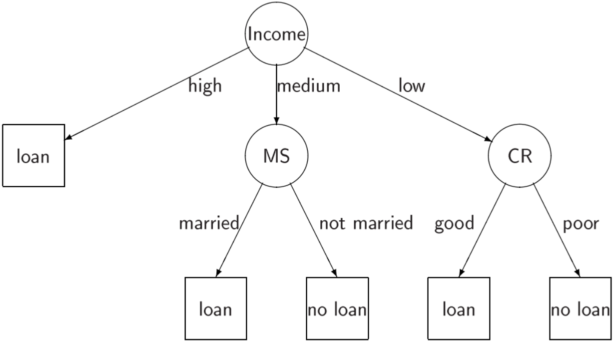
Decision trees

Victor Kitov

Table of Contents

Example of decision tree



Definition of decision tree

- Prediction is performed by tree T:
  - directed graph
  - without loops
  - with single root node

Definition of decision tree

- for each internal node t a check-function $Q_t(x)$ is associated
- for each edge $r_1(t), ...r_{K(t)}(t)$ a set of values of check-function $Q_t(x)$ is associated: $S_1(t), ...S_{K(t)}(t)$ such that:
  - $\bigcup_k S_t(k) = range[Q_t]$
  - $S_t(i) \cap S_t(j) = \emptyset \; \forall i \neq j$

Prediction process

- a set of nodes is divided into:
  - internal nodes $int(T)$, each having ≥ 2 child nodes
  - terminal nodes $terminal(T)$, which do not have child nodes but have associated prediction values.

Prediction process

- a set of nodes is divided into:
  - internal nodes $int(T)$, each having ≥ 2 child nodes
  - terminal nodes $terminal(T)$, which do not have child nodes but have associated prediction values.
- Prediction process for tree T:
  - $t = root(T)$
  - while t is not a leaf node:
    - calculate $Q_t(x)$
    - determine S_j out of $S_1(t), ...S_{K(t)}(t)$, where $Q_t(x)$ belongs: $Q_t(x) \in S_j(t)$
    - follow edge $r_j(t)$ to child node $\tilde{t}_j$: $t = \tilde{t}_j$
  - return prediction, associated with leaf t.

Specification of decision tree

- To define a decision tree one needs to specify:
    - the check-function: $Q_t(x)$
    - the splitting criterion: $K(t)$ and $S_t(1), ...S_t(K(t))$
    - the termination criteria (when node is defined as a terminal node)
    - the predicted value for each leaf node.

Table of Contents

CART version of splitting rule

- single feature value is considered:

$$Q_t(x) = x^{i(t)}$$

- binary splits:

$$K(t) = 2$$

- split based on threshold:

$$S_1 = \{x^{i(t)} \le threshold(t)\},\ S_2 = \{x^{i(t)} > threshold(t)\}$$

- $threshold(t) \in \{x_1^{i(t)}, x_2^{i(t)}, ... x_N^{i(t)}\}$
    - applicable only for real, ordinal and binary features
    - discrete unordered features:

CART version of splitting rule

- single feature value is considered:

$$Q_t(x) = x^{i(t)}$$

- binary splits:

$$K(t) = 2$$

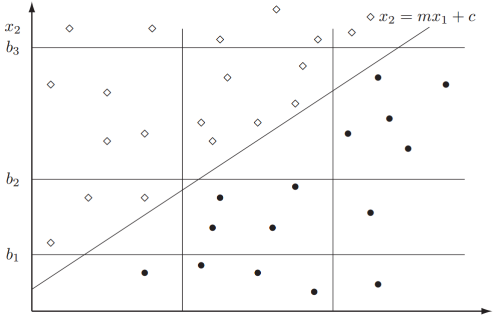
- split based on threshold:

$$S_1 = \{x^{i(t)} \le threshold(t)\},\ S_2 = \{x^{i(t)} > threshold(t)\}$$

- $threshold(t) \in \{x_1^{i(t)}, x_2^{i(t)}, ...x_N^{i(t)}\}$
    - applicable only for real, ordinal and binary features
    - discrete unordered features:may use one-hot encoding.

