Decision Trees

ML Instruction Team, Fall 2022

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Decision Tree

- Decision Tree algorithms can be considered as an iterative, top-down construction method for either classifier or regressor.
- Considering only binary (or Boolean) features, at each node, there are 2^m potential splits to be evaluated given that the dataset has m features.

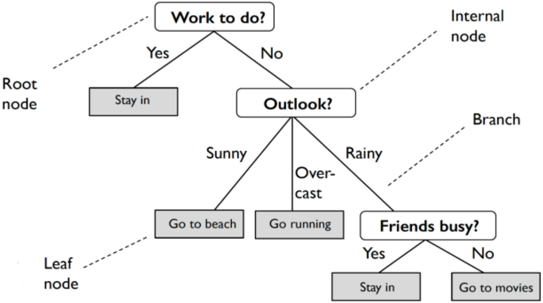


Figure: Decision Tree, Source

Terminology

- Root Node: No incoming edge, zero, or more outgoing edges.
- Internal Node: One incoming edge, two (or more) outgoing edges.
- Leaf Node: Each leaf node is assigned a class label if nodes are pure; otherwise, the class label is determined by majority vote.
- Parent & Child Node: If a node is split, we refer to that given node as the parent node, and the resulting nodes are called child nodes.

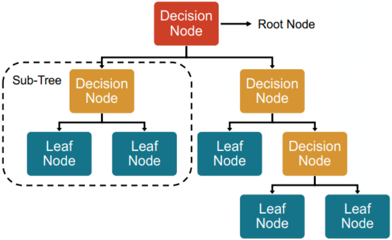


Figure: Terminology, Source

Information Gain

- Entropy: Let X be a random variable over a discrete space Ω with probability mass function $\mathbb{P}$. Then the (Shannon) entropy of X is:

$$H(X) = \mathbb{E}_X[\log(\frac{1}{\mathbb{P}(X)})] = \sum_{x \in X} \mathbb{P}(x) \log \frac{1}{\mathbb{P}(x)} = -\sum_{x \in X} \mathbb{P}(x) \log \mathbb{P}(x)$$

- Upper Bound for $H(x)$:
  - Jensen Inequality:

$$H(X) = \mathbb{E}\left(\log \frac{1}{\mathbb{P}_X(X)}\right) \leq \log \mathbb{E}\left(\frac{1}{\mathbb{P}_X(X)}\right) = \log |X|$$

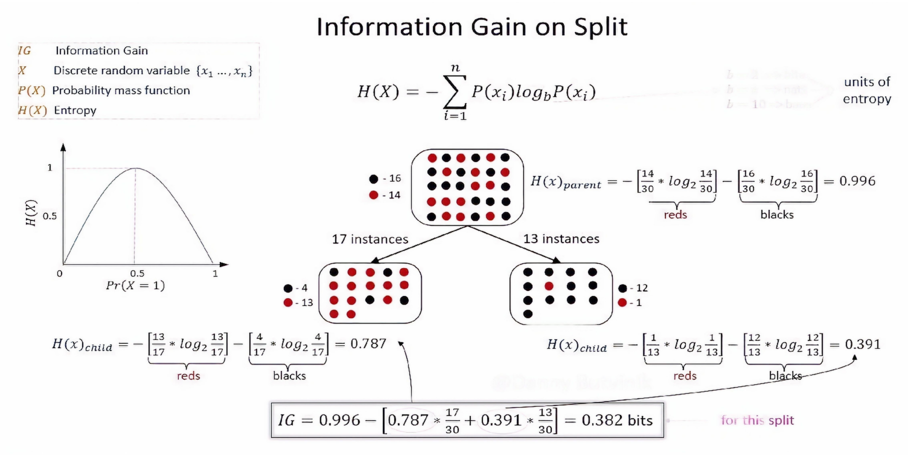
  - Using Lagrange multipliers with the constraint $\sum_x p(x) = 1$:

$$H(x) \leq -\sum_x \frac{1}{|X|} \log(\frac{1}{|X|}) = \log(|X|)$$

- Gini Impurity: Let X be a random variable over a discrete space Ω with probability mass function $\mathbb{P}$. Then the gini coefficient of X is:

$$G(X) = \sum_{x \in X} \mathbb{P}(x)(1 - \mathbb{P}(x)) = 1 - \sum_{x \in X} \mathbb{P}(x)^2$$

