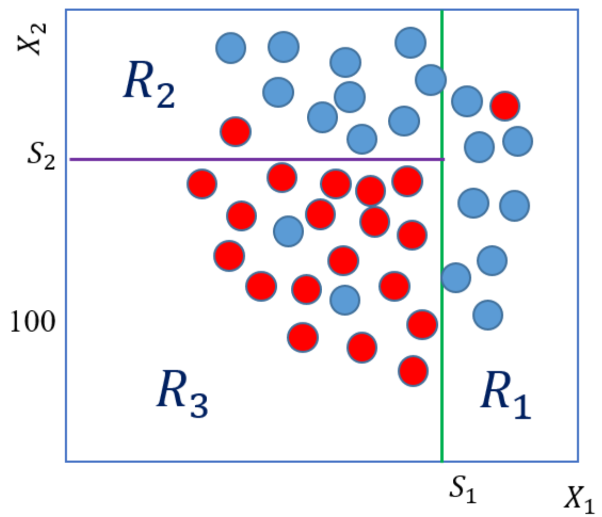
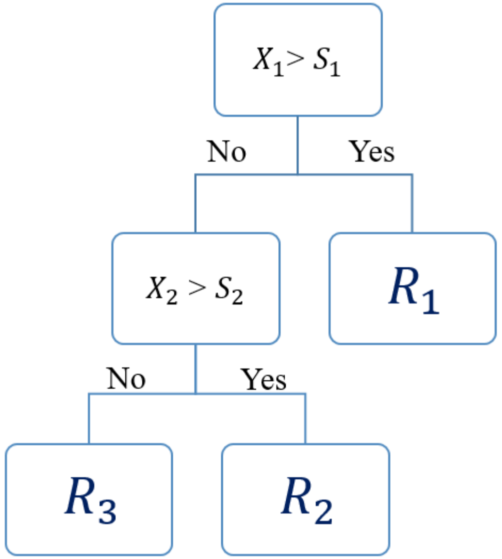
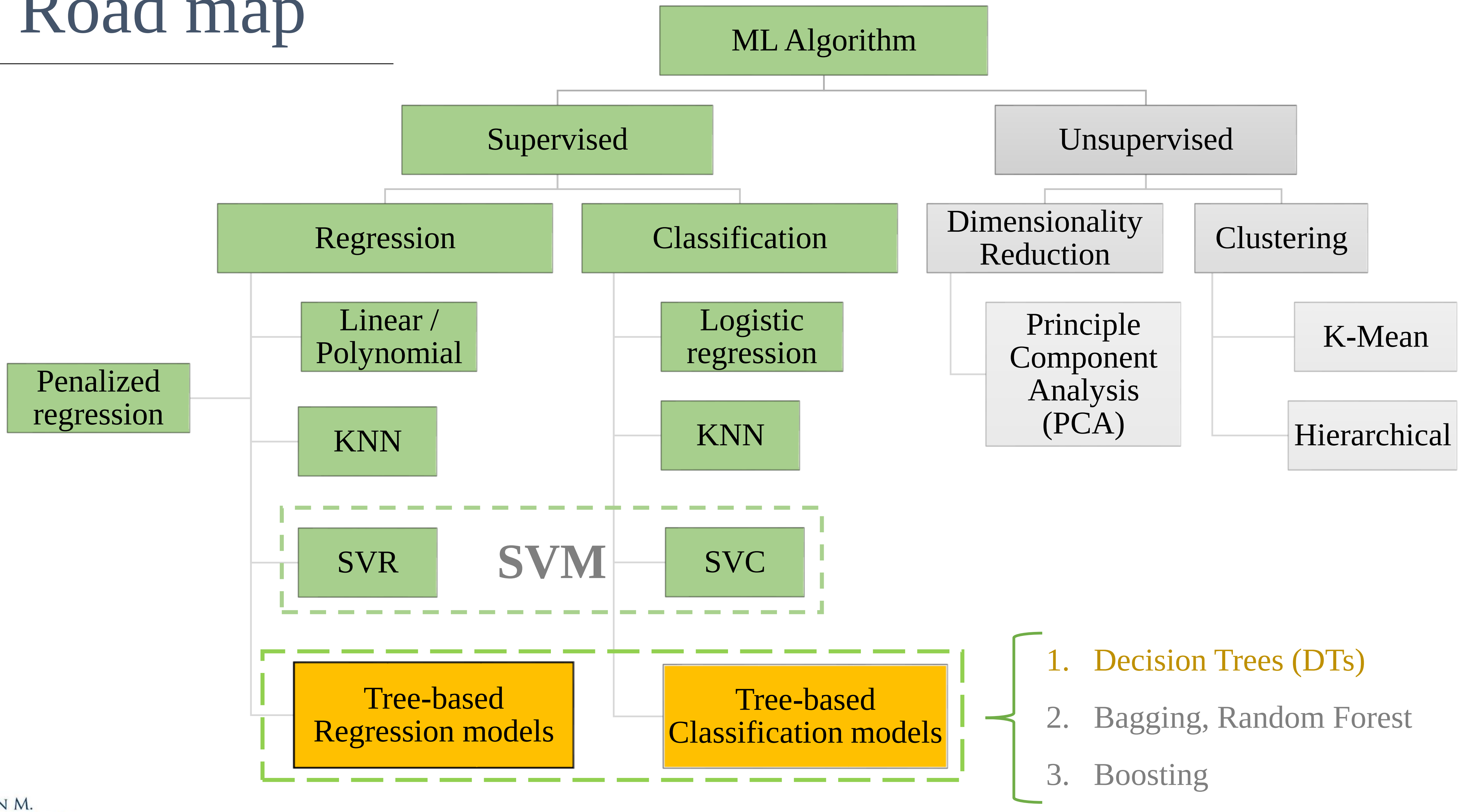
Class -18
Decision Trees (DTs)

Prof. Pedram Jahangiry





Road map


ML Algorithm
Supervised
Unsupervised
Regression
Classification
Dimensionality Reduction
Clustering
Linear / Polynomial
Logistic regression
Principle Component Analysis (PCA)
K-Mean
Penalized regression
KNN
KNN
Hierarchical
SVR
SVM
SVC
Tree-based Regression models
Tree-based Classification models
1. Decision Trees (DTs)
2. Bagging, Random Forest
3. Boosting

Topics

Part I

1. Decision Trees Definitions
2. Decision Trees criteria
   - MSE
   - Error Rate
   - Gini Index
   - Entropy

Part II

1. Regression Trees
2. Classification Trees

Part III

1. Pruning a tree
2. Hyperparameters

Part IV

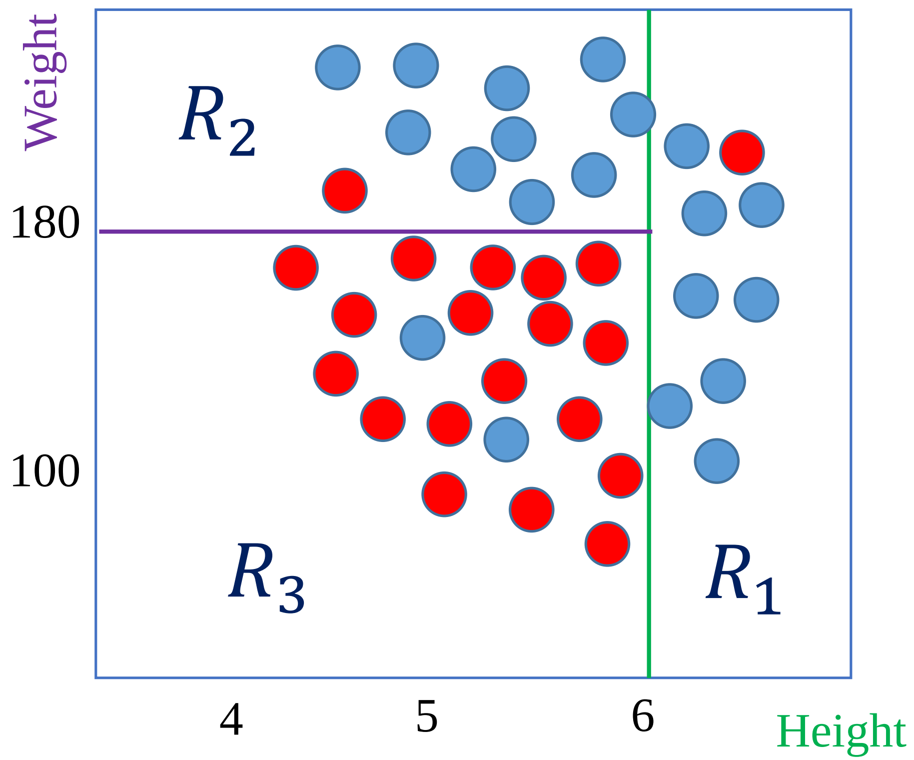
1. Pros and Cons
2. Applications in Finance

