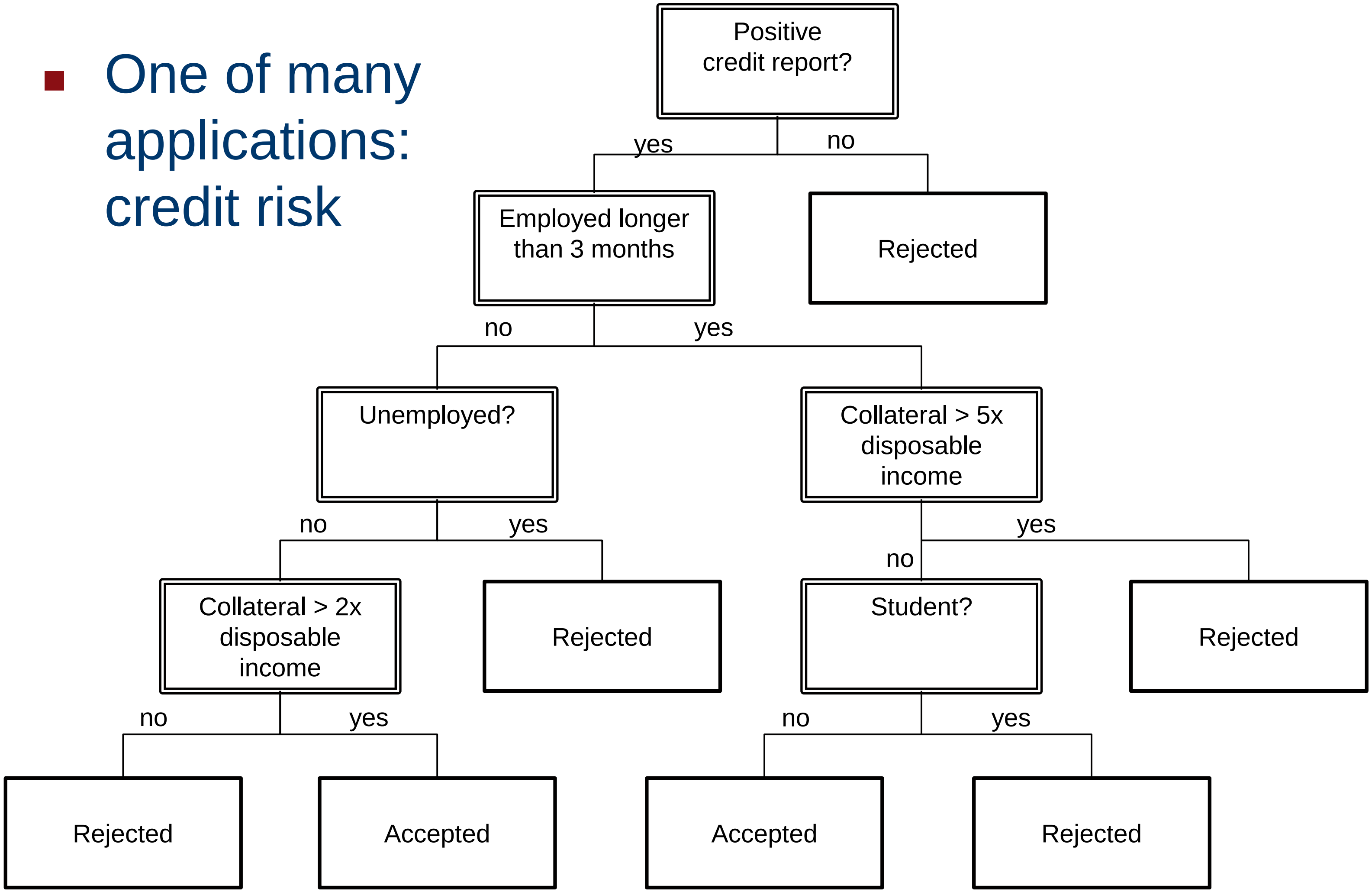
Universität Potsdam
Institut für Informatik
Lehrstuhl Maschinelles Lernen

Decision Trees

Tobias Scheffer

Decision Trees

- One of many applications: credit risk



Overview

- Decision trees.
- Classification with categorical features: ID3.
- Classification with continuous features: C4.5.
- Regression: CART, model trees.
- Bagging.
- Random forests.

Decision Trees – Why?

- Simple to interpret.
  - Provides a classification plus a justification for it.
  - “Rejected, because subject has been employed less than 3 months and has collateral < 2 x disposable income“.
- Fast inference:
  - For each instance, only one branch has to be traversed.
  - Frequently used in image processing.
- Simple, efficient, scalable learning algorithm.
- Numeric and categorical features, no preprocessing
- Works for classification and regression problems.

Classification

- Input: instance $\mathbf{x} \in X$.
  - Instances are represented as a vector of attributes.
  - An instance is an assignment to the attributes.
  - Instances will also be called feature vectors.

$$\mathbf{x} = \begin{pmatrix} x_1 \\ \vdots \\ x_m \end{pmatrix}$$

e.g. features like color, test results,…

- Output: class $y \in Y$; finite set Y.
  - e.g., {accepted, rejected}; {spam, not spam}.
  - The class is also referred to as the target attribute.

Classifier learning

- Input: training data.
  - $L = \langle(\mathbf{x}_1, y_1), \dots, (\mathbf{x}_n, y_n)\rangle$
  - $\mathbf{x}_i = \begin{pmatrix} x_{i1} \\ \vdots \\ x_{n1} \end{pmatrix}$
- Output: Classifier.
  - $f : X \to Y$

e.g. a decision tree:
path along the edges to a leaf
provides the classification

Regression

- Input: instance $\mathbf{x} \in X$.
  - e.g., feature vector

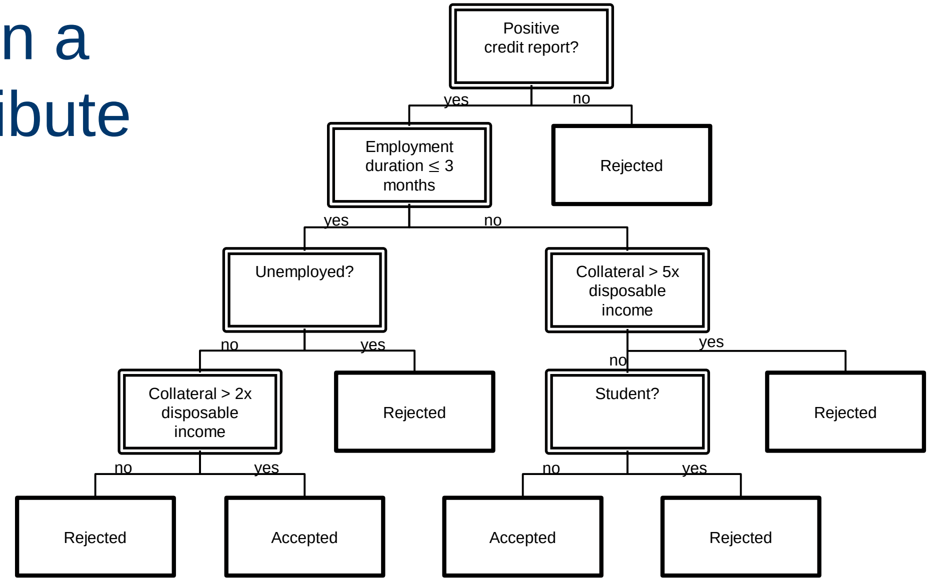
$$\mathbf{x} = \begin{pmatrix} x_1 \\ \vdots \\ x_m \end{pmatrix}$$

- Output: continuous (real) value, $y \in \mathbb{R}$

- Learning problem: training data with continuous target value
  - $L = \langle(\mathbf{x}_1, y_1), \ldots, (\mathbf{x}_n, y_n)\rangle$
  - e.g. $\langle(\mathbf{x}_1, 3.5), \ldots, (\mathbf{x}_n, -2.8)\rangle$

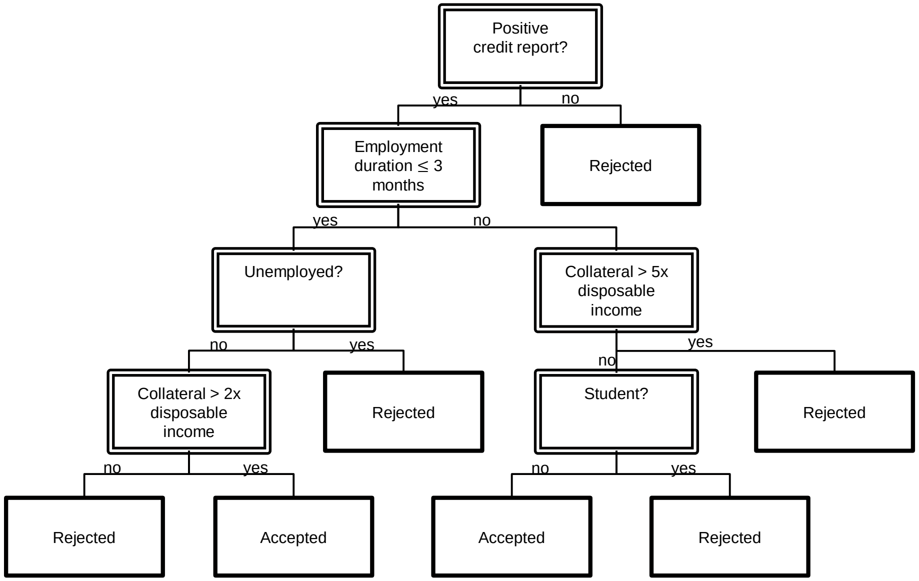
Decision Trees

- Test nodes:
  - Discrete attributes: node contains an attribute, branches are labeled with values.
  - Continuous attributes; nodes contain “≤” comparisons, branches are labeled “yes” and “no”.
- Terminal nodes contain a value of the target attribute



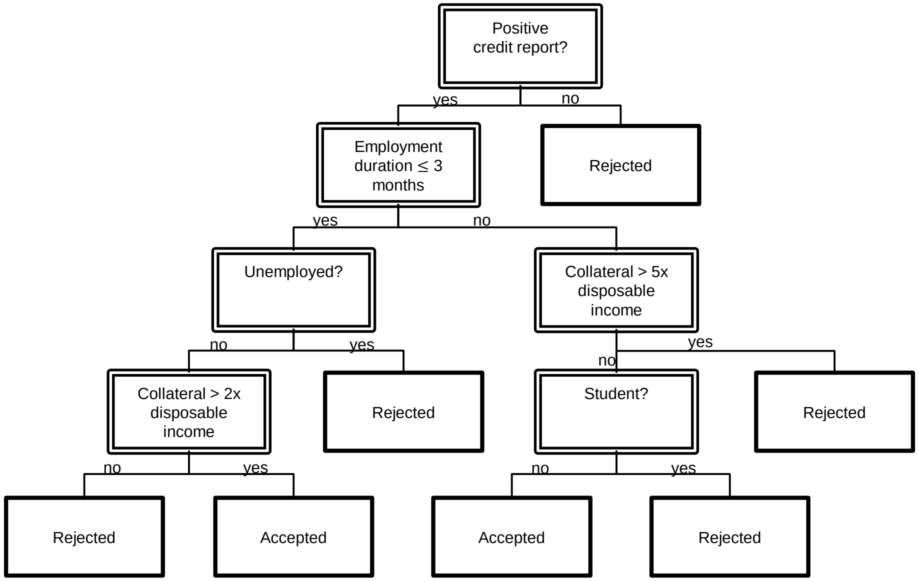
Decision Trees

- Decision trees can be represented as decision rules, each terminal node corresponds to a rule.
  - E.g., Rejected ← positive credit report ∧ employment duration ≤ 3 months ∧ unemployed.



