## Classification and Regression Tree



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## 1 Introduction



- The decision tree is one of the most popular used predictive modelling approaches
- Classification for predicting categorical labels
- Regression for numeric prediction
- The Classification And Regression Tree (CART) [1] is one commonly used algorithm to build binary decision trees



#### Input:

- Years: number of years played in the major leagues
- Hits: number of hits made in the previous year

#### **Output:**

Log salary (in thousands of dollars)

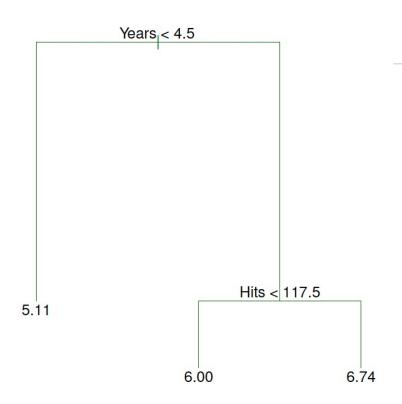


Figure 1: A regression tree for predicting the log salary of a baseball player. From Figure 8.1 in [2].



- **Root node:** the entire training data set
- Internal node: a decision node to conduct splitting
- Leaf node: holds the decision and cannot be further split
- **Depth:** three

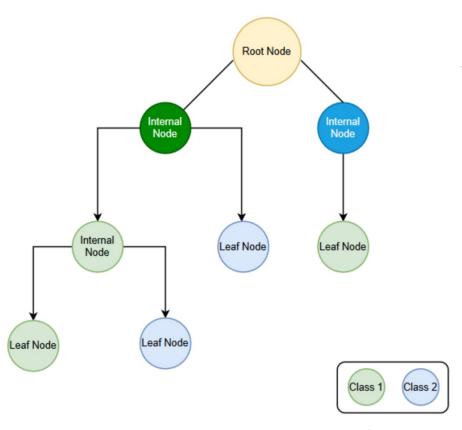


Figure 2 : Decision tree structure. <u>Image Source</u>.

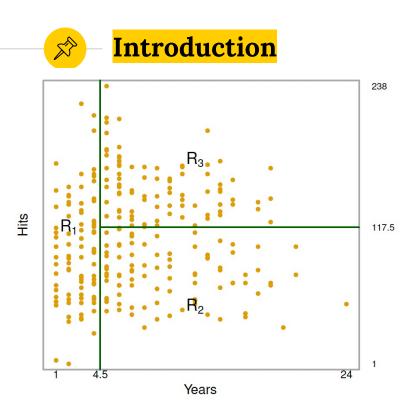


Figure3 : The three-region partition for the example in Figure 1. Adopted from [2.]

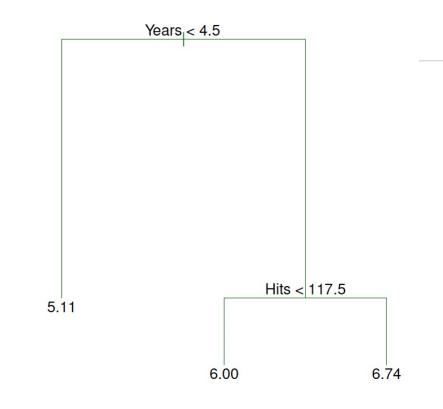


Figure 1: A regression tree for predicting the log salary of a baseball player. Adopted from [2].



#### Advantages of the decision tree:

- Simplicity:
  - trees can be displayed graphically and easy to understand
- Flexibility:
  - non-parametric model;
  - handle both numerical and categorical data;
- High interpretability:
  - mirrors human decision making

## 2 Construction of the tree



How to construct a tree / How to divide the feature space/ how to split a node:

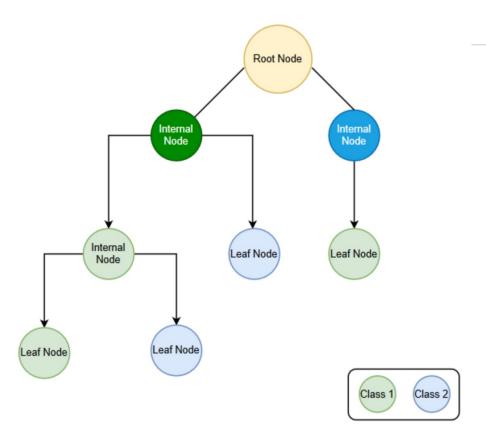
- Which feature
- A cut-off value
- A criterion

#### The CART algorithm



#### The **recursive binary splitting** approach:

- Top-down begin at the top; successively split
- Greedy
  find the best split at each node





