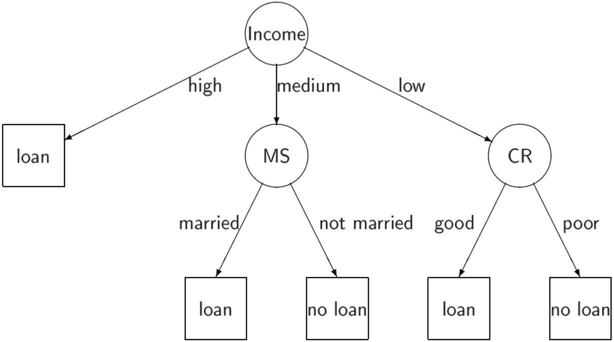
Decision trees

Victor Kitov
v.v.kitov@yandex.ru

Yandex School of Data Analysis

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 $r_t(1), ...r_t(K_t)$ a set of values of check-function $Q_t(x)$ is associated: $S_t(1), ...S_t(K_t)$ 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 j such that $Q_t(x) \in S_t(j)$
    - follow edge $r_t(j)$ to j-th child node: $t = \tilde{t}_j$
  - 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

Possible definitions of splitting rules

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

Most famous decision tree algorithms

- CART (classification and regression trees)
    - implemented in scikit-learn
- C4.5

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 h_t:

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

- $h(t) \in \{x_1^{i(t)}, x_2^{i(t)}, ...x_N^{i(t)}\}$
  - 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:

$$K_t = 2$$

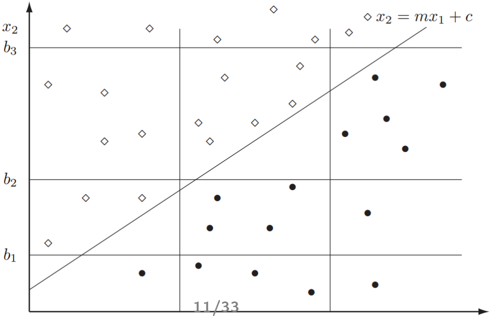
- split based on threshold h_t:

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

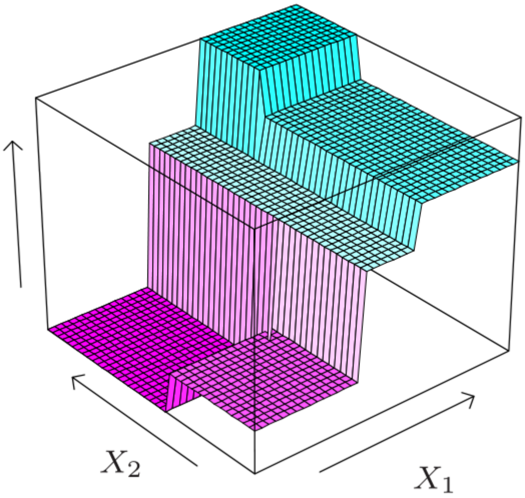
- $h(t) \in \{x_1^{i(t)}, x_2^{i(t)}, \ldots x_N^{i(t)}\}$
    - applicable only for real, ordinal and binary features
    - discrete unordered features:may use one-hot encoding.

Analysis of CART splitting rule

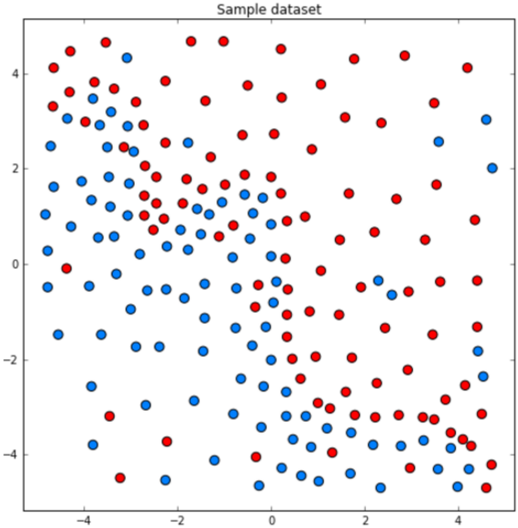
- Advantages:
    - simplicity
    - estimation efficiency
    - interpretability
- Drawbacks:
    - many nodes may be needed to describe boundaries not parallel to axes:



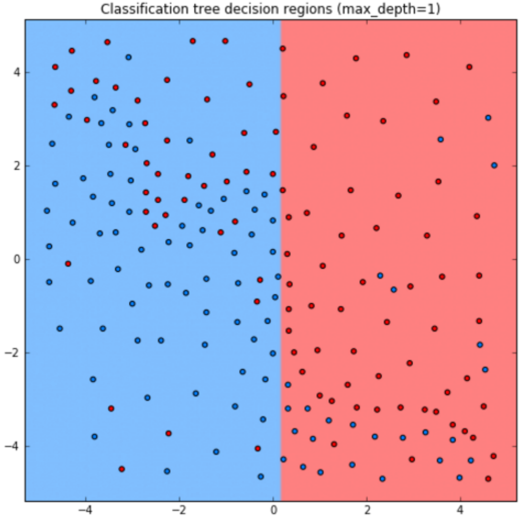
Piecewise constant predictions of decision trees



