Homework Assignment 4

CSE 251A: Introduction to Machine Learning

Due: May 30th, 2023, 9:30am (Pacific Time)

Instructions: Please answer the questions below, attach your code in the document, and insert figures to create **a single PDF file**. You may search information online but you will need to write code/find solutions to answer the questions yourself.

Grade: ____ out of 120 points

1 (40 points) Naïve Bayes

In this question, we would like to build a Naïve Bayes model for a classification task. Assume there is a classification dataset $S = \{(\mathbf{x}^{(i)}, y^{(i)}), i = 1, ..., 8\}$ where each data point $(\mathbf{x}, y)$ contains a feature vector $\mathbf{x} = (x_1, x_2, x_3); x_1, x_2, x_3 \in \{0, 1\}$ and a ground-truth label $y \in \{0, 1\}$. The dataset S can be read from the table below:

i	x_1	x_2	x_3	y
1	0	0	1	1
2	0	1	1	1
3	1	1	0	1
4	0	0	1	1
5	0	1	0	0
6	1	1	0	0
7	1	0	0	0
8	0	0	1	0

In Naïve Bayes model, we use random variable $X_i \in \{0, 1\}$ to represent i-th dimension of the feature vector $\mathbf{x}$, and random variable $Y \in \{0, 1\}$ to represent the class label y. Thus, we can estimate probabilities $P(Y)$, $P(X_i|Y)$ and $P(X_i, Y)$ by counting data points in dataset S, for example:

$$\begin{aligned}
P(Y = 1) &= \frac{\#\{\text{data points with } y = 1\}}{\#\{\text{all data points}\}} = \frac{4}{8} = 0.5 \\
P(X_1 = 1|Y = 0) &= \frac{\#\{\text{data points with } x_1 = 1 \text{ and } y = 0\}}{\#\{\text{data points with } y = 0\}} = \frac{2}{4} = 0.5 \\
P(X_1 = 1, Y = 1) &= P(X_1 = 1|Y = 1)P(Y = 1) \\
&= \frac{\#\{\text{data points with } x_1 = 1 \text{ and } y = 1\}}{\#\{\text{all data points}\}} = \frac{1}{8} = 0.125
\end{aligned}$$

It is noteworthy that **only** probabilities $P(Y)$, $P(X_i|Y)$ and $P(X_i, Y)$ can be **directly** estimated from dataset S in Naïve Bayes model. Other joint probabilities (e.g. $P(X_1, X_2)$ and $P(X_1, X_2, X_3)$) should **not** be estimated by directly counting the data points.

Next, we can use the probabilities $P(Y)$ and $P(X_i|Y)$ to build our Naïve Bayes model for classification: For a feature vector $\mathbf{x} = (x_1, x_2, x_3)$, we can estimate the probability $P(Y = y|X_1 = x_1, X_2 = x_2, X_3 = x_3)$ with the **conditional independence assumptions**:

$$\begin{aligned} P(Y = y|X_1 = x_1, X_2 = x_2, X_3 = x_3) &= \frac{P(X_1 = x_1, X_2 = x_2, X_3 = x_3, Y = y)}{P(X_1 = x_1, X_2 = x_2, X_3 = x_3)} \\ &= \frac{P(X_1 = x_1, X_2 = x_2, X_3 = x_3|Y = y)P(Y = y)}{P(X_1 = x_1, X_2 = x_2, X_3 = x_3)} \\ &= \frac{\left(\prod_{i=1}^{3} P(X_i = x_i|Y = y)\right)P(Y = y)}{P(X_1 = x_1, X_2 = x_2, X_3 = x_3)} \end{aligned}$$

where the joint probability $P(X_1 = x_1, X_2 = x_2, X_3 = x_3)$ can be calculated as:

$$\begin{aligned} P(X_1 = x_1, X_2 = x_2, X_3 = x_3) &= \sum_{y=0}^{1} P(X_1 = x_1, X_2 = x_2, X_3 = x_3, Y = y) \\ &= \sum_{y=0}^{1} \Big(P(X_1 = x_1, X_2 = x_2, X_3 = x_3|Y = y)P(Y = y)\Big) \\ &= \sum_{y=0}^{1} \left(\Big(\prod_{i=1}^{3} P(X_i = x_i|Y = y)\Big)P(Y = y)\right) \end{aligned}$$

