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

$$Life\ Insurance\ Promotion = No$$

- Rules can be expressed using SQL for query.

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

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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.

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.

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Decision Tree Types

Binary trees

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

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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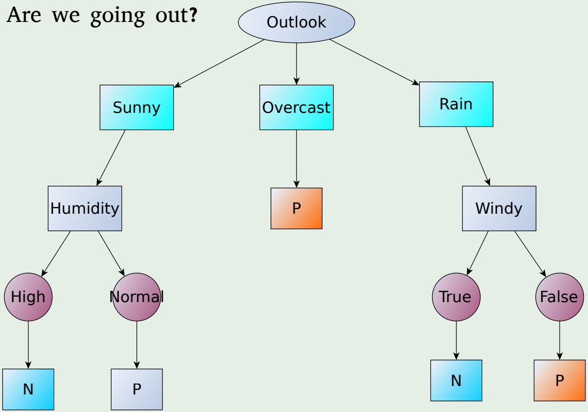
An Example

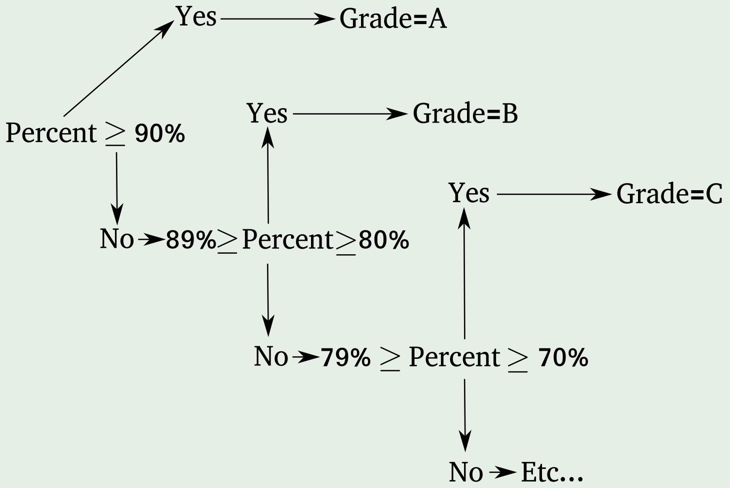
We have

Are we going out?



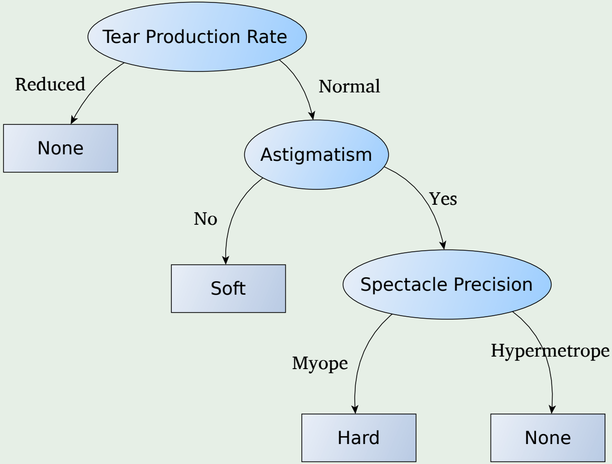
Another Example - Grades

Deciding the grades



Yet Another Example

Decision About Needing Glasses



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First than anything

Assume

Consider a Regression Problem with:

1. Continuous Response y.
2. Inputs x_1 and x_2 taking values in $[0, 1]$.
3. We have only recursive binary decisions/partitions.

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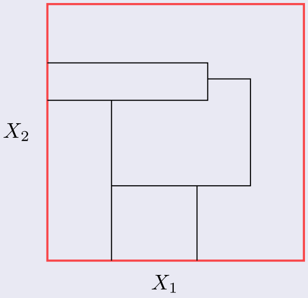

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Although

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

- The Resulting Regions are difficult to describe!!!

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Solving the Issue

We do the following

- 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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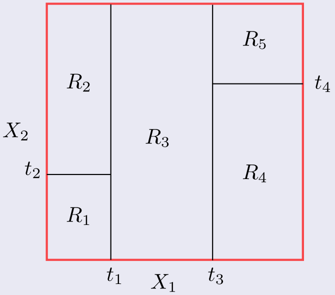

The corresponding Regression Tree

We have

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

This regression can be interpreted as

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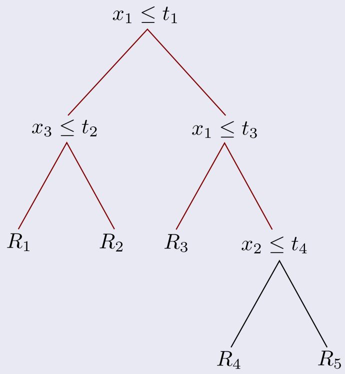

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- Nodes
  - Appear as rectangles or circles
  - Represent test or decision
- Lines or branches - represent outcome of a test
- Circles - terminal (leaf) nodes.