Application of Decision Trees

- Recursively descent along branch.
- In each test node, conduct test, choose the appropriate branch.
- In a terminal node, return the value.



Learning Decision Trees

Loan	Credit report	Employment last 3 months	Collateral > 50% loan	Payed back in full
1	Positive	Yes	No	Yes
2	Positive	No	Yes	Yes
3	Positive	No	No	No
4	Negative	No	Yes	No
5	Negative	Yes	No	No

- Find a decision tree that predicts the correct class for the training data.
- Trivial way: create a tree that merely reproduces the training data.

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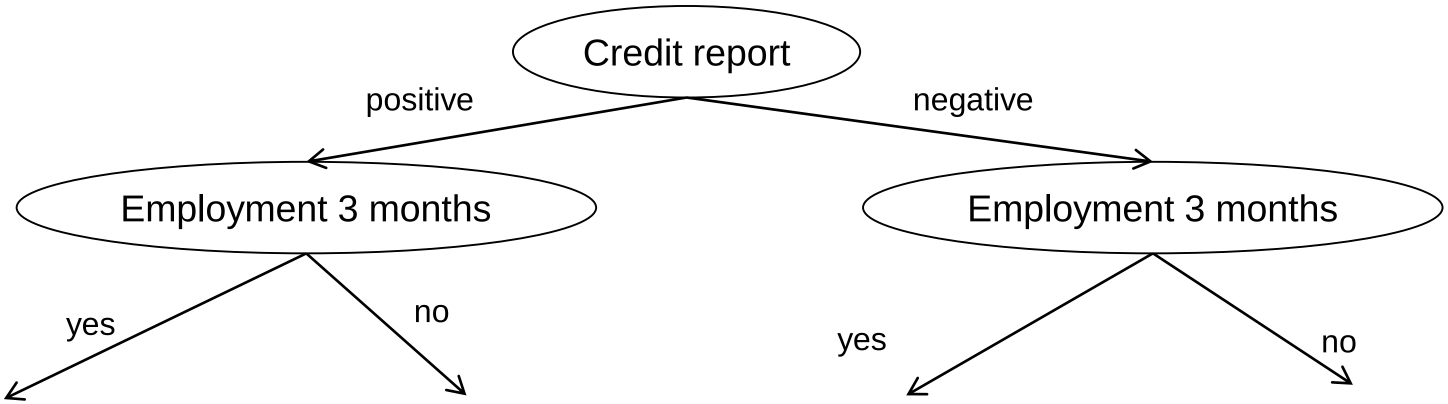

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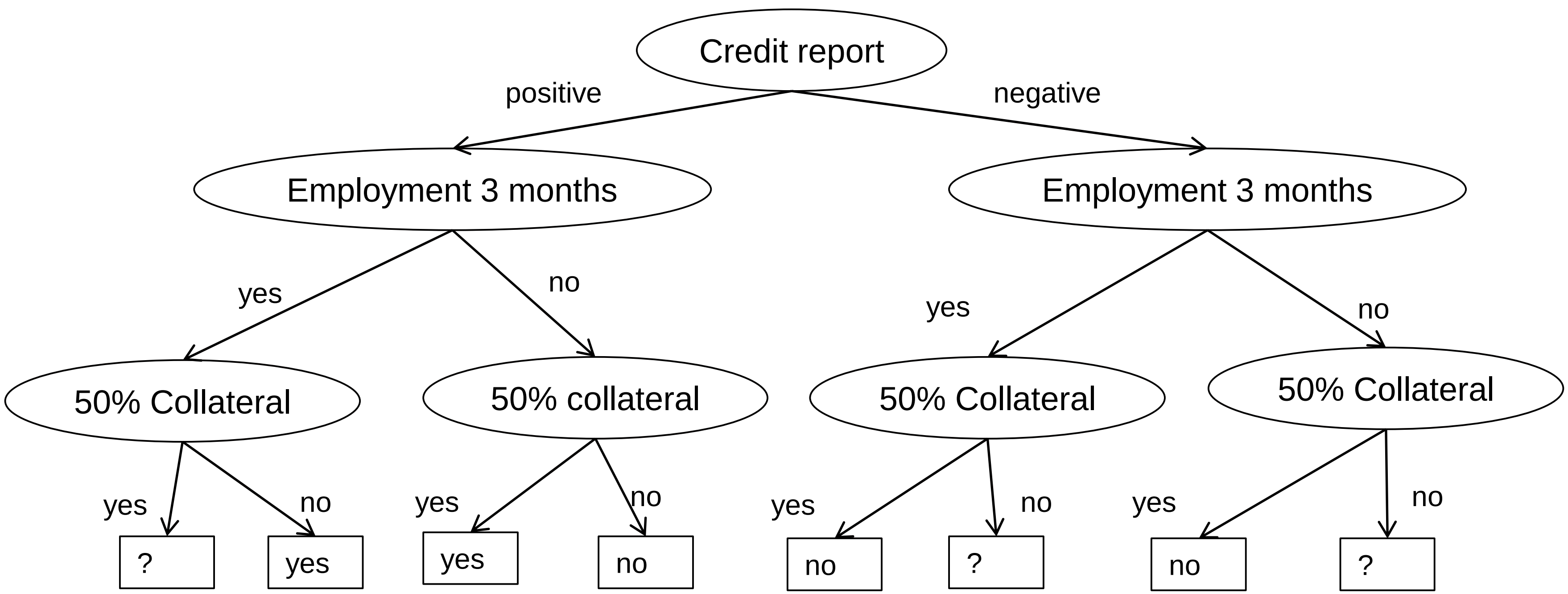

Learning of Decision Trees

- Perhaps more elegant: From the trees that are consistent with the training data, choose the smallest (as few nodes as possible).
- Small trees can be good because:
  - they are easier to interpret;
  - There are more training instances per leaf node. Hence, the class decision in each leaf is better substantiated.

Complete Search for the Smallest Tree

- How many functionally different decision trees are there?
  - Assume m binary attributes and two classes.

- What is the complexity of a complete search for the smallest tree?

Complete Search for the Smallest Tree

- How many functionally different decision trees are there?
  - Assume m binary attributes and two classes.
  - Tree has m layers of test nodes $\rightarrow 2^m - 1$ test nodes.
  - $2^{(2^m)}$ assignments of classes to leaf nodes.

- What is the complexity of a complete search for the smallest tree?
  - Assignments of m attributes (or node can be missing) to $2^m - 1$ test nodes: $O\left((m+1)^{2^m-1}\right)$.
  - Assignments of class labels to leaf nodes: $O(2^{(2^m)})$

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Learning of Decision Trees

- Greedy algorithm that finds a small tree (instead of the smallest tree) but is polynomial in the number of attributes.
- Idea for Algorithm?

Greedy Algorithm – Top-Down Construction

1. `ID3(L)`
   1. `If all data in L have same class y, then return leaf node with class y.`

ID3(

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) = yes

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        1. Choose attribute x_j that separates L into subsets $L_1, \ldots, L_k$ with most homogenous class distributions.
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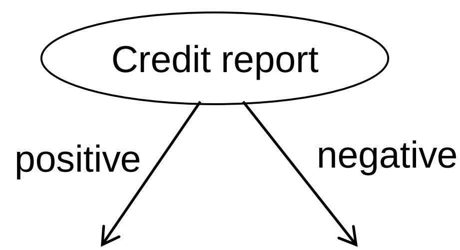
2 x payed back
3 x not payed back



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1 x not payed back

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)

2 x not payed back

Greedy Algorithm – Top-Down Construction

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What does it mean that an attribute splits the sample into subsets with homogenous class distributions?

Information

- Information theory uses models that involve a sender, a channel, a receiver, and a probability distribution over messages.
- Information is a property of messages, measured in units of bit.
- Information in a message (rounded) = number of bits needed to code that message in an optimal code.

Sender $\longrightarrow$ Receiver

Message y

$p(y)$

Information

- Information theory uses models that involve a sender, a channel, a receiver, and a probability distribution over messages.
- The information in a message y that is sent with probability $p(y)$ is $-\log_2 p(y)$.

Sender $\longrightarrow$ Receiver

$p(0) = \frac{1}{2}$
$p(1) = \frac{1}{4}$
$p(2) = \frac{1}{4}$

Message 0

$I(0) = -\log_2 \frac{1}{2}$
$= 1 bit$

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Sender $\longrightarrow$ Receiver

$p(0) = \frac{1}{2}$
$p(1) = \frac{1}{4}$
$p(2) = \frac{1}{4}$

Message 1

$I(1) = -\log_2 \frac{1}{4}$
$= 2bit$

Entropy

- Entropy is the expected information of a message.
  - $H(y) = -\sum_{v=1}^{k} p(y=v) \log_2 p(y=v)$
- Entropy quantifies the receiver's uncertainty regarding the message
- Empirical entropy H_L: use frequencies observed in data L instead of probabilities.

Sender $\longrightarrow$ Receiver

Message y

$p(0) = \frac{1}{2}$

$p(1) = \frac{1}{4}$

$p(2) = \frac{1}{4}$

$$H(y) = -\frac{1}{2}\log_2 \frac{1}{2} - 2\,\frac{1}{4}\log_2 \frac{1}{4}$$
$$= 1.5 bit$$

Entropy of Class Labels in Training Data

- Information / uncertainty of the class labels = expected number of bits needed to send message about class label of an instance to a receiver.

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$$H_L(y) = -\frac{2}{5}\log_2 \frac{2}{5} - \frac{3}{5}\log_2 \frac{3}{5} = 0.97 bit$$

Conditional Entropy

- Information / uncertainty of the class labels under some condition on the features.

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$$H_L(y|x_1 = n) = -\frac{2}{2}\log_2\frac{2}{2} - \frac{0}{2}\log_2\frac{0}{2} = 0bit$$

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$$H_L(y|x_1 = n) = -\frac{2}{2}\log_2\frac{2}{2} - \frac{0}{2}\log_2\frac{0}{2} = 0bit$$

$$H_L(y|x_1 = p) = -\frac{2}{3}\log_2\frac{2}{3} - \frac{1}{3}\log_2\frac{1}{3} = 0.91bit$$

Information Gain of an Attribute

- Reduction of entropy by splitting the data along an attribute
  - $G_L(x_j) = H_L(y) - \sum_{v=1}^{k} p_L(x_j = v) H_L(y|x_j = v)$

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- $G_L(x_1) = H_L(y) - p_L(x_1 = p) H_L(y|x_1 = p) - p_L(x_1 = n) H_L(y|x_1 = n)$
  $= 0.97 - \frac{3}{5} 0.91 - \frac{2}{5} 0 = 0.42 bit$
- Splitting along x_1 reduces the uncertainty regarding the class label y by 0.42 bit.

