CS540 Introduction to Artificial Intelligence
Lecture 6

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A Decision Tree

Motivation

Axes Aligned Decision Boundary

Motivation

Decision Tree

Description

- Find the feature that is the most informative.
- Split the training set into subsets according to this feature.
- Repeat on the subsets until all the labels in the subset are the same.

Binary Entropy

Definition

- Entropy is the measure of uncertainty.
- The value of something uncertain is more informative than the value of something certain.
- For binary labels, $y_i \in \{0, 1\}$, suppose p_0 fraction of labels are 0 and $1 - p_0 = p_1$ fraction of the training set labels are 1, the entropy is:

$$
\begin{aligned}
H(Y) &= p_0 \log_2 \left(\frac{1}{p_0}\right) + p_1 \log_2 \left(\frac{1}{p_1}\right) \\
&= -p_0 \log_2 (p_0) - p_1 \log_2 (p_1)
\end{aligned}
$$

Measure of Uncertainty

Definition

- If $p_0 = 0$ and $p_1 = 1$, the entropy is 0, the outcome is certain, so there is no uncertainty.
- If $p_0 = 1$ and $p_1 = 0$, the entropy is 0, the outcome is also certain, so there is no uncertainty.
- If $p_0 = \frac{1}{2}$ and $p_1 = \frac{1}{2}$, the entropy is the maximum 1, the outcome is the most uncertain.

Entropy

Definition

- If there are K classes and p_y fraction of the training set labels are in class y, with $y \in \{1, 2, ..., K\}$, the entropy is:

$$H(Y) = \sum_{y=1}^{K} p_y \log_2 \left(\frac{1}{p_y}\right)$$

$$= -\sum_{y=1}^{K} p_y \log_2 (p_y)$$

Conditional Entropy

Definition

- Conditional entropy is the entropy of the conditional distribution. Let K_X be the possible values of a feature X and K_Y be the possible labels Y. Define p_x as the fraction of the instances that are x, and $p_{y|x}$ as the fraction of the labels that are y among the ones with instance x.

$$H\left(Y|X=x\right) = -\sum_{y=1}^{K_Y} p_{y|x} \log_2\left(p_{y|x}\right)$$

$$H\left(Y|X\right) = \sum_{x=1}^{K_X} p_x H\left(Y|X=x\right)$$

Aside: Cross Entropy

Definition

- Cross entropy measures the difference between two distributions.

$$H(Y, X) = -\sum_{z=1}^{K} p_{Y=z} \log_2 (p_{X=z})$$

- It is used in logistic regression to measure the difference between actual label Y_i and the predicted label A_i for instance i, and at the same time, to make the cost convex.

$$H(Y_i, A_i) = -y_i \log(a_i) - (1 - y_i) \log(1 - a_i)$$

Information Gain

Definition

- The information gain is defined as the difference between the entropy and the conditional entropy.

$$I\left(Y|X\right) = H\left(Y\right) - H\left(Y|X\right).$$

- The larger than information gain, the larger the reduction in uncertainty, and the better predictor the feature is.

Splitting Discrete Features

Definition

- The most informative feature is the one with the largest information gain.

$$\arg\max_j I\left(Y \middle| X_j\right)$$

- Splitting means dividing the training set into K_{X_j} subsets.

$$\left\{(x_i, y_i) : x_{ij} = 1\right\}, \left\{(x_i, y_i) : x_{ij} = 2\right\}, ..., \left\{(x_i, y_i) : x_{ij} = K_{X_j}\right\}$$

Splitting Continuous Features

Definition

- Continuous features can be (arbitrarily) uniformly split into K_X categories.
- To construct binary splits, all possible splits of the continuous feature can be constructed, and the one that yields the highest information gain is used.

$$\mathbb{1}_{\{X_j \leqslant x_{1j}\}}, \mathbb{1}_{\{X_j \leqslant x_{2j}\}}, \ldots, \mathbb{1}_{\{X_j \leqslant x_{nj}\}}$$

- One of the above binary features is used in place of the original continuous feature X_j.

Choice of Thresholds

Definition

- In practice, the efficient way to create the binary splits uses the midpoint between instances of different classes.
- The instances in the training set are sorted by X_j, say $x_{(1)j}, x_{(2)j}, \dots, x_{(n)j}$, and suppose $x_{(i)j}$ and $x_{(i+1)j}$ have different labels, then $\frac{1}{2}\left(x_{(i)j} + x_{(i+1)j}\right)$ is considered as a possible binary split.

$$\mathbb{1}_{\left\{X_j \leqslant \frac{1}{2}\left(x_{(i)j}+x_{(i+1)j}\right)\right\}}$$

Splitting Continuous Variables Diagram

Definition

ID3 Algorithm (Iterative Dichotomiser 3), Part I

Algorithm

- Input: instances: $\{x_i\}_{i=1}^n$ and $\{y_i\}_{i=1}^n$, feature j is split into K_j categories and y has K categories
- Output: a decision tree
- Start with the complete set of instances $\{x_i\}_{i=1}^n$.
- Suppose the current subset of instances is $\{x_i\}_{i \in S}$, find the information gain from each feature.

$$I\left(Y|X_j\right) = H\left(Y\right) - H\left(Y|X_j\right)$$

ID3 Algorithm (Iterative Dichotomiser 3), Part II

Algorithm

$$H(Y) = -\sum_{y=1}^{K} \frac{\#(Y=y)}{\#(Y)} \log\left(\frac{\#(Y=y)}{\#(Y)}\right)$$

$$H(Y|X_j) = -\sum_{x=1}^{K_j}\sum_{y=1}^{K} \frac{\#(Y=y, X_j=x)}{\#(Y)} \log\left(\frac{\#(Y=y, X_j=x)}{\#(X_j=x)}\right)$$