- 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.

Classification Trees

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

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Classification and Regression Trees (CART)

CART

- The term CART is an umbrella term used to refer to both of the above procedures.

Introduced by

- It was introduced by Breiman et. al in the book
  - **"Classification and Regression Trees"**

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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Data Consists on inputs of dimensionality d

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

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

Here, we want an algorithm

- 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

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

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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The simplest function for c_m

Something Notable

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

Then

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

Problem

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

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What to do?

Consider a splitting variable j and split point s

- Define the pair of half-planes

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

Using an Optimization Problem

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

The nice part of this

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

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We can repeat this process

- Problem, we can finish with an over-fitting tree/a very large tree.

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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.

Given that each R_m is indexed by m

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

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

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Thus

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

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

Finally

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

Properties of α

- Large values of α result in smaller T_{α}
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Furthermore

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

- How do we find T_α?

Using weakest link pruning

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

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

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- T_α is one of the threes in the in the sequence.

Estimation of α is achieved by cross-validation

- We choose the value $\widehat{\alpha}$ to minimize the cross-validated sum of squares.
  - This is the final $T_{\widehat{\alpha}}$

For Details

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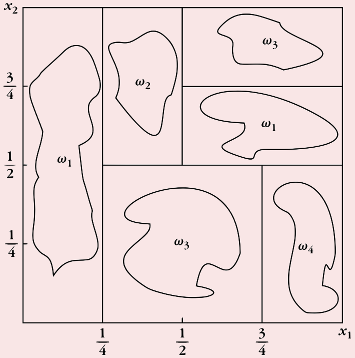

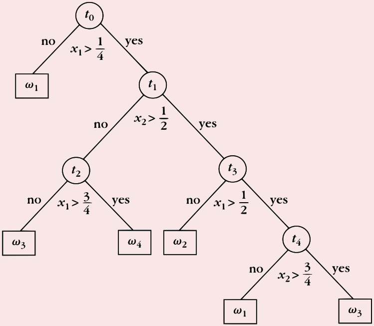

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Training of a OBCT

We need first

- 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.

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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.

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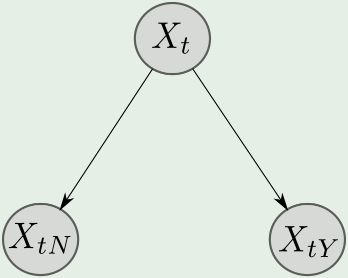
Splitting the Node X_t

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



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

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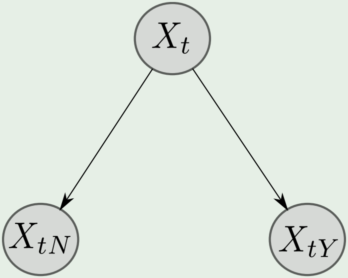

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Given the question for each feature k "Is $x_k \leq \alpha$"

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

Thus in theory

An infinite set of questions has to be asked if α is an interval $Y_\alpha \subseteq \mathbb{R}$.

In practice

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For example

Since the number, N, of training points in X is finite

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

Where

$N_t = |X_t|$ with $X_t \subset X$

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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.

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Outline

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.

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).

Rule

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

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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.

Meaning

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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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.

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We define one of the most common impurities

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

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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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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

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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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For example you can adopt

A threshold T and stop splitting if the maximum value of $\Delta I(t)$ over all possible splits is less than T.

- 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:

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

Outline

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Final Algorithm

Algorithm

1. Begin with the root node, that is, $X_t = X$.
2. For each new node t
3. For every feature x_k, $k = 1, 2, ..., l$:
4. For every value α_{kn}, $n = 1, 2, ..., N_{tk}$
5. Generate X_{tY} and X_{tN} according to the answer in the question:
6. "Is $x_k(i) \leq \alpha_{kn}$," $i = 1, 2, ..., N_t$
7. Compute the impurity decrease
8. Choose α_{kn_0} leading to the maximum decrease w.r. to x_k.
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
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Popular Classification Methods

- Decision trees have emerged as one of the most popular methods of classification.

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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The CART trees are bad at modeling additive structures

- For Example

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

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

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The CART trees are bad at modeling additive structures

- For Example

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

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