

# CS 6350: Machine Learning Fall 2016

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Due date: December 6, 2016

## General Instructions

- You are welcome to talk to other members of the class about the homework. I am more concerned that you understand the underlying concepts. However, you should write down your own solution. Please keep the class collaboration policy in mind.
- Feel free discuss the homework with the instructor or the TAs.
- Your written solutions should be brief and clear. You need to show your work, not just the final answer, but you do *not* need to write it in gory detail. Your assignment should be **no more than 10 pages**. Every extra page will cost a point.
- Handwritten solutions will not be accepted.
- The homework is due by midnight of the due date. Please submit the homework on Canvas.
- Some questions are marked **For 6350 students**. Students who are registered for CS 6350 should do these questions. Of course, if you are registered for CS 5350, you are welcome to do the question too, but you will not get any credit for it.

## 1 Warmup: Probabilities

For the following questions, suppose  $A_1, A_2, A_3, A_4$  are events.

*(Remember that no points will be awarded without explanations.)*

1. [2 points] If  $P(A_1) = P(A_2) = P(A_1 \mid A_2) = \frac{1}{2}$ , then are the events  $A_1$  and  $A_2$  independent? Why?

Events  $A_1$  and  $A_2$  are independent if

$$P(A_1 \mid A_2) = P(A_1)$$

and

$$P(A_2 \mid A_1) = P(A_2)$$

Using Bayes rule

$$\begin{aligned}
 P(A_2 \mid A_1) &= \frac{P(A_1 \mid A_2)P(A_2)}{P(A_1)} \\
 &= \frac{\frac{1}{2} \times \frac{1}{2}}{\frac{1}{2}} \\
 &= \frac{1}{2} \\
 &= P(A_2) \\
 &= P(A_1 \mid A_2) \\
 &= P(A_1)
 \end{aligned}$$

2. [3 points] Suppose  $A_1, A_2$  and  $A_3$  are mutually exclusive. If, for  $i \in \{1, 2, 3\}$ , we have  $P(A_i) = \frac{1}{3}$  and  $P(A_4 \mid A_i) = \frac{i}{6}$ , then what is  $P(A_4)$ ?

Using the theorem of total probability in the above case

$$\begin{aligned}
 P(A_4) &= \sum_{i=1}^3 P(A_4 \mid A_i)P(A_i) \\
 &= \sum_{i=1}^3 \frac{i}{6} \times \frac{1}{3} \\
 &= \frac{1}{3} \times \left( \frac{1}{6} + \frac{2}{6} + \frac{3}{6} \right) \\
 &= \frac{1}{3} \times \frac{6}{6} \\
 &= \frac{1}{3}
 \end{aligned}$$

3. [3 points] Let  $n$  be the number at the top when a fair six-sided die is tossed. If a fair coin is tossed  $n$  times, then what is the probability of exactly two heads?

Let  $H$  be the event of getting a head,  $2H$  be the event of getting exactly two heads when tossing a coin, and let  $D_n$  be the event for the number at the top when a die is tossed.

So the probability of exactly two heads is

$$\begin{aligned}
&= \sum_{n=1}^6 P(2H \mid D_n) \times P(D_n) \\
&= \sum_{n=1}^6 P(2H \mid D_n) \times \frac{1}{6} \\
&= \sum_{n=1}^6 \binom{n}{2} \times (P(H))^2 \times (1 - P(H))^{n-2} \times \frac{1}{6} \\
&= \frac{1}{6} \times \left[ 0 + 1 \times \left(\frac{1}{2}\right)^2 \times \left(\frac{1}{2}\right)^0 + 3 \times \left(\frac{1}{2}\right)^2 \times \left(\frac{1}{2}\right)^1 + 6 \times \left(\frac{1}{2}\right)^2 \times \left(\frac{1}{2}\right)^2 \right. \\
&\quad \left. + 10 \times \left(\frac{1}{2}\right)^2 \times \left(\frac{1}{2}\right)^3 + 15 \times \left(\frac{1}{2}\right)^2 \times \left(\frac{1}{2}\right)^4 \right] \\
&= \frac{1}{6} \times \left[ 0 + \frac{1}{4} + \frac{3}{8} + \frac{6}{16} + \frac{10}{32} + \frac{15}{64} \right] \\
&= \frac{1}{6} \times \left[ \frac{16 + 24 + 24 + 20 + 15}{64} \right] \\
&= \frac{1}{6} \times \frac{99}{64} \\
&= \frac{33}{128}
\end{aligned}$$

