Introduction to Machine Learning

Regression and Classification Trees

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Outline

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Decision Trees

Powerful/popular

For classification and prediction.

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Represent rules

- Rules can be expressed in English.

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  - **IF** $Age \leq 43$ & $Sex == Male$ **AND** $Credit\ Card\ Insurance == No$ **THEN**

$$Life\ Insurance\ Promotion = No$$

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  - **IF** $Age \leq 43$ & $Sex == Male$ **AND** $Credit\ Card\ Insurance == No$ **THEN**

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Useful to explore data to gain insight into relationships

Of a large number of candidate input variables to a target (output) variable.

What are They?

Decision Tree

A structure that can be used to divide up a large collection of records into successively smaller sets of records by applying a sequence of simple decision rules.

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A decision tree model

Consists of a set of rules for dividing a large heterogeneous population into smaller, more homogeneous groups with respect to a particular target variable.

Decision Tree Types

Binary trees

- Only two choices in each split. Can be non-uniform (uneven) in depth.

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Binary trees

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N-way trees or Ternary trees

- Three or more choices in at least one of its splits (3-way, 4-way, etc.).

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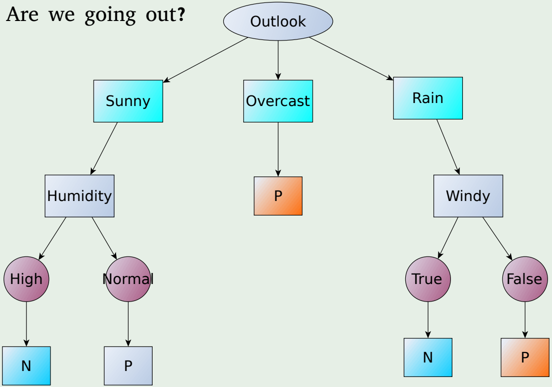
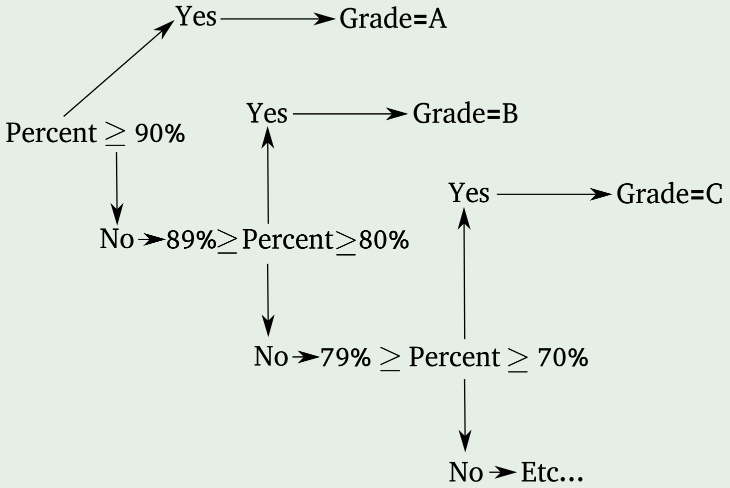
An Example

We have



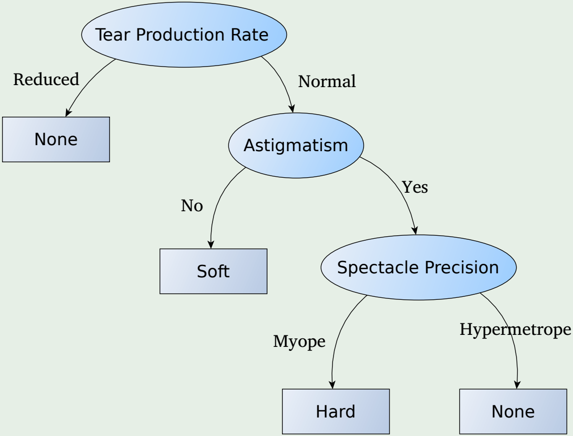
Another Example - Grades

Deciding the grades



Yet Another Example

Decision About Needing Glasses



Outline

First than anything

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Consider a Regression Problem with:

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1. Continuous Response y.

