ECE M146 Homework 3 Solution
Introduction to Machine Learning
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Please upload your homework to Gradescope by April 23, 11:59 pm.
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Note: All log in the decision tree problems is base 2.

1. Consider the modified objective function of regularized logistic regression:

$$J(w) = -\sum_{n=1}^{N} \left[y_n \log h_w(x_n) + (1-y_n)\log(1-h_w(x_n))\right] + \frac{1}{2}\sum_i w_i^2 \tag{1}$$

where $h_w(x) = \sigma(w^T x)$ and the sigmoid function $\sigma(x) = \frac{1}{1+\exp(-x)}$. Find the partial derivative $\frac{\partial J}{\partial w_j}$ and derive the gradient descent update rules for the weights.

Solution:

$$\begin{aligned}
\frac{\partial}{\partial w_j} J(w) &= -\sum_{n=1}^{N}\left[\frac{y_n}{h_w(x_n)} - \frac{1-y_n}{1-h_w(x_n)}\right]\frac{\partial}{\partial w_j} h_w(x_n) + w_j \\
&= -\sum_{n=1}^{N}\left[\frac{y_n}{h_w(x_n)} - \frac{1-y_n}{1-h_w(x_n)}\right] h_w(x_n)(1-h_w(x_n))\frac{\partial}{\partial w_j} w^T x + w_j \\
&= -\sum_{n=1}^{N}\left[y_n(1-h_w(x_n)) - (1-y_n)h_w(x_n)\right] x_j + w_j \\
&= \sum_{n=1}^{N}(h_w(x_n) - y_n)x_j + w_j.
\end{aligned}$$

The gradient descent update rules is therefore:

$$w_j := w_j - \eta\left[\sum_{n=1}^{N}(h_w(x_n) - y_n)x_j + w_j\right],$$

where η denotes the learning rate. You may notice that the update rule is mathematically the same as the result obtained for the gradient descent under quadratic loss and with L2 regularization. This is due to the special choice of the sigmoid function and the cross entropy loss.

2. In class we have seen the probabilistic interpretation of the logistic regression objective, and the derivation of the gradient descent rule for maximizing the conditional likelihood. We have this maximum likelihood (ML) formulation for $w \in \mathbb{R}^m$:

$$w^* = \arg\max_w \prod_{i=1}^{n} P(y_i|x_i, w). \tag{2}$$

To prevent overfitting, we want the weights to be small. To achieve this, we consider some prior distribution of the weights $f(w)$ and use maximum a posteriori (MAP) estimation:

$$w^* = \arg\max_w \prod_{i=1}^{n} P(y_i|x_i, w) f(w). \tag{3}$$

Assuming a standard Gaussian prior $\mathcal{N}(0, I)$ for the weight vector, show that the MAP estimation is equivalent to minimizing the logistic regression objective with L2 regularization as shown in the previous question. Note: For $Z \sim \mathcal{N}(0, I_m)$,

$$f_Z(z) = \frac{1}{(2\pi)^{\frac{m}{2}}} \exp\left(-\sum_{i=1}^{m} \frac{z_i^2}{2}\right).$$

Solution: By assumption, $P(y_i|x_i, w) = (h_w(x_i))^{y_i}(1 - h_w(x_i))^{1-y_i}$. We can write the MAP estimator explicitly as:

$$w^* = \arg\max_w \frac{1}{(2\pi)^{\frac{m}{2}}} \exp\left(-\sum_{i=1}^{m} \frac{w_i^2}{2}\right) \prod_{i=1}^{n} (h_w(x_i))^{y_i}(1 - h_w(x_i))^{1-y_i}.$$

Taking negative log of the argument, the MAP estimator is then:

$$\begin{aligned} w^* &= \arg\min_w - \sum_{n=1}^{N} \left[y_n \log h_w(x_n) + (1 - y_n) \log(1 - h_w(x_n))\right] + \frac{1}{2} \sum_i w_i^2 \\ &= \arg\min_w J(w). \end{aligned}$$

3. You are trying to choose between two restaurants (sample 9 and sample 10) to eat at. To do this, you will use a decision tree that will be trained based on your past experiences (sample 1-8). The features for each restaurants and your judgment on the goodness of sample 1-8 are summarized by the following chart.

Sample #	HasOutdoorSeating	HasBar	IsClean	HasGoodAtmosphere	IsGoodRestaurant
1	0	0	0	1	1
2	1	1	0	0	0
3	0	1	1	1	1
4	1	0	0	1	1
5	1	1	1	0	0
6	1	0	1	0	1
7	1	1	0	1	1
8	0	0	1	1	1
9	0	1	0	1	?
10	1	1	1	1	?