4. [4 points] Prove or disprove: If  $P(A_1) = a_1$  and  $P(A_2) = a_2$ , then  $P(A_1|A_2) \geq \frac{a_1+a_2-1}{a_2}$ .

From the product rule of probability, we know that

$$P(A_1 \wedge A_2) = P(A_1 \mid A_2)P(A_2) \quad (1)$$

From the sum rule of probability, we know that

$$P(A_1 \vee A_2) = P(A_1) + P(A_2) - P(A_1 \wedge A_2) \quad (2)$$

From equation 1,

$$P(A_1 \mid A_2) = \frac{P(A_1 \wedge A_2)}{P(A_2)}$$

Using equation 2,

$$P(A_1 \mid A_2) = \frac{P(A_1) + P(A_2) - P(A_1 \wedge A_2)}{P(A_2)}$$

Since we know that  $P(A_1 \wedge A_2) \leq 1$ ,

$$\begin{aligned}
P(A_1 \mid A_2) &\geq \frac{P(A_1) + P(A_2) - 1}{P(A_2)} \\
&\geq \frac{a_1 + a_2 - 1}{a_2}
\end{aligned}$$

5. [8 points] If  $A_1$  and  $A_2$  are independent events, then show that

(a)  $E[A_1 + A_2] = E[A_1] + E[A_2]$

The expected value (also known as the mean  $\mu$ ) of a random variable  $X$  is defined as

$$E(X) = \sum_{e \in S} X(e)P(e)$$

where  $e$  is a single event in probability space  $S$ .

$$\begin{aligned}
E(A_1 + A_2) &= \sum_{e \in S} \{A_1(e) + A_2(e)\} P(e) \\
&= \sum_{e \in S} A_1(e)P(e) + A_2(e)P(e) \\
&= E(A_1) + E(A_2)
\end{aligned}$$

6.  $var[A_1 + A_2] = var[A_1] + var[A_2]$

Here  $E[\cdot]$  and  $var[\cdot]$  denote the mean and variance respectively.

The variance of a random variable  $X$  is defined as

$$\begin{aligned}
var(X) &= E([X - E(X)]^2) \\
&= E(X^2 - 2XE(X) + E(X)^2) \\
&= E(X^2) - 2E(XE(X)) + E(E(X)^2)
\end{aligned}$$

In the above equations, I have represented  $(E(X))^2$  as  $E(X)^2$  in order to simplify the notation rather than use the explicit version with the extra parentheses.

Based on the definition of  $E(X)$ ,

$$\begin{aligned}
E(XE(X)) &= \sum_{e \in S} X(e)P(e)E(X) \\
&= E(X) \sum_{e \in S} X(e)P(e) \\
&= E(X)^2
\end{aligned}$$

The reason we can take  $E(X)$  out of the summation above, is that it is just a number. By a similar argument,  $E(E(X)^2) = E(X)^2$ , since expected value of a number is that same number.

Going back to the expansion of  $var(X)$ ,

$$\begin{aligned} var(X) &= E(X^2) - 2E(XE(X)) + E(E(X)^2) \\ &= E(X^2) - 2E(X)^2 + E(X)^2 \\ &= E(X^2) - E(X)^2 \end{aligned}$$

Now we can expand  $var[A_1 + A_2]$

$$\begin{aligned} var[A_1 + A_2] &= E([A_1 + A_2]^2) - E(A_1 + A_2)^2 \\ &= E(A_1^2 + 2A_1A_2 + A_2^2) - (E(A_1) + E(A_2))^2 \\ &= E(A_1^2) + 2E(A_1A_2) + E(A_2^2) - (E(A_1)^2 + 2E(A_1)E(A_2) + E(A_2)^2) \end{aligned}$$

