# Chapter ML:III

## III. Decision Trees

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


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# Decision Trees Basics

## Specification of Classification Problems [ML Introduction]

Characterization of the model (model world):

- $X$ 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.


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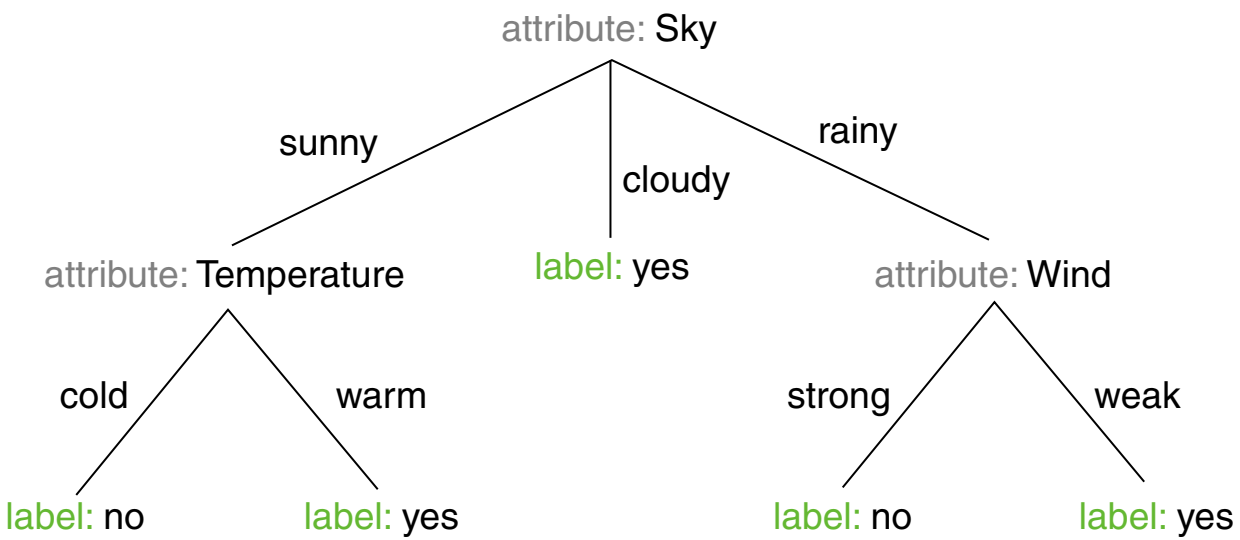
# Decision Trees Basics

## Decision Tree for the Concept “EnjoySport”

| Example | Sky | Temperature | Humidity | Wind | Water | Forecast | EnjoySport |
|---|---|---|---|---|---|---|---|
| 1 | sunny | warm | normal | strong | warm | same | yes |
| 2 | sunny | warm | high | strong | warm | same | yes |
| 3 | rainy | cold | high | strong | warm | change | no |
| 4 | sunny | warm | high | strong | cool | change | yes |





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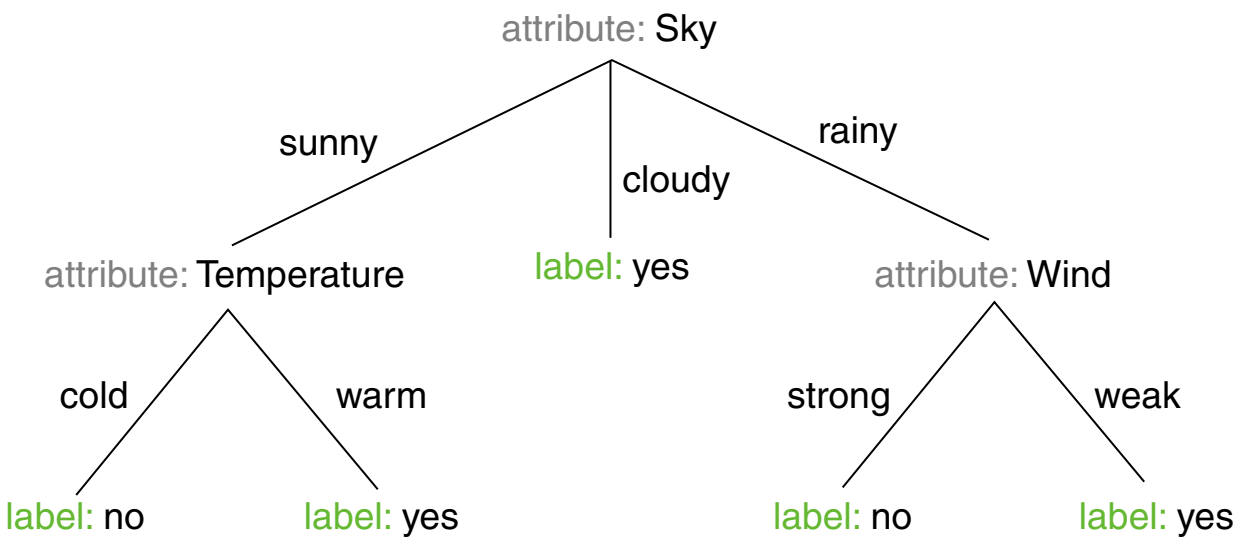


Partitioning of $X$ at the root node:

$$X = \{\mathbf{x} \in X : \mathbf{x}|_{\text{Sky}} = \text{sunny}\} \cup \{\mathbf{x} \in X : \mathbf{x}|_{\text{Sky}} = \text{cloudy}\} \cup \{\mathbf{x} \in X : \mathbf{x}|_{\text{Sky}} = \text{rainy}\}$$


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# Decision Trees Basics

## Definition 1 (Splitting)

Let $X$ be feature space and let $D$ be a set of examples. A splitting of $X$ is a partitioning of $X$ into mutually exclusive subsets $X_1, \ldots, X_s$. I.e., $X = X_1 \cup \ldots \cup X_s$ with $X_j \neq \emptyset$ and $X_j \cap X_{j'} = \emptyset$, where $j, j' \in \{1, \ldots, s\}, j \neq j'$.

