

Chapter ML:III

III. Decision Trees

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

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.
- $c : X \rightarrow C$ is the ideal classifier for X .
- $D = \{(\mathbf{x}_1, c(\mathbf{x}_1)), \dots, (\mathbf{x}_n, c(\mathbf{x}_n))\} \subseteq X \times C$ is a set of examples.

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

Decision Tree Algorithms

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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 $\{a_1, \dots, a_k\}$:

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

2. Splitting criterion is the 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 $\setminus \{A^*\}$, 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()*
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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* = argmax_{A ∈ Attributes} (informationGain(D, A))*
- 6.
- 7.

Decision Tree Algorithms

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

ID3(D, Attributes, Target)

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

 ELSE
 $\text{createEdge}(t, a, \text{ID3}(D_a, \text{Attributes} \setminus \{A^*\}, \text{Target}))$
 ENDIF
 ENDDO
7. $\text{return}(t)$

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. $A^* = \operatorname{argmax}_{A \in \text{Attributes}} (\text{informationGain}(D, A))$
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:

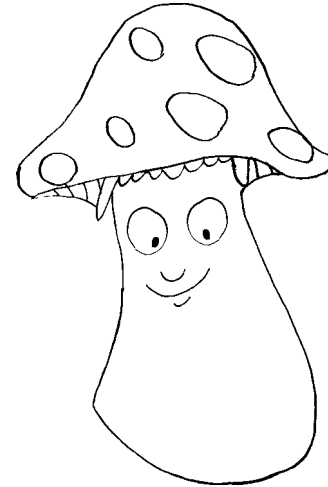
- ❑ “*Target*” designates the feature (= attribute) that is comprised of the labels according to which an example can be classified. Within Mitchell’s algorithm the respective class labels are ‘+’ and ‘−’, modeling the binary classification situation. In the pseudo code version, *Target* may contain multiple (more than two) classes.
- ❑ Step 3 of the [ID3 algorithm](#) checks the purity of D and, given this case, assigns the unique class c , $c \in \text{dom}(\textit{Target})$, 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”:

		toxic	eatable	$\rightarrow \quad D_{\text{red}} = 2, D_{\text{brown}} = 2, D_{\text{green}} = 1$
$D _{\text{color}} =$	red	1	1	
	brown	0	2	
	green	0	1	

Estimated a-priori probabilities:

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

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

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Conditional entropy values for all attributes:

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

$$H(C \mid \text{size}) \approx 0.55$$

$$H(C \mid \text{points}) = 0.4$$

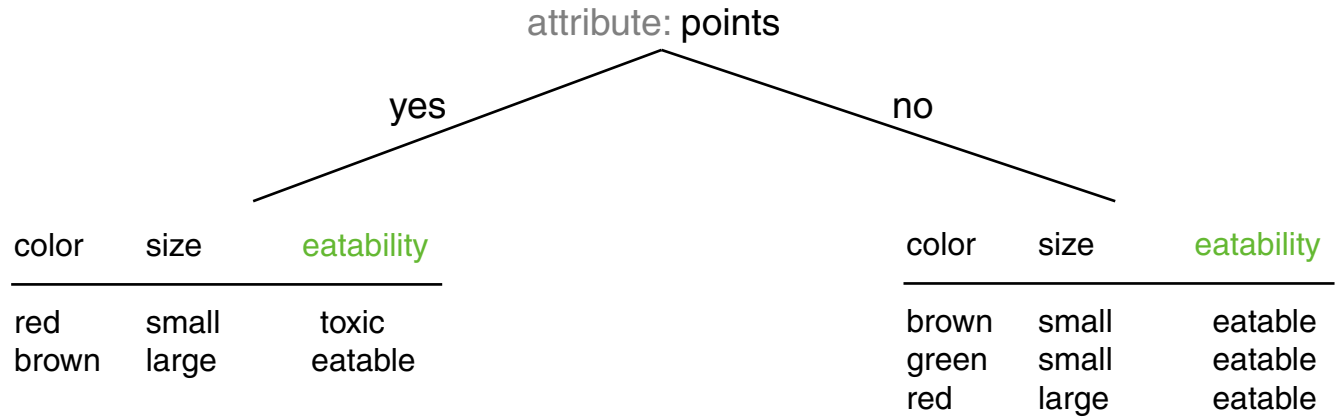
Remarks:

- ❑ 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:

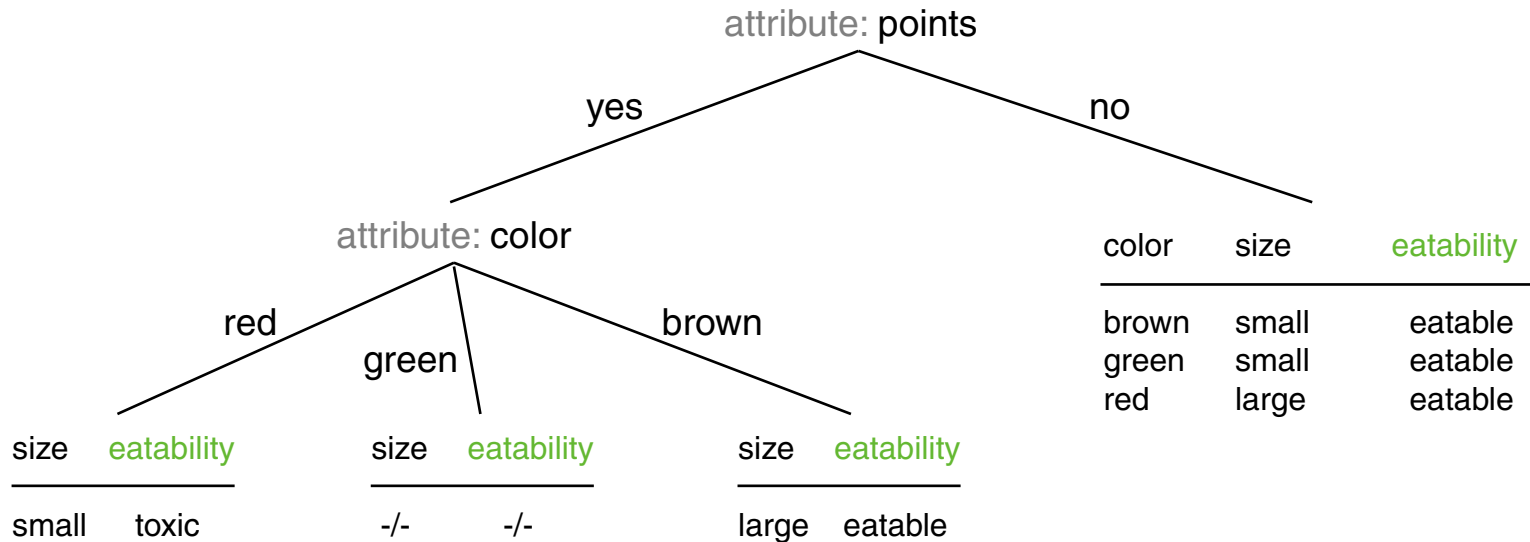


The feature “points” was chosen in Step 5 of the ID3 algorithm.

Decision Tree Algorithms

ID3 Algorithm: Example (continued)

Decision tree before the second recursion step:

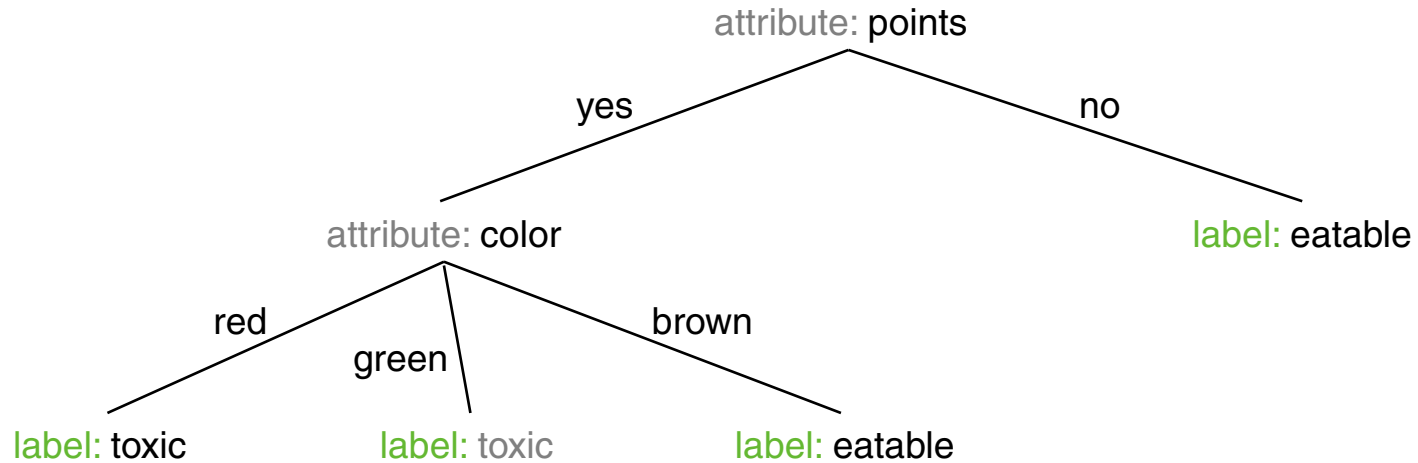


The feature “color” was chosen in Step 5 of the ID3 algorithm.

Decision Tree Algorithms

ID3 Algorithm: Example (continued)

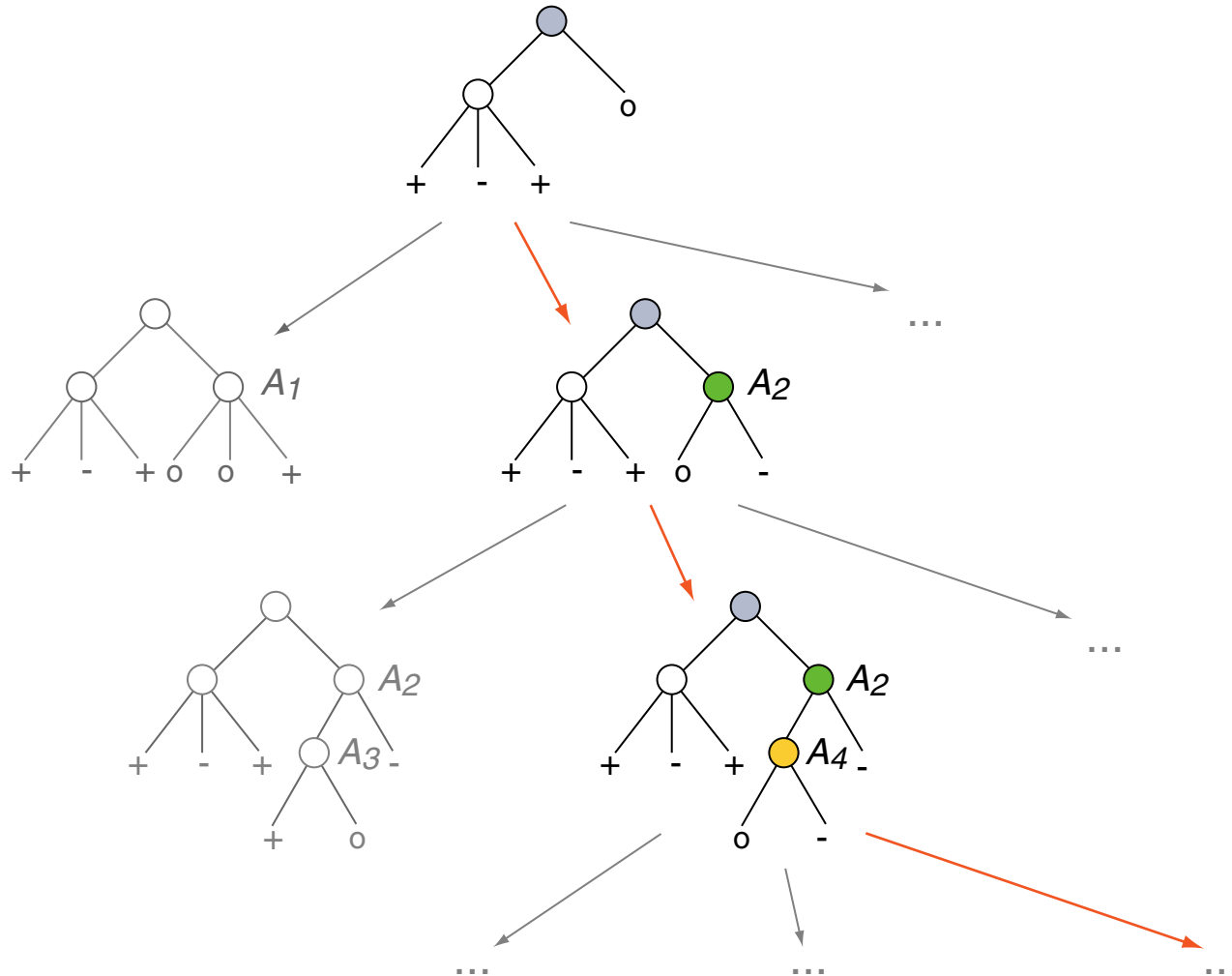
Final decision tree after second recursion step:



Break of a tie: choosing the class “toxic” for D_{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

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 - 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
 - *local* optimization of decision trees

Decision Tree Algorithms

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Where the inductive bias of the ID3 algorithm becomes manifest:

- ❑ Small decision trees are preferred.
- ❑ 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 , $j = 1, \dots, p$, 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 , $h : \mathbf{A}_1 \times \dots \times \mathbf{A}_p \rightarrow C$. 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] :

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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 $x_{\min} < a < x_{\max}$, where x_{\min} , x_{\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

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 - 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 $\Delta \iota$:

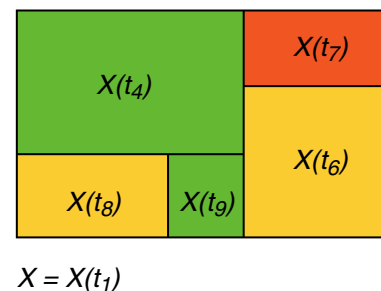
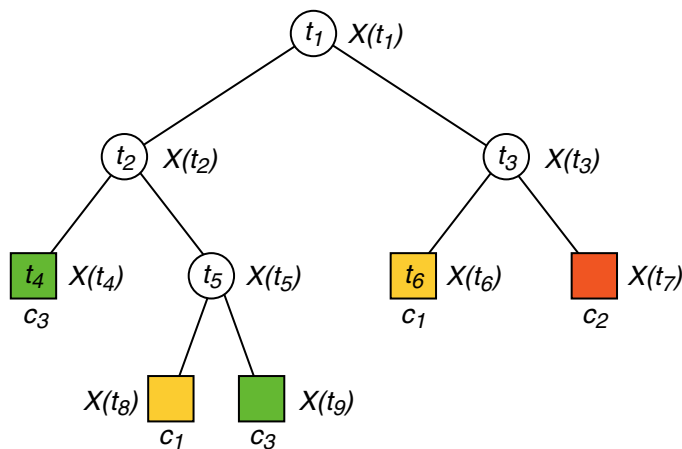
$$\Delta \iota(D(t), \{D(t_L), D(t_R)\}) = \iota(t) - \frac{|D_L|}{|D|} \cdot \iota(t_L) - \frac{|D_R|}{|D|} \cdot \iota(t_R),$$

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.