Based on the definition of  $E(X)$

$$\begin{aligned} E(A_1A_2) &= \sum_{e \in S} A_1(e)A_2(e)P(e) \\ &= \sum_{x \in S, y \in S} A_1(x)A_2(y)P(A_1 = x, A_2 = y) \end{aligned}$$

Since  $A_1$  and  $A_2$  are independent,  $P(A_1 = x, A_2 = y) = P(A_1 = x)P(A_2 = y)$ . Going back to the expansion of  $E(A_1A_2)$ ,

$$\begin{aligned} E(A_1A_2) &= \sum_{x \in S, y \in S} A_1(x)A_2(y)P(A_1 = x, A_2 = y) \\ &= \sum_{x \in S, y \in S} A_1(x)A_2(y)P(A_1 = x)P(A_2 = y) \\ &= \sum_{x \in S} A_1(x)P(A_1 = x) \sum_{y \in S} A_2(y)P(A_2 = y) \\ &= E(A_1)E(A_2) \end{aligned}$$

Going back to the expansion of  $var[A_1 + A_2]$ ,

$$\begin{aligned} var[A_1 + A_2] &= E(A_1^2) + 2E(A_1A_2) + E(A_2^2) - (E(A_1)^2 + 2E(A_1)E(A_2) + E(A_2)^2) \\ &= E(A_1^2) + 2E(A_1)E(A_2) + E(A_2^2) - (E(A_1)^2 + 2E(A_1)E(A_2) + E(A_2)^2) \\ &= E(A_1^2) - E(A_1)^2 + E(A_2^2) - E(A_2)^2 \end{aligned}$$

Since we have already shown above that  $var(X) = E(X^2) - E(X)^2$ , this means that

$$var[A_1 + A_2] = var(A_1) + var(A_2)$$

## 2 Naive Bayes

In this question, we will examine the influence of the conditional independence assumption that the naive Bayes model makes. For this question, we will use the notation  $P$  to denote the true probabilities that generates the data and  $\hat{P}$  to denote probabilities that are learned from data. Assume no smoothing is done.

1. [Part 1] Suppose we have a binary classification problem where the label  $y$  can either be  $-1$  or  $1$ . In the first case, consider the case where we have only one feature  $x_1$  that can also be either  $-1$  or  $1$ . The generative distribution of the data is  $P(x_1, y) = P(y)P(x_1 | y)$ . Note that this satisfies the independence assumption of the naive Bayes model. All features are conditionally independent of each other given the label – of course, there is only one feature so this statement is trivially true.

Suppose we know the true distribution that generated the data as follows:

- $P(y = -1) = 0.1$  and  $P(y = 1) = 0.9$
- $P(x_1 = -1 | y = -1) = 0.8$ ,  $P(x_1 = 1 | y = -1) = 0.2$ ,  $P(x_1 = -1 | y = 1) = 0.1$  and  $P(x_1 = 1 | y = 1) = 0.9$ .

- (a) [2 points] If we have infinite data drawn from this distribution and we train a naive Bayes classifier, what would the values of  $\hat{P}(x_1 | y)$  and  $\hat{P}(y)$  be?

According to *Hoeffdings Inequality* [1], the probability distribution of a random variable  $\nu$  will be very close to its mean value  $\mu$  for large samples. For a sample size of  $N$ ,

$$P[|\nu - \mu| > \epsilon] \leq 2e^{-2\epsilon^2 N}$$

for any  $\epsilon > 0$ .

When  $N$  is  $\infty$ , the values of  $\hat{P}(x_1 | y)$  and  $\hat{P}(y)$  will be the same as  $P(x_1 | y)$  and  $P(y)$ .

- (b) [6 points] Use these learned values probabilities from the previous question to fill up the following table:

Input $x_1$	$\hat{P}(x_1, y = -1)$	$\hat{P}(x_1, y = 1)$	Prediction: $y' = \arg \max_y \hat{P}(x_1, y)$
-1	0.8	0.1	-1
1	0.2	0.9	1

- (c) [3 points] If the probabilities learned above were used to make predictions, what would the error of that classifier be? In other words, what is  $P(y' \neq y)$ ?

