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.
- $c : X \to C$ 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

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

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

2. Splitting criterion is 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 \ {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

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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. $A^* = \text{argmax}_{A \in \textit{Attributes}}(\textit{informationGain}(D, A))$
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Decision Tree Algorithms

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4. **IF** *Attributes* $= \emptyset$ **THEN** *return*(t) **ENDIF**
5. $A^* = \text{argmax}_{A \in \mathit{Attributes}}(\mathit{informationGain}(D, A))$
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:

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

Decision Tree Algorithms

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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:

attribute: points

yes

color	size	eatability
red	small	toxic
brown	large	eatable

no

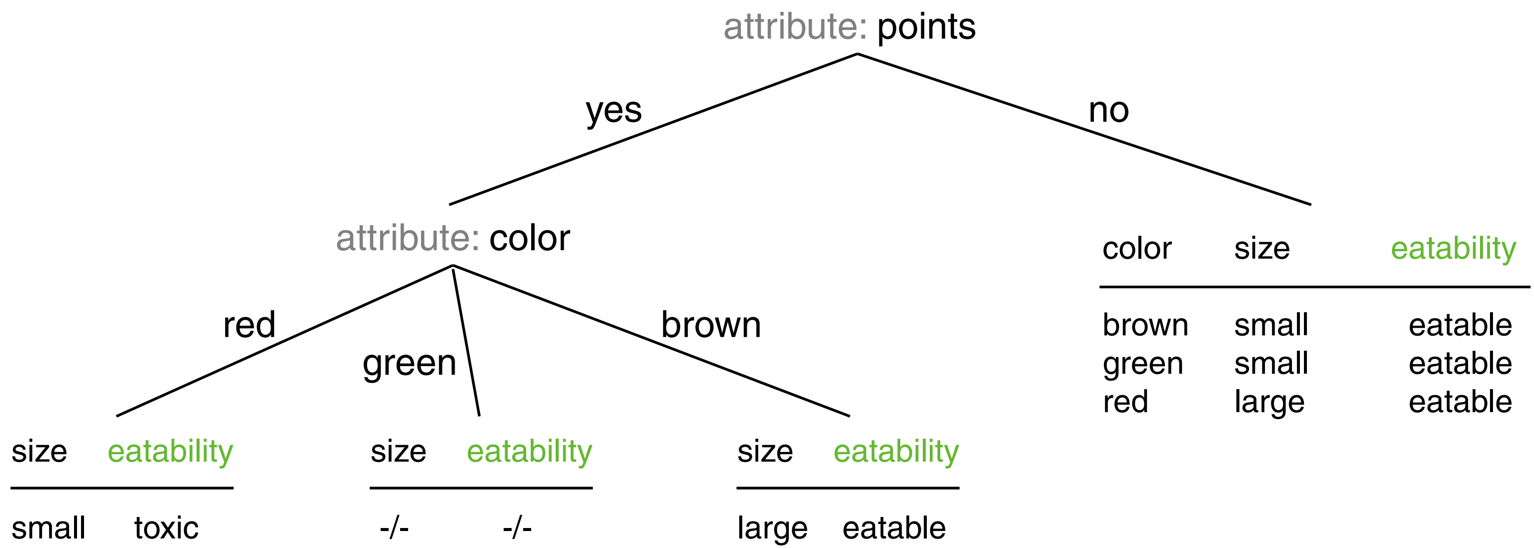
color	size	eatability
brown	small	eatable
green	small	eatable
red	large	eatable

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:

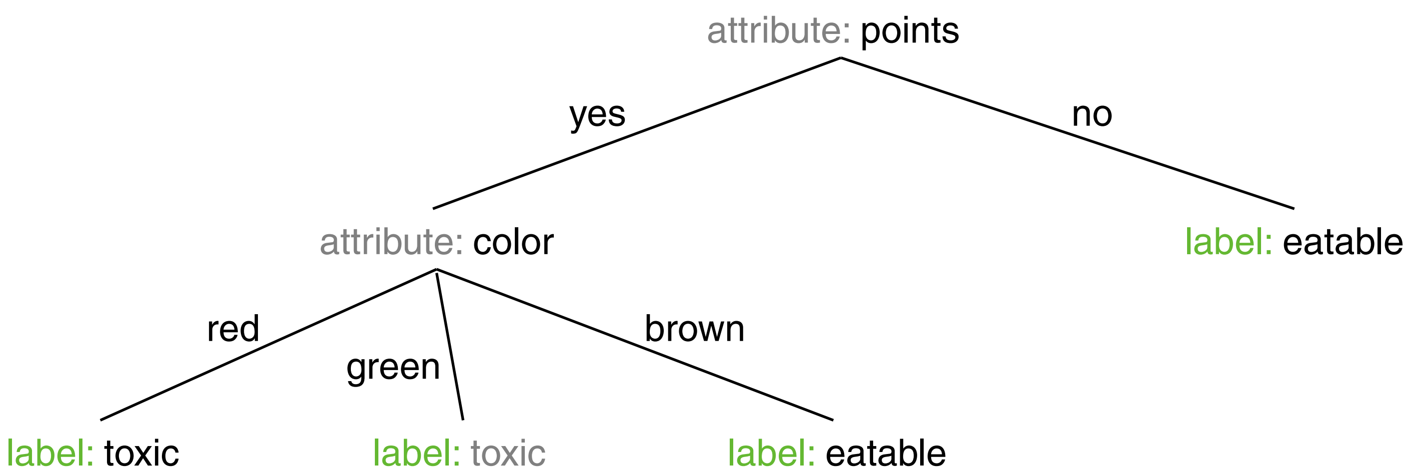


The feature “color” was chosen in Step 5 of the ID3 algorithm.

Decision Tree Algorithms

ID3 Algorithm: Example (continued)

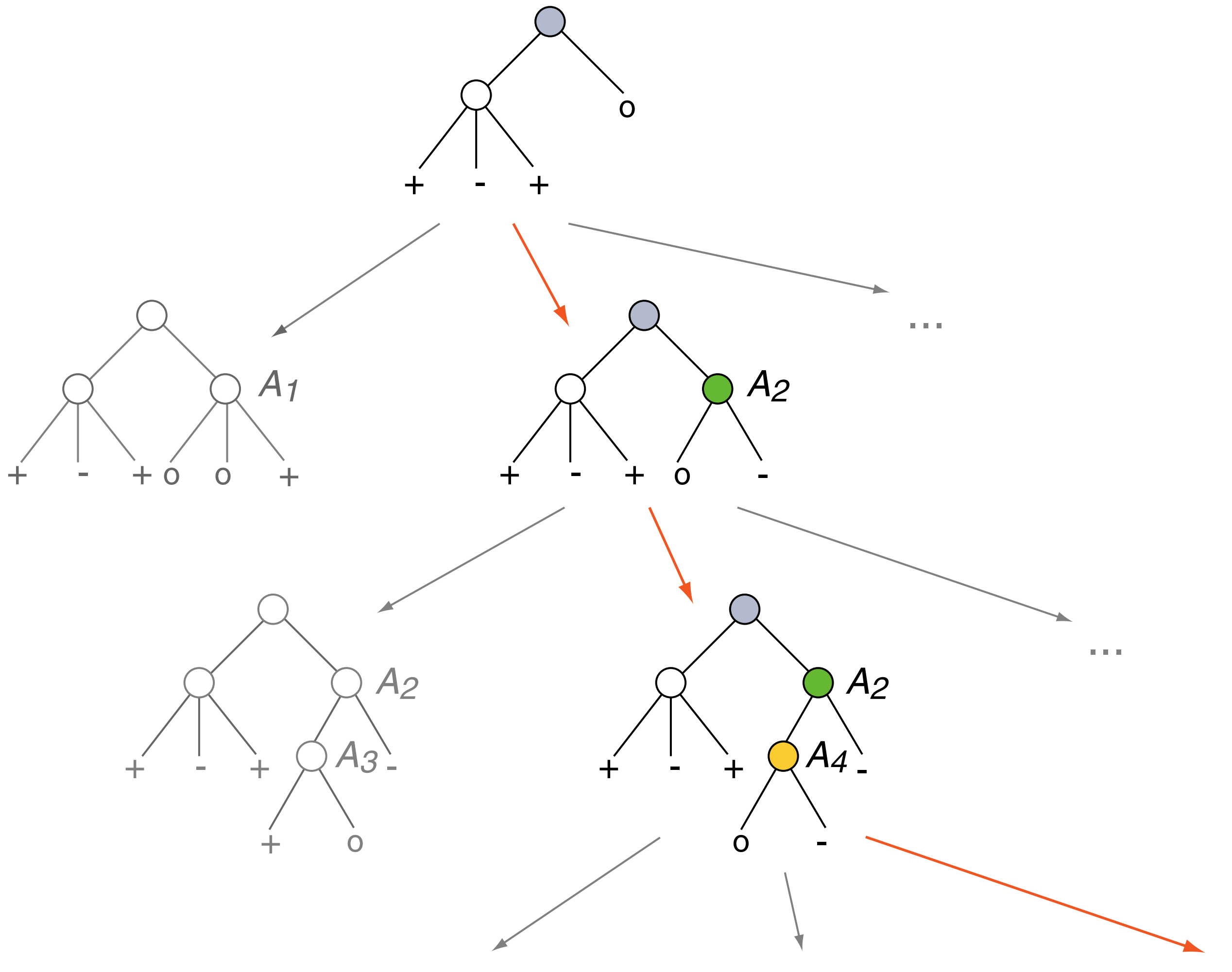
Final decision tree after second recursion step:



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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- 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
  - ➜ *local* optimization of decision trees

Decision Tree Algorithms

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  - ➜ no backtracking takes place
  - ➜ *local* optimization of decision trees

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] :

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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.

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_{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.

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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 $\Delta\iota$:

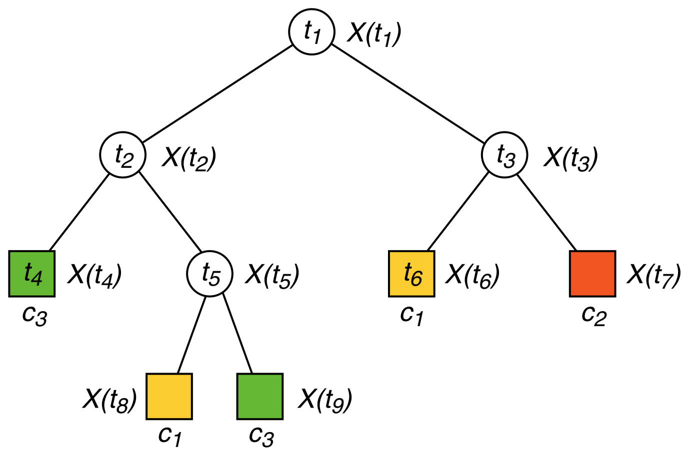
$$\Delta\iota\big(D(t),\ \{D(t_L), D(t_R)\}\big) \ = \ \iota(t) - \frac{|D_L|}{|D|} \cdot \iota(t_L) - \frac{|D_R|}{|D|} \cdot \iota(t_R),$$

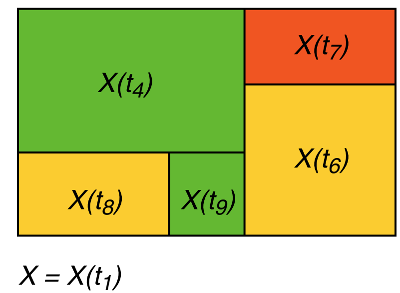
where t_L and t_R denote the left and right successor of t.

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.