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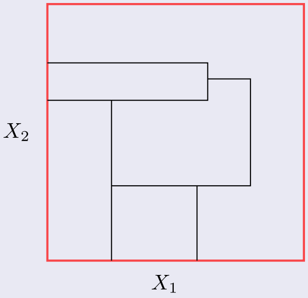
Example of a partition



Everything is fine, but!!!

Although

- In each partition element we can model Y with a different constant.

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Solving the Issue

We do the following

- Chose a variable and split the space using $x_i = c$

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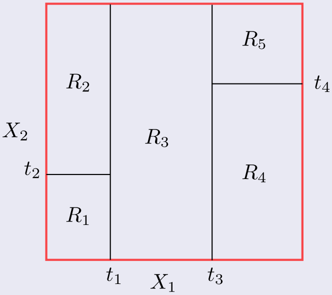
- Chose a variable and split the space using $x_i = c$

Keep doing that using one of the variables until a rules stops the process



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The corresponding Regression Tree

We have

$$\widehat{y} = f(\boldsymbol{x}) = \sum_{m=1}^{5} c_m I\left\{(x_1, x_2) \in R_m\right\}$$

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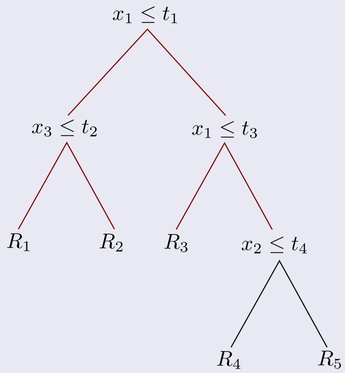
This regression can be interpreted as



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- Nodes
  - Appear as rectangles or circles

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- Internal nodes are used for decisions
- Terminal Nodes or Leaves are the final results

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Types of Decision Trees

Regression Trees

The predicted outcome can be considered a number.

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Classification Trees

- The predicted outcome is the class to which the data belongs.

Classification and Regression Trees (CART)

CART

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Similarities

- Regression and Classification trees have some similarities – nevertheless they differ in the way the splitting at each node is done.

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Setup

Data Consists on inputs of dimensionality d

$$\left\{ (x_i, y_i)_{i=1}^{N} \right\}$$

Where $x_i = (x_{i1}, x_{i2}, ..., x_{id})^T$.

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- To do the splitting automatically

Thus, assume a initial M partition $R_1, R_2, ..., R_M$

- We model the response as a constant c_m in each region

$$f(\boldsymbol{x}) = \sum_{m=1}^{M} c_m I(\boldsymbol{x} \in R_m)$$

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We have then

We adopt as our criterion minimization

$$L\left(c_1, c_2, ..., c_M\right) = \sum_{i=1}^{N}\sum_{i=1}^{M}\left(y_i - f\left(\boldsymbol{x}_i\right)\right)^2$$

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Then using a classic derivative with respect to c_m

$$\frac{\partial L\left(c_1, c_2, ..., c_M\right)}{\partial c_m} = -2 \sum_{i=1}^{N} \left(y_i - \sum_{m=1}^{M} c_m I\left(\boldsymbol{x}_i \in R_m\right)\right) I\left(\boldsymbol{x}_i \in R_m\right)$$

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Then

$$\sum_{y_i | \boldsymbol{x}_i \in R_m} y_i - \sum_{i=1}^{N} I\left(\boldsymbol{x}_i \in R_m\right) \sum_{m=1}^{M} c_m I\left(\boldsymbol{x}_i \in R_m\right) = 0$$

The simplest function for c_m

Something Notable

$$\sum_{\boldsymbol{x}_i \in R_m} c_m = \sum_{y_i | \boldsymbol{x}_i \in R_m} y_i$$

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$$c_m = \frac{1}{N_m} \sum_{y_i | \boldsymbol{x}_i \in R_m} y_i$$

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Problem

- Finding the best binary partition in terms of minimum sum of squares is generally $O\left(2^N\right)$ a NP Problem!!!

