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CS109

Handout #38
May 18, 2016

Problem Set #6

Due: 2:30pm on Wednesday, June 1st

Note: The last day this assignment will be accepted (late) is Friday, June 3rd

As noted above, the last day this assignment will be accepted (one day late) is Friday, June 3rd at 2:30pm sharp, as solutions will be made available then (in the handout bins in Gates).

For each of the written problems, **explain/justify how you obtained your answer** in order to obtain full credit. In fact, most of the credit for each problem will be given for the derivation/model used as opposed to the final answer. Make sure to describe the distribution and parameter values you used, where appropriate.

This problem set has written problems, programming problems and an optional extension.

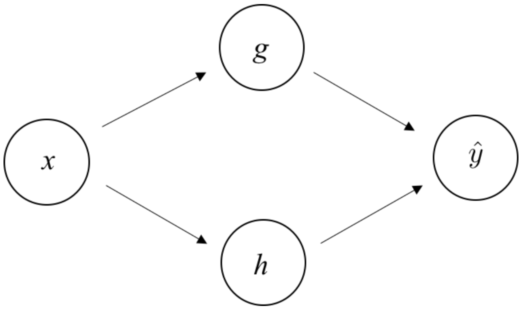
Written problems

1. Consider the Exponential distribution. It is your friend. Specifically, consider a sample of I.I.D. random variables $X_1, X_2, \ldots, X_n$, where each $X_i \sim \text{Exp}(\lambda)$. Derive the maximum likelihood estimate for the parameter λ in the Exponential distribution.

2. Calculate the log-likelihood function of θ for I.I.D. sample pairs $(X_1, Y_1), (X_2, Y_2), \ldots (X_n, Y_n)$ under the assumption that $Y = \theta_1 X + \theta_2 + Z$ and $Z \sim N(0, \sigma^2)$. Note that in this question theta is a vector: $\theta = \{\theta_1, \theta_2\}$. Show your work. You do not need to calculate the maximum likelihood estimates. The solution to this question is the probabilistic derivation for why Linear Regression is solved by minimizing sum-of-squared-error!

3. Say you have a set of binary input features/variables $X_1, X_2, \ldots, X_m$ that can be used to make a prediction about a discrete binary output variable Y (i.e., each of the X_i as well as Y can only take on the values 0 or 1). In using the input features/variables $X_1, X_2, \ldots, X_m$ to make a prediction about Y, recall that the Naïve Bayesian Classifier makes the simplifying assumption that $P(X_1, X_2, \ldots, X_n \mid Y) = \prod_{i=1}^{n} P(X_i \mid Y)$ in order to make it tractable to compute $\arg\max_y P(\boldsymbol{X}, Y) = \arg\max_y P(X_1, X_2, \ldots, X_n \mid Y) P(Y)$. Say that the first *k* input variables $X_1, X_2, \ldots, X_k$ are actually all *identical* copies of each other, so that when one has the value 0 or 1, they all do. Explain informally, but precisely, why this may be problematic for the model learned by the Naïve Bayesian Classifier.

4. Calculate the derivatives of the given log-likelihood function with respect to all four parameters ($\theta_1, \theta_2, \theta_3$, and θ_4) in this neural-network. Each variable is a single neuron:



$$g = \text{sigmoid}(\theta_1 \cdot x)$$
$$h = \text{sigmoid}(\theta_2 \cdot x)$$
$$\hat{y} = \text{sigmoid}(\theta_3 \cdot g + \theta_4 \cdot h)$$
$$LL(\theta) = \sum_{i=1}^{n} y_i \log \hat{y}_i + (1 - y_i) \log(1 - \hat{y}_i)$$

Programming Problems

For the following problems, you will be implementing two learning algorithms: the Naïve Bayesian Classifier and Logistic Regression. You must implement your algorithms in your choice of C, C++, Java, or Python. **Please note that other programming languages (e.g., R, MATLAB, etc.) are not allowed on this assignment**. You can feel free (but are under no obligation) to use the CS106A ACM Java libraries, the CS106B/X C++ libraries, or the C++ Standard Template Libraries (STL) as well as the standard libraries that are part of these languages. You should **not** use any non-standard libraries (e.g., other libraries from the web). Similarly, if you use Python you may only use libraries that are standard in the language (e.g., math, string, collections, etc. libraries), but you may **not** make use of any external non-standard libraries such as NumPy or SciPy. For each algorithm, **you should turn in your source code as well as answers to the questions listed below**. It's fine if your implementation of both algorithms is in a single file or if you use multiple files. In either case, please provide any code you write.