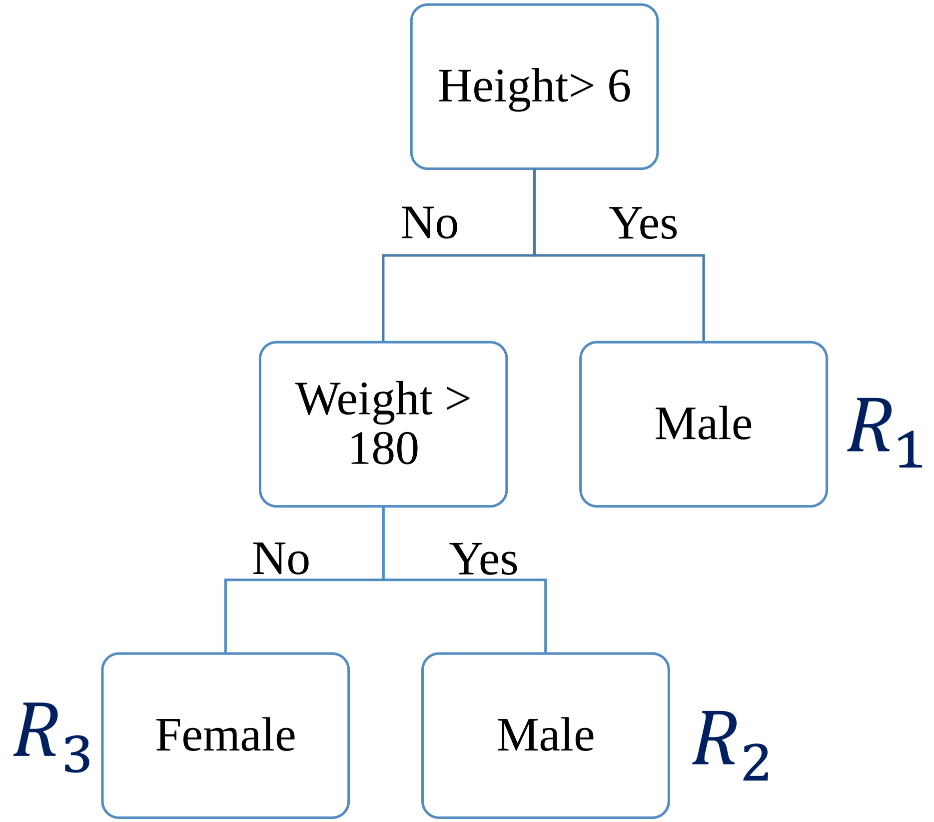
Part I

Decision Trees definitions and criteria

Decision Trees Definitions

- DTs are ML algorithms that progressively divide data sets into smaller data groups based on a descriptive feature, until they reach sets that are small enough to be described by some label.
- DTs apply a top-down approach to data, trying to group and label observations that are similar.

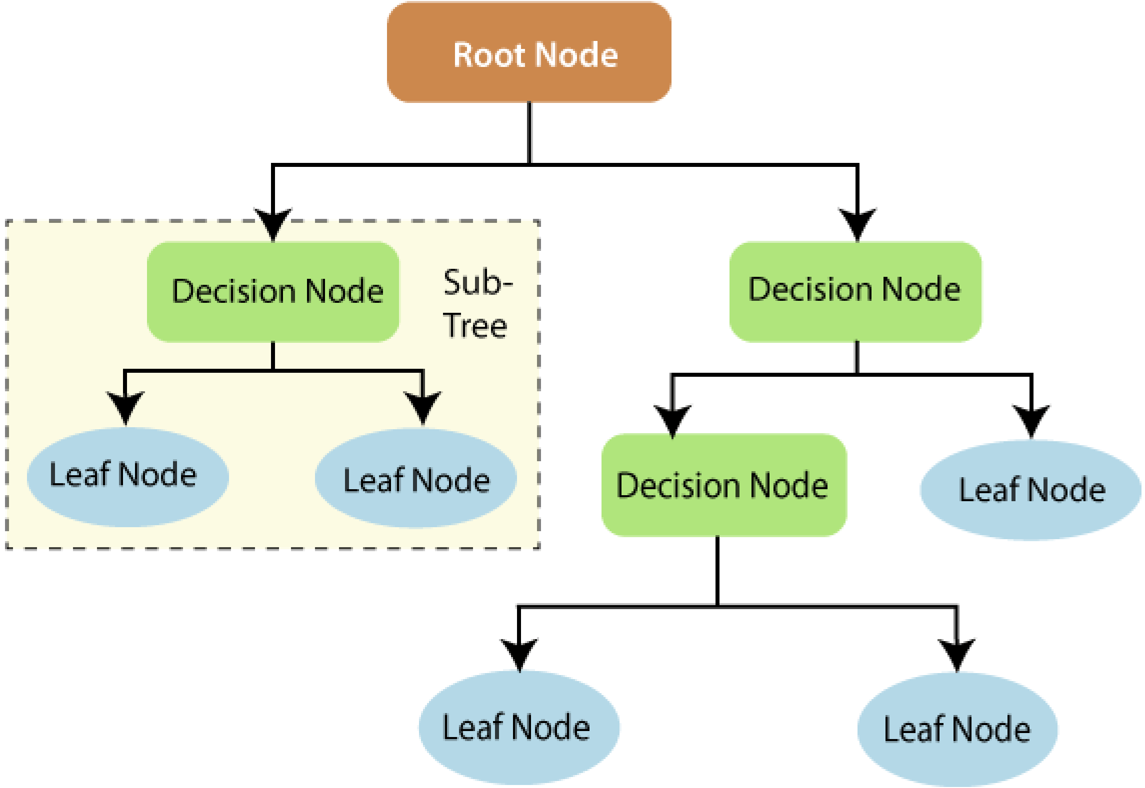




Decision Trees Definitions

- When the target variable consists of real numbers: regression trees
- When the target variable is categorical: classification trees
- Terminology:

  - ✓ Root node
  - ✓ Splitting
  - ✓ Branch
  - ✓ Decision node (internal node)
  - ✓ Leaf node (terminal node)
  - ✓ Sub-tree
  - ✓ Depth (level)
  - ✓ Pruning