(a) What is the entropy of IsGoodRestaurant, i.e., $H(IsGoodRestaurant)$?

Solution: Define the binary entropy function as follows:

$$H_b(p) = -p\log(p) - (1-p)\log(1-p).$$

$$H(IsGoodRestaurant) = H_b(\frac{2}{8}) = -(\frac{6}{8}\log(\frac{6}{8}) + \frac{2}{8}\log(\frac{2}{8})) \approx 0.8113$$

(b) Calculate the conditional entropy of IsGoodRestaurant conditioning on HasOutdoorSeating. To do this, first compute $H(IsGoodRestaurant|HasOutdoorSeating = 0)$ and $H(IsGoodRestaurant|HasOutdoorSeating = 1)$, then weigh each term by the probabilities $P(HasOutdoorSeating = 0)$ and $P(HasOutdoorSeating = 1$, respectively. Namely, calculate the following:

$$\begin{aligned}&H(IsGoodRestaurant|HasOutdoorSeating)\\ =&P(HasOutdoorSeating = 0)H(IsGoodRestaurant|HasOutdoorSeating = 0)\\ +&P(HasOutdoorSeating = 1)H(IsGoodRestaurant|HasOutdoorSeating = 1).\end{aligned}$$

Solution: Use the given equation, we get:

$$\begin{aligned}&H(IsGoodRestaurant|HasOutdoorSeating)\\ =&\frac{3}{8}H_b(\frac{3}{3}) + \frac{5}{8}H_b(\frac{3}{5}) \approx 0.606844.\end{aligned}$$

(c) Similarly, calculate

$$H(IsGoodRestaurant|X), \text{for } X \in \{HasBar, IsClean, HasGoodAtmosphere\},$$

i.e., the conditional entropy of IsGoodRestaurant conditioning on the other three features.

Solution:

$$H(IsGoodRestaurant|HasBar) = \frac{1}{2}H_b(\frac{4}{4}) + \frac{1}{2}H_b(\frac{2}{4}) = 0.5.$$

$$H(IsGoodRestaurant|IsClean) = \frac{1}{2}H_b(\frac{3}{4}) + \frac{1}{2}H_b(\frac{3}{4}) \approx 0.8113.$$

$$H(IsGoodRestaurant|HasGoodAtmosphere) = \frac{3}{8}H_b(\frac{1}{3}) + \frac{5}{8}H_b(\frac{5}{5}) \approx 0.34436.$$

(d) Calculate the information gain:

$$I(IsGoodRestaurant; X) = H(IsGoodRestaurant) - H(IsGoodRestaurant|X),$$

for

$$X \in \{HasOutdoorSeating, HasBar, IsClean, HasGoodAtmosphere\}.$$

Solution:

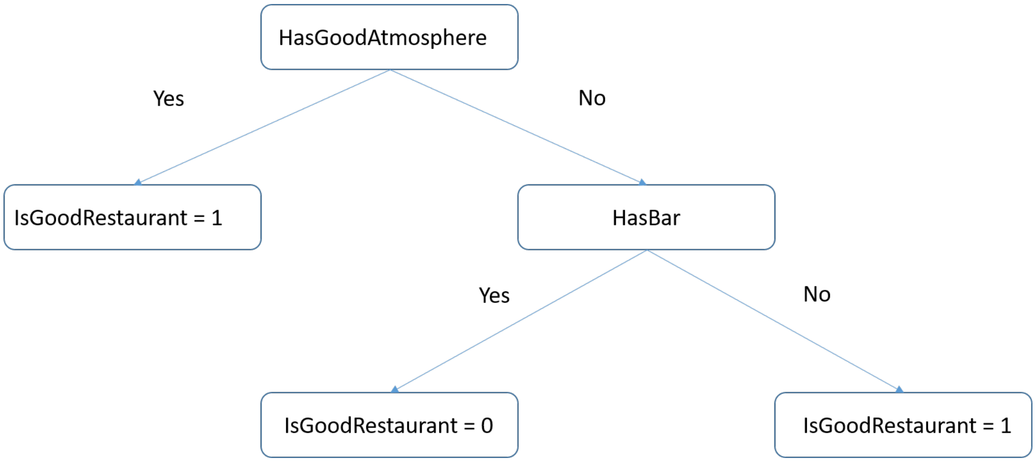
$$\begin{aligned} I(IsGoodRestaurant; HasOutdoorSeating) &= 0.8113 - 0.606844 = 0.204456; \\ I(IsGoodRestaurant; HasBar) &= 0.8113 - 0.5 = 0.3113; \\ I(IsGoodRestaurant; IsClean) &= 0.8113 - 0.8113 = 0; \\ I(IsGoodRestaurant; HasGoodAtmosphere) &= 0.8113 - 0.34436 = 0.46694. \end{aligned}$$

(e) Based on the information gain, determine the first attribute to split on.