For each algorithm you write, you will be testing it with three data sets. A description of the data sets you will be using, the file format for the data files, and instructions on how to obtain the data files are given below. Note: you do **not** need to do any error checking in your file reading code (you can assume the data is always correctly formatted). To simplify your implementation, you can assume that all input features are always binary variables (0 or 1), and the output class is also always a binary variable (0 or 1). For the assignment, our main interest is the results you obtain with the learning algorithms. As a result, you do not need to worry about the generality of your implementation – i.e., you can write your algorithms to only deal with binary input/output features. Your code should, however, be general enough to work for any number of input features or data instances (within reason), as the different datasets you will be dealing with contain different numbers of input features and data instances. We will be grading your code only on functionality, not on programming style. With that said, it is still in your interest to write good modular code as there are many opportunities for code reuse in implementing this assignment.

Data Sets

You will be running your learning algorithms on four data sets (each of which has a respective training data file and testing data file). The data sets are described in more detail online.

Simple (`simple-train.txt`, `simple-test.txt`)

This is a simple dataset provided primarily to help you determine that your code is working correctly. There are two input features, and the output class value is determined by the value of the first feature (i.e., $y = x_1$). The training data set and testing data set are identical, each containing four data vectors. Both your Naïve Bayesian Classifier and Logistic Regression implementations should be able to classify all instances in the simple testing data set with 100% accuracy after training on the simple training set.

Heart tomography diagnosis (`heart-train.txt`, `heart-test.txt`)

This dataset contains data related to diagnosing heart abnormalities based on tomography (X-ray) information. Each input vector represents data extracted from the X-ray of one patient's heart. There are 22 binary input features. The output class value represents the diagnosis of the patient's heart (normal or abnormal, encoded in binary). The training data set contains 80 data vectors, and the testing data set contains 187 data vectors.

(Thanks to Lukasz Kurgan and Krzysztof Cios for providing this data to the UC Irvine Machine Learning Data Repository.)

Genetic ancestry (`ancestry-train.txt`, `ancestry-test.txt`)

This dataset contains DNA nucleotide readings from 467 individuals. Each input vector represents locations in the human genome and whether the individual's nucleotide at given locations matches the human reference genome. The output class value represents the super population of the user.

(Thanks to Jim Notwell and Gill Bejerano for providing this dataset.)

Netflix dataset (`netflix-train.txt`, `netflix-test.txt`)

This dataset contains real user ratings on Netflix.com. Each input vector represents ratings by a single user for the 30 most commonly rated movies (1=ratings of 4 or 5). The output class value represents whether the user rated the target movie (Miss Congeniality) as a 4 or 5.

(This dataset is made available by Reed Hastings with processing by Chris Piech.)

Data file format

All the data files described above adhere to the following file format:

```
<number of input variables per vector>
<number of data vectors in file>
<first data vector>
<second data vector>
...
<n-th data vector>
```

Note that each data vector in the file is comprised of a number of input variable values that are binary (0 or 1). The input variable values are separated by a single space. The last input variable value is immediately followed by a colon character '`:`', then a single space and then the value of the binary output variable for the vector.

For example, here is the annotated **`simple-train.txt`** data file (with annotations in italic font on the right-hand side):

File: `simple-train.txt`	Explanation of lines in data file
`2`	← ***There are 2 input variables per vector in the file***
`4`	← ***There are 4 data vectors in the file***
`0 0: 0`	← ***First data vector (has class 0)***
`0 1: 0`	← ***Second data vector (has class 0)***
`1 0: 1`	← ***Third data vector (has class 1)***
`1 1: 1`	← ***Fourth data vector (has class 1)***

How to get data sets
The data files are available on the CS109 website home page: **`http://cs109.stanford.edu`**.

Actual programming problems

Training and Testing your algorithms
The "training" data files should be used to train your learning algorithm (i.e., determine the model parameters). The "testing" data file should be used to determine the accuracy of your model *after* the training phase is complete. In other words, when we describe *training* an algorithm below, you should take that to mean that you are working *only* with the "**`-train`**" file for a particular dataset to determine the parameters of your model. When we then describe *testing* a model you should take that to mean that you are using only the "**`-test`**" file for a particular dataset to determine how well your model does at classifying the data.

Measuring model accuracy
After a model is trained, we determine its accuracy by testing it on a new set of data (generally not the same data we used to train the model). We measure the model's accuracy by determining how many of the testing vectors were correctly classified – that is, the number of times the output class value predicted by the model was the same as the actual output class value provided in the data. We report accuracy by indicating the number testing data vectors that were tested of each class, and the number that were correctly classified. For example, say we have a testing data set consisting of 12 vectors total, where the first 5 vectors are of class $y = 0$ and the remaining 7 of class $y = 1$. When we then make predictions for each data vector using our model, say we correctly predict class $\hat{y} = 0$ for 4 out of the first 5 vectors and then correctly predict class $\hat{y} = 1$ for 5 out of the next 7 vectors. Our overall accuracy for the model would be 0.75 since we correctly classified a total of 9 out of 12 vectors. We would report these results as follows:

```
Class 0: tested 5, correctly classified 4
Class 1: tested 7, correctly classified 5
Overall: tested 12, correctly classified 9
Accuracy = 0.75
```

You should use this same accuracy reporting scheme for the algorithms you implement below.