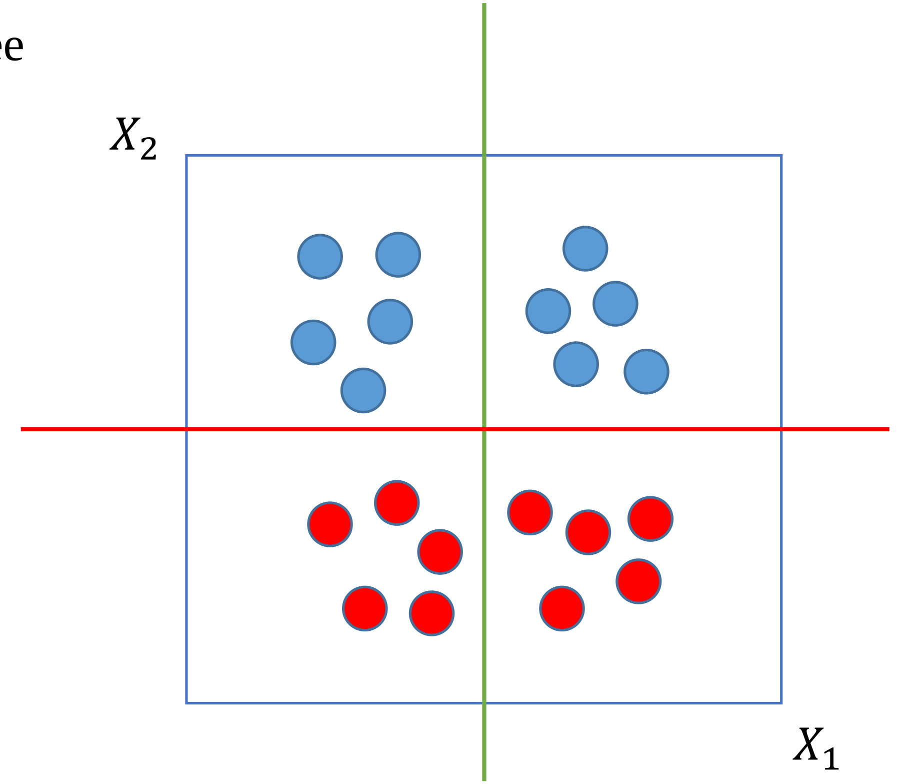


Decision Trees Criteria

- Which split adds the most information gain (minimum impurity)?
- Regression trees: MSE
- Classification trees:
  1. Error rate
  2. Entropy
  3. Gini Index

Control how a Decision Tree decides to split the data

They all measure **impurity**



Decision Trees Criteria

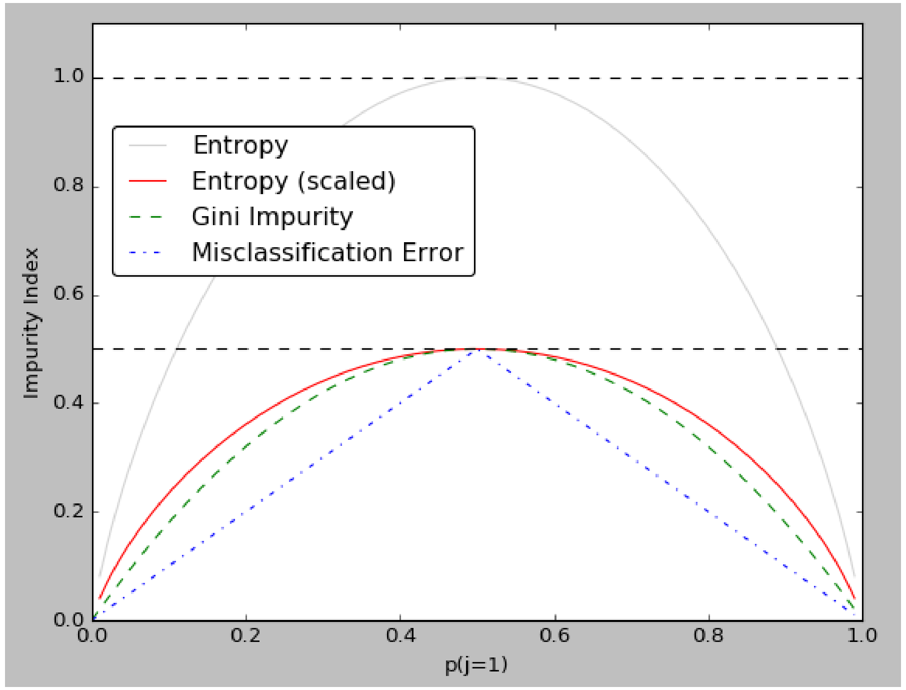
- Entropy: Measures the impurity or randomness (uncertainty) in the data points
- Gini Index: Measure how often a randomly chosen element would be incorrectly labeled

- For both Entropy and Gini, 0 expresses all the elements belong to a specified class (pure)

- Different decision tree algorithms utilize different impurity metrics

$$entropy = -\sum_{j} p_j \log_2(p_j)$$

$$Gini = 1 - \sum_{j} p_j^2$$



Part II

Regression / Classification Trees!

How does a decision tree work?

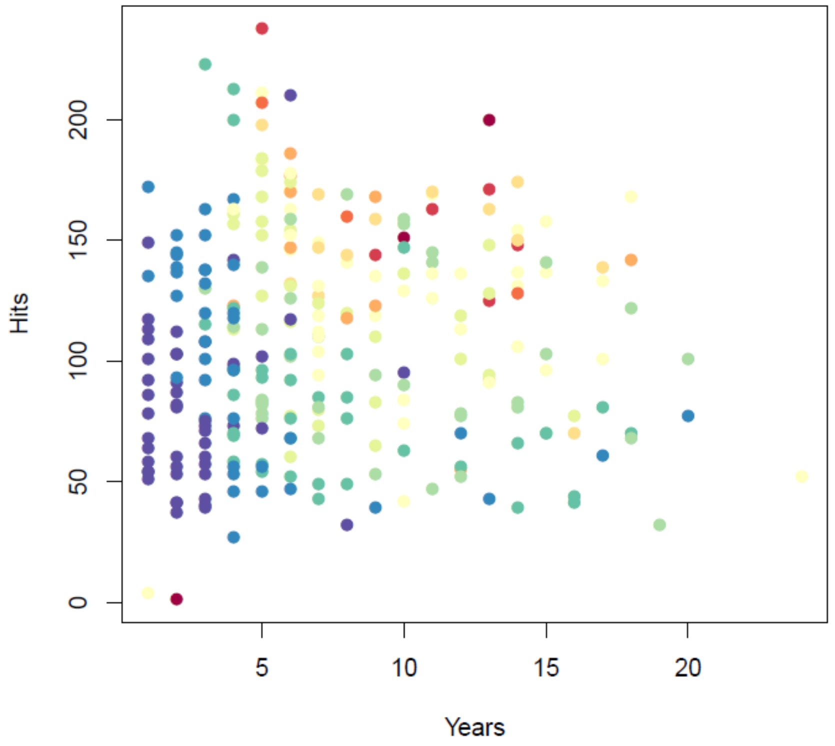
Regression Trees

- Baseball Salary is color-coded from low (blue, green) to high (yellow, red)

- DTs apply a top-down approach to data, trying to group and label observations that are similar.

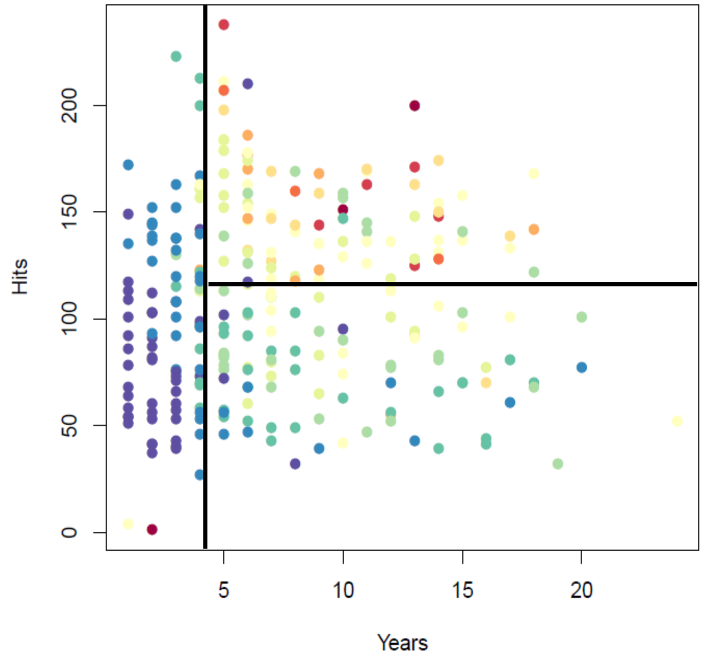
- The main questions in every decision-making process:

1. Which feature to start with?
2. Where to put the split (cut off)?



Interpreting the results

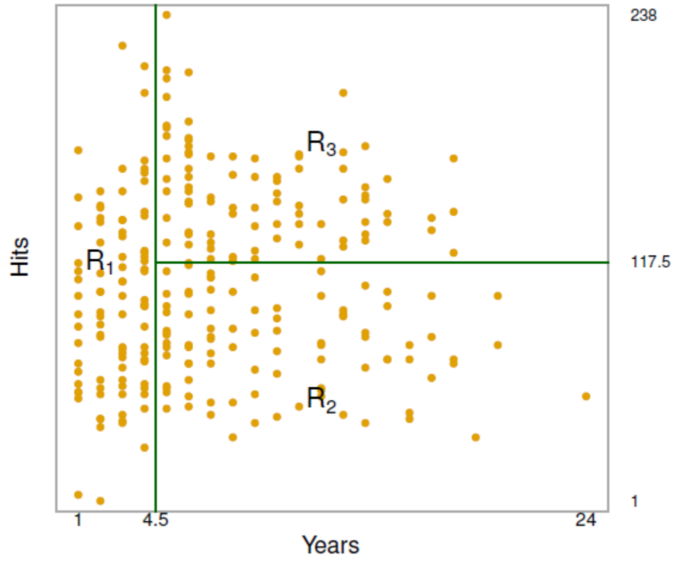
- Based on color-coded salary, it seems that years is the most important factor in determining salary.
- For less experienced players, the number of hits seems irrelevant.
- Among more experienced players thought, players with more hits tend to have higher salaries.
- As one can see, the model is very easy to display, interpret and explain.



Tree building process

- Divide the feature space into J distinct and non-overlapping regions.
- For every observation that falls into the region R_j, we make the same prediction, which is simply the mean of the target values for the training observations in R_j.
- The goal is to find rectangles $R_1, R_2, \ldots, R_j$ that minimize the RSS:

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



- Where $\hat{y}_{R_j}$ is the mean target for the training observations within the j^{th} rectangle.

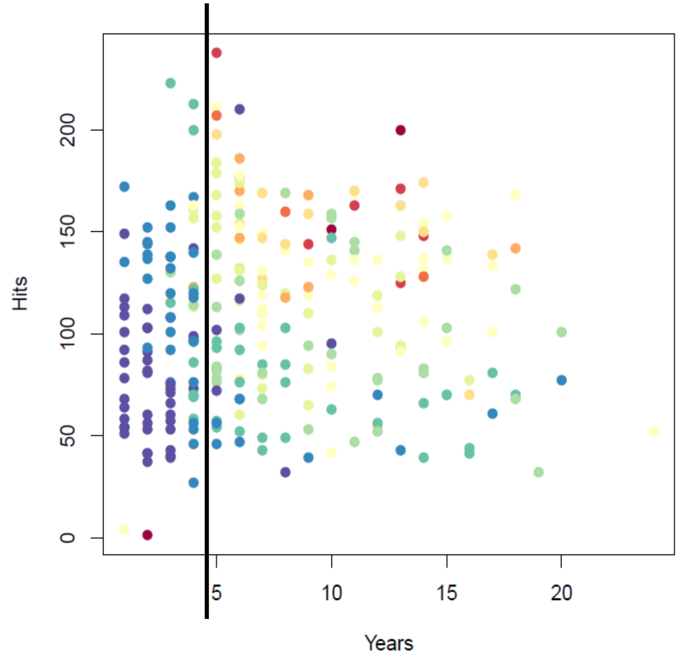
Tree building process: Recursive Binary Splitting

- How does the algorithm select X_j and the split s ?
- X_j and s are selected such that splitting the feature space into the regions $\{X|X_j < s\}$ and $\{X|X_j \geq s\}$ leads to the largest possible reduction in RSS.

$$R_1(j,s) = \{X|X_j < s\} \text{ and } R_2(j,s) = \{X|X_j \geq s\}$$

- Seeking for the value of j and s that minimized the following equation:

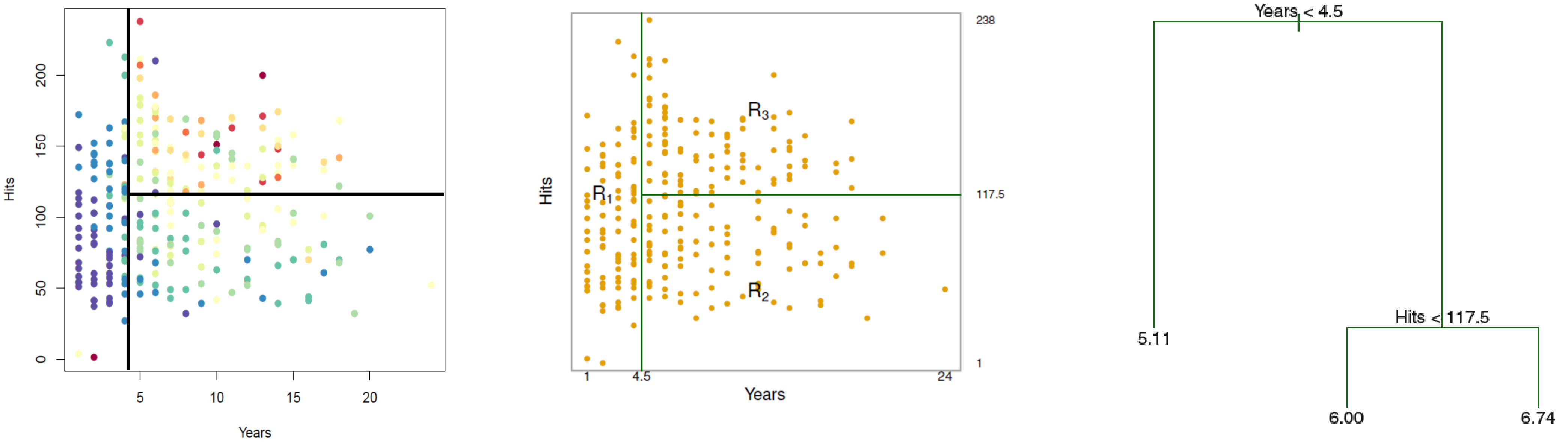
$$\sum_{i:\, x_i \in R_1(j,s)} (y_i - \hat{y}_{R_1})^2 + \sum_{i:\, x_i \in R_2(j,s)} (y_i - \hat{y}_{R_2})^2$$



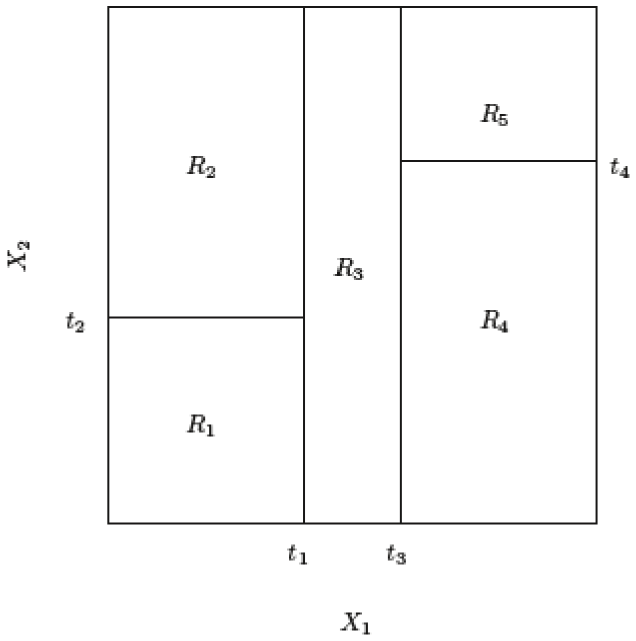
- The best split is made at that particular step, rather than looking ahead and picking a split that will lead to a better tree in some future step.