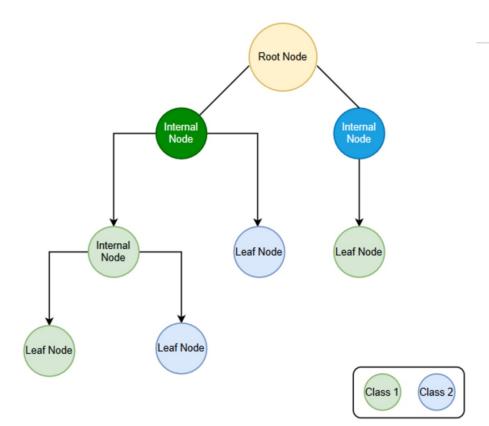
#### How to evaluate the "best"? (criterion)

Regression:

$$RSS = \sum_{j=1}^{J} \sum_{i \in R_j} \left( y_i - \hat{y}_{R_j} \right)^2$$

Classification:

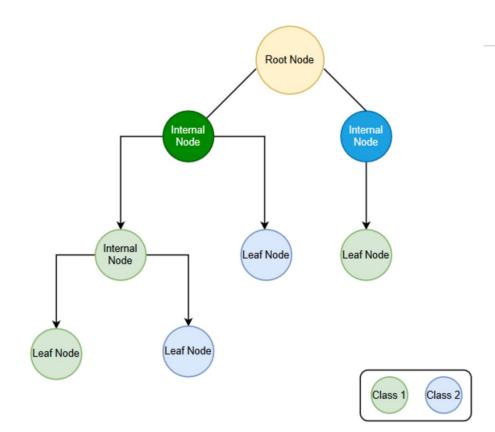
Gini = 
$$\sum_{j=1}^{J} \sum_{k=1}^{K} \hat{p}_{jk} (1 - \hat{p}_{jk})$$





#### How to predict?

- Regression:
  - $\hat{y}_{R_j}$  = sample mean
- Classification:
  - $\hat{y}_{R_i} = \text{most common class}$

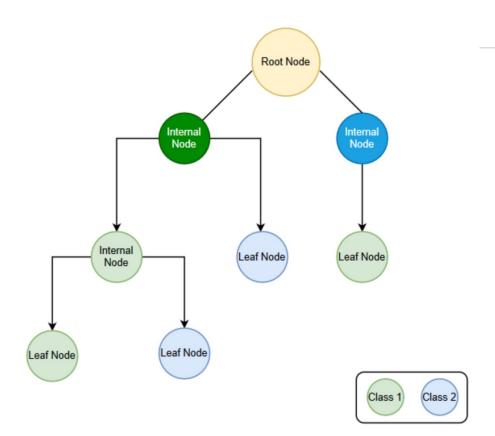




#### How to stop?

- Min\_samples\_leaf
- Min\_samples\_spilt
- Max\_depth

#### Important to avoid overfitting!



## **Construction**

- A set of p feature variables  $S = \{x_1, \dots, x_p\}$ , a response variable y
- Recursively create binary partitions (for regression):
  - Start at the root node.
  - Consider a splitting variable  $x \in S$  and a cut-off value c to divide the space into  $\{x \le c\}$  and  $\{x > c\}$ , then model the response y by its sample mean over each region.
  - Choose the splitting variable and cut-off value that achieves the best fit in a least squares sense.
  - Stop the splitting once a stopping rule is satisfied.



#### Advantages of the decision tree:

- Simplicity:
  trees can also be displayed graphically
- Flexibility:
   non-parametric model;
   handle both numerical and categorical data;
- High interpretability:mirrors human decision making

## — Cross validation



#### Tuning tree complexity: cross-validation

- As the number of features increases, the size of the tree grows rapidly
  - An overly complex model
  - Nullify the model's attractive interpretability
  - Overfitting problem
- Balance between the tree complexity and the model's goodness-of-fit



#### K-Fold Cross-Validation Procedure:

- Suppose we wish to select a maximal tree depth  $\gamma$  from a set  $\{\gamma_1, \dots, \gamma_m\}$
- Given a sample of data, randomly split the full dataset into K roughly equal-sized groups. Set aside one group as the validation set and use the remaining K-1 groups as the training set.
- Build a tree model on the training set for each  $\gamma_j$  for  $j=1,\cdots,m$ . Then calculate the mean squared prediction error of each fitted model on the hold-out validation set.
- The process is repeated K times, and we obtain K estimates of the prediction error for each  $\gamma_j$  for  $j=1,\cdots,m$ .
- Select the maximal depth  $\gamma_i$  that minimizes the average prediction error.

## Python implementation



#### Non-robustness:

A small change in the training data could cause a large change in the tree

#### Predictive accuracy:

Trees generally do not have the same level of predictive accuracy as some of the other regression and classification approaches

bagging or boosting



- [1]. Leo Breiman, Jerome Friedman, Charles J Stone, and Richard A Olshen. Classification and Regression Trees. CRC press, 1984.
- [2]. Gareth, James, Witten Daniela, Hastie Trevor, and Tibshirani Robert. An introduction to statistical learning: with applications in R. Spinger, 2013.



# Thanks!