# Chapter ML:III

## III. Decision Trees

- Decision Trees Basics
- Impurity Functions
- Decision Tree Algorithms
- Decision Tree Pruning

## ID3 Algorithm [Quinlan 1986] [CART Algorithm]

Characterization of the model (model world) [ML Introduction] :

- $X$ is a set of feature vectors, also called feature space.
- $C$ is a set of classes.
- $c : X \to C$ is the ideal classifier for $X$.
- $D = \{(\mathbf{x}_1, c(\mathbf{x}_1)), \ldots, (\mathbf{x}_n, c(\mathbf{x}_n))\} \subseteq X \times C$ is a set of examples.

Task: Based on $D$, construction of a decision tree $T$ to approximate $c$.

# Decision Tree Algorithms

## ID3 Algorithm [Quinlan 1986] [CART Algorithm]

Characterization of the model (model world) [ML Introduction] :

- $X$ is a set of feature vectors, also called feature space.
- $C$ is a set of classes.
- $c : X \to C$ is the ideal classifier for $X$.
- $D = \{(\mathbf{x}_1, c(\mathbf{x}_1)), \ldots, (\mathbf{x}_n, c(\mathbf{x}_n))\} \subseteq X \times C$ is a set of examples.

Task: Based on $D$, construction of a decision tree $T$ to approximate $c$.

Characteristics of the ID3 algorithm:

1. Each splitting is based on one nominal feature and considers its complete domain. Splitting based on feature $A$ with domain $\{a_1, \ldots, a_k\}$ :

$$X = \{\mathbf{x} \in X : \mathbf{x}|_A = a_1\} \cup \ldots \cup \{\mathbf{x} \in X : \mathbf{x}|_A = a_k\}$$

2. Splitting criterion is information gain.

# Decision Tree Algorithms

## ID3 Algorithm [Mitchell 1997] [algorithm template]

ID3(D, Attributes, Target)

1. Create a node t for the tree.
2. Label t with the most common value of Target in D.
3. If all examples in D are positive, return the single-node tree t, with label “+”.

   If all examples in D are negative, return the single-node tree t, with label “–”.
4. If Attributes is empty, return the single-node tree t.

- Otherwise:

  5. Let A* be the attribute from Attributes that best classifies examples in D.

     Assign t the decision attribute A*.
  6. For each possible value “a” in A* do:
     - Add a new tree branch below t, corresponding to the test A* = “a”.
     - Let D_a be the subset of D that has value “a” for A*.
     - If D_a is empty:
       Then add a leaf node with label of the most common value of Target in D.
       Else add the subtree ID3(D_a, Attributes \ {A*}, Target).

7. Return t.

# Decision Tree Algorithms

## ID3 Algorithm (pseudo code) [algorithm template]

*ID3*$(D,$ *Attributes*, *Target*$)$

1. $t =$ *createNode*$()$
2. *label*$(t) =$ *mostCommonClass*$(D,$ *Target*$)$
3. **IF** $\forall \langle \mathbf{x}, c(\mathbf{x}) \rangle \in D : c(\mathbf{x}) = c$ **THEN** *return*$(t)$ **ENDIF**
4. **IF** *Attributes* $= \emptyset$ **THEN** *return*$(t)$ **ENDIF**
5. 
6. 
7. 

# Decision Tree Algorithms

## ID3 Algorithm (pseudo code) [algorithm template]

*ID3*$(D,$ *Attributes*, *Target*$)$

1. $t =$ *createNode*$()$
2. *label*$(t) =$ *mostCommonClass*$(D,$ *Target*$)$
3. **IF** $\forall\langle \mathbf{x}, c(\mathbf{x})\rangle \in D : c(\mathbf{x}) = c$ **THEN** *return*$(t)$ **ENDIF**
4. **IF** *Attributes* $= \emptyset$ **THEN** *return*$(t)$ **ENDIF**
5. $A^* = \text{argmax}_{A \in \textit{Attributes}}(\textit{informationGain}(D, A))$
6. 
7. 