A splitting $X_1, \ldots, X_s$ of $X$ induces a splitting $D_1, \ldots, D_s$ of $D$, where $D_j$, $j = 1, \ldots, s$, is defined as $\{(\mathbf{x}, c(\mathbf{x})) \in D \mid \mathbf{x} \in X_j\}$.


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A splitting depends on the measurement scale of a feature:

1. $m$-ary splitting induced by a (nominal) feature $A$ with finite domain:

   $$A = \{a_1, \ldots, a_m\}: \quad X = \{\mathbf{x} \in X : \mathbf{x}|_A = a_1\} \cup \ldots \cup \{\mathbf{x} \in X : \mathbf{x}|_A = a_m\}$$


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2. Binary splitting induced by a (nominal) feature $A$:
   $$A' \subset A: \qquad X = \{\mathbf{x} \in X : \mathbf{x}|_A \in A'\} \cup \{\mathbf{x} \in X : \mathbf{x}|_A \notin A'\}$$

3. Binary splitting induced by an ordinal feature $A$:
   $$v \in \mathit{dom}(A): \qquad X = \{\mathbf{x} \in X : \mathbf{x}|_A \succeq v\} \cup \{\mathbf{x} \in X : \mathbf{x}|_A \prec v\}$$


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Remarks:

- The syntax $\mathbf{x}|_A$ denotes the projection operator, which returns that vector component (dimension) of $\mathbf{x} = (x_1, \ldots, x_p)$ that is associated with $A$. Without loss of generality this projection can be presumed being unique.
- A splitting of $X$ into two disjoint, non-empty subsets is called a binary splitting.
- We consider only splittings of $X$ that are induced by a splitting of a single feature $A$ of $X$. Keyword: monothetic splitting


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# Decision Trees Basics

## Definition 2 (Decision Tree)

Let $X$ be feature space and let $C$ be a set of classes. A decision tree $T$ for $X$ and $C$ is a finite tree with a distinguished root node. A non-leaf node $t$ of $T$ has assigned (1) a set $X(t) \subseteq X$, (2) a splitting of $X(t)$, and (3) a one-to-one mapping of the subsets of the splitting to its successors.

$X(t) = X$ iff $t$ is root node. A leaf node of $T$ has assigned a class from $C$.


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# Decision Trees Basics

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$X(t) = X$ iff $t$ is root node. A leaf node of $T$ has assigned a class from $C$.

Classification of some $\mathbf{x} \in X$ given a decision tree $T$:

1. Find the root node of $T$.
2. If $t$ is a non-leaf node, find among its successors that node whose subset of the splitting of $X(t)$ contains $\mathbf{x}$. Repeat this step.
3. If $t$ is a leaf node, label $\mathbf{x}$ with the respective class.

➜ The set of possible decision trees forms the hypothesis space $H$.


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Remarks:

- The classification of an $\mathbf{x} \in X$ determines a unique path from the root node of $T$ to some leaf node of $T$.
- At each non-leaf node a particular feature of $\mathbf{x}$ is evaluated in order to find the next node along with a possible next feature to be analyzed.
- Each path from the root node to some leaf node corresponds to a conjunction of feature values, which are successively tested. This test can be formulated as a decision rule. Example:

  IF Sky=rainy AND Wind=weak THEN EnjoySport=yes

  If all tests in $T$ are of the kind shown in the example, namely, a comparison with a single feature value, all feature domains must be finite.
- If in all non-leaf nodes of $T$ only one feature is evaluated at a time, $T$ is called a *monothetic* decision tree. Examples for *polythetic* decision trees are the so-called oblique decision trees.
- Decision trees became popular in 1986, with the introduction of the ID3 Algorithm by J. R. Quinlan.


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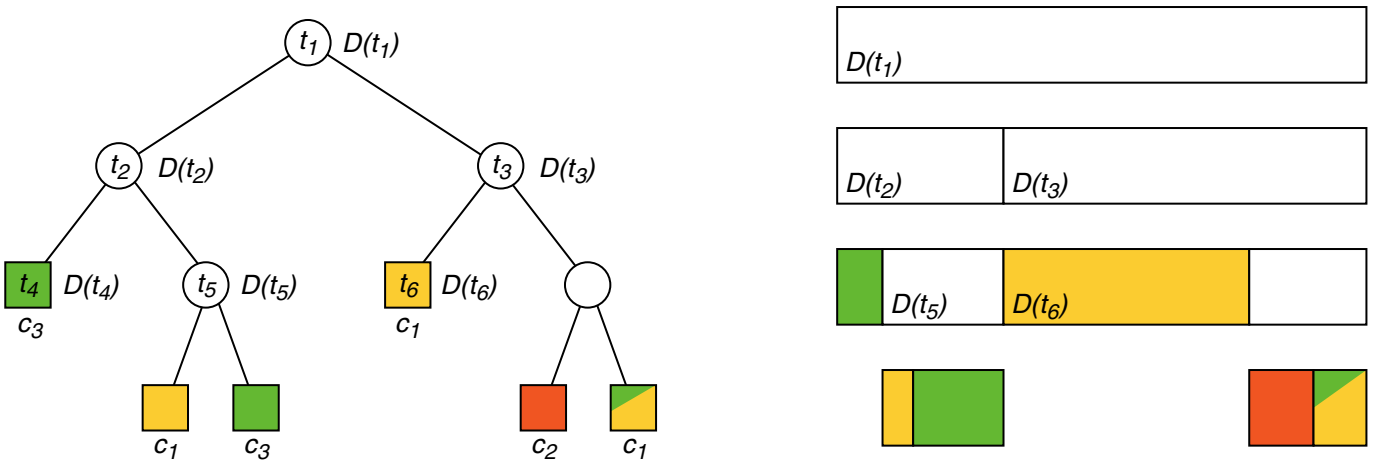
# Decision Trees Basics