5. Implement the Naïve Bayesian Classifier for binary input/output data. Specifically, your classifier should make predictions for the output variable using the rule: $\hat{Y} = \arg\max_{y} P(\boldsymbol{X} \mid Y)P(Y)$, by employing the Naïve Bayes assumption, which states that:

$$P(\boldsymbol{X} \mid Y) = P(X_1, X_2, \ldots X_m \mid Y) = \prod_{i=1}^{m} P(X_i \mid Y).$$

Thus, your program will need to estimate the values P(Y) as well as P(X_i | Y) for all $1 \leq i \leq m$ from the training data. Note that to estimate the probability mass function P(X_i | Y), you will need to estimate both P(X_i | Y = 0) and P(X_i | Y = 1). For each of parts (a)-(c) below, you should run your algorithm **twice**, the first time computing your probability estimates using Maximum Likelihood Estimators and the second time computing your probability estimates using Laplace Estimators.

a. Train your algorithm on the data file **`simple-train.txt`**. Test your algorithm on the data file **`simple-test.txt`** and report your classification accuracy. Remember to do this once with Maximum Likelihood Estimators and once with Laplace Estimators. As a sanity check, you should be able to achieve 100% classification accuracy on the testing data using a model trained with Maximum Likelihood Estimators.

b. Train and test your algorithm on each of the remaining datasets (heart, ancestry and netflix). Report your classification accuracies for each dataset. Remember to do this once with Maximum Likelihood Estimators and once with Laplace Estimators.

c. Did did you see any difference between using Maximum Likelihood Estimators versus Laplace Estimators in your accuracy results? In general, under what conditions (i.e., characteristics of the data sets) do you think using Laplace Estimators (rather than Maximum Likelihood Estimators) would be better (e.g., likely improve classification accuracy)? Under what conditions do you think using Maximum Likelihood Estimators (rather than Laplace Estimators) would be better?

d. Make sure to turn in a copy of your code for the Naïve Bayes Classifier.

Continued on back

6. Implement Logistic Regression for binary input/output data. Specifically, you should implement the "batch" gradient algorithm described in class. In each case below, you should train your classifier for 10,000 epochs (passes through the training data).

   Note that you will need to use an exponential function (e^x) to implement Logistic Regression. In C/C++, you will find the function **`double exp(double x)`** from the library **`<math.h>`** helpful. Similarly, for those working in Java, the static method **`double exp(double x)`** from the class **`java.lang.Math`** computes e^x.

   a. Train your algorithm on the data file **`simple-train.txt`**. Use learning rate $\eta = 0.0001$. Test your algorithm on the data file **`simple-test.txt`** and report your classification accuracy. You should be able to achieve 100% classification accuracy on the testing data.

   b. Train and test your algorithm on each of the remaining datasets (heart, ancestry and netflix). Use learning rate $\eta = 0.0001$. Report your classification accuracies for each dataset. **Were you able to obtain a higher classification accuracy than with the Naïve Bayes classifier on this data? Briefly explain why or why not this may be the case.**

   c. Train your algorithm on the data file `heart-train.txt`. Experiment with using different learning rates η, where you are still testing your algorithm on the data file **`heart-test.txt`**. As a starting point for experimenting, try $\eta = 0.0005$ and $\eta = 0.00002$ (i.e., values for η that are larger and smaller than 0.0001 by a factor of 5), and then continue experimenting from there. **Report the highest classification accuracy you could obtain on the testing data, and what was the value of the learning rate η you used to obtain it. Explain why different learning rates have an effect on your classification accuracy.**

   d. Make sure to turn in a copy of your code for Logistic Regression.

Optional Extension

You can optionally implement a neural network and see if you can improve your testing accuracy on the Netflix dataset. For this extension you may use any math libraries you like – for example you can use Python's numpy and scipy libraries. The only restriction is that you can't use a neural network library (like TensorFlow, Torch or Lasagne).

Warning: implementing a neural network can be hard. Here are some protips:

1. Try a simple network with one hidden layer first.
2. Graph your training log-loss over time. It should be decreasing.
3. Use learning rate $\eta = 0.001$
4. Look at the difference between training error and testing error. If training error is much higher than testing error you are over fitting. You may want to include dropout.

Submit your code and report your accuracy on the Netflix dataset. This extension is optional. If you manage to get a working neural network we will award extra credit.