# Decision Tree Algorithms

## ID3 Algorithm (pseudo code) [algorithm template]

*ID3*$(D,$ *Attributes*, *Target*$)$

1. $t =$ *createNode*$()$
2. *label*$(t) =$ *mostCommonClass*$(D,$ *Target*$)$
3. **IF** $\forall \langle \mathbf{x}, c(\mathbf{x}) \rangle \in D : c(\mathbf{x}) = c$ **THEN** *return*$(t)$ **ENDIF**
4. **IF** *Attributes* $= \emptyset$ **THEN** *return*$(t)$ **ENDIF**
5. $A^* = \text{argmax}_{A \in \textit{Attributes}}(\textit{informationGain}(D, A))$
6. **FOREACH** $a \in A^*$ **DO**

   $D_a = \{(\mathbf{x}, c(\mathbf{x})) \in D : \mathbf{x}|_{A^*} = a\}$

   **IF** $D_a = \emptyset$ **THEN**

   **ELSE**

   *createEdge*$(t, a,$ *ID3*$(D_a,$ *Attributes* $\setminus \{A^*\},$ *Target*$))$

   **ENDIF**

   **ENDDO**
7. *return*$(t)$

# Decision Tree Algorithms

## ID3 Algorithm (pseudo code) [algorithm template]

*ID3*$(D,$ *Attributes*, *Target*$)$

1. $t =$ *createNode*$()$
2. *label*$(t) =$ *mostCommonClass*$(D,$ *Target*$)$
3. **IF** $\forall \langle \mathbf{x}, c(\mathbf{x}) \rangle \in D : c(\mathbf{x}) = c$ **THEN** *return*$(t)$ **ENDIF**
4. **IF** *Attributes* $= \emptyset$ **THEN** *return*$(t)$ **ENDIF**
5. $A^* = \text{argmax}_{A \in \textit{Attributes}}(\textit{informationGain}(D, A))$
6. **FOREACH** $a \in A^*$ **DO**

   $D_a = \{(\mathbf{x}, c(\mathbf{x})) \in D : \mathbf{x}|_{A^*} = a\}$

   **IF** $D_a = \emptyset$ **THEN**

   $t' =$ *createNode*$()$

   *label*$(t') =$ *mostCommonClass*$(D,$ *Target*$)$

   *createEdge*$(t, a, t')$

   **ELSE**

   *createEdge*$(t, a,$ *ID3*$(D_a,$ *Attributes* $\setminus \{A^*\},$ *Target*$))$

   **ENDIF**

   **ENDDO**
7. *return*$(t)$

Remarks:

- "*Target*" designates the feature (= attribute) that is comprised of the labels according to which an example can be classified. Within Mitchell's algorithm the respective class labels are '+' and '–', modeling the binary classification situation. In the pseudo code version, *Target* may contain multiple (more than two) classes.

- Step 3 of of the ID3 algorithm checks the purity of $D$ and, given this case, assigns the unique class $c$, $c \in$ *dom*$($*Target*$)$, as label to the respective node.

# Decision Tree Algorithms

## ID3 Algorithm: Example

Example set $D$ for mushrooms, implicitly defining a feature space $X$ over the three dimensions color, size, and points:

| | Color | Size | Points | Eatability |
|---|---|---|---|---|
| 1 | red | small | yes | toxic |
| 2 | brown | small | no | eatable |
| 3 | brown | large | yes | eatable |
| 4 | green | small | no | eatable |
| 5 | red | large | no | eatable |

# Decision Tree Algorithms

## ID3 Algorithm: Example (continued)

Top-level call of ID3. Analyze a splitting with regard to the feature "color" :

$D|_{\text{color}} =$

| | toxic | eatable |
|---|---|---|
| red | 1 | 1 |
| brown | 0 | 2 |
| green | 0 | 1 |

➜ $|D_{\text{red}}| = 2, \ |D_{\text{brown}}| = 2, \ |D_{\text{green}}| = 1$

Estimated a-priori probabilities:

$$p_{\text{red}} = \frac{2}{5} = 0.4, \quad p_{\text{brown}} = \frac{2}{5} = 0.4, \quad p_{\text{green}} = \frac{1}{5} = 0.2$$