## Notation

Let $T$ be decision tree for $X$ and $C$, let $D$ be a set of examples, and let $t$ be a node of $T$. Then we agree on the following notation:

- $X(t)$ denotes the subset of the feature space $X$ that is represented by $t$. (as used in the decision tree definition)
- $D(t)$ denotes the subset of the example set $D$ that is represented by $t$, where $D(t) = \{(\mathbf{x}, c(\mathbf{x})) \in D \mid \mathbf{x} \in X(t)\}$. (see the splitting definition)

Illustration:





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Remarks:

- The set $X(t)$ is comprised of those members $\mathbf{x}$ of $X$ that are filtered by a path from the root node of $T$ to the node $t$.
- *leaves*$(T)$ denotes the set of all leaf nodes of $T$.
- A single node $t$ of a decision tree $T$, and hence $T$ itself, encode a piecewise constant function. This way, $t$ as well as $T$ can form complex non-linear classifiers. The functions encoded by $t$ and $T$ differ in the number of evaluated features of $\mathbf{x}$, which is one for $t$ and the tree height for $T$.
- In the following we will use the symbols "$t$" and "$T$" to denote also the classifiers that are encoded by a node $t$ and a tree $T$ respectively:

$$t, T : X \to C \quad \text{(instead of } y_t, y_T : X \to C\text{)}$$


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# Decision Trees Basics

## Algorithm Template: Construction

| | | |
|---|---|---|
| Algorithm: | *DT-construct* | Decision Tree Construction |
| Input: | $D$ | (Sub)set of examples. |
| Output: | $t$ | Root node of a decision (sub)tree. |

*DT−construct*$(D)$

1. $t =$ *newNode*$()$
   *label*$(t) =$ *representativeClass*$(D)$
2. **IF** *impure*$(D)$
   **THEN** *criterion* $=$ *splitCriterion*$(D)$
   **ELSE** *return*$(t)$
3. $\{D_1, \ldots, D_s\} =$ *decompose*$(D,$ *criterion*$)$
4. **FOREACH** $D'$ **IN** $\{D_1, \ldots, D_s\}$ **DO**
   *addSuccessor*$(t,$ *DT−construct*$(D'))$
   **ENDDO**
5. *return*$(t)$

[Illustration]


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# Decision Trees Basics

## Algorithm Template: Classification

| | | |
|---|---|---|
| Algorithm: | *DT-classify* | Decision Tree Classification |
| Input: | $\mathbf{x}$ | Feature vector. |
| | $t$ | Root node of a decision (sub)tree. |
| Output: | $y(\mathbf{x})$ | Class of feature vector $\mathbf{x}$ in the decision (sub)tree below $t$. |

*DT*$-$*classify*$(\mathbf{x}, t)$

```
1. IF isLeafNode(t)
   THEN return(label(t))
   ELSE return(DT-classify(x, splitSuccessor(t, x))
```


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Remarks:

- Since *DT-construct* assigns to each node of a decision tree $T$ a class, each subtree of $T$ (as well as each pruned version of a subtree of $T$) represents a valid decision tree on its own.
- Functions of *DT-construct*:
  - *representativeClass*$(D)$
    Returns a representative class for the example set $D$. Note that, due to pruning, each node may become a leaf node.
  - *impure*$(D)$
    Evaluates the (im)purity of a set $D$ of examples.
  - *splitCriterion*$(D)$
    Returns a split criterion for $X(t)$ based on the examples in $D(t)$.
  - *decompose*$(D, \textit{criterion})$
    Returns a splitting of $D$ according to *criterion*.
  - *addSuccessor*$(t, t')$
    Inserts the successor $t'$ for node $t$.
- Functions of *DT-classify*:
  - *isLeafNode*$(t)$
    Tests whether $t$ is a leaf node.
  - *splitSuccessor*$(t, \mathbf{x})$
    Returns the (unique) successor $t'$ of $t$ for which $\mathbf{x} \in X(t')$ holds.


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# Decision Trees Basics

## When to Use Decision Trees

Problem characteristics that may suggest a decision tree classifier:

- the objects can be described by feature-value combinations.
- the domain and range of the target function are discrete
- hypotheses take the form of disjunctions
- the training set contains noise

Selected application areas:

- medical diagnosis
- fault detection in technical systems
- risk analysis for credit approval
- basic scheduling tasks such as calendar management
- classification of design flaws in software engineering


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# Decision Trees Basics

## On the Construction of Decision Trees

- How to exploit an example set both efficiently and effectively?
- According to what rationale should a node become a leaf node?
- How to assign a class for nodes of impure example sets?
- How to evaluate decision tree performance?


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# Decision Trees Basics

## Performance of Decision Trees

1. Size

2. Classification error


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# Decision Trees Basics

## Performance of Decision Trees

1. Size

   Among those theories that can explain an observation, the most simple one is to be preferred *(Ockham's Razor)*:

   *Entia non sunt multiplicanda sine necessitate.*

   [Johannes Clauberg 1622-1665]

   Here: among all decision trees of minimum classification error we choose the one of smallest size.

2. Classification error

   Quantifies the rigor according to which a class label is assigned to $\mathbf{x}$ in a leaf node of $T$, based on the examples in $D$.

   If all leaf nodes of a decision tree $T$ represent a single example of $D$, the classification error of $T$ with respect to $D$ is zero.


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# Decision Trees Basics

## Performance of Decision Trees: Size

- Leaf node number
- Tree height
- External path length
- Weighted external path length


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# Decision Trees Basics

## Performance of Decision Trees: Size

- Leaf node number

  The leaf node number corresponds to number of rules that are encoded in a decision tree.

- Tree height

  The tree height corresponds to the maximum rule length and bounds the number of premises to be evaluated to reach a class decision.