Solution: We choose HasGoodAtmosphere which has the largest information gain.

(f) Make the full decision tree. After each split, treat the sets of samples with $X = 0$ and $X = 1$ as two separate sets and redo (b), (c), (d) and (e) on each of them. X is the feature for previous split and is thus excluded from the available features which can be split on next. Terminate splitting if after the previous split, the entropy of IsGoodRetaurant in the current set is 0. For example, if we choose HasGoodAtmosphere as our first feature to split, we get $H(IsGoodRetaurant|HasGoodAtmosphere = 1) = 0$. We thus stop splitting the tree in this branch. Draw the tree and indicate the split at each node.

Solution: Below show the decision tree if we choose HasGoodAtmosphere as the first splitting feature.



After the first split, $H(IsGoodRetaurant|HasGoodAtmosphere = 1) = 0$ so the tree stops growing on that branch. We are left with the samples that have $HasGoodAtmosphere = 0$ which is summarized in the following table.

Sample #	HasOutdoorSeating	HasBar	IsClean	IsGoodRestaurant
2	1	1	0	0
5	1	1	1	0
6	1	0	1	1

By observation, Feature HasBar has the highest information gain. Then the next split should be HasBar. After this split, every leaf is pure, i.e., IsGoodRestaurant is either 0 or 1. Therefore, we stop growing the tree.

(g) Now, determine if restaurants 9 and 10 are good or not.

Solution:

Restaurant 9: Good

Restaurant 10: Good

4. When training decision trees for classification, we generally use entropy or gini index to help determine good splits. These functions are examples of impurity measures. We can formally define impurity measures as follows.

   Assume we are performing binary classification. Let V be a set of data points and let $\{y_i \in \{+1, -1\}\ ,\ \forall i \in V\}$ be the set of labels. Let $V_1 \subseteq V$. We define p and q as follows:

$$p(V_1, V) = \frac{|V_1|}{|V|} \quad q(V_1) = \frac{|\{i : i \in V_1, y_i = 1\}|}{|V_1|}$$

   where $|\cdot|$ is the cardinality of a set.
   Let $i(q(V))$ measure the impurity of a set V. Two desired properties of $i(q(V))$ are:

   - $i(q(V)) = 0$ when the set has only one class
   - $i(q(V))$ reaches its maximum value for sets where the two classes are perfectly balanced.

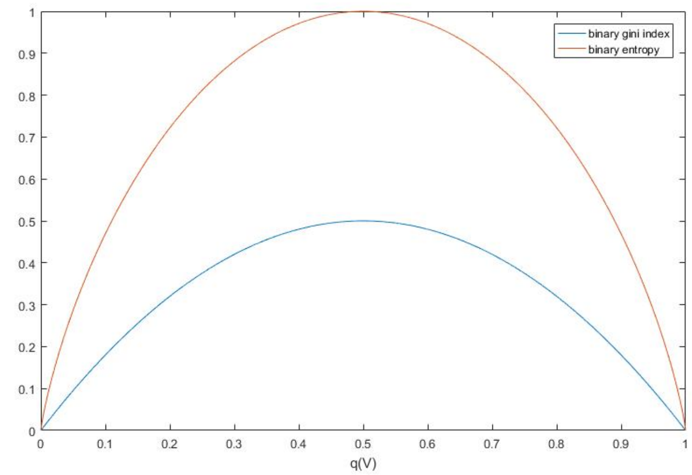
   When a split is performed of a set V, the result is two sets $V_1 \cup V_2 = V$ such that $V_1 \cap V_2 = \emptyset$. The information gain of this split is defined as

$$I(V_1, V_2, V) = i(q(V)) - (p(V_1, V)i(q(V_1)) + p(V_2, V)i(q(V_2))).$$

   Using the previous notation, we define the binary gini Index and binary entropy as:

$$\begin{aligned} gini(q(V)) &= 2q(V)(1 - q(V)) \\ H(q(V)) &= -(q(V)\log(q(V)) + (1 - q(V))\log(1 - q(V))) \end{aligned}$$

   (a) Like binary entropy, gini index is an alternative impurity measure that is commonly used. Plot both the Gini index and the binary entropy function for $q(V)$ from 0 to 1. Comment on their similarities.
   Solution:



   They both attains the maximum value at $q(V) = \frac{1}{2}$. They are both 0 when $q(V) = 0$ or $q(V)1$.