Information Gain Ratio

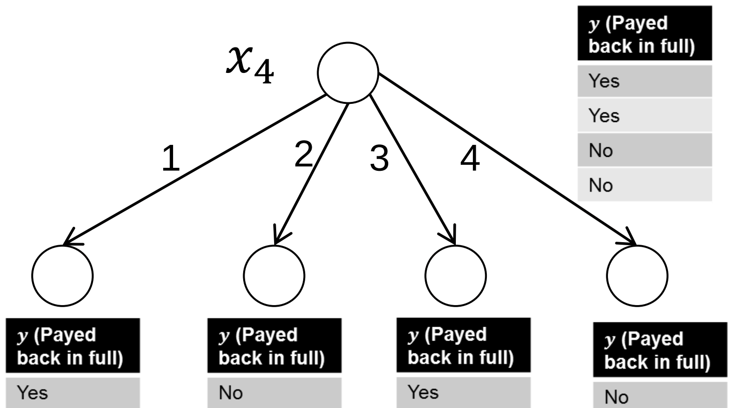
- Motivation:
  - Predicting whether a student will pass an exam.
  - How high is the information gain of the attribute “Matriculation number“?
- Information gain favors attributes with many values.
- Not necessarily an indicator of good generalization.
- Idea: factor the information that is contained in the attribute values into the decision
  - $H_L(x_j) = -\sum_{v=1}^{k} p_L(x_j = v) \log_2 p_L(x_j = v)$

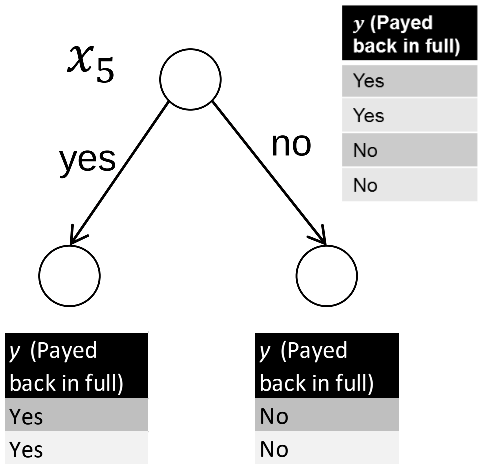
Information Gain Ratio

- Idea: factor the information that is contained in the attribute values into the decision
  - $H_L(x_j) = -\sum_{v=1}^{k} p_L(x_j = v) \log_2 p_L(x_j = v)$
- Information gain ratio:
  - $GR_L(x_j) = \frac{G_L(x_j)}{H_L(x_j)}$

Example: Info Gain Ratio

- Which split is better?





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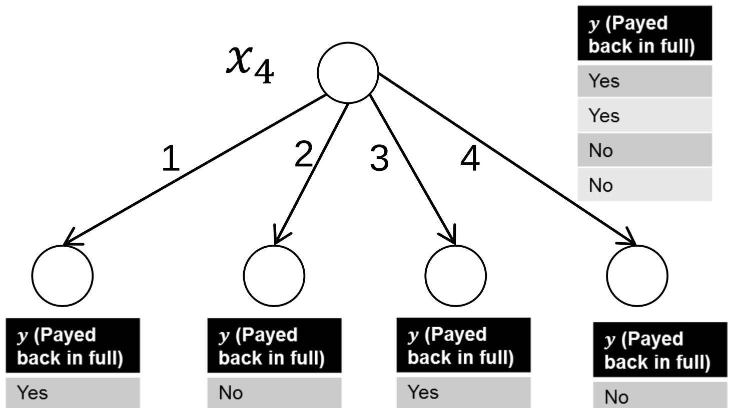

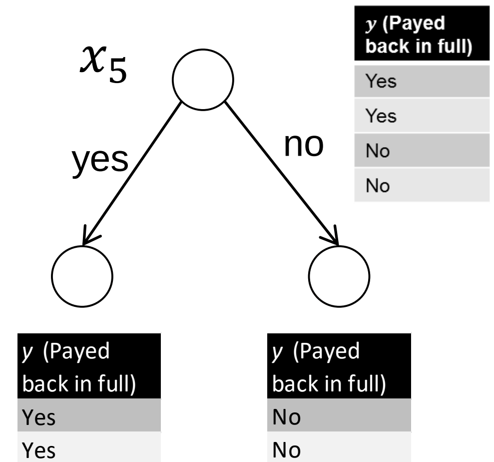

$$IG_L(x_4) = 1 - 4\tfrac{1}{4}0 = 1$$
$$H_L(x_4) = -4\left(\tfrac{1}{4}\log_2\tfrac{1}{4}\right) = 2$$
$$GR_L(x_4) = \frac{IG_L(x_4)}{H_L(x_4)} = \frac{1}{2}$$

$$IG_L(x_5) = 1 - \tfrac{1}{2}0 - \tfrac{1}{2}0 = 1$$
$$H_L(x_5) = -2\left(\tfrac{1}{2}\log_2\tfrac{1}{2}\right) = 1$$
$$GR_L(x_5) = \frac{IG_L(x_5)}{H_L(x_5)} = 1$$

Algorithm ID3

- Preconditions:
  - Classification problems
  - All attributes have fixed, discrete ranges of values.
- Idea: recursive algorithm.
  - Choose attribute that conveys highest information regarding the class label (Use information gain, gain ratio, or Gini index).
  - Split the training data according to the attribute.
  - Recursively call algorithm for branches.
  - In each branch, use each attribute only once; if all attributes have been used, return leaf node.

Learning Decision Trees with ID3

ID3(L, X)

1. If all data in L have same class y or X={}, then return leaf node with majority class y.
2. Else
   1. For all attributes $x_j \in X$, calculate split criterion $G_L(x_j)$ or $GR_L(x_j)$.
   2. Choose attribute $x_j \in X$ with highest $G_L(x_j)$ or $GR_L(x_j)$.
   3. Let $L_i = \{(x, y) \in L : x_j = i\}$.
   4. Return test node with attribute x_j and children ID3(L_1, $X \setminus x_j$), …, ID3(L_k, $X \setminus x_j$).

ID3: Example

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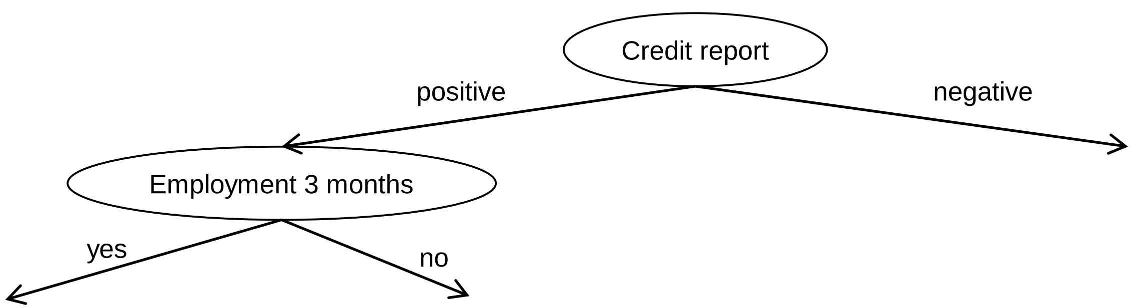

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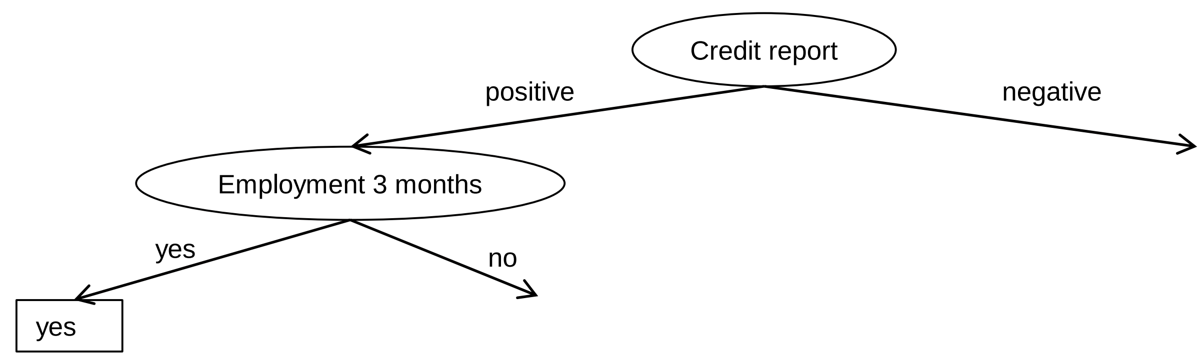

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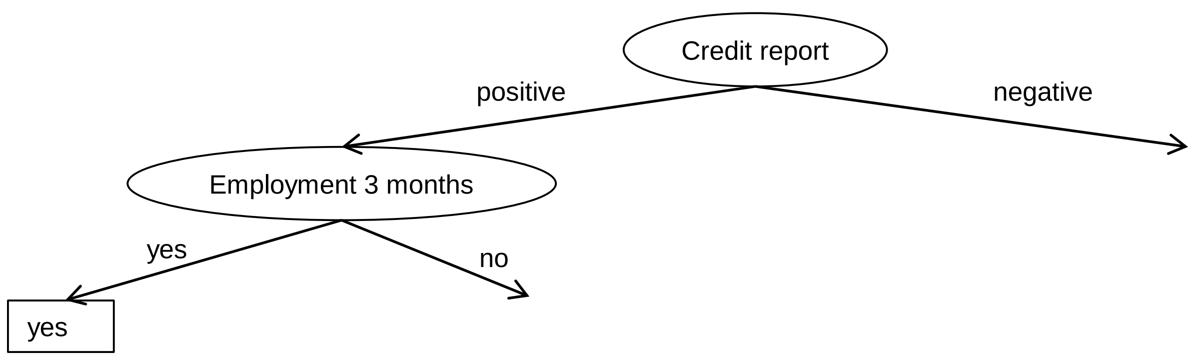
2	Positive	No	Yes	Yes
3	Positive	No	No	No
4	Negative	No	Yes	No
5	Negative	Yes	No	No

ID3(L, X)

1. If all data in L have same class y or X={}, then return leaf node with majority class y.
2. Else
    1. For all $x_j \in X$, calculate $G_L(x_j)$.
    2. Choose attribute $x_j \in X$ with highest $G_L(x_j)$.
    3. Let $L_i = \{(x, y) \in L : x_j = i\}$.
    4. Return test node with attribute x_j and children ID3(L_1, $X \setminus x_j$), …, ID3(L_k, $X \setminus x_j$).



ID3: Example

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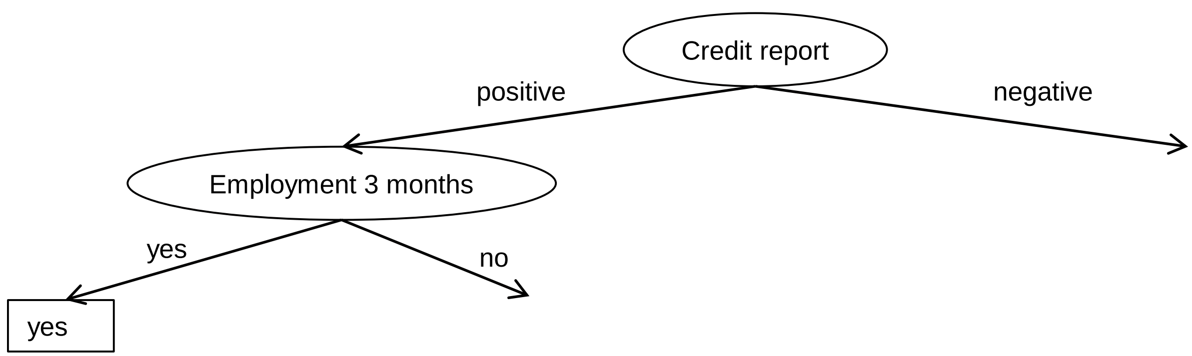