Top-level call of ID3. Analyze a splitting with regard to the feature "color" :

$D|_{\text{color}} =$

| | toxic | eatable |
|---|---|---|
| red | 1 | 1 |
| brown | 0 | 2 |
| green | 0 | 1 |

➜ $|D_{\text{red}}| = 2, \ |D_{\text{brown}}| = 2, \ |D_{\text{green}}| = 1$

Estimated a-priori probabilities:

$$p_{\text{red}} = \frac{2}{5} = 0.4, \quad p_{\text{brown}} = \frac{2}{5} = 0.4, \quad p_{\text{green}} = \frac{1}{5} = 0.2$$

Conditional entropy values for all attributes:

$$\begin{aligned} H(C \mid \text{color}) \quad &= \quad -(\, 0.4 \cdot (\tfrac{1}{2} \cdot \log_2 \tfrac{1}{2} + \tfrac{1}{2} \cdot \log_2 \tfrac{1}{2}) + \\ &\qquad\quad 0.4 \cdot (\tfrac{0}{2} \cdot \log_2 \tfrac{0}{2} + \tfrac{2}{2} \cdot \log_2 \tfrac{2}{2}) + \\ &\qquad\quad 0.2 \cdot (\tfrac{0}{1} \cdot \log_2 \tfrac{0}{1} + \tfrac{1}{1} \cdot \log_2 \tfrac{1}{1}) \,) \ = \ 0.4 \end{aligned}$$

$$\begin{aligned} H(C \mid \text{size}) \quad &\approx \quad 0.55 \\ H(C \mid \text{points}) \quad &= \quad 0.4 \end{aligned}$$

Remarks:

- The smaller $H(C \mid \textit{feature})$ is, the larger becomes the information gain. Hence, the difference $H(C) - H(C \mid \textit{feature})$ needs not to be computed since $H(C)$ is constant within each recursion step.
- In the example, the information gain in the first recursion step becomes maximum for the two features "color" and "points".

# Decision Tree Algorithms

## ID3 Algorithm: Example (continued)

Decision tree before the first recursion step:

attribute: points

yes

| color | size | eatability |
|---|---|---|
| red | small | toxic |
| brown | large | eatable |

no

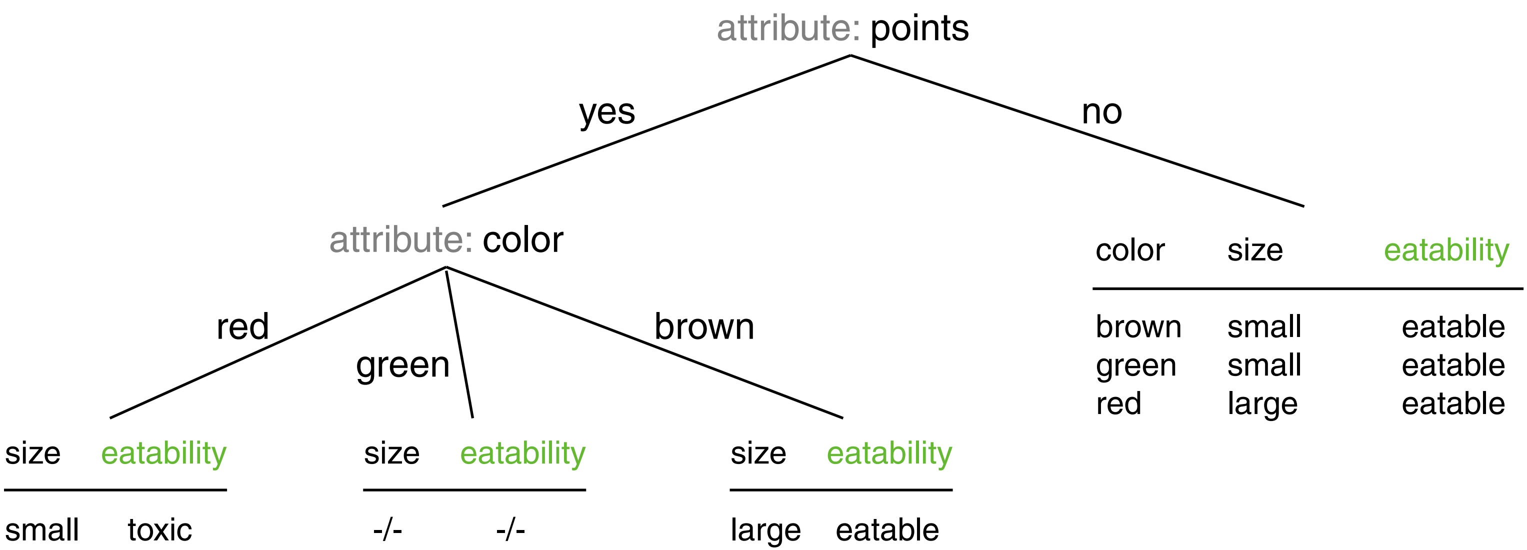
| color | size | eatability |
|---|---|---|
| brown | small | eatable |
| green | small | eatable |
| red | large | eatable |