Tree building process: Recursive Binary Splitting

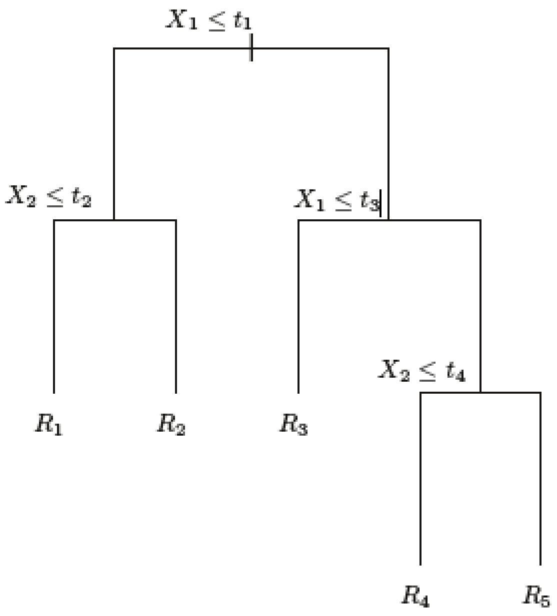
- Next, the algorithm repeats the process, looking for the best feature and best split in order to split the data further to minimize the RSS within each of the resulting regions.
- The process continues until a stopping criterion is reached; for instance, continues until no region contains more than a fixed number of observations.



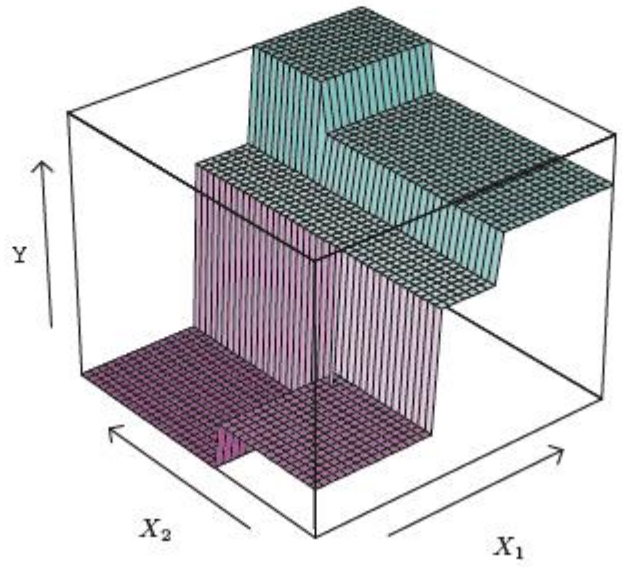
A Five-Region Example of Recursive Binary Splitting



The output of recursive binary splitting on a two-dimensional example



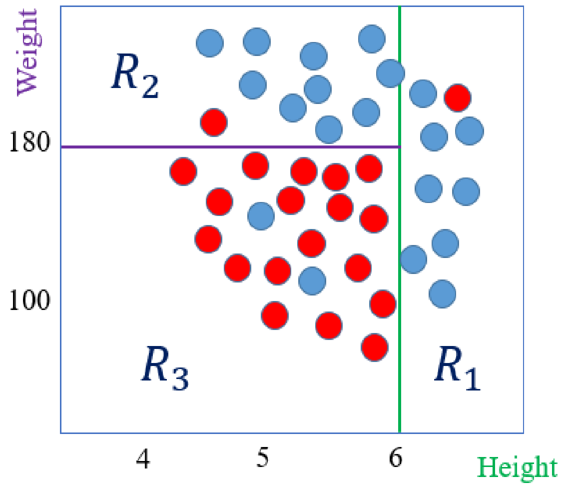
A tree corresponding to the partition in the left panel.

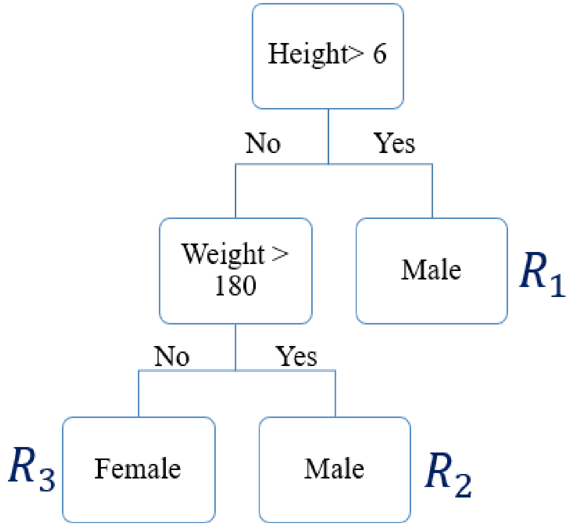


A perspective plot of the prediction surface corresponding to that tree.

Classification Trees

- Classification trees are very similar to regression trees, except that it is used to predict a qualitative response rather thana quantitative one.
- The prediction of the algorithm at each terminal node will be the category with the majority of data points i.e., the most commonly occurring class.

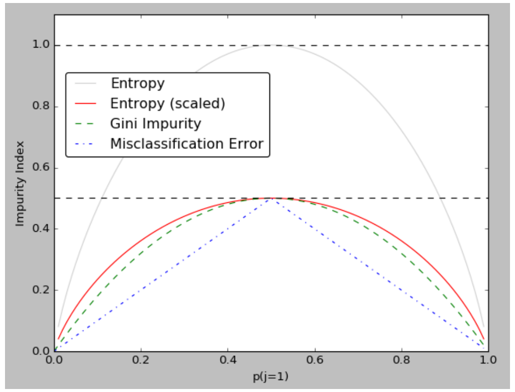




Classification Trees (details)

- Just as in the regression setting, the recursive binary splitting is used to grow a classification tree. However, instead of RSS we will be using one of the following impurity criteria:

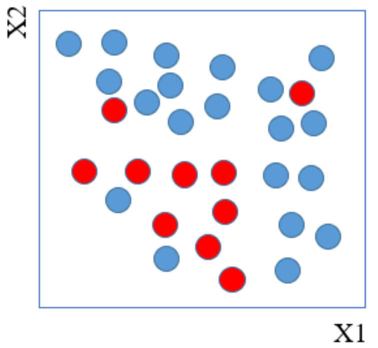
  1. Classification error rate: $E = 1 - \max_{k}(\hat{p}_{mk})$
  2. Gini index: $G = \sum_{k=1}^{K} \hat{p}_{mk}(1 - \hat{p}_{mk})$
  3. Cross entropy: $D = -\sum_{k=1} \hat{p}_{mk} \log \hat{p}_{mk}$

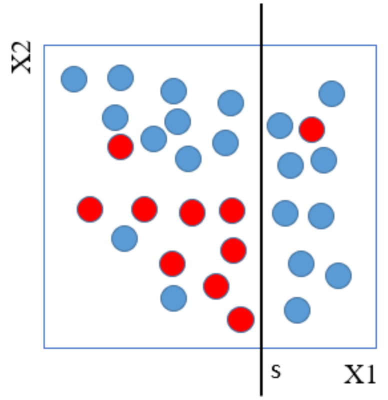


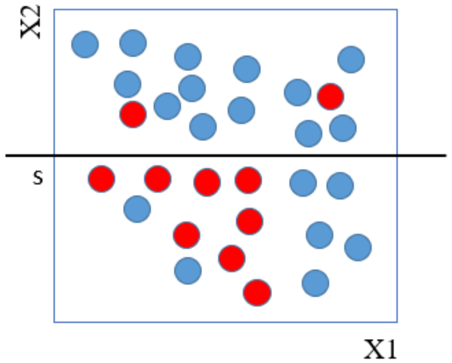
- $\hat{p}_{mk}$ represents the proportion of training observations in the m^{th} region from the k^{th} class.
- Classification error rate is not sufficiently sensitive to node purity and in practice either Gini or Cross entropy is preferred.