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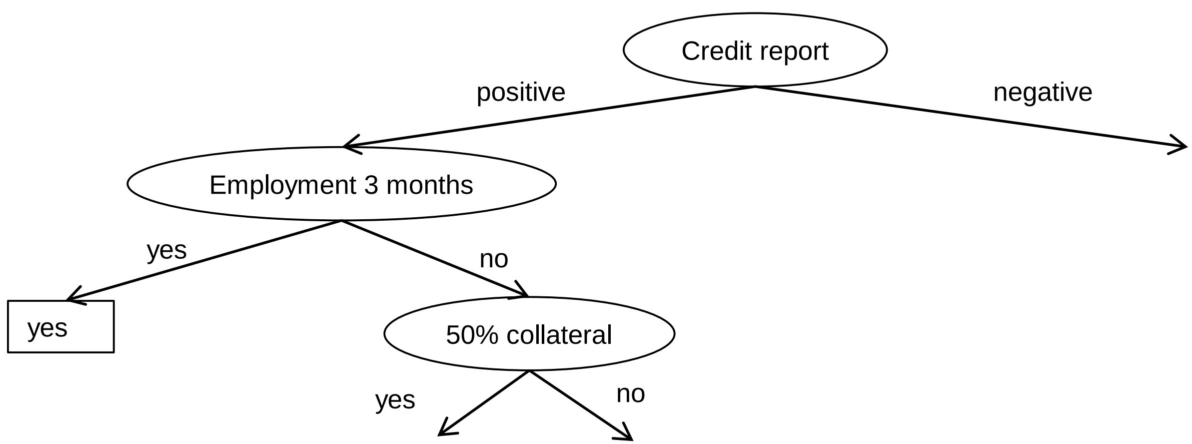

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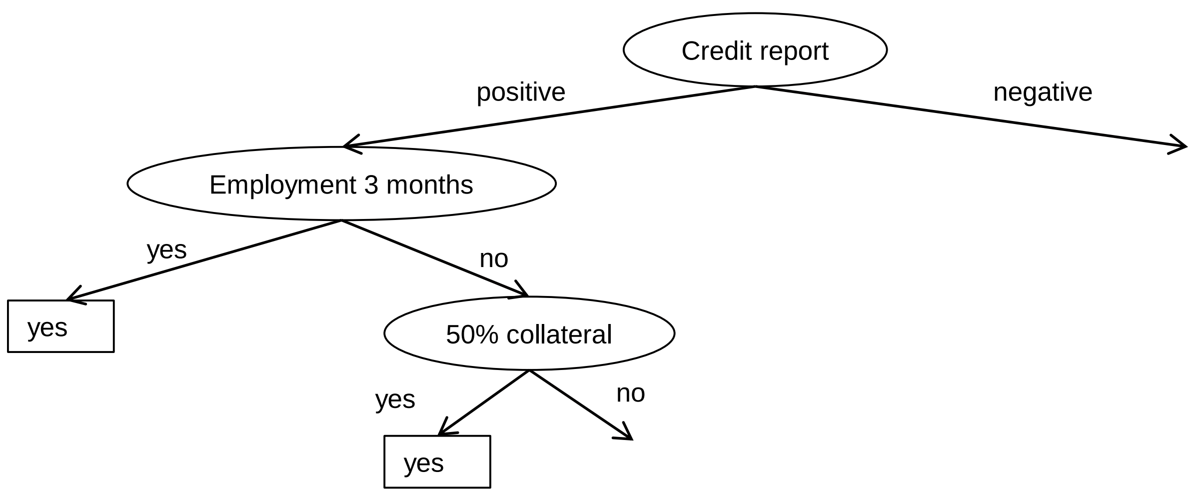

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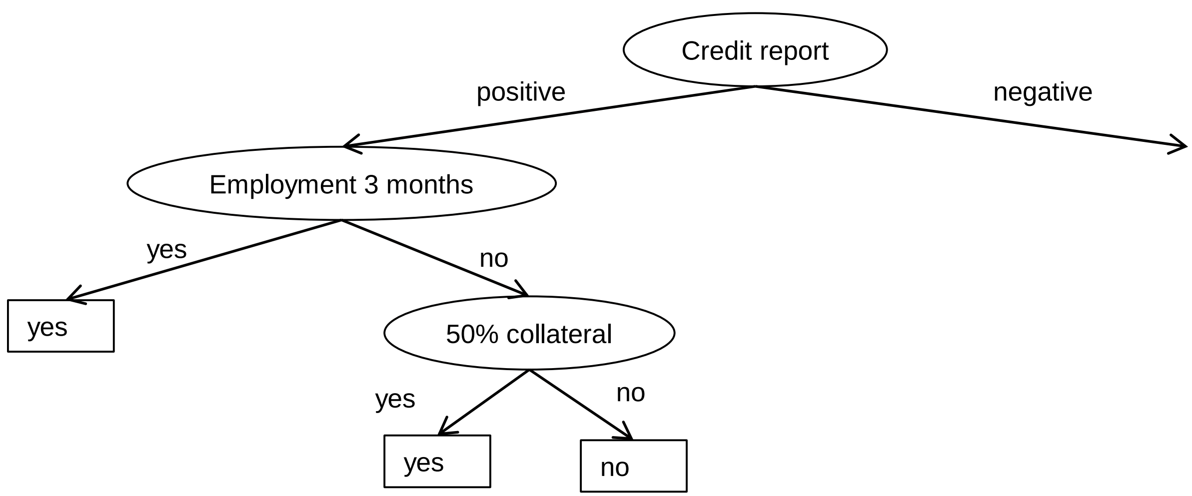

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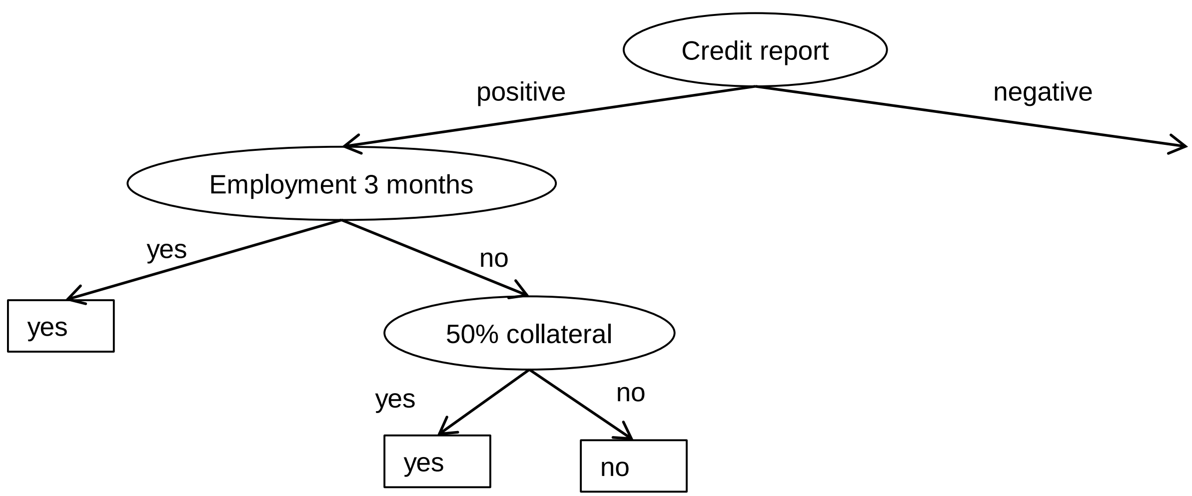

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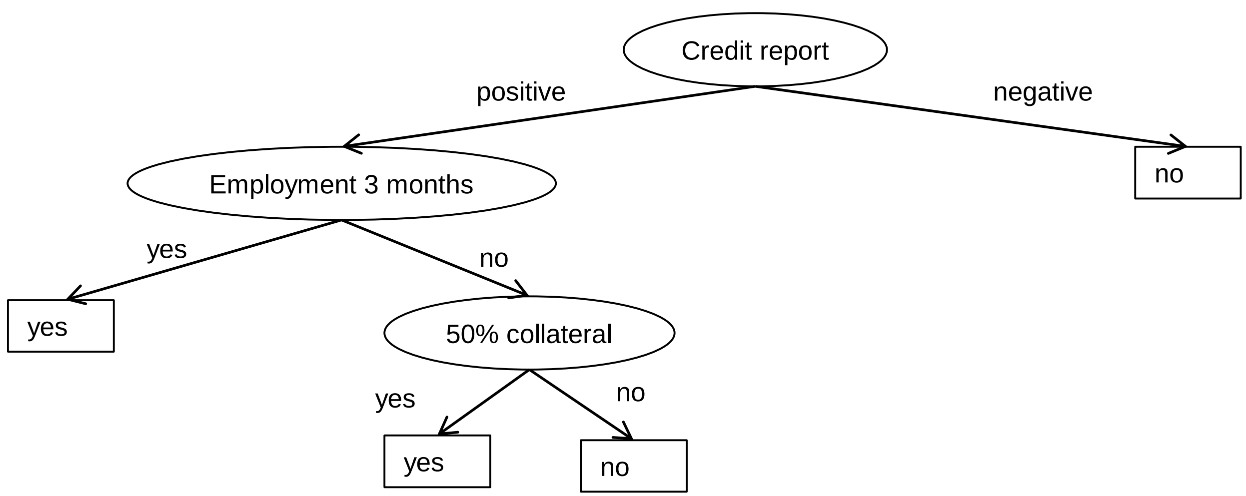

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2	Positive	No	Yes	Yes
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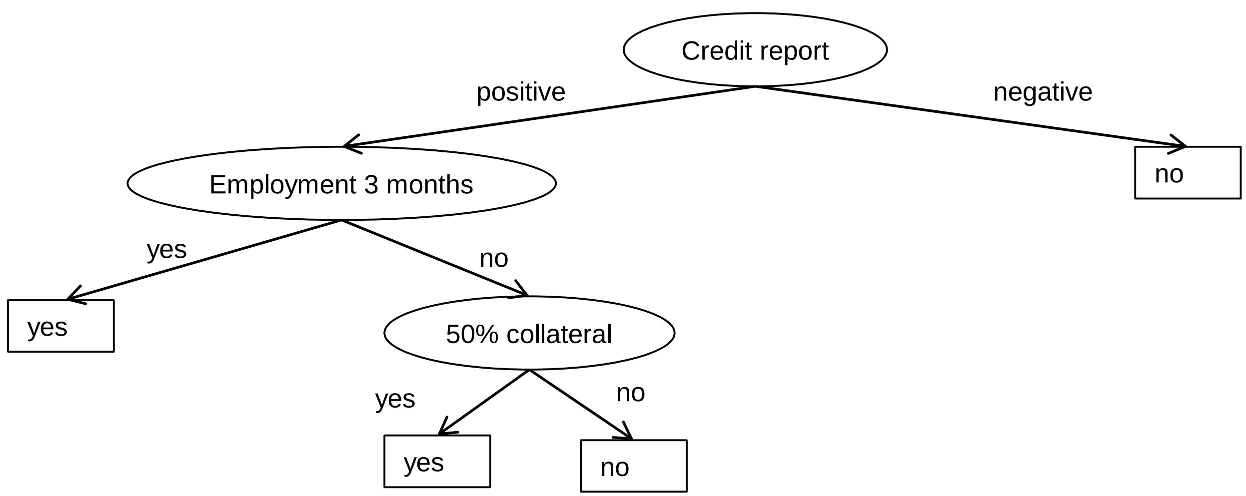


Overview

- Decision trees.
- Classification with categorical features: ID3.
- Classification with continuous features: C4.5.
- Regression: CART, model trees.
- Bagging.
- Random forests.