Finally, if we find:

$$P(Y = 1|X_1 = x_1, X_2 = x_2, X_3 = x_3) > P(Y = 0|X_1 = x_1, X_2 = x_2, X_3 = x_3)$$

then we can predict the class of feature vector $\mathbf{x} = (x_1, x_2, x_3)$ to be 1, otherwise 0. It is noteworthy that although conditional independence assumptions are made in Naïve Bayes model, $P(Y = 1|X_1 = x_1, X_2 = x_2, X_3 = x_3) + P(Y = 0|X_1 = x_1, X_2 = x_2, X_3 = x_3)$ should **still be** 1.

1. (15 pts) Please estimate the following probabilities:

   $$(1)\ P(X_1 = 1, Y = 0), \quad (2)\ P(Y = 0), \quad (3)\ P(X_1 = 1|Y = 1).$$

   Note that these probabilities can be directly estimated by counting from dataset S.

1) $\frac{2}{8} = \frac{1}{4} = .25$ 2) $\frac{4}{8} = .5$ 3) $\frac{2}{4} = .5$

2. (18 pts) Please calculate the probability $P(Y = 1|X_1 = 1, X_2 = 1, X_3 = 0)$ in Naïve Bayes model using conditional independence assumptions.

$P(X_1=1|Y=1) = \frac{1}{4} = .25$ $\quad P(X_3=0|Y=1) = \frac{1}{4} = .25$

$P(X_2=1|Y=1) = \frac{2}{4} = .5$

$P(Y=1) = .5$

$P(X_1=1, X_2=1, X_3=0) = .25 \cdot .25 \cdot .5$

$= .03125 \cdot .5$

$= .015625$

$$\frac{.03125 \cdot .5}{.015625} = \boxed{.5}$$

3. (7 pts) Please calculate the probability $P(Y = 0|X_1 = 1, X_2 = 1, X_3 = 0)$ in Naïve Bayes model and predict the class of feature vector $\mathbf{x} = (1, 1, 0)$.

$P(X_1=1|Y=0) = .5$ $\quad P(X_3=0|Y=0) = .75$

$P(X_2=1|Y=0) = .5$ $\quad P(Y=0) = .5$

$$\frac{.5 \cdot .5 \cdot .75}{.5} = .375$$

2 (40 points) Decision Tree

In this question, we would like to create a decision tree model for a binary classification task. Assume there is a classification dataset $T = \{(\mathbf{x}^{(i)}, y^{(i)}), i = 1, ..., 5\}$ where each data point $(\mathbf{x}, y)$ contains a feature vector $\mathbf{x} = (x_1, x_2) \in \mathbb{R}^2$ and a ground-truth label $y \in \{0, 1\}$. The dataset T can be read from the table below:

i	x_1	x_2	y
1	1.0	2.0	1
2	2.0	2.0	1
3	3.0	2.0	0
4	2.0	3.0	0
5	1.0	3.0	0

To build the decision tree model, we use a simplified CART algorithm, which is a recursive procedure as follows:

- Initialize a root node with dataset T and set it as current node.
- Start a procedure for current node:
  - **Step 1**: Assume the dataset in current node is T_{cur}. Check if all data points in T_{cur} are in the same class:
    - If it is true, set current node as a *leaf node* to predict the common class in T_{cur}, and then terminate *current* procedure.
    - If it is false, continue the procedure.
  - **Step 2**: Traverse all possible splitting rules. Each splitting rule is represented by a vector (j, t), which compares feature x_j and threshold t to split the dataset T_{cur} into two subsets T_1, T_2:

    $$T_1 = \{(\mathbf{x}, y) \in T_{\text{cur}} \text{ where } x_j \le t\},$$
    $$T_2 = \{(\mathbf{x}, y) \in T_{\text{cur}} \text{ where } x_j > t\}.$$