Information Gain



Information Gain on Split

IG	Information Gain
X	Discrete random variable $\{x_1 \dots, x_n\}$
$P(X)$	Probability mass function
$H(X)$	Entropy

$$H(X) = -\sum_{i=1}^{n} P(x_i) log_b P(x_i)$$

$b = 2$ -> bits
$b = e$ -> nats
$b = 10$ -> bans

units of entropy

$$H(x)_{parent} = -\underbrace{\left[\frac{14}{30} * log_2 \frac{14}{30}\right]}_{\text{reds}} - \underbrace{\left[\frac{16}{30} * log_2 \frac{16}{30}\right]}_{\text{blacks}} = 0.996$$

$$H(x)_{child} = -\underbrace{\left[\frac{13}{17} * log_2 \frac{13}{17}\right]}_{\text{reds}} - \underbrace{\left[\frac{4}{17} * log_2 \frac{4}{17}\right]}_{\text{blacks}} = 0.787$$

$$H(x)_{child} = -\underbrace{\left[\frac{1}{13} * log_2 \frac{1}{13}\right]}_{\text{reds}} - \underbrace{\left[\frac{12}{13} * log_2 \frac{12}{13}\right]}_{\text{blacks}} = 0.391$$

$$\boxed{IG = 0.996 - \left[0.787 * \frac{17}{30} + 0.391 * \frac{13}{30}\right] = 0.382 \text{ bits}}$$

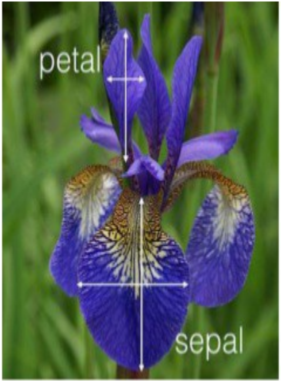
for this split

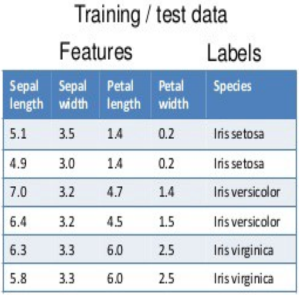
Figure: Information Gain, Source

CART Algorithm

- The algorithm first splits the training set in two subsets using a single feature k and a threshold t_k.
- How does it choose k and t_k?
  It searches for the pair (k, t_k) producing the purest subsets, which are weighted by their size.
- Once it has successfully split the training set in two, it splits the subsets using the same logic, then the sub-subsets and so on, recursively.
- CART algorithm is a greedy algorithm: it greedily searches for an optimum split at the top level, then repeats the process at each level.
- It does not check whether or not the split will lead to the lowest possible impurity several levels down.

Decision Trees in Practice





Training / test data

Features				Labels
Sepal length	Sepal width	Petal length	Petal width	Species
5.1	3.5	1.4	0.2	Iris setosa
4.9	3.0	1.4	0.2	Iris setosa
7.0	3.2	4.7	1.4	Iris versicolor
6.4	3.2	4.5	1.5	Iris versicolor
6.3	3.3	6.0	2.5	Iris virginica
5.8	3.3	6.0	2.5	Iris virginica

Figure: Iris Dataset, Source

Decision Trees in Practice

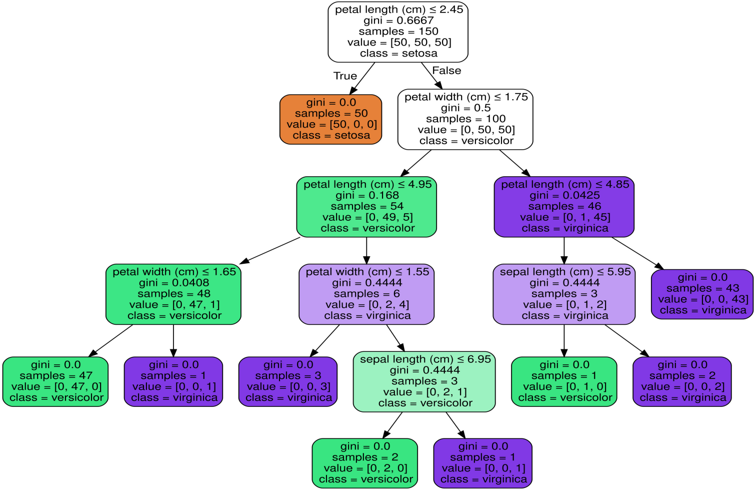


Figure: Decision Trees on Iris Dataset, Source

Misclassifications Error

- Misclassification error seems to be another reasonable choice, where:

  $$ERR(\mathcal{D}) = \frac{1}{n} \sum_{i=1}^{n} L(\hat{y}^{[i]}, y^{[i]})$$

  with the 0-1 Loss,

  $$L(\hat{y}, y) = \{ \begin{array}{l} 0 \text{ if } \hat{y} = y, \\ 1 \text{ if } \hat{y} \neq y \end{array}$$

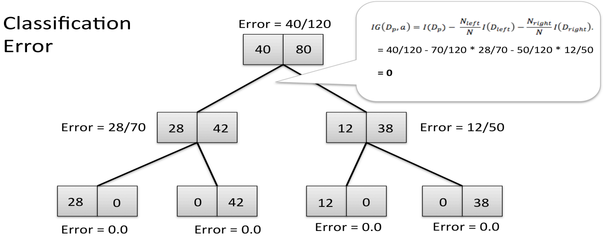
- This, in case of the training set, is equal to

  $$ERR(p) = 1 - \max_i(p(i \mid x_j))$$

  for a given node if we use majority voting at this node.

- Can we apply this measure as the criteria for splitting?

Misclassifications Error

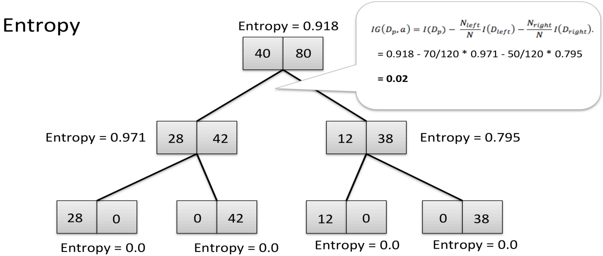


$IG(D_p, a) = I(D_p) - \frac{N_{left}}{N} I(D_{left}) - \frac{N_{right}}{N} I(D_{right}).$

= 40/120 - 70/120 * 28/70 - 50/120 * 12/50

= 0

(a) Misclassification Error, Source



$IG(D_p, a) = I(D_p) - \frac{N_{left}}{N} I(D_{left}) - \frac{N_{right}}{N} I(D_{right}).$

= 0.918 - 70/120 * 0.971 - 50/120 * 0.795

= 0.02

Positiveness of Information Gain

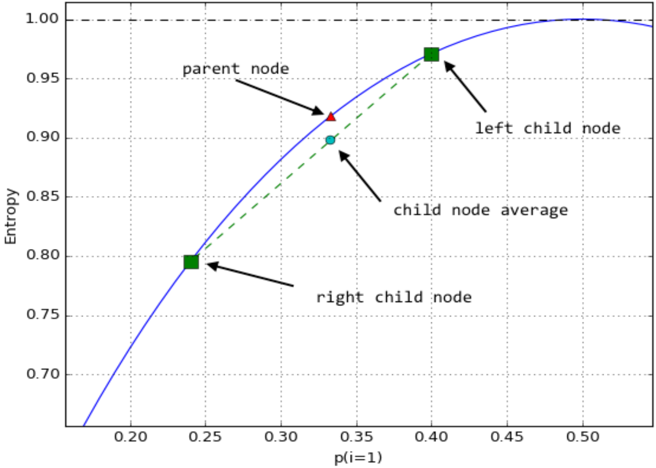


Figure: Concavity of Entropy, Source

Overfitting

- Decision Trees make very few assumptions about the training data!
- If left unconstrained, their structure will adapt itself to the training data, fitting it very closely, and most likely overfitting it!
- To avoid overfitting the training data, you need to restrict the Decision Tree's freedom during training.
- Which parameters can be restricted?
  - Max Tree Depth: Maximum depth of the tree.
  - Max Leaf Nodes: Maximum number of leaf nodes.
  - Min Sample Leaf: Minimum number of samples a leaf node must have.
  - Min Sample Split: Minimum number of samples a node must have before it can be split.
  - Max Features: Maximum number of features that are evaluated for splitting at each node)