Continuous Attributes

- ID3 constructs a branch for every value of the selected attribute.
- This only works for discrete attributes.
- Idea: Choose attribute value pair, use test $x_j \leq v$.
  - $G_L(x_j \leq v)$
    $= H_L(y) - p_L(x_j \leq v) H_L(y|x_j \leq v) - p_L(x_j > v) H_L(y|x_j > v)$

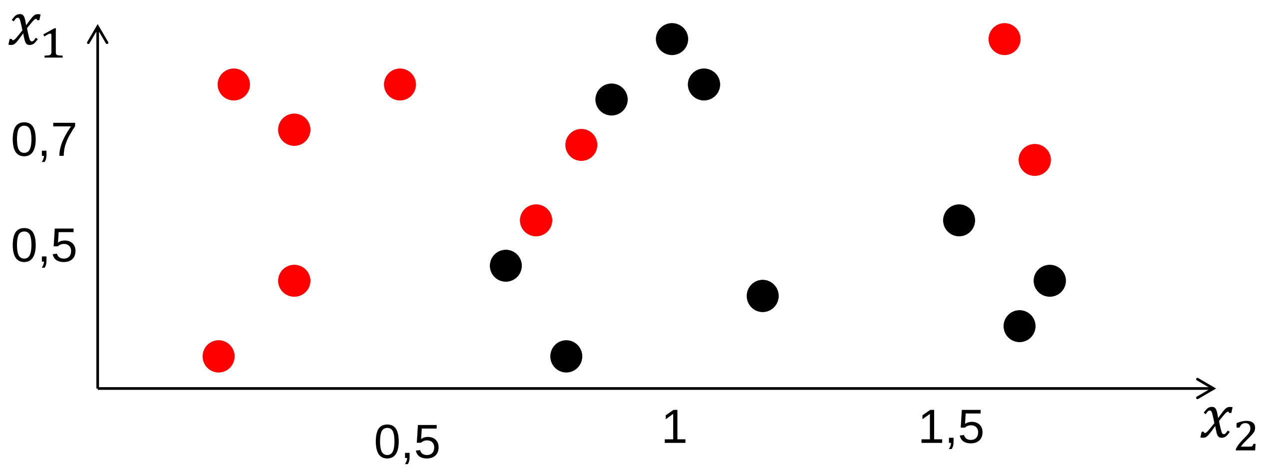
- Problem: there are infinitely many values.
- Idea: use only values that occur for that attribute in the training data.

Learning Decision Trees with C4.5

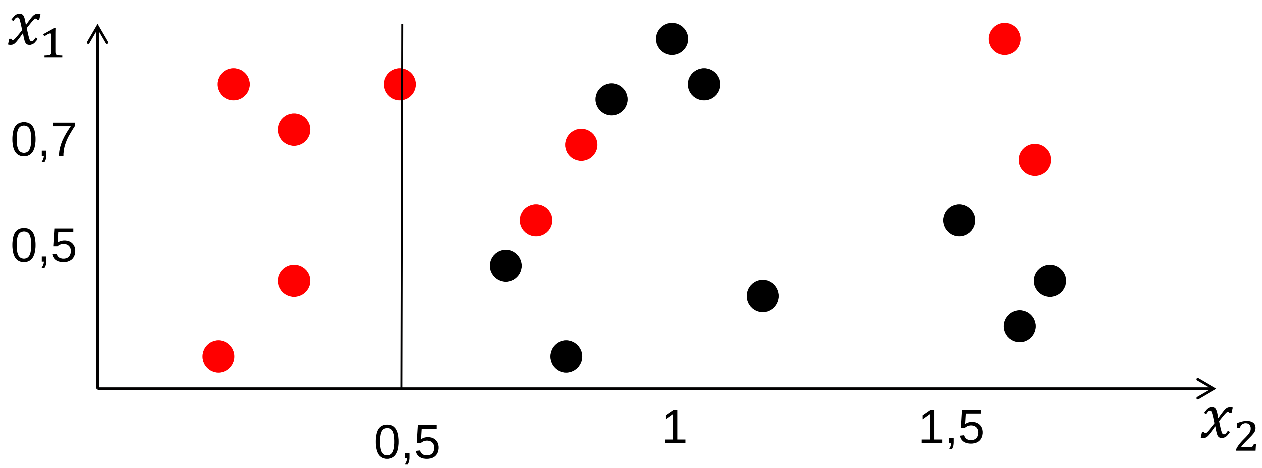
C4.5(L)

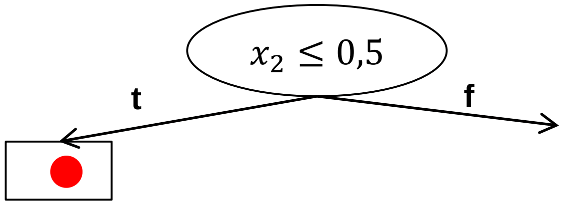
1. If all data in L have same class y or are identical, then return leaf node with majority class y.
2. Else
    1. For all discrete attributes $x_j \in X$: calculate $G_L(x_j)$.
    2. For all continuous attributes $x_j \in X$ and all values v that occur for x_j in L: calculate $G_L(x_j \leq v)$.
    3. If discrete attribute has highest $G_L(x_j)$:
        1. Let $L_i = \{(x, y) \in L: x_j = i\}$.
        2. Return test node with attribute x_j and children $C4.5(L_1)$, …, $C4.5(L_k)$.
    4. If continuous attribute has highest $G_L(x_j \leq v)$:
        1. Let $L_\leq = \{(x, y) \in L: x_j \leq v\}$, $L_> = \{(x, y) \in L: x_j > v\}$
        2. Return test node with test $x_j \leq v$ and children $C4.5(L_\leq)$, $C4.5(L_>)$.