Hint: To answer this, you should use the fact that  $P(y' \neq y) = P(y' \neq y, x_1 = -1) + P(y' \neq y, x_1 = 1)$ .

$$\begin{aligned}
P(y' \neq y) &= P(y' \neq y, x_1 = -1) + P(y' \neq y, x_1 = 1) \\
P(y' \neq y) &= P(y = 1, x_1 = -1) + P(y = -1, x_1 = 1) \\
P(y' \neq y) &= P(x_1 = -1, y = 1) + P(x_1 = 1, y = -1) \\
P(y' \neq y) &= P(x_1 = -1 \mid y = 1)P(y = 1) + P(x_1 = 1 \mid y = -1)P(y = -1) \\
&= 0.1 \times 0.9 + 0.2 \times 0.1 \\
&= 0.09 + 0.02 \\
&= 0.11
\end{aligned}$$

2. [Part 2] Now, suppose we have a binary classification problem with two features  $x_1, x_2$  both of which can be  $-1$  or  $1$ . However, the second feature  $x_2$  is actually identical to the first feature  $x_1$ . And we have the same true probabilities  $P(x_1 \mid y)$  and  $P(y)$  as in Part 1 above.

- (a) [1 point] Are  $x_1$  and  $x_2$  conditionally independent given  $y$ ? Prove your answer formally using the definition of conditional independence.

Since the features  $x_1$  and  $x_2$  are identical,

$$P(x_1, x_2 \mid y) = P(x_1 \mid y) = P(x_2 \mid y)$$

For  $x_1$  and  $x_2$  to be conditionally independent given  $y$ , the following should hold true

$$P(x_1, x_2 \mid y) = P(x_1 \mid y)P(x_2 \mid y)$$

The only cases where the product of two probabilities is the same as the individual probabilities is when both are 0 or when both are 1. This means that the above two equations cannot be true for all cases of probability values and so  $x_1$  and  $x_2$  are not conditionally independent given  $y$ .

- (b) [8 points] Let  $\hat{P}(x_1 \mid y)$ ,  $\hat{P}(x_2 \mid y)$  and  $\hat{P}(y)$  represent the learned parameters of a naive Bayes classifier that is learned on infinite data generated according to the above distribution. Using these parameters, fill up the following table:

$x_1$	$x_2$	$\hat{P}(x_1, x_2, y = -1)$	$\hat{P}(x_1, x_2, y = 1)$	<b>Prediction:</b> $y' = \arg \max_y \hat{P}(x_1, x_2, y)$
-1	-1	0.64	0.01	-1
-1	1	0.16	0.09	-1
1	-1	0.16	0.09	-1
1	1	0.04	0.81	1

- (c) [3 points] If the probabilities learned above were used to make predictions, what would the error of that classifier be? In other words, what is  $P(y' \neq y)$ ?

$$\begin{aligned}
P(y' \neq y) &= P(y' \neq y, x_1 = -1, x_2 = -1) + P(y' \neq y, x_1 = -1, x_2 = 1) \\
&\quad + P(y' \neq y, x_1 = 1, x_2 = -1) + P(y' \neq y, x_1 = 1, x_2 = 1)
\end{aligned}$$

- (d) [2 points] Do you expect a logistic regression classifier to have the same performance as the naïve Bayes classifier when the variable is duplicated? Give an intuitive explanation (no more than 2 sentences) for your answer.