What to do?

Consider a splitting variable j and split point s

- Define the pair of half-planes

$$R_1(j,s) = \{\boldsymbol{x} | x_j \leq s\} \text{ and } R_2(j,s) = \{\boldsymbol{x} | x_j > s\}$$

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Using an Optimization Problem

$$\min_{j,s}\left\{\min_{c_1}\sum_{\boldsymbol{x}_i\in R_1(j,s)}(y_i-c_1)^2+\min_{c_2}\sum_{\boldsymbol{x}_i\in R_2(j,s)}(y_i-c_2)^2\right\}$$

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The nice part of this

- For any choice j and s, the inner minimization is solved by

$$\widehat{c}_1=\frac{1}{N_1}\sum_{y_i|\boldsymbol{x}_i\in R_1(j,s)}y_i \text{ and } \widehat{c}_2=\frac{1}{N_1}\sum_{y_i|\boldsymbol{x}_i\in R_2(j,s)}y_i$$

Therefore

For each splitting variable j

- Finding s is done quickly!!!

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We can repeat this process

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How do we solve?

- Tree size is an hyper-parameter governing the model's complexity.

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We have that

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A preferred strategy

- Grow the tree until some minimum size node is done.

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Then

- This large tree is pruned using cost-complexity pruning.

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We need to define something

Definition

- We define a subtree $T \subseteq T_0$ to be any tree that can be obtained by pruning T_0:
  - By collapsing any number of its internal (non-terminal) nodes.

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- We define a subtree $T \subseteq T_0$ to be any tree that can be obtained by pruning T_0:
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Given that each R_m is indexed by m

- Let $|T|$ denote the number of terminal nodes in T:

$$N_m = |R_m|\,,\ \widehat{c}_m = \frac{1}{N_m} \sum_{y_i | \boldsymbol{x}_i \in R_m} y_i \text{ and } Q_m\left(T\right) = \frac{1}{N_m}\left(\widehat{c}_m - y_i\right)^2$$

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Thus

Define the cost complexity criterion with $\alpha \geq 0$

$$C_{\alpha}(T) = \sum_{m=1}^{|T|} N_m Q_m(T) + \alpha |T|$$

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Finally

- The idea is to find, for each α, the subtree $T_{\alpha} \subseteq T_0$ to minimize $C_{\alpha}\left(T\right)$

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Properties of α

- Large values of α result in smaller T_α
- Small values of α result in larger T_α

Furthermore

For each α one can show the existence of unique smallest subtree T_α

- How do we find T_α?

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Using weakest link pruning

- We successively collapse the internal node that produces the smallest per-node increase in

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Using weakest link pruning

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Until you get a single-node (root) and a sequence

$$T \supseteq T_1 \supseteq T_2 \supseteq \cdots \supseteq T_N$$

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Then

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For Details

- "Pattern Recognition and Neural Networks" by Brian D. Ripley

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Most of the work

It focuses on deciding which property test or query should be performed at the node!!!

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If the data test is numerical in nature

There is a way to visualize the decision boundaries produced by the decision trees.