(b) Show that if $i(q(V))$ is concave in $q(V)$ then $I(V_1, V_2, V) \geq 0 \; \forall \; V_1 \cup V_2 = V, V_1 \cap V_2 = \emptyset$. This means that every split does not lose any information. Recall that a function is concave if $\forall \lambda \in [0, 1]$ and $\forall q_1, q_2$ then $i(\lambda q_1 + (1 - \lambda) q_2) \geq \lambda i(q_1) + (1 - \lambda) i(q_2)$.

Solution: For simplicity, let $q = q(V), q_1 = q(V_1), q_2 = q(V_2), p_1 = p(V_1, V), p_2 = p(V_2, V)$.

$$\begin{aligned} q &= \frac{|\{i : i \in V, y_i = 1\}|}{|V|} \\ &= \frac{|\{i : i \in V_1, y_i = 1\}|}{|V|} + \frac{|\{i : i \in V_2, y_i = 1\}|}{|V|} \\ &= \frac{|V_1|}{|V|} \frac{|\{i : i \in V_1, y_i = 1\}|}{|V_1|} + \frac{|V_2|}{|V|} \frac{|\{i : i \in V_2, y_i = 1\}|}{|V_2|} \\ &= p_1 * q_1 + p_2 * q_2 \end{aligned}$$

Due to concavity, we have

$$i(q) = i(p_1 q_1 + p_2 q_2) \geq p_1 i(q_1) + p_2 i(q_2).$$

Hence, $I(V_1, V_2, V) \geq 0$

(c) Show that binary entropy is concave. Hint: Show that the 2nd derivative is always non-positive.

Solution:

$$\begin{aligned} \frac{dH(q)}{dq} &= \log(\frac{1}{q} - 1) \\ \frac{d^2 H(q)}{dq^2} &= -\frac{1}{q - q^2} \end{aligned}$$

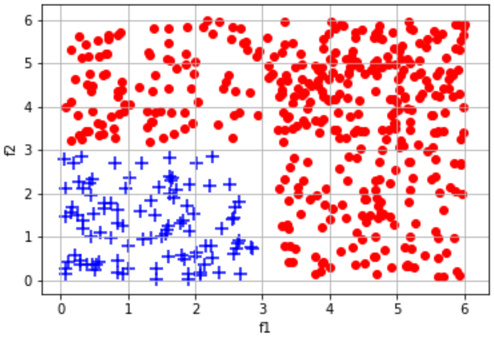
Since $q \in [0, 1]$, then $q \geq q^2$. As such, the second derivative is always non-positive.

(d) Show that the binary Gini index is concave.

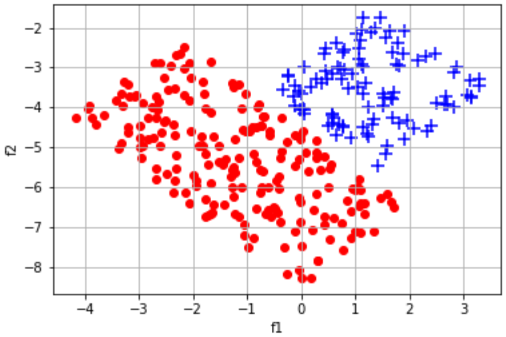
Solution: Similarly,

$$\begin{aligned} \frac{dgini(q)}{dq} &= 2(1 - 2q) \\ \frac{d^2 gini(q)}{dq^2} &= -4 \end{aligned}$$

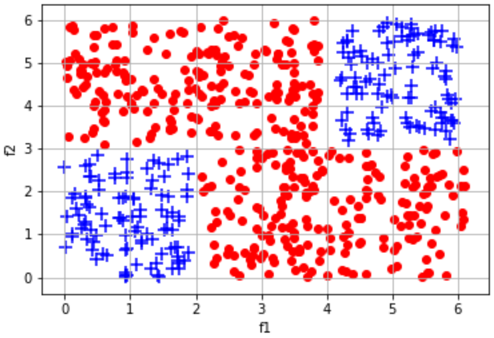
5. Consider the following plots:



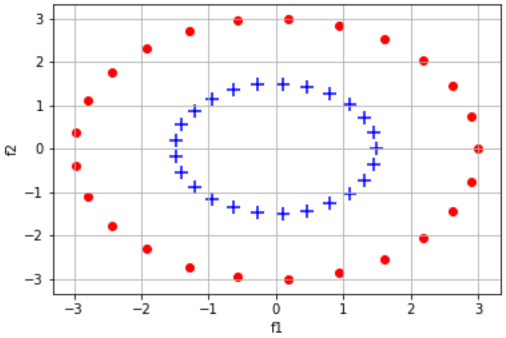
(1) Decision Tree Example 1



(2) Decision Tree Example 2



(3) Decision Tree Example 3



(4) Decision Tree Example 4

Assume that you are using a binary split decision tree to classify the points. At each node, you may ask questions like: "Is $f_1 \geq 3$?" or "Is $f_2 \leq 1.8$?". Here, $f1$ and $f2$ are the variables on the horizontal axis and vertical axis of the examples, respectively.

(a) Which examples can be fully separated using a depth 2 decision tree?

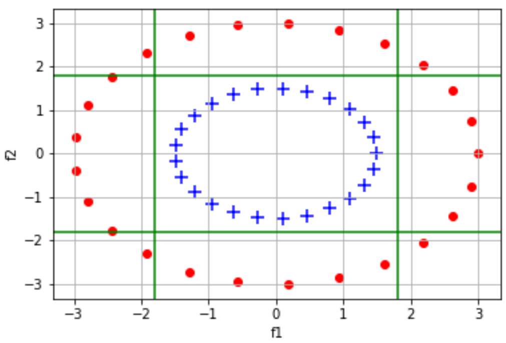
Solution: Examples 1 and 3. For example 1, the first question to ask is "Is $f1 \geq 3$?". If "No", ask the second question "Is $f2 \geq 3$?". For example 2, ask the first question "Is $f2 \geq 3$?" . If "No", ask the second question "Is $f1 \geq 2$?". If "Yes", ask the second question "Is $f1 \geq 4$?".

(b) Which example would have the most complex decision tree in terms of the number of splits? Explain why.

Solution: Example 2 because the points are separated by a non-axis aligned hyperplane which would require a lot of binary splits to model. Decision tree works well only when the decision boundaries are axis-aligned.

(c) If you used a depth 4 decision tree, is one more example now separable? If so, show how you can separate it using a depth 4 decision tree.

Solution: Example 4. You may ask these four questions: "Is $f1 \geq -1.8$?", "Is $f1 \leq 1.8$?", "Is $f1 \geq -1.8$?" and "Is $f1 \leq 1.8$?". If all answers are "Yes", then we decide the class is the blue one. See illustration in the next figure.


3
2
1
0
−1
−2
−3
f2
−3
−2
−1
0
1
2
3
f1

6. On April 15, 1912, the largest passenger liner ever made collided with an iceberg during her maiden voyage. When the Titanic sank it killed 1502 out of 2224 passengers and crew. This sensational tragedy shocked the international community and led to better safety regulations for ships. One of the reasons that the shipwreck resulted in such loss of life was that there were not enough lifeboats for the passengers and crew. Although there was some element of luck involved in surviving the sinking, some groups of people were more likely to survive than others.

   In this section, you will use decision trees to predict whether a person survives or not. You will be using the data set provided in *dataTesting_X.csv, dataTesting_Y.csv*, *dataTraining_X.csv* and *dataTraining_Y.csv* which contains feature values and labels for both training and testing data. The data is normalized so that all feature values are between 0 and 1. If you are interested in the actual meaning of each feature, we provide the original data in *titanic.csv* where we use the mapping (Female:0, Male:1). (For python, feel free to use the following libraries: math, collections, numpy, matplotlib and sklearn.)

   (a) Before starting, it is useful to have a baseline accuracy to compare against. A simple baseline to consider is majority voting where the classifier always outputs the class with the majority in the training set. Provide the accuracy of this classifier on both the training and the testing set. To find the accuracy, calculate the fraction in both the training and the testing set that has the same class as the majority class in the training set.

   Solution: Baseline by predicting everyone dies for test set is 0.6949. Baseline by predicting everyone dies for training set is 0.5944.

   (b) Now, use **fitctree** (**sklearn.tree.DecisionTreeClassifier** for python user) to train a decision tree classifier on the training data. Make sure to set the splitting criteria to "deviance" ("entropy" for python user) to make it use cross entropy. What is the training and testing accuracy of this model?

   Solution: Training error:0.0901 (0.0183 for python). Testing error:0.1808 (0.18 to 0.23 for python).