### 3 [25 points, Extra Credit for the holidays] Naïve Bayes and Linear Classifiers

In this problem you will show that a Gaussian naïve Bayes classifier is a linear classifier. We will denote inputs by  $d$  dimensional vectors,  $\mathbf{x} = (x_1, x_2, \dots, x_d)^T$ . We will assume that each feature  $x_j$  is a real number. Our classifier will predict the label 1 if  $\Pr(y = 1|\mathbf{x}) \geq \Pr(y = 0|\mathbf{x})$ . Or equivalently,

$$\frac{\Pr(\mathbf{x}|y = 1) \Pr(y = 1)}{\Pr(\mathbf{x}|y = 0) \Pr(y = 0)} \geq 1$$

Remember the naïve Bayes assumption we saw in class:

$$\Pr(\mathbf{x}|y) = \prod_{j=0}^d \Pr(x_j|y)$$

Suppose each  $P(x_j|y)$  is defined using a Gaussian/Normal probability density function, one for each value of  $y$  and  $j$ . Each Gaussian distribution has mean  $\mu_{j,y}$  and variance  $\sigma^2$  (Note that they will all have same variance). As a reminder, the Gaussian distribution is represented by the following probability density function:

$$f(x_j | \mu_{j,y}, \sigma) = \frac{1}{\sqrt{2\sigma^2\pi}} e^{-\frac{(x_j - \mu_{j,y})^2}{2\sigma^2}}$$

Show that this naïve Bayes classifier has a linear decision boundary.

[Hint: Refer to the notes on the naïve Bayes classifier and Linear models in the class website to see how to do this with binary features]

The classifier will predict a label of 1 if

$$P(y = 1 | \mathbf{x}) \geq P(y = 0 | \mathbf{x})$$

or equivalently if

$$\frac{P(y = 1 | \mathbf{x})}{P(y = 0 | \mathbf{x})} \geq 1$$

$$\frac{P(y = 1)P(\mathbf{x} | y = 1)}{P(y = 0)P(\mathbf{x} | y = 0)} \geq 1$$

Using the Naïve Bayes assumption



$$\frac{P(y=1) \prod_{j=0}^d P(\mathbf{x}_j \mid y=1)}{P(y=0) \prod_{j=0}^d P(\mathbf{x}_j \mid y=0)} \geq 1$$

As per the normal probability distribution assumption described above in the question, the classifier will predict a label of 1 if,

$$\begin{aligned} \frac{P(y=1)}{P(y=0)} \prod_{j=0}^d \frac{\frac{1}{\sqrt{2\sigma^2\pi}} \exp\left(\frac{-(x_j - \mu_{1,j,y})^2}{2\sigma^2}\right)}{\frac{1}{\sqrt{2\sigma^2\pi}} \exp\left(\frac{-(x_j - \mu_{2,j,y})^2}{2\sigma^2}\right)} &\geq 1 \\ \frac{P(y=1)}{P(y=0)} \prod_{j=0}^d \frac{\exp\left(\frac{-(x_j - \mu_{1,j,y})^2}{2\sigma^2}\right)}{\exp\left(\frac{-(x_j - \mu_{2,j,y})^2}{2\sigma^2}\right)} &\geq 1 \\ \ln\left(\frac{P(y=1)}{P(y=0)}\right) + \sum_{j=0}^d \left(-\frac{(x_j - \mu_{1,j,y})^2}{2\sigma^2} + \frac{(x_j - \mu_{2,j,y})^2}{2\sigma^2}\right) &\geq 0 \\ \ln\left(\frac{P(y=1)}{P(y=0)}\right) + \sum_{j=0}^d \left(\frac{-x_j^2 + 2x_j\mu_{1,j,y} - \mu_{1,j,y}^2 + x_j^2 - 2x_j\mu_{2,j,y} + \mu_{2,j,y}^2}{2\sigma^2}\right) &\geq 0 \\ \ln\left(\frac{P(y=1)}{P(y=0)}\right) + \sum_{j=0}^d \left(\frac{\mu_{2,j,y}^2 - \mu_{1,j,y}^2 + 2(\mu_{1,j,y} - \mu_{2,j,y})x_j}{2\sigma^2}\right) &\geq 0 \\ b + \sum_{j=0}^d x_j w_j &\geq 0 \end{aligned}$$

where

$$b = \ln\left(\frac{P(y=1)}{P(y=0)}\right) + \sum_{j=0}^d \left(\frac{\mu_{2,j,y}^2 - \mu_{1,j,y}^2}{2\sigma^2}\right)$$

and

$$w_j = \sum_{j=0}^d \frac{\mu_{1,j,y} - \mu_{2,j,y}}{\sigma^2}$$

This means that the classifier has a linear decision boundary.

