appears together.