- External path length

  The external path length totals the lengths of all paths from the root of a tree to its leaf nodes. It corresponds to the space to store all rules that are encoded in a decision tree.

- Weighted external path length

  The weighted external path length is defined as the external path length whereas each length value is weighted by the number of examples in $D$ that are classified by this path.


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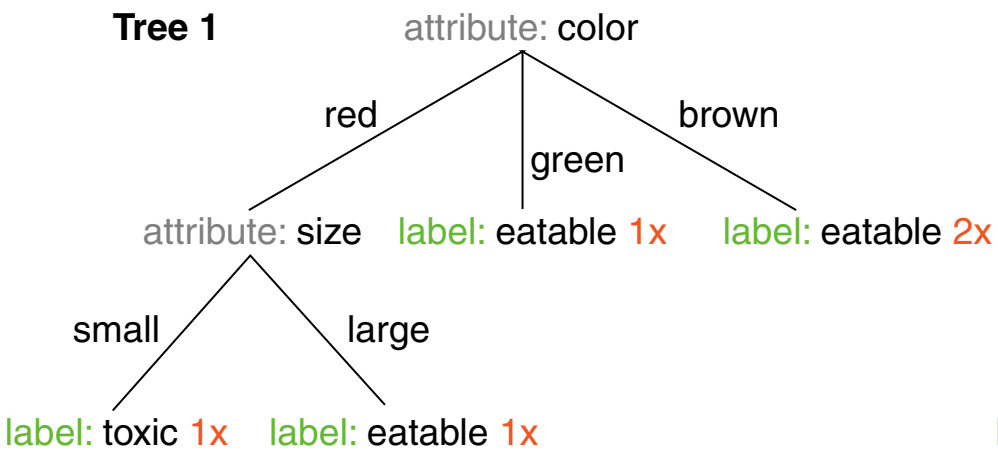
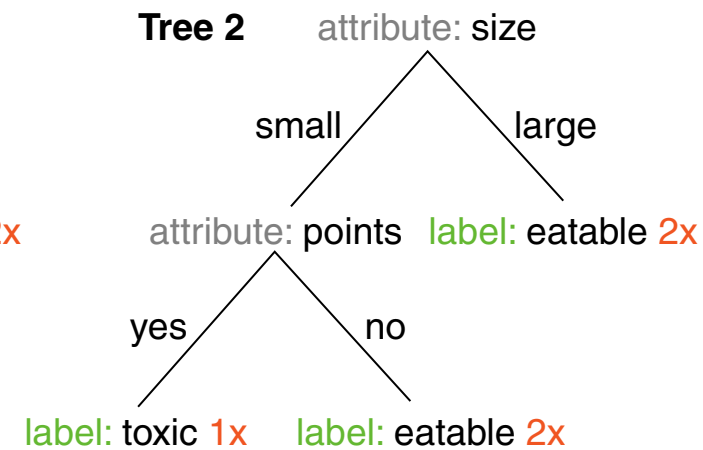
# Decision Trees Basics

## Performance of Decision Trees: Size (continued)

Both trees below correctly classify all examples in $D$:




| Criterion | Tree 1 | Tree 2 |
|---|---|---|
| Leaf node number | 4 | 3 |
| Tree height | 2 | 2 |
| External path length | 6 | 5 |
| Weighted external path length | 7 | 8 |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# Decision Trees Basics

## Performance of Decision Trees: Size (continued)

**Theorem 3 (External Path Length Bound)**

The problem to decide for a set of examples $D$ whether or not a decision tree exists whose external path length is bounded by $b$, is NP-complete.


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# Decision Trees Basics

## Performance of Decision Trees: Classification Error

Given a decision tree $T$, a set of examples $D$, and a node $t$ of $T$ that represents the example subset $D(t) \subseteq D$. Then, the class that is assigned to $t$, *label*$(t)$, is defined as follows:

$$\textit{label}(t) = \operatorname*{argmax}_{c \in C} \frac{|\{(\mathbf{x}, c(\mathbf{x})) \in D(t) : c(\mathbf{x}) = c\}|}{|D(t)|}$$


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Misclassification rate of node classifier $t$ wrt. $D(t)$:

$$\textit{Err}(t, D(t)) = \frac{|\{(\mathbf{x}, c(\mathbf{x})) \in D(t) : c(\mathbf{x}) \neq \textit{label}(t)\}|}{|D(t)|} = 1 - \max_{c \in C} \frac{|\{(\mathbf{x}, c(\mathbf{x})) \in D(t) : c(\mathbf{x}) = c\}|}{|D(t)|}$$


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Misclassification rate of decision tree classifier $T$ wrt. $D(t)$:

$$\textit{Err}(T, D) = \sum_{t \in \textit{leaves}(T)} \frac{|D(t)|}{|D|} \cdot \textit{Err}(t, D(t))$$


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Remarks:

- Observe the difference between $\max(f)$ and $\operatorname{argmax}(f)$. Both expressions maximize $f$, whereas the former returns the maximum $f$-value (the image) while the latter returns the argument (the preimage) for which $f$ becomes maximum:
  - $\max_{c \in C}(f(c)) = \max\{f(c) \mid c \in C\}$
  - $\operatorname{argmax}_{c \in C}(f(c)) = c^* \quad \Rightarrow \; f(c^*) = \max_{c \in C}(f(c))$

- The classifiers $t$ and $T$ may not have been constructed using $D(t)$ as training data. Stated another way, the example set $D(t)$ is in the role of a holdout test set.

- The true misclassification rate $\mathit{Err}^*(T)$ is based on a probability measure $P$ on $X \times C$ (and not on relative frequencies). For a node $t$ of $T$ this probability becomes minimum iff:

$$\mathit{label}(t) = \operatorname*{argmax}_{c \in C} \; P(c \mid X(t))$$

- If $D$ has been used as training set, a reliable interpretation of the (training) error $\mathit{Err}(T, D)$ in terms of $\mathit{Err}^*(T)$ requires the Inductive Learning Hypothesis to hold. This implies, among others, that the distribution of $C$ over the feature space $X$ corresponds to the distribution of $C$ over the training set $D$.