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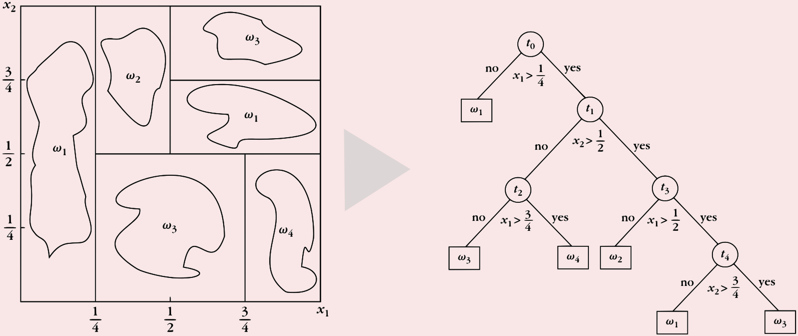
Example



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Training of a OBCT

We need first

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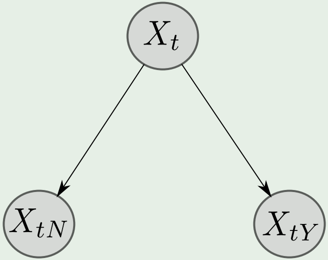
- At each node, the set of candidate questions to be asked has to be decided.
- Each question corresponds to a specific binary split into two descendant nodes.
- Each node, t, is associated with a specific subset X_t of the training set X.

Splitting the Node X_t

Basically, we want to split the node into two groups with questions $t_Y == "YES"$ and $t_N = "NO"$



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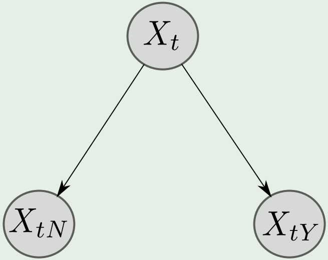

With Properties

- $X_{tY} \cap X_{tN} = \emptyset$.
- $X_{tY} \cup X_{tN} = X_t$

Important

Given the question for each feature k "Is $x_k \leq \alpha$"

For each feature, every possible value of the threshold α defines a specific split of the subset X_t.

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In practice

only a finite set of questions can be considered.

For example

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Any of the features x_k with $k = 1, ..., l$ can take at most $N_t \leq N$ different values

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Where

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Then

For feature x_k, one can use α_{kn} with $n = 1, 2, ..., N_{tk}$ and $N_{tk} \leq N_t$ where α_{kn} are taken halfway between consecutive distinct values of x_k in the training subset X_t.

Then

We repeat this with all features

In such a case, the total number of candidate questions is

$$\sum_{k=1}^{l} N_{tk} \tag{1}$$

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- The best split is decided according to a **splitting criterion**.

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Criterion's to be Found

Splitting criterion

- A splitting criterion must be adopted according to which the best split from the set of candidate ones is chosen.

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Stop-splitting rule

A stop-splitting rule is required that controls the growth of the tree,and a node is declared as a terminal one (leaf).

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Rule

A rule is required that assigns each leaf to a specific class.

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Looking for Homogeneity!!!

In order for the tree growing methodology

From the root node down to the leaves every split must generate a subsets that are more homogeneous compared to the ancestor's subset X_t.

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The training feature vectors in each one of the new subsets show, whereas data in X_t are more equally distributed among the classes.

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The training feature vectors in each one of the new subsets show, whereas data in X_t are more equally distributed among the classes.

For example

Consider the task of classifying four classes $\{\omega_1, \omega_2, \omega_3, \omega_4\}$ and assume that the vectors in subset X_t are distributed among the classes with equal probability.

Thus

If we split the node so

- ω_1 and ω_2 form X_{tY}
- ω_3 and ω_4 form X_{tN}

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In other words

"Purer" in the decision tree terminology.

Our Goal

We need

To define a measure that quantifies node impurity.

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To define a measure that quantifies node impurity.

Thus

The Overall Impurity of the descendant nodes is optimally decreased with respect to the ancestor node's impurity.

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Probabilistic Impurity

Probabilistic Impurity

Assume the following probability of a vector in X_t belongs to class ω_i

$$P(\omega_i|t) \text{ for } i = 1, \cdots, M \tag{2}$$

A Common Impurity

We define one of the most common impurities

$$I(t) = -\sum_{i=1}^{M} P(\omega_i|t) \log_2 P(\omega_i|t)$$

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This is nothing more than the Shannon's Entropy!!!