Decision Tree Metrics (Simple Example)

Node	*Gini* $1-\sum_j p_j^2$	*Cross entropy* $-\sum_j p_j \log(p_i)$	*Error rate* $1-\max(p_i)$
Entire training data before split	$\left\{1-\left(\left(\frac{10}{30}\right)^2+\left(\frac{20}{30}\right)^2\right)\right\} = 0.44$	$-\left\{\left(\frac{10}{30} log \frac{10}{30}+\frac{20}{30} log \frac{20}{30}\right)\right\} = 0.64$	$1-\max\left\{\frac{10}{30},\frac{20}{30}\right\}$ $= 1-\frac{20}{30} = 0.333$
Root node: X1 > s	$\frac{20}{30} * \left\{1-\left(\left(\frac{9}{20}\right)^2+\left(\frac{11}{20}\right)^2\right)\right\} +$ $\frac{10}{30} * \left\{1-\left(\left(\frac{1}{10}\right)^2+\left(\frac{9}{10}\right)^2\right)\right\} =$ $\frac{20}{30} * 0.495 + \frac{10}{30} * 0.18 = \mathbf{0.39}$	$-\frac{20}{30}\left\{\left(\frac{9}{20}\log_2\frac{9}{20}+\frac{11}{20}\log_2\frac{11}{20}\right)\right\} +$ $-\frac{10}{30}\left\{\left(\frac{1}{10}\log_2\frac{1}{10}+\frac{9}{10}\log_2\frac{9}{10}\right)\right\} =$ $\frac{20}{30} * 0.69 + \frac{10}{30} * 0.325 = \mathbf{0.57}$	$\frac{20}{30} * \frac{9}{20} +$ $\frac{10}{30} * \frac{1}{10} =$ $\mathbf{0.333}$
Root node: X2 > s	$\frac{15}{30} * \left\{1-\left(\left(\frac{2}{15}\right)^2+\left(\frac{13}{15}\right)^2\right)\right\} +$ $\frac{15}{30} * \left\{1-\left(\left(\frac{8}{15}\right)^2+\left(\frac{7}{15}\right)^2\right)\right\} =$ $\frac{15}{30} * 0.231 + \frac{15}{30} * 0.497 = \mathbf{0.37}$	$-\frac{15}{30}\left\{\left(\frac{2}{15}\log_2\frac{2}{15}+\frac{13}{15}\log_2\frac{13}{15}\right)\right\} +$ $-\frac{15}{30}\left\{\left(\frac{8}{15}\log_2\frac{8}{15}+\frac{7}{15}\log_2\frac{7}{15}\right)\right\} =$ $\frac{15}{30} * 0.39 + \frac{15}{30} * 0.69 = \mathbf{0.54}$	$\frac{15}{30} * \frac{2}{15} +$ $\frac{15}{30} * \frac{7}{15} =$ $\mathbf{0.3}$



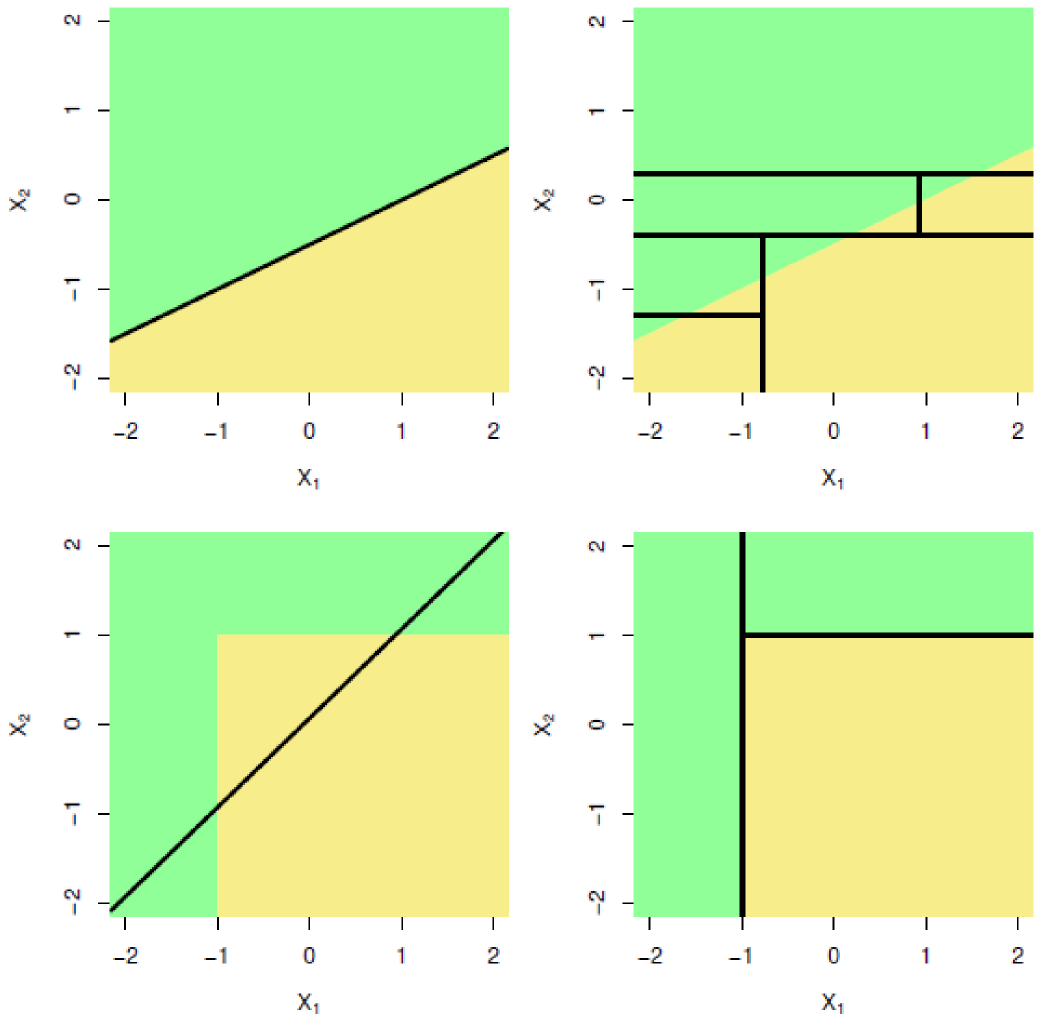




Trees Versus Linear Models

Left column: linear model; Right column: tree-based model

Top Row: True linear boundary
Bottom row: true non-linear boundary.



Part III

Pruning a tree

Tunning hyper parameters

Pruning a tree

- Decision tree may produce good predictions on the training set, but is likely to overfit the data, leading to poor test set performance. (why?)
- A smaller tree with fewer splits may lead to lower variance and better interpretation at the cost of a little bias.
- This strategy may result in smaller trees, but is too short-sighted:

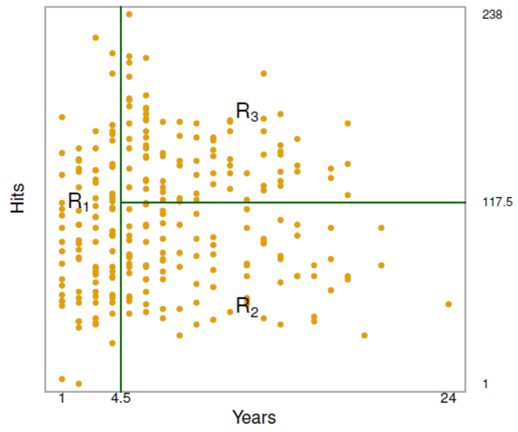
" a seemingly worthless split early on in the tree might be followed by a very good split, a split that leads to a large reduction in RSS/impurity index later on"

- A better strategy is to grow a very large tree T_0, and then prune it back in order to obtain a subtree.
- Cost complexity pruning is used to do this.

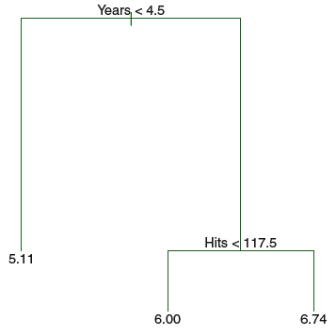
Cost complexity pruning (weakest link pruning)

- Consider a sequence of trees indexed by a nonnegative tuning parameter α.
- For each value of α there corresponds a subtree $T \subset T_0$ such that the following objective function is minimized.

$$\sum_{m=1}^{|T|} \sum_{i:\, x_i \in R_m} (y_i - \hat{y}_{R_m})^2 + \alpha|T|$$



  - $|T|$ indicates the number of terminal nodes of the tree T
  - R_m is the rectangle corresponding to m^{th} terminal node and
  - $\hat{y}_{Rm}$ is the mean of the training observations in R_m



- α controls the bias variance trade off and is determined by cross validation.
- Lastly, we return to full data set and obtain the subtree corresponding to α

Building a Regression Tree algorithm

Algorithm 8.1 *Building a Regression Tree*

1. Use recursive binary splitting to grow a large tree on the training data, stopping only when each terminal node has fewer than some minimum number of observations.