The feature “points” was chosen in Step 5 of the ID3 algorithm.

# Decision Tree Algorithms

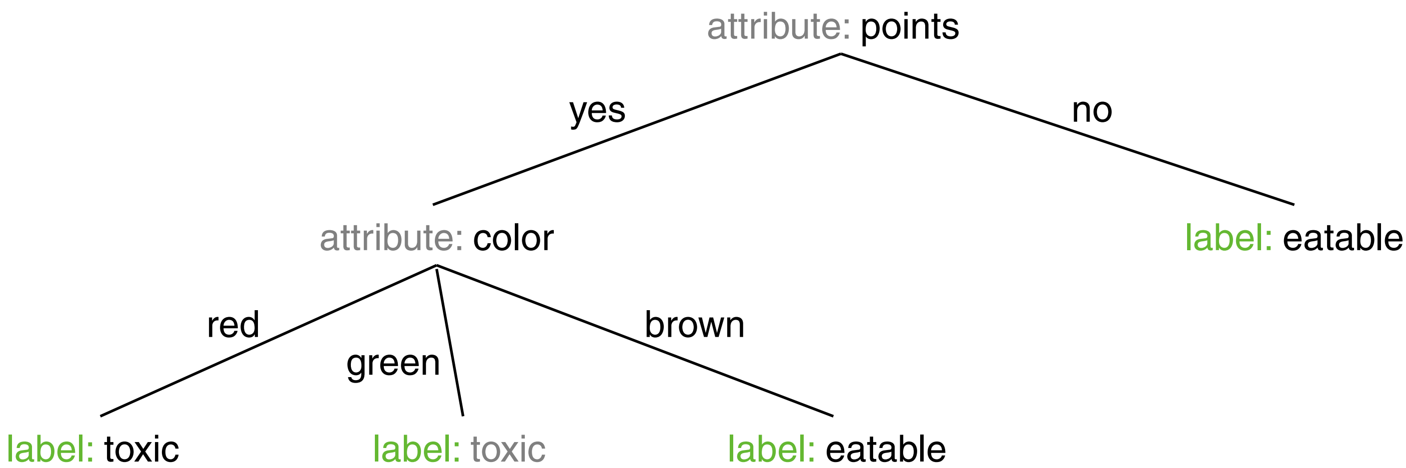
## ID3 Algorithm: Example (continued)

Decision tree before the second recursion step:




The feature “color” was chosen in Step 5 of the ID3 algorithm.