C4.5: Example

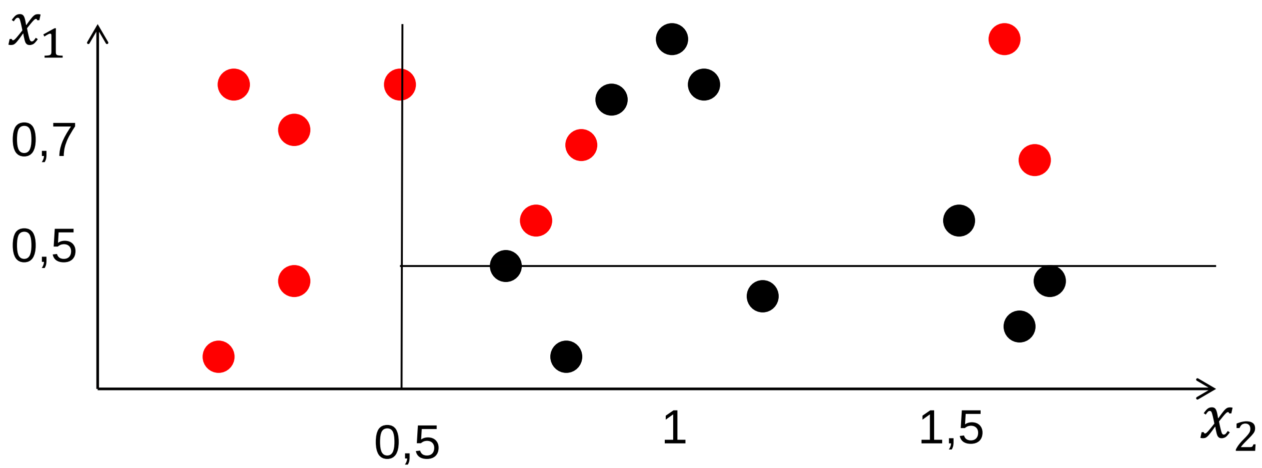


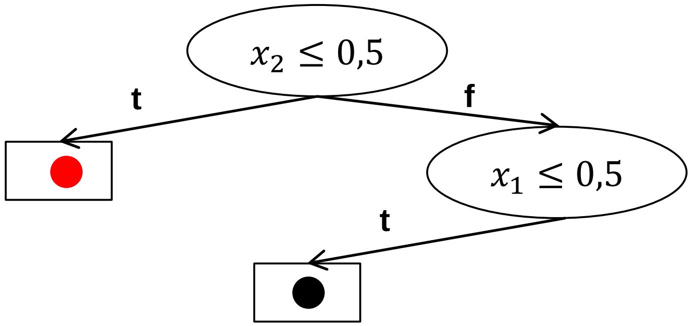
C4.5: Example



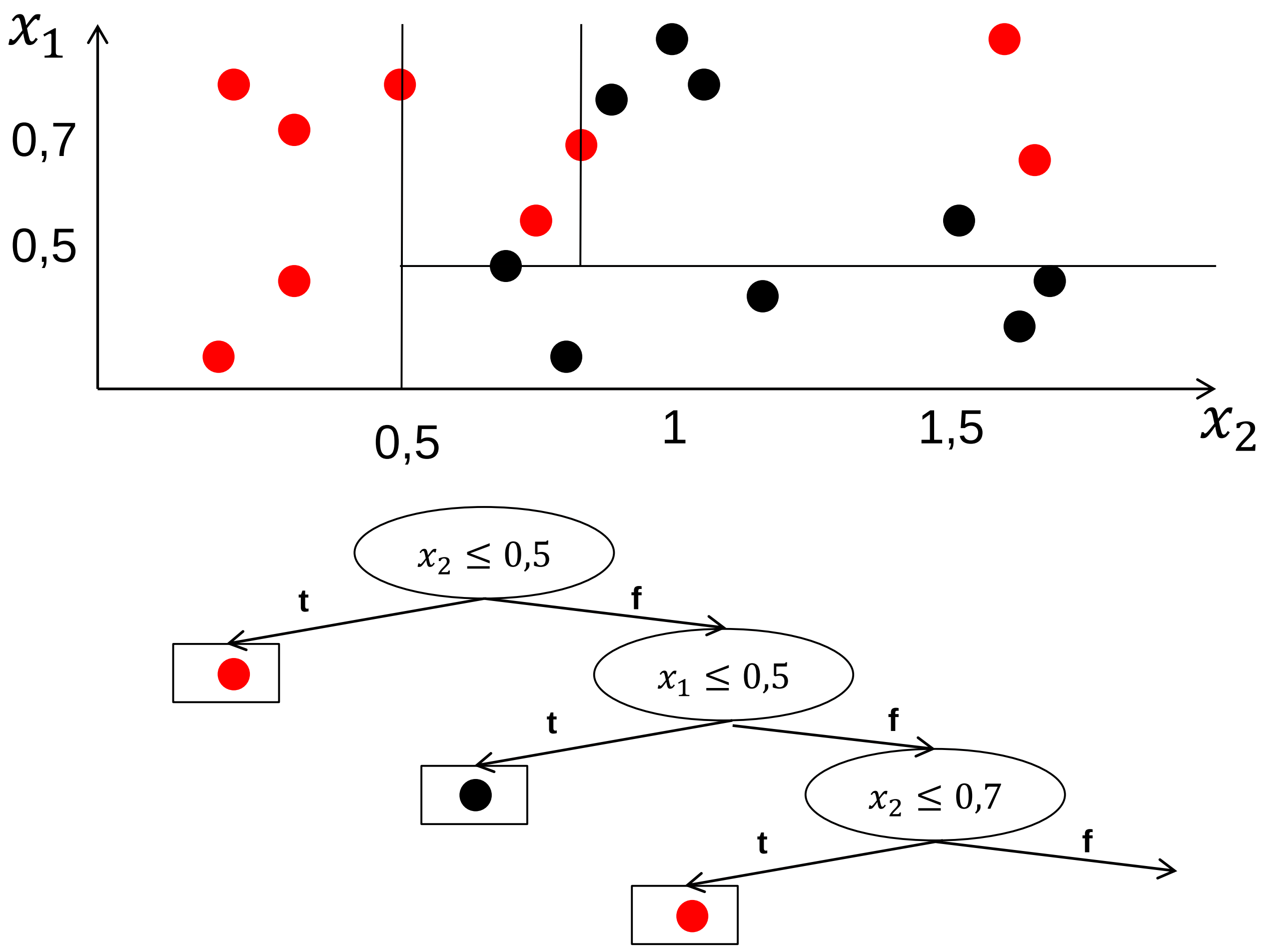


C4.5: Example

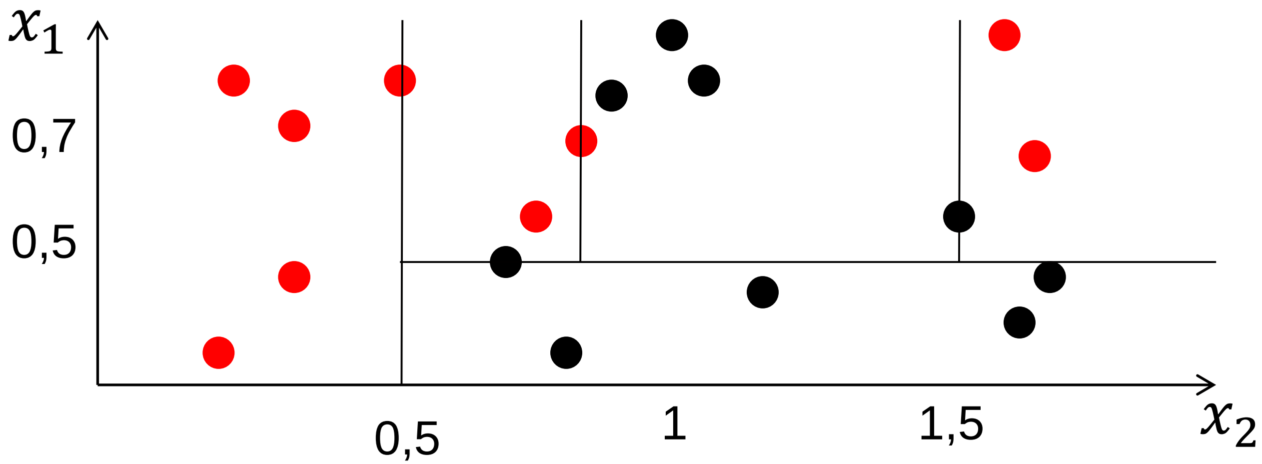


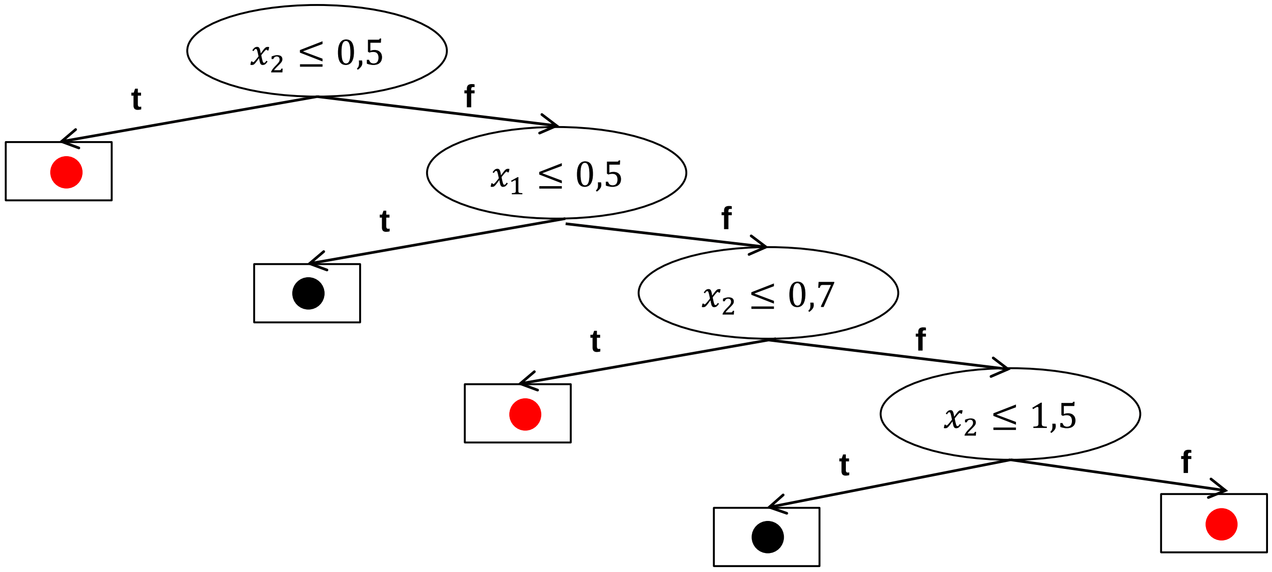


C4.5: Example



C4.5: Example



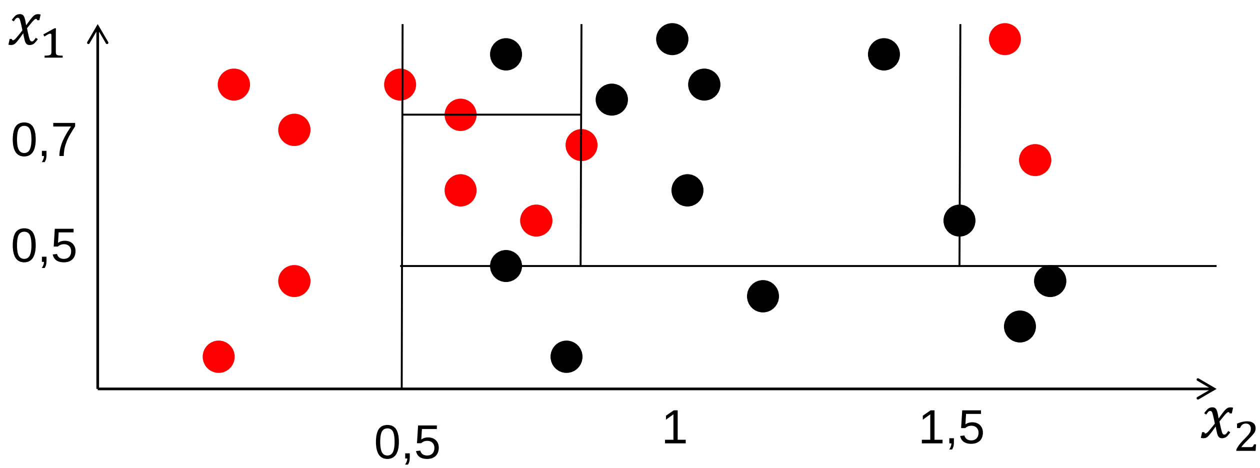


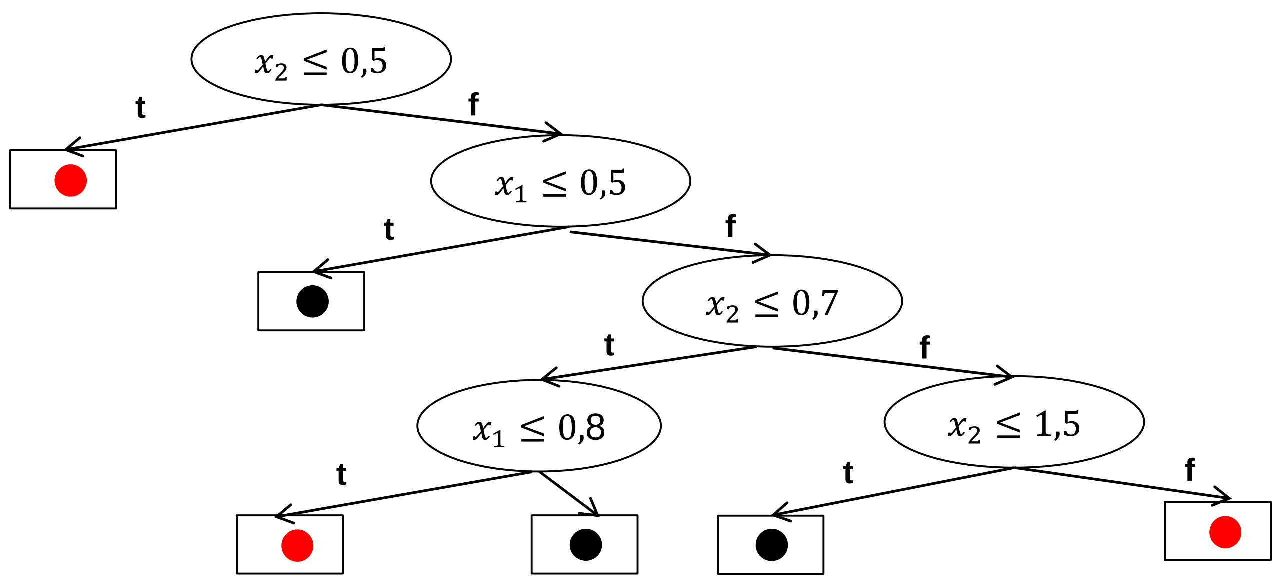
Pruning

- Leaf nodes that only are supported by a single (or very few) instances, often do not provide a good classification.
- Pruning:
  - Remove test nodes whose leaves have less than τ instances.
  - Collect in new leaf node that is labeled with the majority class

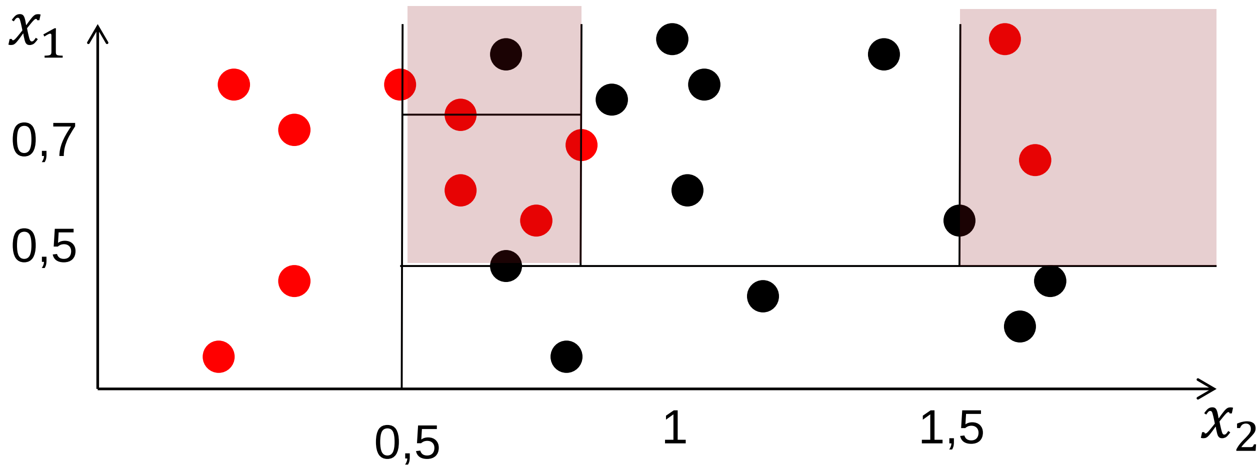
- Pruning parameter τ is a regularization parameter that has to be tuned (e.g., by cross validation).