    We will traverse the rules over all feature dimensions $j \in \{0, 1\}$ and thresholds $t \in \{x_j | (\mathbf{x}, y) \in T_{\text{cur}}\}$.
  - **Step 3**: Decide the best splitting rule. The best splitting rule (j^*, t^*) minimizes the weighted sum of Gini indices of T_1, T_2:

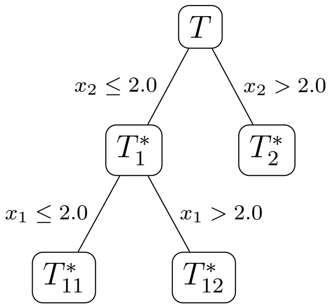
    $$(j^*, t^*) = \arg\min_{j,t} \frac{|T_1|\text{Gini}(T_1) + |T_2|\text{Gini}(T_2)}{|T_1| + |T_2|}$$

    where the Gini$(\cdot)$ is defined as:

    $$\text{Gini}(T_i) = 1 - \sum_{y=0}^{1} P(Y = y)^2,$$

    $$P(Y = y) = \frac{\#\{\text{data points with label } y \text{ in } T_i\}}{\#\{\text{data points in } T_i\}}.$$
  - **Step 4**: We split the dataset T_{cur} into two subsets T_1^*, T_2^* following the best splitting rule (j^*, t^*). Then we set current node as a *branch* node and create child nodes with the subsets T_1^*, T_2^* respectively. For each child node, start from **Step 1** again recursively.

If we run the above decision tree building procedure on dataset T and find the generated tree is shown below:



Please answer the questions:

1. (16 pts) Calculate the subsets $T_1^*, T_2^*, T_{11}^*, T_{12}^*$ using the given decision tree.

$T_1 = \{(1,2,1),(2,2,1),(3,2,0)\}$

$T_2 = \{(2,3,0),(1,3,0)$

$T_{11} = \{(1,2,1),(2,2,1)\}$

$T_{12} = \{(3,2,0)\}$

2. (12 pts) Calculate Gini(T_1^*) and Gini(T_2^*).

class 0 class 1

Gini(T_1) $T_1 = 1$ $T_1 = 2$ $1-(\frac{1}{3})^2 - (\frac{2}{3})^2$

$\frac{1}{3}$ $\frac{2}{3}$ $1 - \frac{1}{9} - \frac{4}{9}$

$\boxed{= \frac{4}{9}}$

Gini(T_2)

class 0 class 1

2 0 $1 - 1^2 - 0$

$\frac{2}{2} = 1$ $\frac{0}{2} = 0$ $\boxed{= 0}$

3. (12 pts) With the given tree, we can predict the class of a feature vector $\mathbf{x} = (x_1, x_2)$:

   - Start from the root node of the tree:
     - **Step 1**: If current node is a *branch* node, we evaluate conditions on branch edges with $\mathbf{x}$, choose the satisfied branch to go through, and repeat **Step 1**.
     - **Step 2**: If current node is a *leaf* node, the common class of the subset in the leaf node will be used as prediction.

   Please predict the following feature vectors using the given tree:

   (1) $\mathbf{x} = (2, 1)$,

   (2) $\mathbf{x} = (3, 1)$,

   (3) $\mathbf{x} = (3, 3)$.

1) T_{12} node : class 0

2) T_{12} node : class 0

3) T_2 node : class 0

4. (**Bonus Question, 10 pts extra**) In this question, you need to implement the decision tree algorithm. Please download the Jupyter notebook `HW4_Decision_Tree.ipynb` and fill in the blanks. Note that since the same dataset T is used in the notebook, you can use the code to check if your previous answers are correct or not. Please attach your **code** and **results** in Gradescope submission.