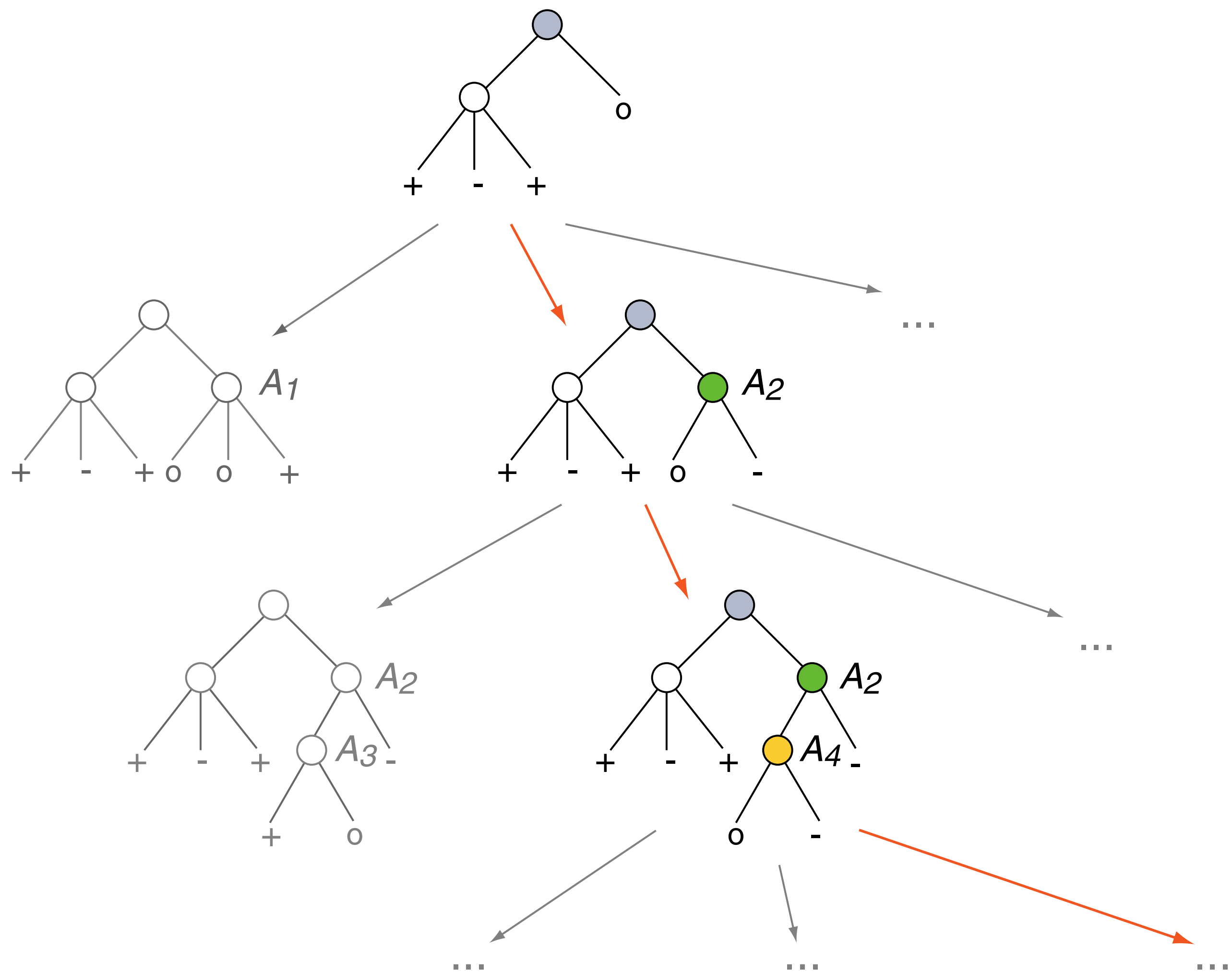
Final decision tree after second recursion step:




Break of a tie: choosing the class “toxic” for $D_{\text{green}}$ in Step 6 of the ID3 algorithm.

# Decision Tree Algorithms

## ID3 Algorithm: Hypothesis Space



# Decision Tree Algorithms

## ID3 Algorithm: Inductive Bias

Inductive bias is the rigidity in applying the (little bit of) knowledge learned from a training set for the classification of unseen feature vectors.

Observations:

- Decision tree search happens in the space of *all* hypotheses.