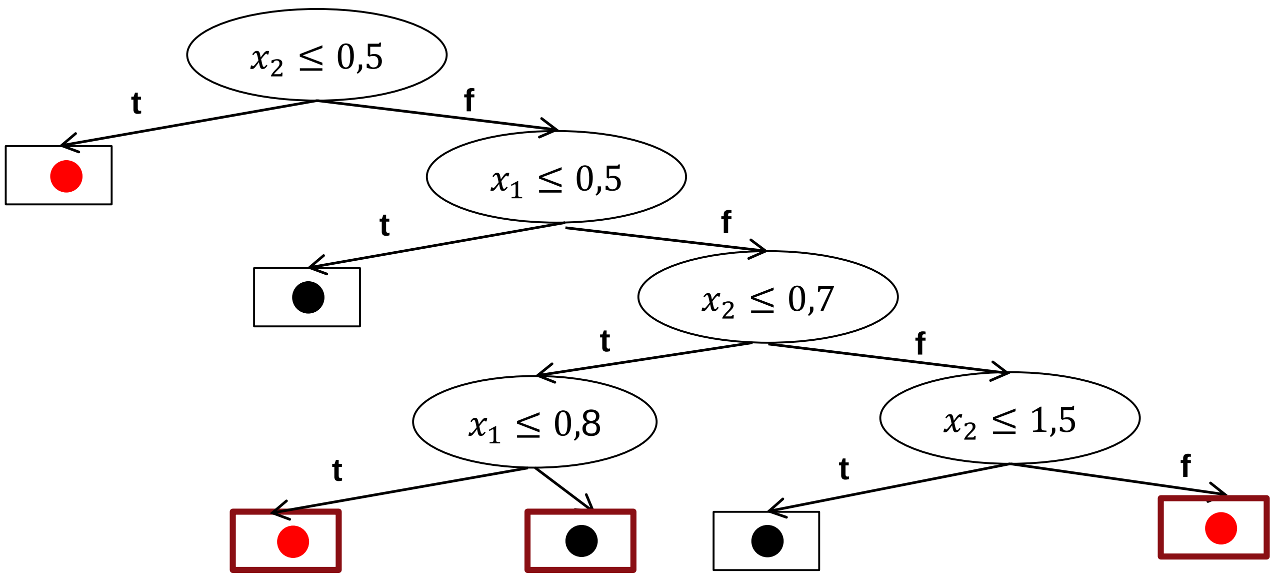
Pruning with Threshold 5: Example



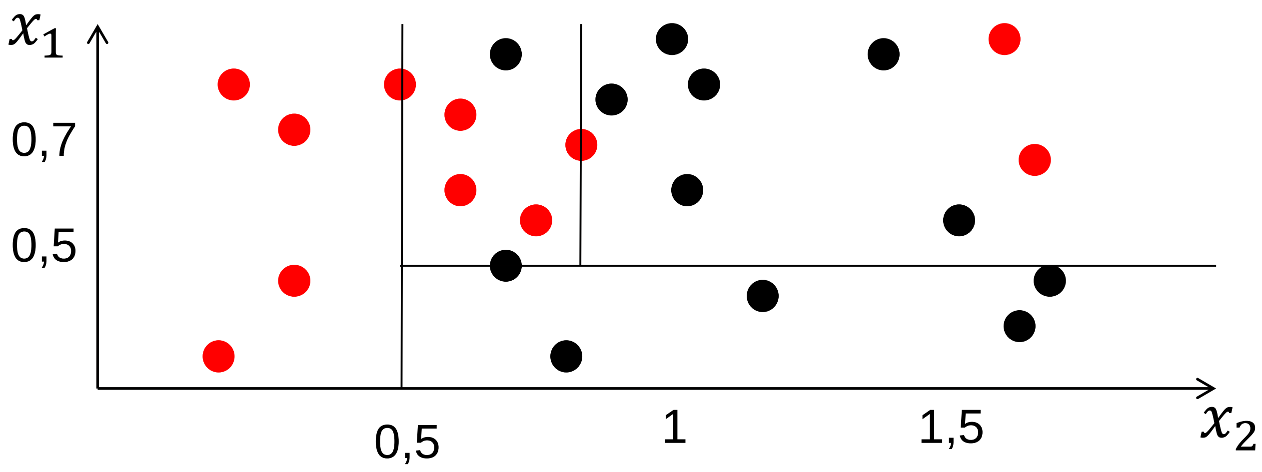


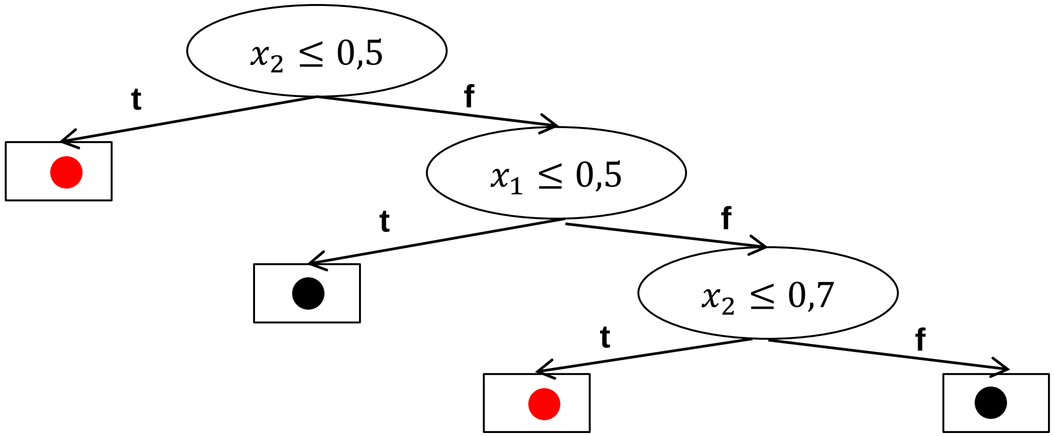
Pruning with Threshold 5: Example





Pruning with Threshold 5: Example





Reduced Error Pruning

- Split training data into a training set and a pruning validation set.
- Construct a decision tree using the training set (for instance, with C4.5).
- Starting from the bottom layer, iterate over all test nodes whose children are leaf nodes.
  - If removing the test node and replacing it with a leaf node that predicts the majority class reduces the error rate on the pruning set, then do it!

Overview

- Decision trees.
- Classification with categorical features: ID3.
- Classification with continuous features: C4.5.
- Regression: CART, model trees.
- Bagging.
- Random forests.

Regression

- Input: instance $\mathbf{x} \in X$.
  - e.g., feature vector

$$\mathbf{x} = \begin{pmatrix} x_1 \\ \vdots \\ x_m \end{pmatrix}$$

- Output: continuous (real) value, $y \in \mathbb{R}$
- Learning problem: training data with continuous target value
  - $L = \langle (\mathbf{x}_1, y_1), \dots, (\mathbf{x}_n, y_n) \rangle$
  - e.g. $\langle (\mathbf{x}_1, 3.5), \dots, (\mathbf{x}_n, -2.8) \rangle$

Regression

- Input: instance $\mathbf{x} \in X$.
  - e.g., feature vector

$$\mathbf{x} = \begin{pmatrix} x_1 \\ \vdots \\ x_m \end{pmatrix}$$

- Output: continuous (real) value, $y \in \mathbb{R}$
- Learning goal:
  - Low quadratic error rate + simple model.
  - $SSE = \sum_{i=1}^{n} \left(y_i - f(x_i)\right)^2$; $MSE = \frac{1}{n} \sum_{i=1}^{n} \left(y_i - f(x_i)\right)^2$
- Split criterion for regression?

Regression Trees

- Variance of the target attribute on sample L:
  - $Var(L) = \frac{1}{n}\sum_{i=1}^{n}(y_i - \bar{y})^2$
- Variance = MSE of predicting the mean value.
- Splitting criterion: variance reduction of $[x_j \leq v]$:
  - $R_L[x_j \leq v]$
    $= Var(L) - \frac{n_{[x_j \leq v]}}{n} Var\left(L_{[x_j \leq v]}\right) - \frac{n_{[x_j > v]}}{n} Var\left(L_{[x_j > v]}\right)$
- Stopping criterion:
  - Do not create a new test node if $nVar(L) \leq \tau$.

Learning Regression Trees with CART

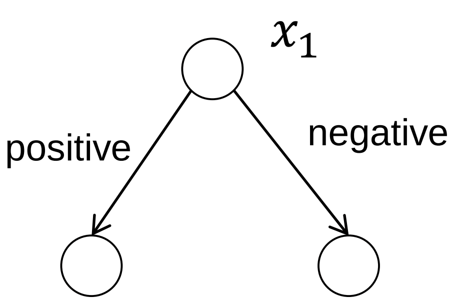
CART(L)

1. If $\sum_{i=1}^{n}(y_i - \bar{y})^2 < \tau$, then return leaf node with prediction $\bar{y}$.
2. Else
   1. For all discrete attributes $x_j \in X$: calculate $R_L(x_j)$.
   2. For all continuous attributes $x_j \in X$ and all values v that occur for x_j in L: calculate $R_L(x_j \leq v)$.
   3. If discrete attribute has highest $R_L(x_j)$:
      1. Let $L_i = \{(x, y) \in L: x_j = i\}$.
      2. Return test node with attribute x_j and children CART(L_1), …, CART(L_k).
   4. If continuous attribute has highest $R_L(x_j \leq v)$:
      1. Let $L_\leq = \{(x, y) \in L: x_j \leq v\}$, $L_> = \{(x, y) \in L: x_j > v\}$
      2. Return test node with test $x_j \leq v$ and children CART($L_\leq$), CART($L_>$).

CART- Example

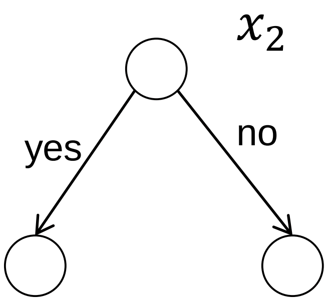
Loan	x_1 (Credit report)	x_2 (Employment last 3 months)	y (recovery rate)
1	Positive	Yes	0.8
2	Positive	No	0.9
3	Positive	No	0.4
4	Negative	No	0.1
5	Negative	Yes	0.2

- Which split is better?
- $Var(L) = \frac{1}{5}\left((0.8-0.48)^2 + \cdots + (0.2-0.48)^2\right) = 0.1148$



y (recovery rate)
0.8
0.9
0.4

y (recovery rate)
0.1
0.2



y (recovery rate)
0.8
0.2

y (recovery rate)
0.9
0.4
0.1

$$Var_{pos} = \frac{1}{3}\left((0.8-0.7)^2 + (0.9-0.7)^2 + (0.4-0.7)^2\right) = 0.0466$$

$$Var_{neg} = \frac{1}{2}\left((0.1-0.15)^2 + (0.2-0.15)^2\right) = 0.0025$$

$$0.1148 - \frac{3}{5} \times 0.0466 - \frac{2}{5} \times 0.0025 = \mathbf{0.085}$$

$$Var_{yes} = \frac{1}{2}\left((0.8-0.5)^2 + (0.2-0.5)^2\right) =$$

$$Var_{no} = \frac{1}{3}\left((0.9-0.46)^2 + (0.4-0.46)^2 + (0.1-0.46)^2\right) =$$

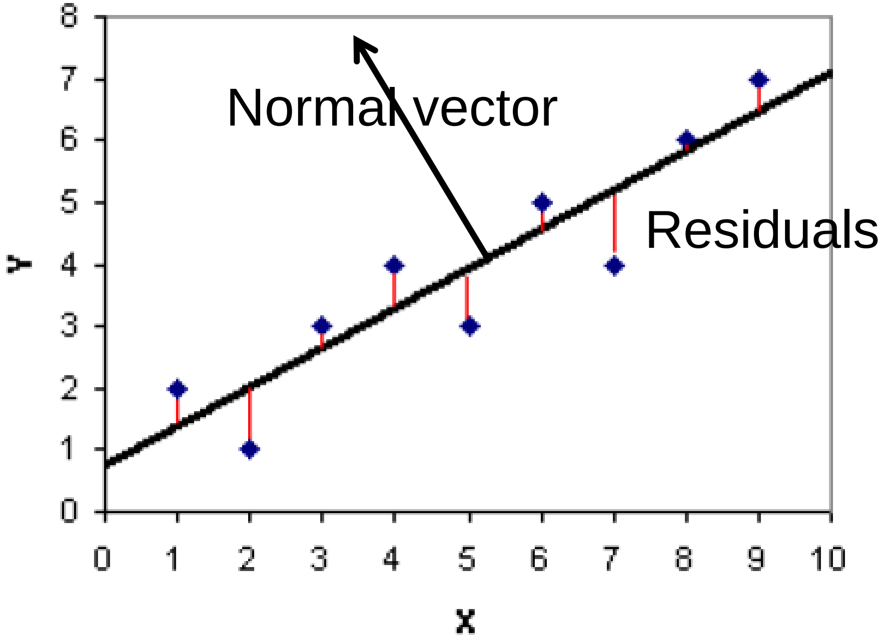
$$0.1148 - \frac{2}{5} \times \qquad - \frac{3}{5} \times \qquad =$$

Model Trees

- Nodes in regression trees are labeled with the mean value of their training instances.
- Idea: Instead train local linear regression model using the instances that fall into the leaf.