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# Decision Trees Basics

## Performance of Decision Trees: Misclassification Costs

Given a decision tree $T$, a set of examples $D$, and a node $t$ of $T$ that represents the example subset $D(t) \subseteq D$. In addition, we are given a cost measure for the misclassification. Then, the class that is assigned to $t$, *label*$(t)$, is defined as follows:

$$\textit{label}(t) = \operatorname*{argmin}_{c' \in C} \sum_{c \in C} \frac{|\{(\mathbf{x}, c(\mathbf{x})) \in D(t) : c(\mathbf{x}) = c\}|}{|D(t)|} \cdot \textit{cost}(c' \mid c)$$


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# Decision Trees Basics

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Misclassification costs of node classifier $t$ wrt. $D(t)$ :

$$\textit{Err}_{\textit{cost}}(t, D(t)) = \frac{1}{|D_t|} \cdot \sum_{(\mathbf{x}, c(\mathbf{x})) \in D(t)} \textit{cost}(\textit{label}(t) | c(\mathbf{x})) = \min_{c' \in C} \sum_{c \in C} \frac{|\{(\mathbf{x}, c(\mathbf{x})) \in D(t) : c(\mathbf{x}) = c\}|}{|D(t)|} \cdot \textit{cost}(c' | c)$$


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Misclassification costs of node classifier $t$ wrt. $D(t)$:

$$\textit{Err}_{\textit{cost}}(t, D(t)) = \frac{1}{|D_t|} \cdot \sum_{(\mathbf{x}, c(\mathbf{x})) \in D(t)} \textit{cost}(\textit{label}(t) | c(\mathbf{x})) = \min_{c' \in C} \sum_{c \in C} \frac{|\{(\mathbf{x}, c(\mathbf{x})) \in D(t) : c(\mathbf{x}) = c\}|}{|D(t)|} \cdot \textit{cost}(c' | c)$$

Misclassification costs of decision tree classifier $T$ wrt. $D(t)$:

$$\textit{Err}_{\textit{cost}}(T, D) = \sum_{t \in \textit{leaves}(T)} \frac{|D(t)|}{|D|} \cdot \textit{Err}_{\textit{cost}}(t, D(t))$$


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Remarks:

- Again, observe the difference between $\min(f)$ and $\operatorname{argmin}(f)$. Both expressions minimize $f$, whereas the former returns the minimum $f$-value (the image) while the latter returns the argument (the preimage) for which $f$ becomes minimum.


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# Impurity Functions

## Splitting

Let $t$ be a leaf node of an incomplete decision tree, and let $D(t)$ be the subset of the example set $D$ that is represented by $t$. [Illustration]

Possible criteria for a splitting of $X(t)$ :

1. Size of $D(t)$.

2. Purity of $D(t)$.

3. Ockham's Razor.


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# Impurity Functions

## Splitting

Let $t$ be a leaf node of an incomplete decision tree, and let $D(t)$ be the subset of the example set $D$ that is represented by $t$. [Illustration]

Possible criteria for a splitting of $X(t)$ :

1. Size of $D(t)$.
   $D(t)$ will not be partitioned further if the number of examples, $|D(t)|$, is below a certain threshold.

2. Purity of $D(t)$.
   $D(t)$ will not be partitioned further if all examples in $D$ are members of the same class.

3. Ockham's Razor.
   $D(t)$ will not be partitioned further if the resulting decision tree is not improved significantly by the splitting.


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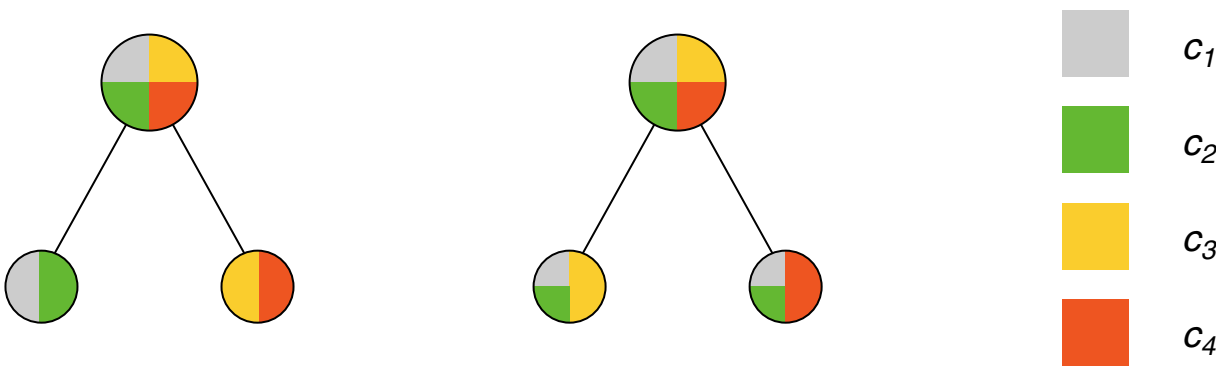
# Impurity Functions

## Splitting (continued)

Let $D$ be a set of examples over a feature space $X$ and a set of classes $C = \{c_1, c_2, c_3, c_4\}$. Distribution of $D$ for two possible splittings of $X$ :





