

Survey of Machine Learning models, cont'd

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April 7, 2025

Outline

Decision Trees

Intro

Decision trees are another example of a powerful model function for machine learning.

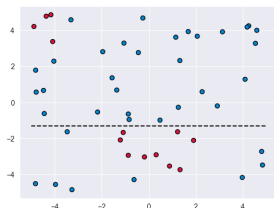
- ▶ Often used for classification (binary or multi-label); however, they can be used for regression tasks as well.
- ▶ Similar to neural networks which are capable of approximating any function, if the “size” of the decision tree is unrestrained then it can, in theory, produce an arbitrarily close approximation to any desired classification of points.

Construction of a decision tree

To build a decision tree, begin with a **decision stump** on \mathbb{R}^d .

Let $\omega = (b, \theta, j)$ be a triple consisting of $b \in \mathbb{R}$, $\theta \in \{1, -1\}$, and j an integer with $1 \leq j \leq d$. Then, define $f_\omega(\mathbf{x}) = \text{sign}(\theta(b - \mathbf{x}_j))$, where $\text{sign}(z)$ is 1 if $z \geq 0$ and is -1 otherwise. Such functions are called decision stumps.

Note that a decision stump is a special type of half-space model that has normal vector with a single non-zero component (i.e., $\mathbf{w} = (0, \dots, 0, -\theta, 0, \dots, 0)$).



Construction

Given sample data, $\mathcal{S} = \{(\mathbf{x}_i, y_i)\}_{i=1}^n$ with $\mathbf{x}_i \in \mathbb{R}^d$, the decision stump which is the best fit may be found simply by minimizing error – that is, find the values of b , θ , and j that achieves the highest accuracy on \mathcal{S} .

If there is no point \mathbf{x}_i between $\{x_{i,j} = b\}$ and $\{x_{i,j} = b'\}$, then the accuracy for (b, θ, j) and (b', θ, j) are the same. So, one can consider just values of b that are an average of two “consecutive” $x_{i,j}$ (and one less than all such j^{th} coordinates, and one larger than all of them). This gives a finite set of decision stumps to check.

A naive algorithm to determine the most accurate among this finite set of decision stumps takes on the order of dn^2 operations.

However, there is a more efficient approach, taking only $dn \log(n)$ time.

Construction of a decision tree

A decision stump is a decision tree with “depth” 1. That is, can think of a decision tree as a collection of nested decision stumps, on smaller and smaller subsets of the data.

Begin with a decision stump on all the data; i.e., find a hyperplane $x_j = b$, where $1 \leq j \leq d$ and b is some number and each data point is on one side: for each $\mathbf{x}_i \in \mathcal{S}$, either $x_{i,j} < b$ or $x_{i,j} > b$. This partitions the data into two subsets. How do you choose where to make a split? You could use the highest accuracy approach described for stumps, but this has disadvantages when the proportion of y_i that are positive, compared to negative, are unbalanced.

Often, something called **Information Gain** is used, which is defined via an entropy function e . That is, set $e(r) = -r \log(r) - (1 - r) \log(1 - r)$. Now, before making a split, set r to be the proportion of y_i that are 1 and m the number of points.

Next, define r_+ (resp. r_-) to be the proportion of points on the positive (resp. negative) side of the split that will have label 1, and let m_+ (resp. m_-) be the numbers of points on the positive (resp. negative) side. The information gain of the split is

$$e(r) - \left(\frac{m_+}{m} e(r_+) + \frac{m_-}{m} e(r_-) \right).$$

Multiple branches

The goal of the process is to recursively partition each side. On each step, one chooses the split with maximum Information Gain, at each step restricting to the two subset of data points on one side. The process ends when points in the same part have the same label, or until some predetermined depth is reached. An innermost region (where points have the same label) corresponds to a **leaf** of the tree.



Decision tree model

Start by determining a decision tree on training data, as above. Then, given test data (not yet "seen" by the model), the decision tree model will check in which partition the test point resides. Then, it labels the test point with the label of the corresponding leaf.

Often (to avoid overfitting), you decide beforehand on the depth of the tree (the maximal number of splits to get to a leaf). Since this will result in having more than one label in some of the partitions (and possibly all), the label given to a test point in each leaf is a function of the training labels in that partition – if the goal is classification, with some categorical labels, the label that has majority; if the goal is regression, with numerical labels, the mean, or the median, could be used.

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What is clustering?

Applications of clustering

K-means

DBSCAN