Linear Regression

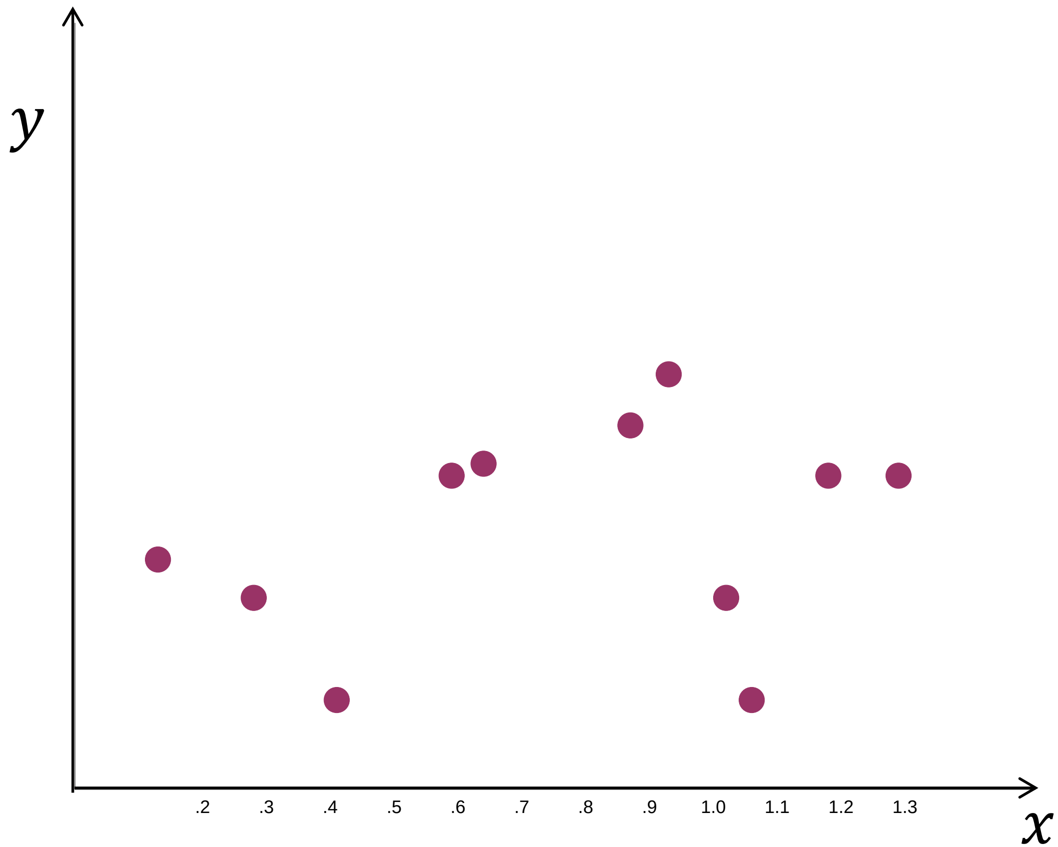
- Input: $L = \langle(\mathbf{x}_1, y_1), \dots, (\mathbf{x}_n, y_n)\rangle$
- Linear regression model $f(\mathbf{x}) = \boldsymbol{\theta}^{\mathrm{T}}\mathbf{x} + \theta_0$
- Will be discussed in later lectue.



Points along the Regression plane are perpendicular to the normal vector.

Model Trees

- Decision trees but with a linear regression model at each leaf node.



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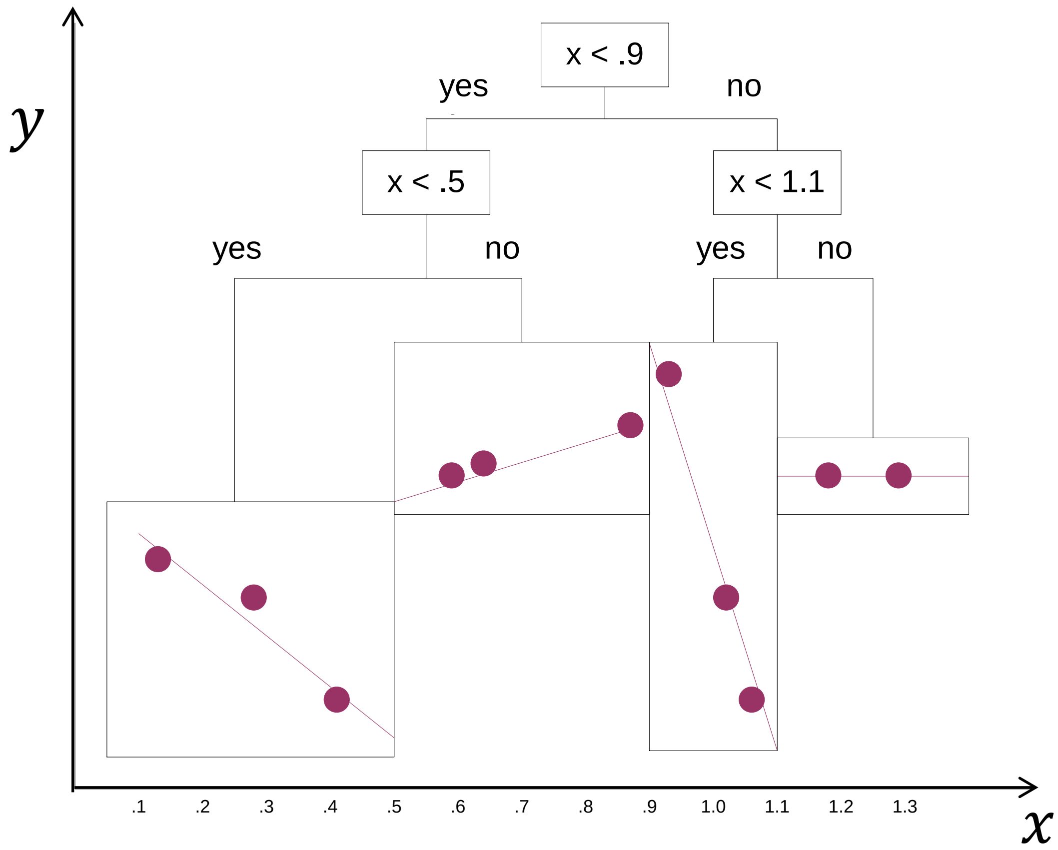

Overview

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Ensemble Learning

- Assume that we have 3 models $f_i(\mathbf{x})$.
- Each model has an error probability of 0.1.
- Let $f(\mathbf{x})$ be the majority vote among the $f_i(\mathbf{x})$:
  - $f(\mathbf{x}) = \arg\max_y |\{i: f_i(\mathbf{x}) = y\}|$.
- What is the error probability of $f(\mathbf{x})$?

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  - $f(\mathbf{x}) = \arg\max_y |\{i: f_i(\mathbf{x}) = y\}|$.
- What is the error probability of $f(\mathbf{x})$?
  - Depends on how correlated the models are.
  - If they always make identical prediction, the error rate of the ensemble is 0.1 as well.

Ensemble Learning

- Assume that we have 3 models $f_i(\mathbf{x})$.
- Each model has an error probability of 0.1.
- Let $f(\mathbf{x})$ be the majority vote among the $f_i(\mathbf{x})$:
  - $f(\mathbf{x}) = \arg\max_y |\{i: f_i(\mathbf{x}) = y\}|$.
- What is the error probability of $f(\mathbf{x})$ if the models are independent?
  - 2 out of 3 models have to err.
  - There are 3 subsets of 2 models.
  - $R \leq 3 \times 0.1^2 = 0.03$.
- Ensemble is much better than individual models.

Ensemble Learning

- Assume that we have n models $f_i(\mathbf{x})$.
- Each model has an error probability of $0.5 - \varepsilon$.
- Let $f(\mathbf{x})$ be the majority vote among the $f_i(\mathbf{x})$:
  - $f(\mathbf{x}) = \arg\max_y |\{i: f_i(\mathbf{x}) = y\}|$.
- Ensemble $f(\mathbf{x})$ may be much better than individual models if
  - Each model's error probability is below 0.5
  - The models are sufficiently uncorrelated.

Ensemble Learning

- Ensemble methods differ in how they try to obtain uncorrelated classifiers from given training data.
- Bagging: sample random subsets of training instances.
- Random forests: sample random subsets of training instances and random subsets of features.
- Boosting: iteratively draw subsets of the training instances such that instances that are misclassified by the current ensemble receive a higher weight.

Bootstrapping

- The bootstrapping procedure draws n instances from a set of n instances *with replacement*.
- Instances can be drawn multiple times.

1. Input: sample L of size n.
2. For i=1…k
    1. Draw n instances uniformly with replacement from L into set L_i.
    2. Learn model f_i on sample L_i.
3. Return models $(f_1, \ldots, f_k)$.

Bagging – Bootstrap Aggregating

- Input: sample L of size n.

1. For i=1…k
    1. Draw n instances uniformly with replacement from L into set L_i.
    2. Learn model f_i on sample L_i.
2. For classification:
    1. Let $f(\mathbf{x})$ be the majority vote among $(f_1(\mathbf{x}), \ldots, f_k(\mathbf{x}))$.
3. For regression:
    1. Let $f(\mathbf{x}) = \frac{1}{\mathrm{k}} \sum_{i=1}^{k} f_i(\mathbf{x})$.

Bagging – Bootstrap Aggregating

- Models are somewhat uncorrelated because they have been trained on different subsets of the data.
- But all models use the same attributes and share a good part of the training data.

- Idea: also vary the attributes.

Random Forests

- Input: sample L of size n, attributes X.

1. For i=1…k
   1. Draw n instances uniformly with replacement from L into set L_i.
   2. Draw m attributes from all attributes X into X_i.
   3. Learn model f_i on sample L_i using attributes X_i.
2. For classification:
   1. Let $f(\mathbf{x})$ be the majority vote among $(f_1(\mathbf{x}), \dots, f_k(\mathbf{x}))$.
3. For regression:
   1. Let $f(\mathbf{x}) = \frac{1}{k}\sum_{i=1}^{k} f_i(\mathbf{x})$.

Random Forests

- Number of sampled attributes is a hyperparameter.
- Decision trees are sometimes trained with depth-bound.
- Decision trees are usually trained without pruning.
- The number of trees is a hyperparameter; often, large, fixed values are used (e.g., 1000 trees).

Random Forests

- Require little to no preprocessing—decision tree algorithm can handle combinations of numeric, categorical, string attributes.
- Powerful non-linear classifiers.
- Quick and easy to apply.
- Perform well in practice for many problems when training data is not large enough to effectively apply neural networks.
- Downside: random forests are not interpretable.

Summary of Decision Trees

- Classification
  - Discrete attributes: ID3.
  - Continuous attributes: C4.5.
- Regression:
  - CART: mean value in each leaf.
  - Model trees: linear regression model in each leaf.
- Applying a decision tree is fast, requires no preprocessing; popular for many applications.
- Random forests are easy to apply, powerful, non-linear prediction models.