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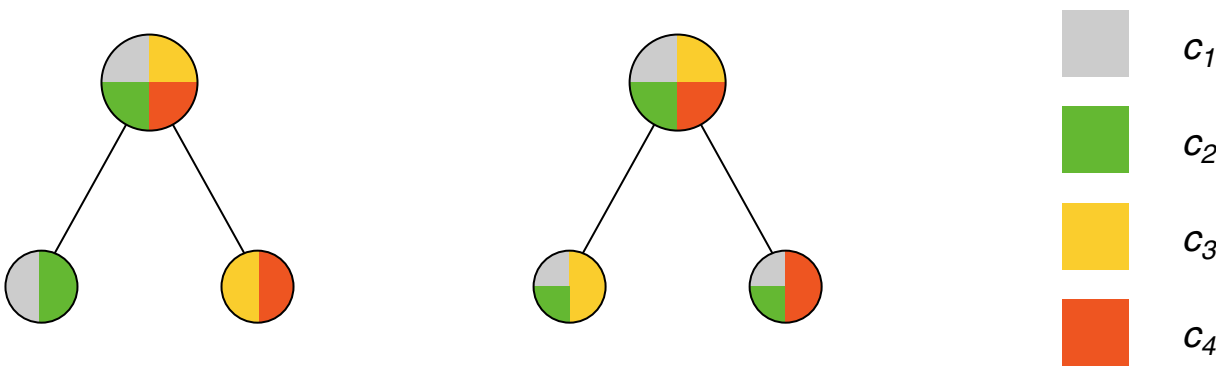
# Impurity Functions

## Splitting (continued)

Let $D$ be a set of examples over a feature space $X$ and a set of classes $C = \{c_1, c_2, c_3, c_4\}$. Distribution of $D$ for two possible splittings of $X$ :




- The left splitting should be preferred, since it minimizes the *impurity* of the subsets of $D$ in the leaf nodes. The argumentation presumes that the misclassification costs are independent of the classes in $C$.
- The impurity is a function defined on $\mathcal{P}(D)$, the set of all subsets of an example set $D$.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# Impurity Functions

**Definition 4 (Impurity Function $\iota$)**

Let $k \in \mathbf{N}$. An impurity function $\iota : [0;1]^k \to \mathbf{R}$ is a partial function defined on the standard $k-1$-simplex $\Delta^{k-1}$ for which the following properties hold:

(a) $\iota$ becomes minimum at points $(1, 0, \ldots, 0), (0, 1, \ldots, 0), \ldots, (0, \ldots, 0, 1)$.

(b) $\iota$ is symmetric with regard to its arguments, $p_1, \ldots, p_k$.

(c) $\iota$ becomes maximum at point $(1/k, \ldots, 1/k)$.


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# Impurity Functions

**Definition 5 (Impurity of an Example Set $\iota(D)$)**

Let $D$ be a set of examples, let $C = \{c_1, \ldots, c_k\}$ be set of classes, and let $c : X \to C$ be the ideal classifier for $X$. Moreover, let $\iota : [0; 1]^k \to \mathbf{R}$ an impurity function. Then, the impurity of $D$, denoted as $\iota(D)$, is defined as follows:

$$\iota(D) = \iota\left(\frac{|\{(\mathbf{x}, c(\mathbf{x})) \in D : c(\mathbf{x}) = c_1\}|}{|D|}, \ldots, \frac{|\{(\mathbf{x}, c(\mathbf{x})) \in D : c(\mathbf{x}) = c_k\}|}{|D|}\right)$$


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# Impurity Functions

**Definition 5 (Impurity of an Example Set $\iota(D)$)**

Let $D$ be a set of examples, let $C = \{c_1, \ldots, c_k\}$ be set of classes, and let $c : X \to C$ be the ideal classifier for $X$. Moreover, let $\iota : [0;1]^k \to \mathbf{R}$ an impurity function. Then, the impurity of $D$, denoted as $\iota(D)$, is defined as follows:

$$\iota(D) = \iota\left(\frac{|\{(\mathbf{x}, c(\mathbf{x})) \in D : c(\mathbf{x}) = c_1\}|}{|D|}, \ldots, \frac{|\{(\mathbf{x}, c(\mathbf{x})) \in D : c(\mathbf{x}) = c_k\}|}{|D|}\right)$$

**Definition 6 (Impurity Reduction $\Delta\iota$)**

Let $D_1, \ldots, D_s$ be a partitioning of an example set $D$, which is induced by a splitting of a feature space $X$. Then, the resulting impurity reduction, denoted as $\Delta\iota(D, \{D_1, \ldots, D_s\})$, is defined as follows:

$$\Delta\iota(D, \{D_1, \ldots, D_s\}) = \iota(D) - \sum_{j=1}^{s} \frac{|D_j|}{|D|} \cdot \iota(D_j)$$


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Remarks:

- The standard $k-1$-simplex comprises all $k$-tuples with non-negative elements that sum to $1$: $\Delta^{k-1} = \left\{(p_1, \ldots, p_k) \in \mathbf{R}^k : \sum_{i=1}^{k} p_i = 1 \text{ and } p_i \geq 0 \text{ for all } i\right\}$
- Observe the different domains of the impurity function $\iota$ in the Definitions 4 and 5, namely, $[0;1]^k$ and $D$. The domains correspond to each other: the set of examples, $D$, defines via its class portions an element from $[0;1]^k$ and vice versa.
- The properties in the definition of $\iota$ suggest to minimize the external path length of $T$ with respect to $D$ in order to minimize the overall impurity characteristics of $T$.
- Within the *DT-construct* algorithm usually a greedy strategy (local optimization) is employed to minimize the overall impurity characteristics of a decision tree $T$.