Analysis of CART splitting rule

- Advantages:
    - simplicity
    - interpretability
- Drawbacks:
    - many nodes may be needed to describe boundaries not parallel to axes:



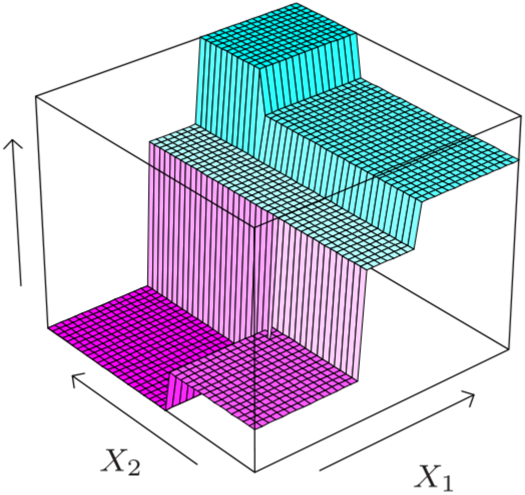
Alternative definitions of splitting rules

- $S_t(i) = \{h_i < x^{k(t)} \le h_{i+1}\}$ for set of partitioning thresholds $h_1, h_2, ...h_{K+1}$.
- $S_t(1) = \{x : \langle x, v\rangle \le 0\}, \quad S_t(2) = \{x : \langle x, v\rangle > 0\}$
- $S_t(1) = \{x : \|x\| \le h\}, \quad S_t(2) = \{x : \|x\| > h\}$
- $Q_t(x) = x^{i(t)}$, where $S_t(j) = v_j$, where $v_1, ...v_K$ are unique values of feature $x^{i(t)}$.

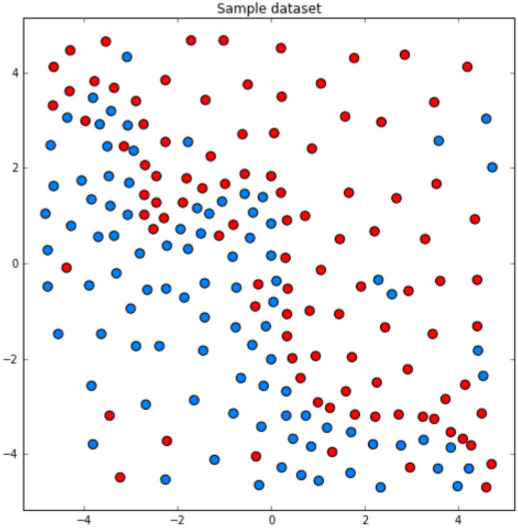
Alternative definitions of splitting rules

- $S_t(i) = \{h_i < x^{k(t)} \le h_{i+1}\}$ for set of partitioning thresholds $h_1, h_2, ...h_{K+1}$.
- $S_t(1) = \{x : \langle x, v\rangle \le 0\}, \quad S_t(2) = \{x : \langle x, v\rangle > 0\}$
- $S_t(1) = \{x : \|x\| \le h\}, \quad S_t(2) = \{x : \|x\| > h\}$
- $Q_t(x) = x^{i(t)}$, where $S_t(j) = v_j$, where $v_1, ...v_K$ are unique values of feature $x^{i(t)}$.
- Properties:
    - may need much fewer nodes than binary splits by threshold
    - less interpretable

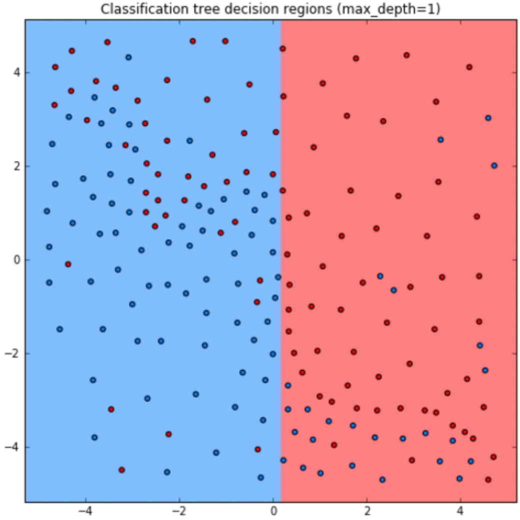
Piecewise constant predictions of decision trees