3 (20 points) Bagging and Boosting

Assume we obtain T linear classifiers $\{h_t, t = 1, ..., T\}$ where each classifier $h : \mathbb{R}^2 \to \{+1, -1\}$ predicts the class $\hat{y} \in \{+1, -1\}$ with given feature vector $\mathbf{x} = (x_1, x_2)$ as follows:

$$\hat{y} = h(\mathbf{x}) = \text{sign}(w_1 x_1 + w_2 x_2 + b) \qquad \text{where} \qquad \text{sign}(a) = \begin{cases} +1 & \text{if } a \geq 0, \\ -1 & \text{if } a < 0. \end{cases}$$

where $w_1, w_2, b \in \mathbb{R}$ are the parameters.

- In a bagging model H_{bagging} of the T linear classifiers, we calculate the average prediction using classifiers $\{h_t\}$, and then use it to predict the class $\hat{y}_{\text{bagging}}$:

$$\hat{y}_{\text{bagging}} = H_{\text{bagging}}(\mathbf{x}) = \text{sign}\Big(\frac{1}{T}\sum_{t=1}^{T} h_t(\mathbf{x})\Big)$$

- In a boosting model H_{boosting} of the T linear classifiers, we calculate the weighted sum of predictions using classifiers $\{h_t\}$, and then use it to predict the class $\hat{y}_{\text{boosting}}$:

$$\hat{y}_{\text{boosting}} = H_{\text{boosting}}(\mathbf{x}) = \text{sign}\Big(\sum_{t=1}^{T} \alpha_t h_t(\mathbf{x})\Big)$$

  where $\{\alpha_t, t = 1, ..., T\}$ are the weight coefficients.

In this problem, suppose we have 3 linear classifiers (i.e. $T = 3$):

$$h_1(\mathbf{x}) = \text{sign}(x_1 + x_2 + 1), \quad h_2(\mathbf{x}) = \text{sign}(x_1 - x_2), \quad h_3(\mathbf{x}) = \text{sign}(x_1 - 2x_2 + 1).$$

Please answer the questions below:

1. (10 pts) Please calculate the $\hat{y}_{\text{bagging}}$ of feature vector $\mathbf{x} = (1, 2)$ using bagging on these three classifiers.

$$h_1(x) = \text{sign}(1+2+1) = \text{Sign}(4)$$

$$h_2(x) = \text{sign}(1-2) = \text{sign}(-1) = -1$$

$$h_3(x) = \text{sign}(1-2\cdot 2+1) = \text{sign}(-2) = -1$$

$$\frac{+1-1-1}{3} = \text{sign}\left(-\frac{1}{3}\right) = -1$$

2. (10 pts) Please calculate the $\hat{y}_{\text{boosting}}$ of feature vector $\mathbf{x} = (1, 2)$ using boosting on these three classifiers. The weight coefficients are $\alpha_1 = 0.8,\ \alpha_2 = 0.2,\ \alpha_3 = 0.3$.

$.8(1) + .2(-1) + .3(-1)$

$.8 - .2 - .3$

$= .3$

$\text{sign}(.3) = 1$

4 (20 points, Open Question) Overfitting of Bagging

Following the last question, suppose in the general case, we train T linear classifiers, each trained on a randomly sampled subset of the training data (assume dataset size is N, subset size is N_p). Is this model more prone to overfitting than the original model? (Could we overfit our final model by increasing N_p? Could we overfit our final model by increasing T?) Explain your reasoning.

The bagging model is more robust to overfitting due to the classifiers being trained on multiple subsets of data. Unlike adding complexity to a single model, adding more classifiers does not introduce new parameters or complexity. Subset size increase also doesn't lead to overfitting since each classifier is trained on a different subset of data. Bagging inherently reduces dependency on individual data points and reduces the effect of outliers.