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# Impurity Functions

## Impurity Functions Based on the Misclassification Rate

Definition for two classes:

$$\iota_{misclass}(p_1, p_2) = 1 - \max\{p_1, p_2\} = \begin{cases} p_1 & \text{if } 0 \leq p_1 \leq 0.5 \\ 1 - p_1 & \text{otherwise} \end{cases}$$

$$\iota_{misclass}(D) = 1 - \max\left\{ \frac{|\{(\mathbf{x}, c(\mathbf{x})) \in D : c(\mathbf{x}) = c_1\}|}{|D|}, \frac{|\{(\mathbf{x}, c(\mathbf{x})) \in D : c(\mathbf{x}) = c_2\}|}{|D|} \right\}$$


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# Impurity Functions

## Impurity Functions Based on the Misclassification Rate

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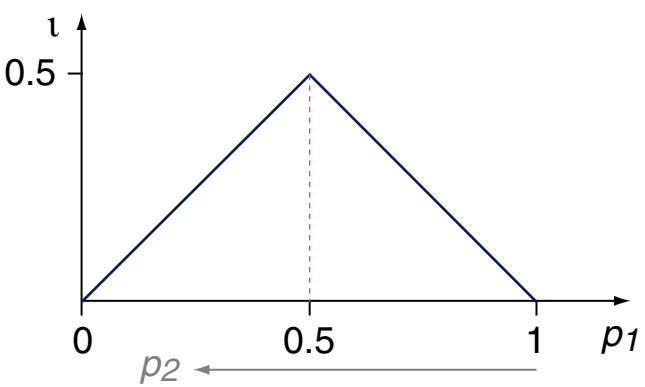
$$\iota_{misclass}(p_1, p_2) = 1 - \max\{p_1, p_2\} = \begin{cases} p_1 & \text{if } 0 \leq p_1 \leq 0.5 \\ 1 - p_1 & \text{otherwise} \end{cases}$$

$$\iota_{misclass}(D) = 1 - \max\left\{ \frac{|\{(\mathbf{x}, c(\mathbf{x})) \in D : c(\mathbf{x}) = c_1\}|}{|D|}, \frac{|\{(\mathbf{x}, c(\mathbf{x})) \in D : c(\mathbf{x}) = c_2\}|}{|D|} \right\}$$

Graph of the function $\iota_{misclass}(p_1, 1 - p_1)$:




[Graph: Entropy, Gini]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# Impurity Functions

## Impurity Functions Based on the Misclassification Rate (continued)

Definition for $k$ classes:

$$\iota_{misclass}(p_1, \ldots, p_k) = 1 - \max_{i=1,\ldots,k} p_i$$

$$\iota_{misclass}(D) = 1 - \max_{c \in C} \frac{|\{(\mathbf{x}, c(\mathbf{x})) \in D : c(\mathbf{x}) = c\}|}{|D|}$$


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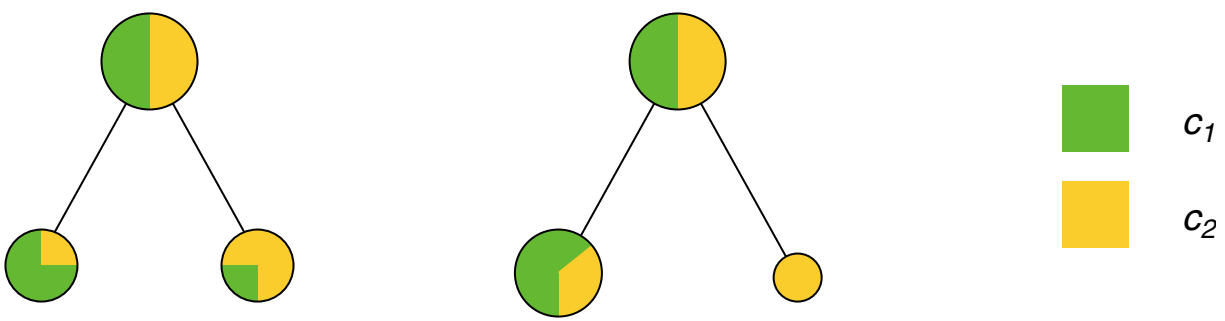
# Impurity Functions

## Impurity Functions Based on the Misclassification Rate (continued)

Problems:

- $\Delta\iota_{misclass} = 0$ may hold for all possible splittings.
- The impurity function that is induced by the misclassification rate underestimates pure nodes (see splitting on the right-hand side):





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# Impurity Functions

## Impurity Functions Based on the Misclassification Rate (continued)

Problems:

- $\Delta\iota_{misclass} = 0$ may hold for all possible splittings.
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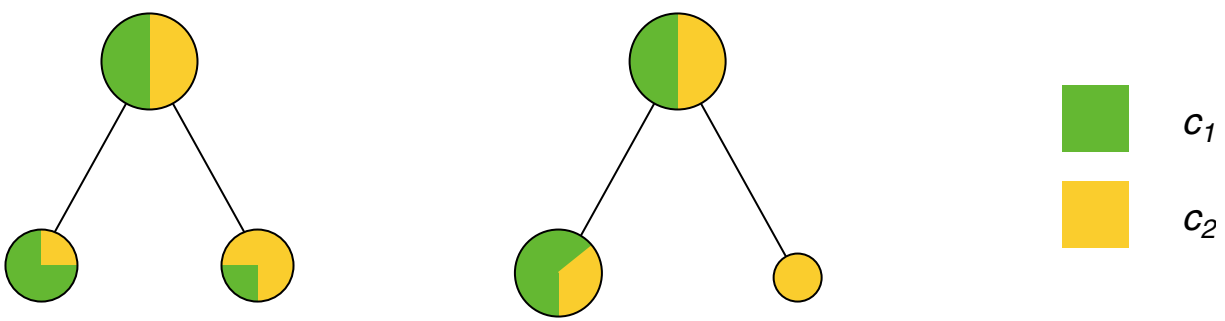


$$\Delta\iota_{misclass} = \iota_{misclass}(D) - \left(\frac{|D_1|}{|D|} \cdot \iota_{misclass}(D_1) + \frac{|D_2|}{|D|} \cdot \iota_{misclass}(D_2)\right)$$

left splitting: $\Delta\iota_{misclass} = \frac{1}{2} - (\frac{1}{2} \cdot \frac{1}{4} + \frac{1}{2} \cdot \frac{1}{4}) = \frac{1}{4}$

right splitting: $\Delta\iota_{misclass} = \frac{1}{2} - (\frac{3}{4} \cdot \frac{1}{3} + \frac{1}{4} \cdot 0) = \frac{1}{4}$