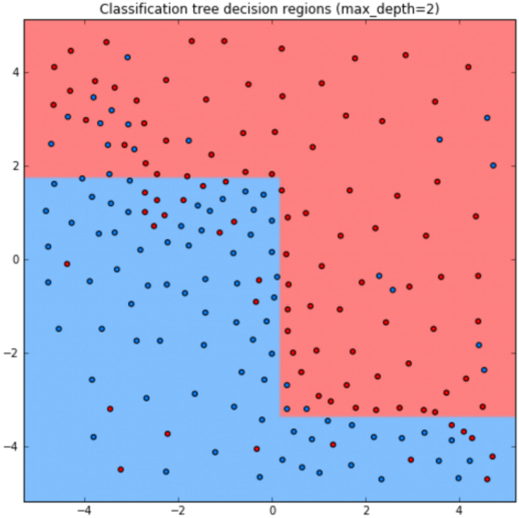
Sample dataset



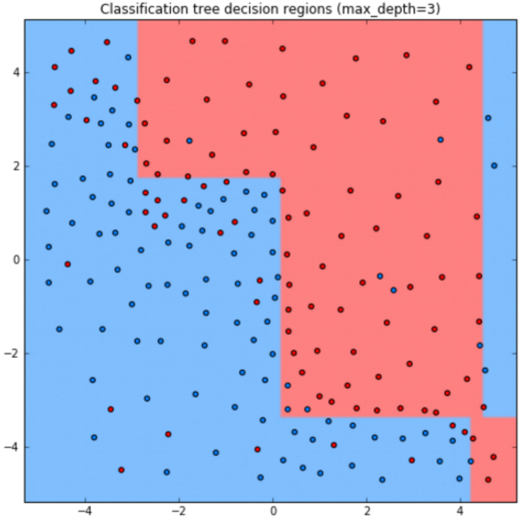
Example: Decision tree classification



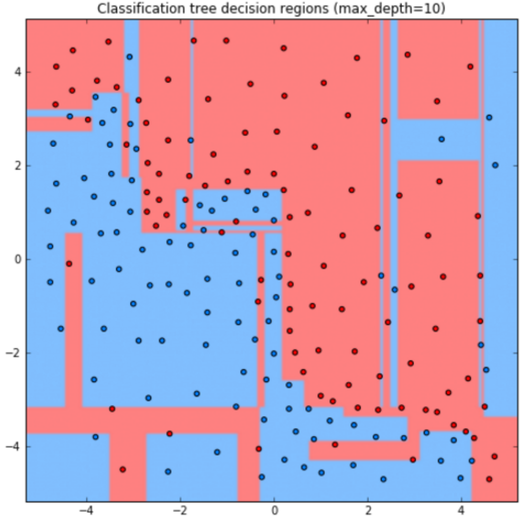
Example: Decision tree classification



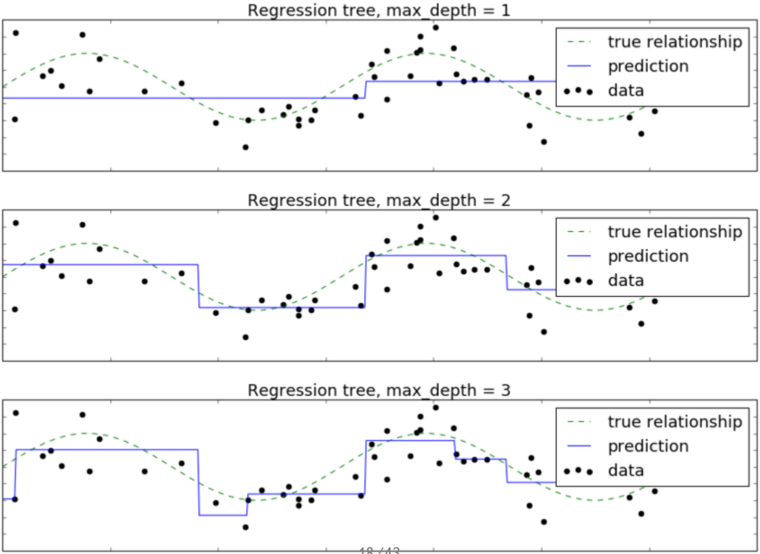
Example: Decision tree classification



Example: Decision tree classification



Example: Regression tree



Example: Regression tree

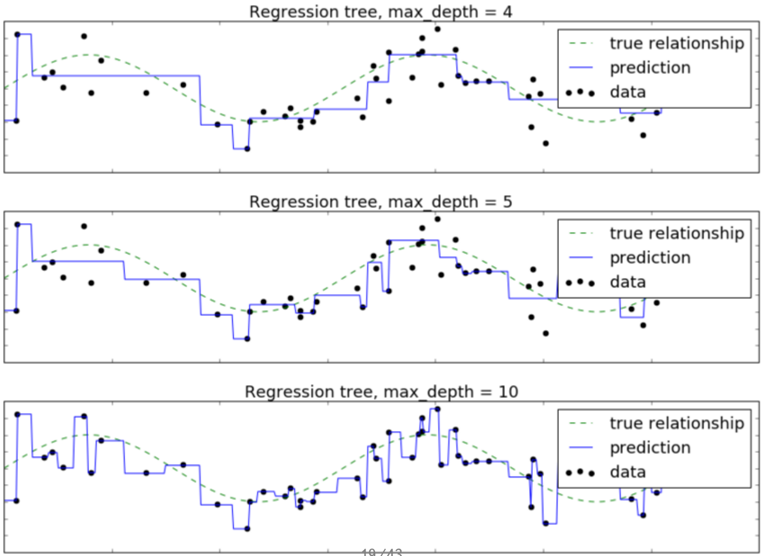


Table of Contents

Impurity function

- Let t be any node and $u(t)$ - associated objects with node t,
- $N(t)$ - total number of objects and $N_j(t)$ - number of objects of class j in t
- Probabilities of classes within node t:

$$p(\omega_j|x \in u(t)) = p(\omega_j|t) \approx \frac{N_j(t)}{N(t)}$$

- Impurity function $I(t) = \phi(p(\omega_1|t), ...p(\omega_C|t))$ has the following properties:
    - $\phi(q_1, q_2, ...q_C)$ is defined for $q_j \geq 0$ and $\sum_j q_j = 1$.