2. Apply cost complexity pruning to the large tree in order to obtain a sequence of best subtrees, as a function of α.

3. Use K-fold cross-validation to choose α. That is, divide the training observations into K folds. For each $k = 1, \ldots, K$:

   (a) Repeat Steps 1 and 2 on all but the kth fold of the training data.

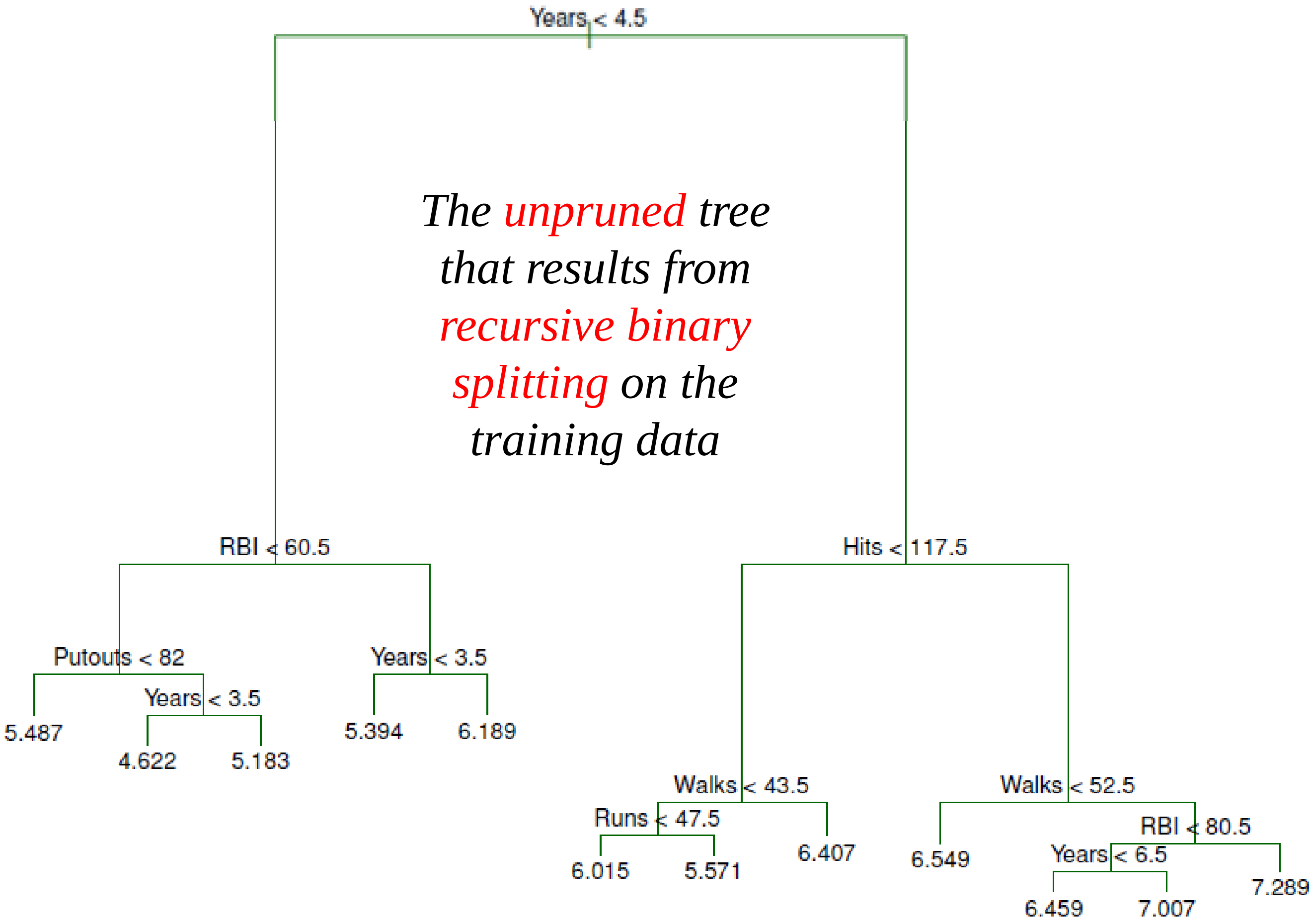
   (b) Evaluate the mean squared prediction error on the data in the left-out kth fold, as a function of α.

   Average the results for each value of α, and pick α to minimize the average error.

4. Return the subtree from Step 2 that corresponds to the chosen value of α.

Source: An introduction to Statistical Learning

Salary example continued



The unpruned tree that results from recursive binary splitting on the training data

Finding the optimal α or T

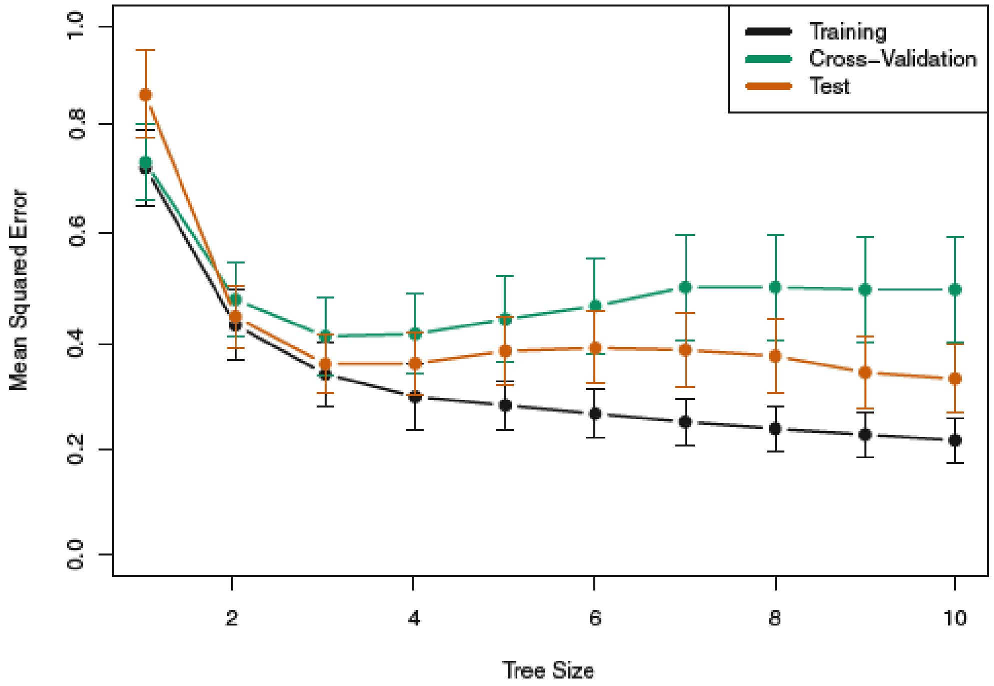
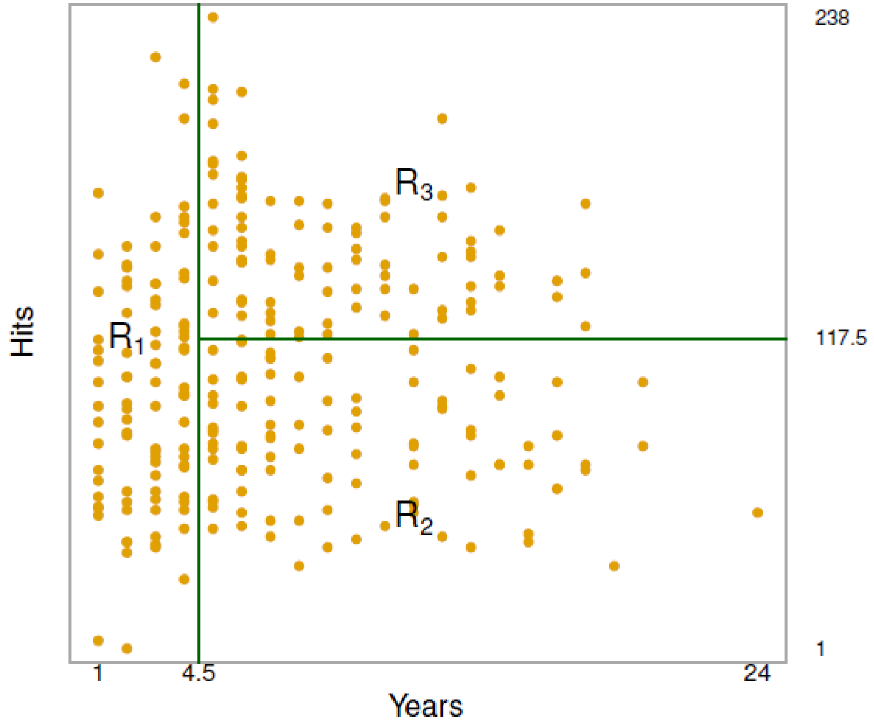