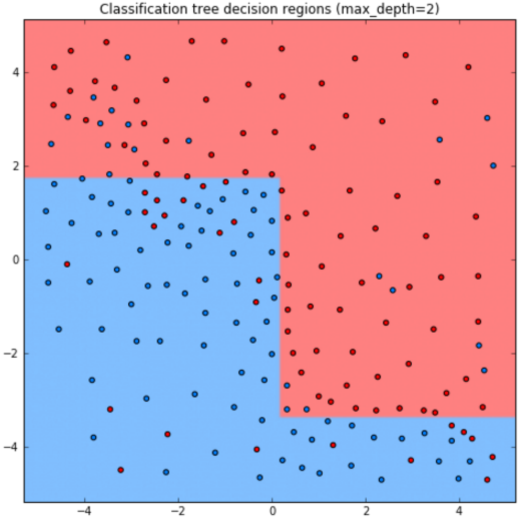
Sample dataset



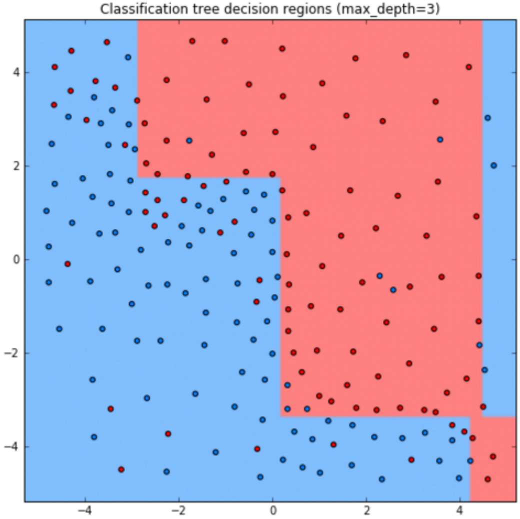
Example: Decision tree classification



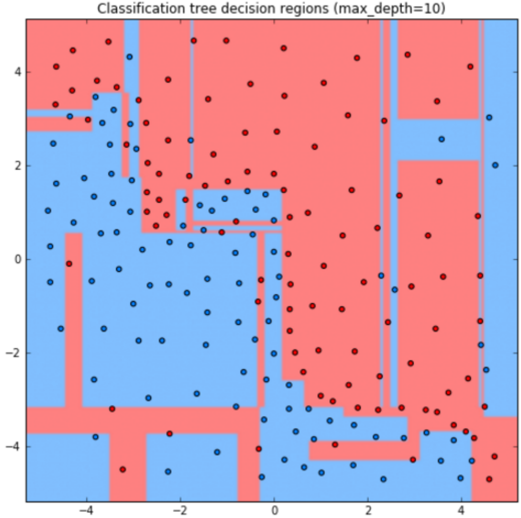
Example: Decision tree classification



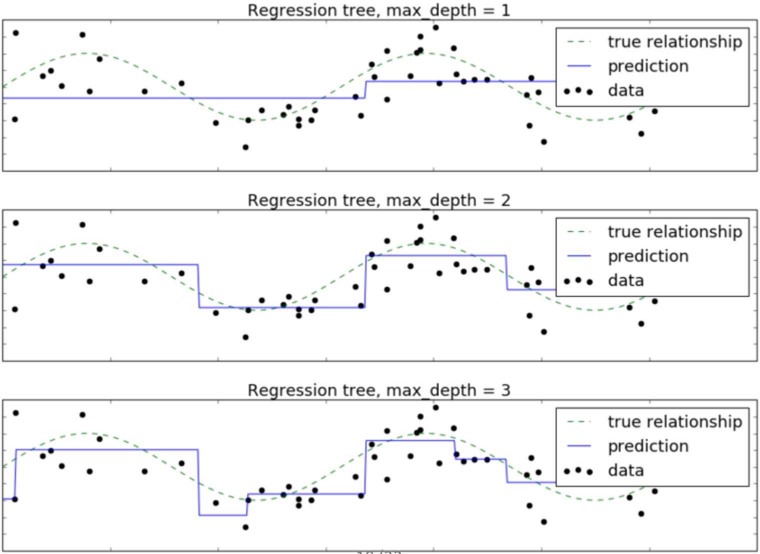
Example: Decision tree classification



Example: Decision tree classification



Example: Regression tree



Example: Regression tree

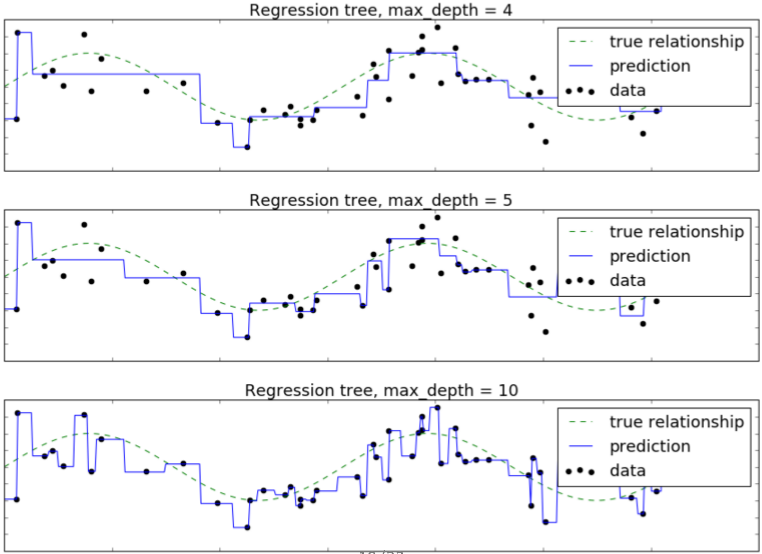


Table of Contents

Impurity functions

- Impurity function measures uncertainty in y for objects falling inside node t.
- Regression:
  - let objects falling inside node$t$ be $I = \{i_1, ...i_K\}$. We may define

$$\phi(t) = \frac{1}{K}\sum_{i\in I}(y_i - \mu)^2$$

$$\phi(t) = \frac{1}{K}\sum_{i\in I}|y_i - \mu|$$

where $\mu = \frac{1}{K}\sum_{i\in I} y_i$.

Classification impurity functions

- For classification: let $p_1, ...p_C$ be class probabilities for objects in node t.
- Then impurity function $\phi(t) = \phi(p_1, p_2, ...p_C)$ should satisfy:
  - ϕ is defined for $p_j \geq 0$ and $\sum_j p_j = 1$.
  - ϕ attains maximum for $p_j = 1/C$, $k = 1, 2, ...C$.
  - ϕ attains minimum when $\exists j : \ p_j = 1, \ p_i = 0 \ \forall i \neq j$.
  - ϕ is symmetric function of $p_1, p_2, ...p_C$.

Typical classification impurity functions

- **Gini criterion**
  - interpretation: probability to make mistake when predicting class 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

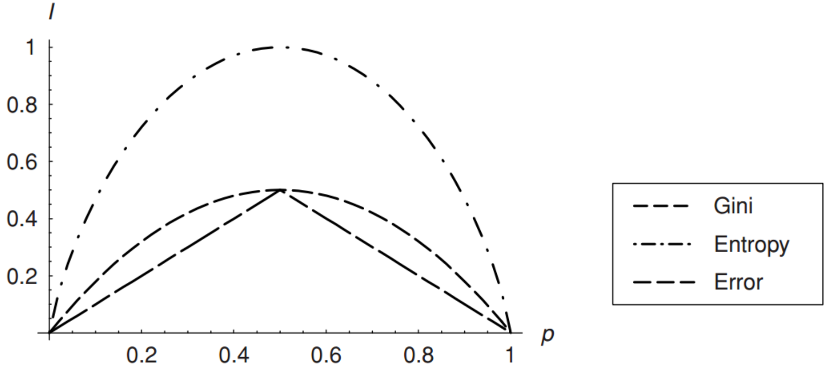
$$I(t) = -\sum_i p(\omega_i|t) \ln p(\omega_i|t)$$

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

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

Typical classification 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

- Define $\Delta I(t)$ - is the quality of the split[1] of node t into child nodes $t_1, ... t_R$.

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

- CART optimization (regression, classification): select feature i_t and threshold h_t, which maximize $\Delta I(t)$:

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

- CART decision making: from node t follow:

$$\begin{cases} \text{left child } t_1, & \text{if } x^{i_t} \leq h_t \\ \text{right child } t_2, & \text{if } x^{i_t} > h_t \end{cases}$$

[1] If $I(t)$ is entropy, then $\Delta I(t)$ is called *information gain*.

Table of Contents

Prediction assignment to leaves

- Regression:
    - mean (optimal for MSE loss)
    - median (optimal for MAE loss)
- Classification
    - most common class (optimal for constant misclassification cost)

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 (not considered here)

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

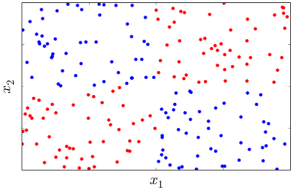
Analysis of rule-based termination

Advantages:

- simplicity
- interpretability

Disadvantages:

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



Tree feature importances

- Tree feature importances (*clf.feature_importances_* in sklearn).
    - Consider feature f
    - Let $T(f)$ be the set of all nodes, relying on feature f when making split.
    - efficiency of split at node t: $\Delta I(t) = I(t) - \sum_{c \in childen(t)} \frac{n_c}{n_t} I(c)$
    - feature importance of f: $\sum_{t \in T(f)} n_t \Delta I(t)$

- Alternative: difference in decision tree prediction quality for
    1. original validation set
    2. validation set with j-th feature randomly shuffled

Analysis of decision trees

- **Advantages:**
  - simplicity of algorithm
  - interpretability of model
  - implicit feature selection
  - good for features of different nature:
    - naturally handles both discrete and real features
    - prediction is invariant to monotone transformations of features for $Q_t(x) = x^{i(t)}$
- **Disadvantages:**
  - not very high accuracy:
    - high overfitting of tree structure up to top
    - 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.