- Facts:
  - $I(t)$reaches its maximum when
  $$P(\omega_i|t) = \frac{1}{M}$$
  - $I(t) = 0$ if all data belongs to a single class i.e. $P(\omega_i|t) = 1$ for only one class, and $P(\omega_j|t, j \neq i) = 0$ for everybody else.

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A Common Impurity

We define one of the most common impurities

$$I(t) = -\sum_{i=1}^{M} P(\omega_i|t) \log_2 P(\omega_i|t)$$

This is nothing more than the Shannon's Entropy!!!

- Facts:
  - $I(t)$reaches its maximum when

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In reality...

We estimate

$$P\left(\omega_i|t\right) = \frac{N_t^i}{N_t}$$

Where $|\omega_i| = N_t^i$ as the number of points in $X_t$that belongs to class ω_i.

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Assume now

If we perform a split, N_{tY} points are sent into the "YES" node X_{tY} and N_{tN} into the "NO" node X_{tN}

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Decrease in node impurity

Then

In a recursive way we define the term decrease in node impurity as:

$$\Delta I(t) = I(t) - \frac{N_{tY}}{N_t} I(t_Y) - \frac{N_{tN}}{N_t} I(t_N) \tag{3}$$

where $I(t_Y)$ and $I(t_N)$ are the impurities of the t_Y and t_N nodes.

The Final Goal

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To adopt from the set of candidate questions the one that performs the split with the highest decrease of impurity.

Stop-Splitting Rule

Now

The natural question that now arises is when one decides to stop splitting a node and declares it as a leaf of the tree.

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- If the subset X_t is small enough.

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Other posibilities

- If the subset X_t is small enough.
- If the subset X_t is pure, in the sense that all points in it belong to a single class.

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Once a node is declared to be a leaf

Class Assignment Rule

Once a node is declared a leaf, we assign the leaf to a class using the rule:

$$j = \arg\max_{i} P\left(\omega_i | t\right).$$

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Outline

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9. Choose x_{k_0} and associated $\alpha_{k_0 n_0}$ for overall maximum decrease of impurity.
10. If the stop-splitting rule is met, declare node t as a leaf and label a class
11. If not, generate two descendant nodes t_Y and t_N with subsets X_{tY} and X_{tN} ,
12. depending on the answer to the question: is $x_{k_0} \leq \alpha$?

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Outline

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Remarks

Popular Classification Methods

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More Impurity Measures

- A variety of node impurity measures can be defined.

The size of the three need to be controlled

- The threshold T leads incorrect sizes.

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- We could consider a Multi-way split

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However

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- That will fragment the data too fast.

We would rather do only split when necessary

- After all a Multi-way split can be achieved with multiple binary split.

Remark

Linear Combination Splits

- Instead of doing simple splittings, we could use

$$\sum_{j=1}^{d} a_i x_i < s$$

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Better use

- Hierarchical Mixture of Experts (HME).

Outline

Issues

One of the biggest issues

- One major problem with trees is their high variance.

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- One major problem with trees is their high variance.

A small change in the data can result in a very different series of splits

- Making interpretability precarious!!!

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Lack of Smoothness

- Another limitation of trees is the lack of smoothness of the prediction surface

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- Another limitation of trees is the lack of smoothness of the prediction surface

Thus strategies to alleviate this problem are necessary

- Multivariate Adaptive Regression Splines (MARS) procedure

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Issue

The CART trees are bad at modeling additive structures

- For Example

$$y = c_1 I\left(x_1 < t_1\right) + c_2 I\left(x_2 < t_2\right) + \epsilon \text{ with } \epsilon \sim N\left(0, \sigma^2\right)$$

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Problem, CART has no special encouragement to capture this model

- Again MARS can help for this given its no dependency to the binary tree structure