- To generate a decision tree, the ID3 algorithm needs per branch at most as many decisions as features are given.

# Decision Tree Algorithms

## ID3 Algorithm: Inductive Bias

Inductive bias is the rigidity in applying the (little bit of) knowledge learned from a training set for the classification of unseen feature vectors.

Observations:

- Decision tree search happens in the space of *all* hypotheses.
  - ➜ The target concept is a member of the hypothesis space.
- To generate a decision tree, the ID3 algorithm needs per branch at most as many decisions as features are given.
  - ➜ no backtracking takes place
  - ➜ the decision tree is a result of *local* optimization

# Decision Tree Algorithms

## ID3 Algorithm: Inductive Bias

Inductive bias is the rigidity in applying the (little bit of) knowledge learned from a training set for the classification of unseen feature vectors.

Observations:

- Decision tree search happens in the space of *all* hypotheses.
  - ➜ The target concept is a member of the hypothesis space.
- To generate a decision tree, the ID3 algorithm needs per branch at most as many decisions as features are given.
  - ➜ no backtracking takes place
  - ➜ the decision tree is a result of *local* optimization

Where the inductive bias of the ID3 algorithm becomes manifest:

1. Small decision trees are preferred.
2. Highly discriminative features tend to be closer to the root.

Is this justified?

Remarks:

- Let $\mathbf{A}_j$ be the finite domain (the possible values) of feature $A_j,\ j = 1, \ldots, p$, and let $C$ be a set of classes. Then, a hypothesis space $H$ that is comprised of all decision trees corresponds to the set of all functions $h,\ h : \mathbf{A}_1 \times \ldots \times \mathbf{A}_p \to C$. Typically, $C = \{0, 1\}$.

- The inductive bias of the ID3 algorithm is of a different kind than the inductive bias of the candidate elimination algorithm (version space algorithm):

  1. The underlying hypothesis space $H$ of the candidate elimination algorithm is incomplete. $H$ corresponds to a coarsened view onto the space of all hypotheses since $H$ contains only conjunctions of attribute-value pairs as hypotheses.

     However, this restricted hypothesis space is searched completely by the candidate elimination algorithm. Keyword: restriction bias

  2. The underlying hypothesis space $H$ of the ID3 algorithm is complete. $H$ corresponds to the set of all discrete functions (from the Cartesian product of the feature domains onto the set of classes) that can be represented in the form of a decision tree.

     However, this complete hypothesis space is searched incompletely (following a preference). Keyword: preference bias or search bias

- The inductive bias of the ID3 algorithm renders the algorithm robust regarding noise.

# Decision Tree Algorithms

## CART Algorithm [Breiman 1984] [ID3 Algorithm]

Characterization of the model (model world) [ML Introduction] :

- $X$ is a set of feature vectors, also called feature space.
  No restrictions are presumed for the features' measurement scales.
- $C$ is a set of classes.
- $c : X \to C$ is the ideal classifier for $X$.
- $D = \{(\mathbf{x}_1, c(\mathbf{x}_1)), \ldots, (\mathbf{x}_n, c(\mathbf{x}_n))\} \subseteq X \times C$ is a set of examples.

Task: Based on $D$, construction of a decision tree $T$ to approximate $c$.

# Decision Tree Algorithms

## CART Algorithm [Breiman 1984] [ID3 Algorithm]

Characterization of the model (model world) [ML Introduction] :

- $X$ is a set of feature vectors, also called feature space.
  No restrictions are presumed for the features' measurement scales.
- $C$ is a set of classes.
- $c : X \to C$ is the ideal classifier for $X$.
- $D = \{(\mathbf{x}_1, c(\mathbf{x}_1)), \ldots, (\mathbf{x}_n, c(\mathbf{x}_n))\} \subseteq X \times C$ is a set of examples.

Task: Based on $D$, construction of a decision tree $T$ to approximate $c$.

Characteristics of the CART algorithm:

1. Each splitting is binary and considers one feature at a time.
2. Splitting criterion is the information gain or the Gini index.