Other Algorithms

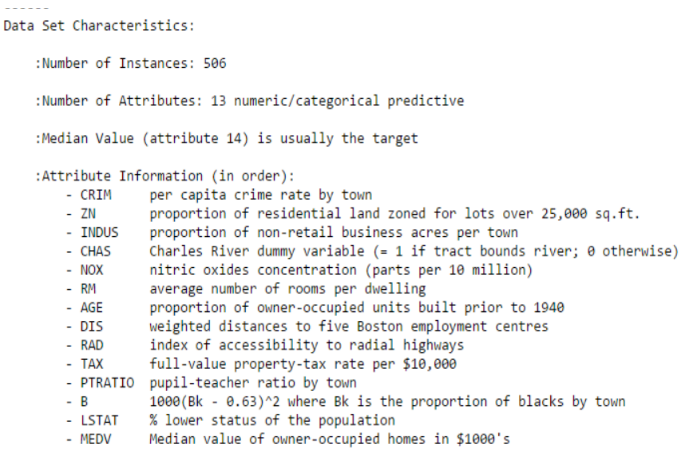
- ID3: Iterative Dichotomizer 3
  - It can only be used for discrete features, and cannot handle numeric features!
  - It supports multi-category splits.
  - It does not apply any pruning, and is prone to overfitting.
  - It results in short and wide trees (compared to CART).
  - It maximizes information gain/minimizes entropy.

- C4.5:
  - It supports Continuous and discrete features (continuous feature splitting is very expensive because must consider all possible ranges).
  - It can handles missing attributes (ignores them in information gain computation)
  - It performs post-pruning

Decision Trees for Regression

- It is the same as classification with a few subtle modifications:
  - The main difference is that instead of predicting a class in each node, it predicts a value.
  - The prediction for each node is simply the average target value of the all training instances associated to this leaf node.
  - Instead of trying to split the training set in a way that minimizes impurity, CART algorithm now tries to split the training set in a way that minimizes the MSE.
  - The MSE at a given node is also often referred to as intra-node variance, and the splitting criterion is thus called variance reduction.
  - Likewise to classification tasks, decision trees are prone to overfitting when dealing with regression tasks.

Positiveness of Information Gain



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Data Set Characteristics:

    :Number of Instances: 506

    :Number of Attributes: 13 numeric/categorical predictive

    :Median Value (attribute 14) is usually the target

    :Attribute Information (in order):
        - CRIM     per capita crime rate by town
        - ZN       proportion of residential land zoned for lots over 25,000 sq.ft.
        - INDUS    proportion of non-retail business acres per town
        - CHAS     Charles River dummy variable (= 1 if tract bounds river; 0 otherwise)
        - NOX      nitric oxides concentration (parts per 10 million)
        - RM       average number of rooms per dwelling
        - AGE      proportion of owner-occupied units built prior to 1940
        - DIS      weighted distances to five Boston employment centres
        - RAD      index of accessibility to radial highways
        - TAX      full-value property-tax rate per $10,000
        - PTRATIO  pupil-teacher ratio by town
        - B        1000(Bk - 0.63)^2 where Bk is the proportion of blacks by town
        - LSTAT    % lower status of the population
        - MEDV     Median value of owner-occupied homes in $1000's
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Figure: Boston Dataset, Source

Decision Trees for Regression

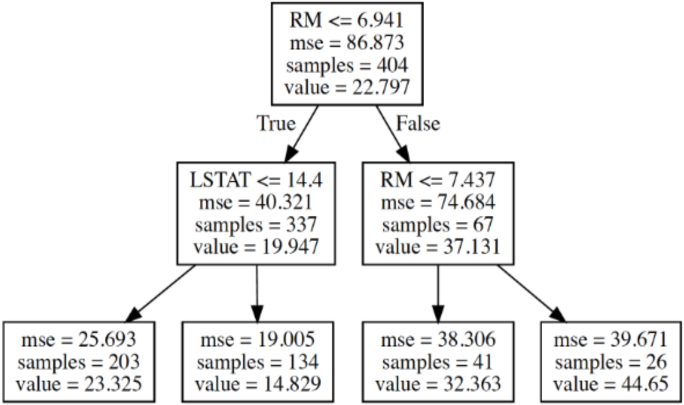

Figure: Concavity of Entropy, Source

Thank You!

Any Question?