FIGURE 8.5. *Regression tree analysis for the* Hitters *data. The training, cross-validation, and test MSE are shown as a function of the number of terminal nodes in the pruned tree. Standard error bands are displayed. The minimum cross-validation error occurs at a tree size of three.*

The optimal (pruned) tree



Other hyperparameters

- ✓ To avoid overfitting, regularization parameters can be added to the model such as:
  - Maximum depth of the tree
  - Minimum population at a node
  - Maximum number of decision nodes
  - Minimum impurity decrease (info gain)
  - Alpha (complexity parameter)
- ✓ Other hyperparameters are:
  - Criterion: gini, entropy
  - Splitter: best, random
  - Class weight: balanced, none

Part IV

Pros and Cons

Applications in finance

DTs' Pros and Cons

Pros:

- Easy to interpret and visualize
- Can easily handle categorical data without the need to create dummy variables
- Can easily capture Non-linear patterns
- Can handle data in its raw form (no preprocessing needed). Why?
- Has no assumptions about distribution because of the non-parametric nature of the algorithm

Cons:

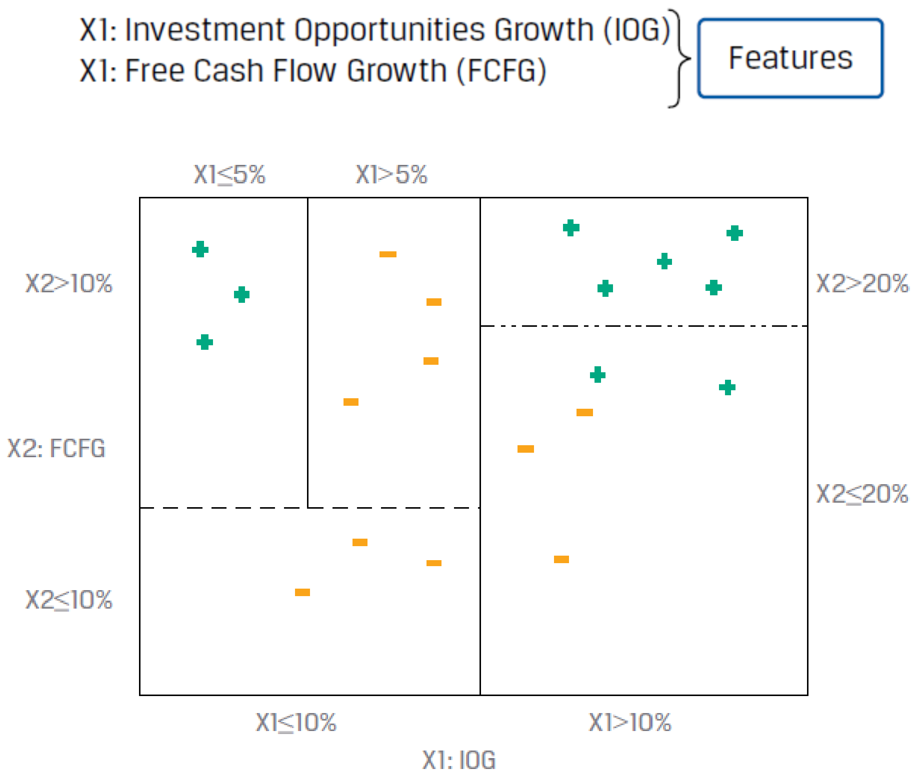
- Poor level of predictive accuracy.
- Sensitive to noisy data. It can overfit noisy data. Small variations in data can result in the different decision tree*.

*This can be reduced by bagging and boosting algorithms.

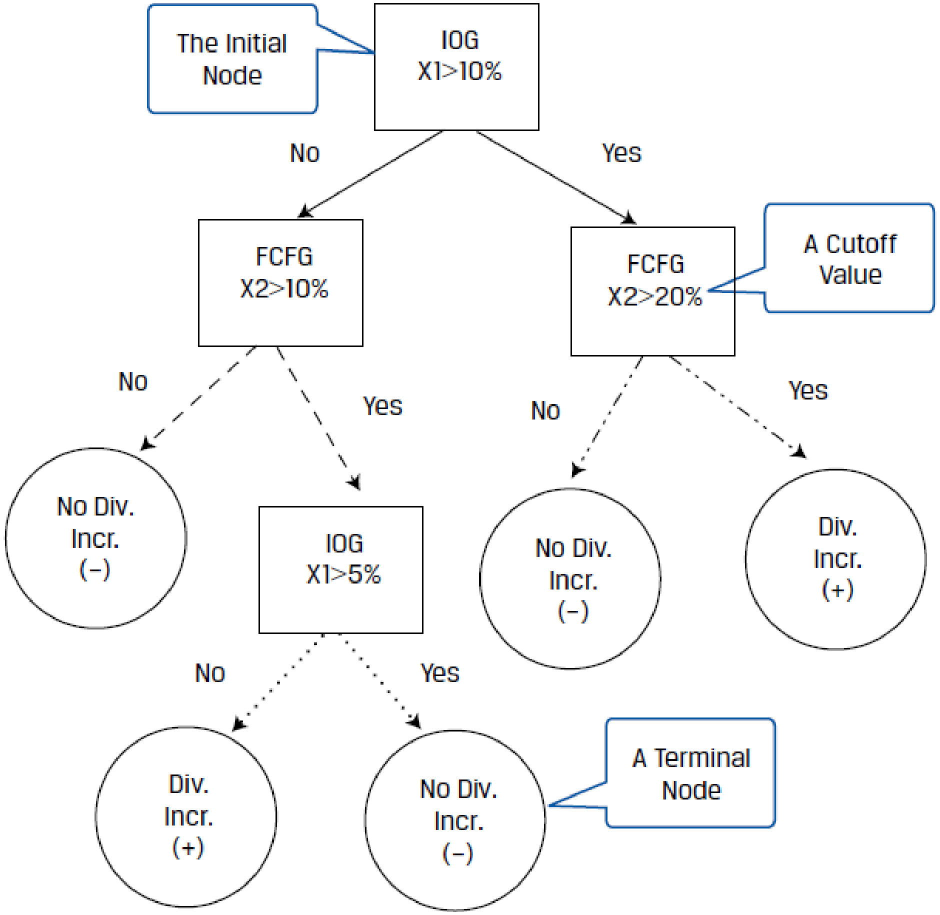
DTs' Applications in finance

- Enhancing detection of fraud in financial statements,
- Generating consistent decision processes in equity and fixed-income selection
- Simplifying communication of investment strategies to clients.
- Portfolio allocation problems.

DT example in finance



Source: CFA PROGRAM. Level II . Reading 7



Students’ questions

1. Should we be concerned about the computational expense of ‘MSE' when working with large trees of continuous data?
2. Having hard time understanding gini impurity and what conceptually the value means.
3. What is the Gini impurity role in classification?
4. A little confused on how to pick which method should be used for a given data set.
5. Would like to go over when the algorithm decides to create a leaf node vs continuing the decision tree.