    - ϕ attains maximum for $q_j = 1/C$, $k = 1, 2, ...C$.
    - ϕ attains minimum when $\exists j: \; q_j = 1, \; q_i = 0 \; \forall i \neq j$.
    - ϕ is symmetric function of $q_1, q_2, ...q_C$.

Typical impurity functions

- **Gini criterion**
  - interpretation: probability to make mistake when classifying object randomly with class probabilities $[p(\omega_1|t), ...p(\omega_C|t)]$:

$$I(t) = \sum_i p(\omega_i|t)(1 - p(\omega_i|t)) = 1 - \sum_i [p(\omega_i|t)]^2$$

- **Entropy**
  - interpretation: measure of uncertainty of random variable

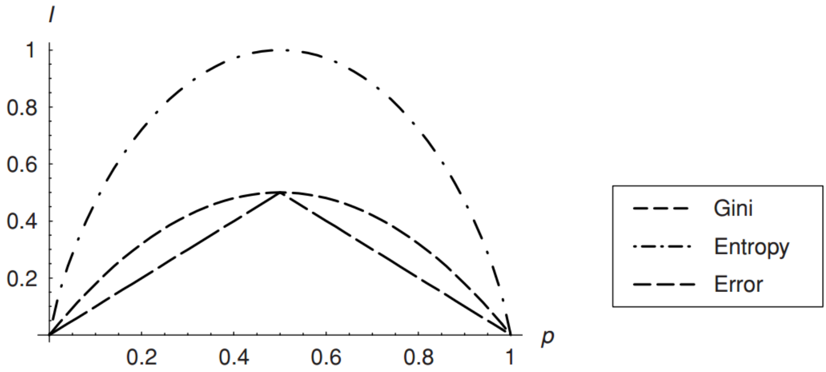
$$I(t) = -\sum_i p(\omega_i|t) \ln p(\omega_i|t)$$

- **Classification error**
  - interpretation: frequency of errors when classifying with the most common class

$$I(t) = 1 - \max_i p(\omega_i|t)$$

Typical impurity functions

Impurity functions for binary classification with class probabilities $p = p(\omega_1|t)$ and $1 - p = p(\omega_2|t)$.