## 4 Experiment

We looked maximum a posteriori learning of the logistic regression classifier in class. In particular, we showed that learning the classifier is equivalent to the following optimization

problem:

$$\min_{\mathbf{w}} \left\{ \sum_{i=1}^m \log(1 + \exp(-y_i \mathbf{w}^T \mathbf{x}_i)) + \frac{1}{\sigma^2} \mathbf{w}^T \mathbf{w} \right\}$$

In this question, you will derive the stochastic gradient descent algorithm for the logistic regression classifier, and also implement it with cross-validation.

1. [5 points] What is the derivative of the function  $g(\mathbf{w}) = \log(1 + \exp(-y_i \mathbf{w}^T \mathbf{x}_i))$  with respect to the weight vector?

$$\begin{aligned} \nabla g(\mathbf{w}) &= \nabla \log(1 + \exp(-y_i \mathbf{w}^T \mathbf{x}_i)) \\ &= \frac{1}{1 + \exp(-y_i \mathbf{w}^T \mathbf{x}_i)} \exp(-y_i \mathbf{w}^T \mathbf{x}_i) (-y_i \mathbf{x}_i) \\ &= \frac{-y_i \mathbf{x}_i \exp(-y_i \mathbf{w}^T \mathbf{x}_i)}{1 + \exp(-y_i \mathbf{w}^T \mathbf{x}_i)} \\ &= \frac{-y_i \mathbf{x}_i}{1 + \exp(y_i \mathbf{w}^T \mathbf{x}_i)} \end{aligned}$$

2. [5 points] The inner most step in the SGD algorithm is the gradient update where we use a single example instead of the entire dataset to compute the gradient. Write down the objective where the entire dataset is composed of a single example, say  $(\mathbf{x}_i, y_i)$ . Derive the gradient of this objective with respect to the weight vector.

We need to find the weight  $\mathbf{w}$  that minimizes the expression given above in the question. The objective when the entire dataset consists of a single example  $(\mathbf{x}_i, y_i)$  is

$$J(\mathbf{w}) = \log(1 + \exp(-y_i \mathbf{w}^T \mathbf{x}_i)) + \frac{1}{\sigma^2} \mathbf{w}^T \mathbf{w}$$

The derivative of the first part has already been derived above. The gradient of this objective with respect to the weight vector is

$$\nabla J(\mathbf{w}) = \frac{-y_i \mathbf{x}_i}{1 + \exp(y_i \mathbf{w}^T \mathbf{x}_i)} + \frac{2\mathbf{w}}{\sigma^2}$$

3. [10 points] Write down the pseudo code for the stochastic gradient algorithm using the gradient from previous part.
4. [20 points] Implement your pseudo code as a training algorithm with cross-validation on the  $\sigma$  parameter. This parameter basically helps trade off between generalizability and model fit.

Use the Adult data set from the UCI Machine Learning repository which you used in homework 2 to train and evaluate the learner. (For a description of the data, see homework 2.) In your writeup, please report on the accuracy of your system, what value of sigma you chose based on cross validation, how many epochs you chose to run SGD, and a plot of the NEGATIVE log likelihood after each epoch of SGD.

## Experiment Submission Guidelines

1. The report should detail your experiments. For each step, explain in no more than a paragraph or so how your implementation works. You may provide the results for the final step as a table or a graph.
2. *Your code should run on the CADE machines.* You should include a shell script, `run.sh`, that will execute your code in the CADE environment. Your code should produce similar output to what you include in your report.

You are responsible for ensuring that the grader can execute the code using only the included script. If you are using an esoteric programming language, you should make sure that its runtime is available on CADE.

3. Please do not hand in binary files! We will *not* grade binary submissions.

## References

- [1] Abu-Mostafa, Yaser S., Malik Magdon-Ismail, and Hsuan-Tien Lin. *Learning from Data: A Short Course*. United States: AMLBook.com, 2012. Print.