# Decision Tree Algorithms

## CART Algorithm (continued)

1. Let $A$ be a feature with domain $\mathbf{A}$. Ensure a finite number of binary splittings for $X$ by applying the following domain partitioning rules:

   – If $A$ is nominal, choose $\mathbf{A}' \subset \mathbf{A}$ such that $0 < |\mathbf{A}'| \leq |\mathbf{A} \setminus \mathbf{A}'|$.

   – If $A$ is ordinal, choose $a \in \mathbf{A}$ such that $x_{\text{min}} < a < x_{\text{max}}$, where $x_{\text{min}}$, $x_{\text{max}}$ are the minimum and maximum values of feature $A$ in $D$.

   – If $A$ is numeric, choose $a \in \mathbf{A}$ such that $a = (x_k + x_l)/2$, where $x_k$, $x_l$ are consecutive elements in the ordered value list of feature $A$ in $D$.

# Decision Tree Algorithms

## CART Algorithm (continued)

1. Let $A$ be a feature with domain $\mathbf{A}$. Ensure a finite number of binary splittings for $X$ by applying the following domain partitioning rules:

   – If $A$ is nominal, choose $\mathbf{A}' \subset \mathbf{A}$ such that $0 < |\mathbf{A}'| \leq |\mathbf{A} \setminus \mathbf{A}'|$.

   – If $A$ is ordinal, choose $a \in \mathbf{A}$ such that $x_{\text{min}} < a < x_{\text{max}}$, where $x_{\text{min}}$, $x_{\text{max}}$ are the minimum and maximum values of feature $A$ in $D$.

   – If $A$ is numeric, choose $a \in \mathbf{A}$ such that $a = (x_k + x_l)/2$, where $x_k$, $x_l$ are consecutive elements in the ordered value list of feature $A$ in $D$.

2. For node $t$ of a decision tree generate all splittings of the above type.

3. Choose a splitting from the set of splittings that maximizes the impurity reduction $\Delta\iota$ :

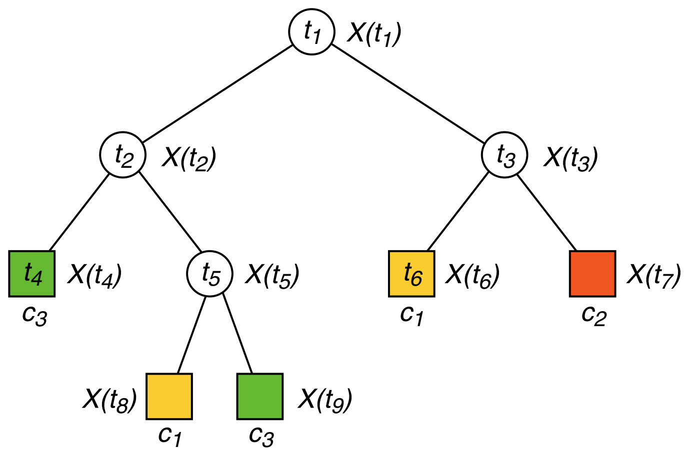
$$\Delta\iota\big(D(t),\ \{D(t_L), D(t_R)\}\big) \ = \ \iota(t) - \frac{|D_L|}{|D|} \cdot \iota(t_L) - \frac{|D_R|}{|D|} \cdot \iota(t_R),$$

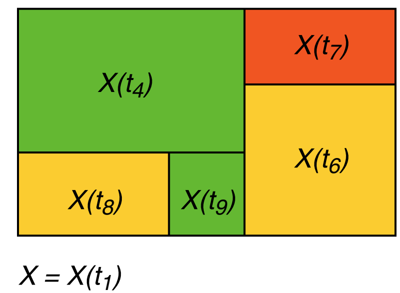
where $t_L$ and $t_R$ denote the left and right successor of $t$.

# Decision Tree Algorithms

## CART Algorithm (continued)

Illustration for two numeric features, i.e., the feature space $X$ corresponds to a two-dimensional plane:




By a sequence of splittings the feature space $X$ is partitioned into rectangles that are parallel to the two axes.