Splitting criterion selection

$$\Delta I(t) = I(t) - \sum_{i=1}^{S} I(t_i) \frac{N(t_i)}{N(t)}$$

- $\Delta I(t)$ is the quality of the split of node t into child nodes $t_1, ...t_S$.
- If $I(t)$ is entropy, then $\Delta I(t)$ is called *information gain*.

Splitting criterion selection

$$\Delta I(t) = I(t) - \sum_{i=1}^{S} I(t_i) \frac{N(t_i)}{N(t)}$$

- $\Delta I(t)$ is the quality of the split of node t into child nodes $t_1, ...t_S$.
- If $I(t)$ is entropy, then $\Delta I(t)$ is called *information gain*.
- CART selection: select feature $k(t)$ and threshold $h(t)$, which maximize $\Delta I(t)$:

$$k(t),\, h(t) = \arg\max_{k,h} \Delta I(t)$$

- CART decision making: from node t follow:
  $$\begin{cases} \text{child } t_1, & \text{if } x^{k(t)} \geq h(t) \\ \text{child } t_2, & \text{if } x^{k(t)} < h(t) \end{cases}$$

Table of Contents

Prediction assignment for leaf nodes

- Define $I_t = \{i : x_i \in u(t)\}$, N_t - number of elements in I_t.
- **Regression:** for quadratic loss $(\widehat{y} - y)^2$:

$$\widehat{y} = \arg\min_{\mu} \sum_{i \in I} (y_i - \mu)^2 = \frac{1}{N_t} \sum_{i \in I} y_i,$$

- **Classification:** the most common class may be associated with the leaf node:

$$c = \arg\max_{\omega} \left| \{ i \in I_t : \; y_i = \omega \} \right|$$

Table of Contents

Termination criterion

- Bias-variance tradeoff:
    - very large complex trees -> overfitting
    - very short simple trees -> underfitting
- Approaches to stopping:
    - rule-based
    - based on pruning

5. Termination criterion
   - Rule based termination
   - CART pruning algorithm

Rule-base termination criteria

- Rule-based: a criterion is compared with a threshold.
- Variants of criterion:
    - depth of tree
    - number of objects in a node
    - minimal number of objects in one of the child nodes
    - impurity of classes
    - change of impurity of classes after the split

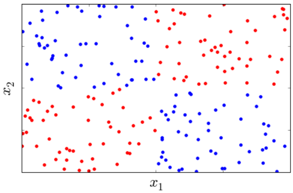
Analysis of rule-based termination

Advantages:

- simplicity
- interpretability

Disadvantages:

- specification of threshold is needed
- impurity change is suboptimal: further splits may become better than current one
    - example:



5 Termination criterion

- Rule based termination
- CART pruning algorithm

Pruning

- C4.5 pruning
- CART pruning

CART

- General idea: build tree up to pure nodes and then prune.
- Let T be some subtree of out tree, $\tilde{T}$ be a set of leaf nodes of tree T.
- Define $R(t)$ the number of misclassifications loss for leaf node $t \in \tilde{T}$ on the training set and N is the training set size.
- Also define

error-rate loss :	$R(T) = \sum_{t \in \tilde{T}} R(t)$
complexity+error-rate loss:	$R_\alpha(T) = \sum_{t \in \tilde{T}} R_\alpha(t) = R(T) + \alpha \lvert \tilde{T} \rvert$

- Condition when $R_{\alpha_t}(T_t) = R_{\alpha_t}(t)$:

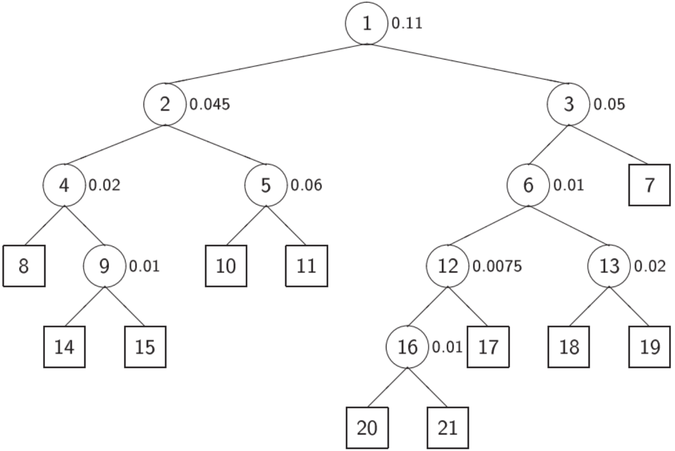
$$\alpha_t = \frac{R(t) - R(T_t)}{\lvert \tilde{T}_t \rvert - 1}$$

Pruning algorithm

1. Build tree until each node contains representatives of only single class - obtain tree T.
2. Build a sequence of nested trees $T = T_0 \supset T_1 \supset ... \supset T_{|T|}$ containing $|T|$, $|T|-1$,...1 nodes, repeating the procedure:
   - replace the tree T_t with smallest α_t with its root t
   - recalculate α_t for all ancestors of t.
3. For trees $T_0, T_1, ...T_{|T|}$ calculate their validation set error-rates $R(T_0), R(T_1), ...R(T_{|T|})$.
4. Select T_i, giving minimum error-rate on the validation set:

$$i = \arg\min_i R(T_i)$$

Example


1
0.11
2
0.045
3
0.05
4
0.02
5
0.06
6
0.01
7
8
9
0.01
10
11
12
0.0075
13
0.02
14
15
16
0.01
17
18
19
20
21

Example

Logs of the performance metrics of the pruning process:

step num.	α_k	$\|\tilde{T}^k\|$	$R(T^k)$
1	0	11	0.185
2	0.0075	9	0.2
3	0.01	6	0.22
4	0.02	5	0.25
5	0.045	3	0.34
6	005	2	0.39
7	0.11	1	0.5

Analysis of decision trees

- Advantages:
  - simplicity
  - interpretability
  - implicit feature selection
  - naturally handles both discrete and real features
  - prediction is invariant to monotone transformations of features for $Q_t(x) = x^{i(t)}$
    - in particular, to normalization of features
- Disadvantages:
  - non-parallel to axes class separating boundary may lead to many nodes in the tree for $Q_t(x) = x^{i(t)}$
  - one step ahead lookup strategy for split selection may be insufficient (XOR example)
  - not online - slight modification of the training set will require full tree reconstruction.

Table of Contents

6. Tree based ensemble methods
    - Bagging and random forest

Bagging& random subspaces

- Bagging
  - random selection of samples (with replacement)
  - *what is the probability that observation will not belong to bootstrap sample?*
  - *what is the limit of this probability with $N \to \infty$?*
- Random subspace method:
  - random selection of features (without replacement)
- We can apply both methods jointly

Random forests

Input: training dataset $TDS = \{(x_i, y_i), 1 = 1, 2, ...N\}$; the number of trees B and the size of feature subsets m.

1. for $b = 1, 2, ...B$:
   1. generate random training dataset TDS^b of size n by sampling (x_i, y_i) pairs from TDS with replacement.
   2. build a tree using TDS^b training dataset with feature selection for each node from random subset of features of size m (generated individually for each node).
2. Evaluate the quality by assigning output to x_i, $i = 1, 2, ...n$ using majority vote (classification) or averaging (regression) among trees with $b \in \{b : (x_i, y_i) \notin T^b\}$

Output: B trees. Classification is done using majority vote and regression using averaging of B outputs.

Comments

- Random forests use random selection on both samples and features
- Left out samples are used for evaluation of model performance.
- Less interpretable than individual trees
- +: Parallel implementation
- -: different trees are not targeted to correct mistakes of each other
- Extra-Random trees: more bias and less variance by random sampling (feature,value) pairs.