- Find the more informative feature $j^\star$.

$$j^\star = \arg\max_j I(Y|X_j)$$

ID3 Algorithm (Iterative Dichotomiser 3), Part III

Algorithm

- Split the subset S into $K_{j^\star}$ subsets.

$$
\begin{aligned}
S_1 &= \{(x_i, y_i) \in S : x_{ij^\star} = 1\} \\
S_2 &= \{(x_i, y_i) \in S : x_{ij^\star} = 2\} \\
&\dots \\
S_{K_{X_{j^\star}}} &= \left\{(x_i, y_i) \in S : x_{ij^\star} = K_{X_{j^\star}}\right\}
\end{aligned}
$$

- Recurse over the subsets until $p_y = 1$ for some y on the subset.

Pruning Diagram

Discussion

Pruning

Discussion

- Use the validation set to prune subtrees by making them a leaf. The leaf created by pruning a subtree has label equal to the majority of the training examples reaching this subtree.
- If making a subtree a leaf does not decrease the accuracy on the validation set, then the subtree is pruned.
- This is one of the simplest ways to prune a decision tree, called Reduced Error Pruning.

D

Bagging

Discussion

- Create many smaller training sets by sampling with replacement from the complete training set.
- Train different decision trees using the smaller training sets.
- Predict the label of new instances by majority vote from the decision trees.
- This is called bootstrap aggregating (bagging).

Random Forest

Discussion

- When training the decision trees on the smaller training sets, only a random subset of the features are used. The decision trees are created without pruning.
- This algorithm is called random forests.

Boosting

Discussion

- The idea of boosting is to combine many weak decision trees, for example, decision stumps, into a strong one.
- Decision trees are trained sequentially. The instances that are classified incorrectly by previous trees are made more important for the next tree.

Adaptive Boosting, Part I

Discussion

- The weights w for the instances are initialized uniformly.

$$w = \left(\frac{1}{n}, \frac{1}{n}, ..., \frac{1}{n}\right)$$

- In each iteration, a decision tree f_k is trained on the training instances weighted by w.

$$f_k = \arg\min_{f} \sum_{i=1}^{n} w_i \mathbb{1}_{\{f(x_i) \neq y_i\}}$$

$$\varepsilon_k = \min_{f} \sum_{i=1}^{n} w_i \mathbb{1}_{\{f_k(x_i) \neq y_i\}}$$

Adaptive Boosting, Part II

Discussion

- The weights for the tree f_k is computed.

$$\alpha_k = \log\left(\frac{1-\varepsilon_k}{\varepsilon_k}\right)$$

- The weights are updated according to the error ε made by f_k, and normalized so that the sum is 1.

$$w_i = w_i e^{-\alpha_k\left(2\cdot\mathbb{1}_{\{f_k(x_i)=y_i\}}-1\right)}$$

Adaptive Boosting, Part II

Discussion

- The label of a new test instance x_i is the α weighted majority of the labels produced by all K trees: $f_1\left(x_i\right), f_2\left(x_i\right), ..., f_K\left(x_i\right)$.
- For example, if there are only two classes $\{0, 1\}$, and α is normalized so that the sum is 1, then the prediction is the following.

$$\hat{y}_i = \mathbb{1}_{\left\{\sum_{k=1}^{K} \alpha_k f_k\left(x_i\right) \geqslant 0.5\right\}}$$

K Nearest Neighbor

Description

- Given a new instance, find the K instances in the training set that are the closest.
- Predict the label of the new instance by the majority of the labels of the K instances.

Distance Function

Definition

- Many distance functions can be used in place of the Euclidean distance.

$$\rho\left(x, x'\right) = \left\|x - x'\right\|_2 = \sqrt{\sum_{j=1}^{m} \left(x_j - x'_j\right)^2}$$

- An example is Manhattan distance.

$$\rho\left(x, x'\right) = \sum_{j=1}^{m} \left|x_j - x'_j\right|$$

Manhattan Distance Diagram

Definition

P Norms

Definition

- Another group of examples is the p norms.

$$\rho\left(x, x'\right) = \left(\sum_{j=1}^{m} \left|x_j - x'_j\right|^p\right)^{\dfrac{1}{p}}$$

- $p = 1$ is the Manhattan distance.
- $p = 2$ is the Euclidean distance.
- $p = \infty$ is the sup distance, $\rho\left(x, x'\right) = \max_{i=1,2,\ldots,m} \left\{\left|x_j - x'_j\right|\right\}$.
- p cannot be less than 1.

K Nearest Neighbor

Algorithm

- Input: instances: $\{x_i\}_{i=1}^n$ and $\{y_i\}_{i=1}^n$, and a new instance $\hat{x}$.
- Output: new label $\hat{y}$.
- Order the training instances according to the distance to $\hat{x}$.

$$\rho\left(\hat{x}, x_{(i)}\right) \leqslant \rho\left(\hat{x}, x_{(i+1)}\right), i = 1, 2, \ldots, n-1$$

- Assign the majority label of the closest k instances.

$$\hat{y} = \text{ mode } \left\{y_{(1)}, y_{(2)}, \ldots, y_{(k)}\right\}$$