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# Impurity Functions

**Definition 7 (Strict Impurity Function)**

Let $\iota : [0;1]^k \to \mathbf{R}$ be an impurity function and let $\mathbf{p}, \mathbf{p}' \in \Delta^{k-1}$. Then $\iota$ is called strict, if it is strictly concave:

(c) $\to$ (c') $\quad \iota(\lambda\mathbf{p} + (1-\lambda)\mathbf{p}') > \lambda\,\iota(\mathbf{p}) + (1-\lambda)\,\iota(\mathbf{p}'), \quad 0 < \lambda < 1,\ \mathbf{p} \neq \mathbf{p}'$


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# Impurity Functions

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Let $\iota : [0;1]^k \to \mathbf{R}$ be an impurity function and let $\mathbf{p}, \mathbf{p}' \in \Delta^{k-1}$. Then $\iota$ is called strict, if it is strictly concave:

(c) $\to$ (c') $\quad \iota(\lambda\mathbf{p} + (1-\lambda)\mathbf{p}') > \lambda\,\iota(\mathbf{p}) + (1-\lambda)\,\iota(\mathbf{p}'), \quad 0 < \lambda < 1,\ \mathbf{p} \neq \mathbf{p}'$

**Lemma 8**

Let $\iota$ be a strict impurity function and let $D_1, \ldots, D_s$ be a partitioning of an example set $D$, which is induced by a splitting of a feature space $X$. Then the following inequality holds:

$$\Delta\iota(D, \{D_1, \ldots, D_s\}) \geq 0$$

The equality is given iff for all $i \in \{1, \ldots, k\}$ and $j \in \{1, \ldots, s\}$ holds:

$$\frac{|\{(\mathbf{x}, c(\mathbf{x})) \in D : c(\mathbf{x}) = c_i\}|}{|D|} = \frac{|\{(\mathbf{x}, c(\mathbf{x})) \in D_j : c(\mathbf{x}) = c_i\}|}{|D_j|}$$


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Remarks:

- Strict concavity entails Property (c) of the impurity function definition.
- For two classes, strict concavity means $\iota(p_1, 1-p_1) > 0$, where $0 < p_1 < 1$.
- If $\iota$ is a twice differentiable function, strict concavity is equivalent with a negative definite Hessian of $\iota$.
- With properly chosen coefficients, polynomials of second degree fulfill the properties (a) and (b) of the impurity function definition as well as strict concavity. See impurity functions based on the Gini index in this regard.
- The impurity function that is induced by the misclassification rate is concave, but it is not strictly concave.
- The proof of Lemma 8 exploits the strict concavity property of $\iota$.


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# Impurity Functions

## Impurity Functions Based on Entropy

**Definition 9 (Entropy)**

Let $A$ denote an event and let $P(A)$ denote the occurrence probability of $A$. Then the entropy (self-information, information content) of $A$ is defined as $-\log_2(P(A))$.

Let $\mathcal{A}$ be an experiment with the exclusive outcomes (events) $A_1, \ldots, A_k$. Then the mean information content of $\mathcal{A}$, denoted as $H(\mathcal{A})$, is called Shannon entropy or entropy of experiment $\mathcal{A}$ and is defined as follows:

$$H(\mathcal{A}) = -\sum_{i=1}^{k} P(A_i) \log_2(P(A_i))$$


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Remarks:

- The smaller the occurrence probability of an event, the larger is its entropy. An event that is certain has zero entropy.
- The Shannon entropy combines the entropies of an experiment's outcomes, using the outcome probabilities as weights.
- In the entropy definition we stipulate the identity $0 \cdot \log_2(0) = 0$.


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# Impurity Functions

## Impurity Functions Based on Entropy (continued)

**Definition 10 (Conditional Entropy, Information Gain)**

Let $\mathcal{A}$ be an experiment with the exclusive outcomes (events) $A_1, \ldots, A_k$, and let $\mathcal{B}$ be another experiment with the outcomes $B_1, \ldots, B_s$. Then the conditional entropy of the combined experiment $(\mathcal{A} \mid \mathcal{B})$ is defined as follows:

$$H(\mathcal{A} \mid \mathcal{B}) = \sum_{j=1}^{s} P(B_j) \cdot H(\mathcal{A} \mid B_j),$$

$$\text{where} \quad H(\mathcal{A} \mid B_j) = -\sum_{i=1}^{k} P(A_i \mid B_j) \log_2(P(A_i \mid B_j))$$


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# Impurity Functions

## Impurity Functions Based on Entropy (continued)

**Definition 10 (Conditional Entropy, Information Gain)**

Let $\mathcal{A}$ be an experiment with the exclusive outcomes (events) $A_1, \ldots, A_k$, and let $\mathcal{B}$ be another experiment with the outcomes $B_1, \ldots, B_s$. Then the conditional entropy of the combined experiment $(\mathcal{A} \mid \mathcal{B})$ is defined as follows:

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$$\text{where} \quad H(\mathcal{A} \mid B_j) = -\sum_{i=1}^{k} P(A_i \mid B_j) \log_2(P(A_i \mid B_j))$$


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# Impurity Functions

## Impurity Functions Based on Entropy (continued)

**Definition 10 (Conditional Entropy, Information Gain)**

Let $\mathcal{A}$ be an experiment with the exclusive outcomes (events) $A_1, \ldots, A_k$, and let $\mathcal{B}$ be another experiment with the outcomes $B_1, \ldots, B_s$. Then the conditional entropy of the combined experiment $(\mathcal{A} \mid \mathcal{B})$ is defined as follows:

$$H(\mathcal{A} \mid \mathcal{B}) = \sum_{j=1}^{s} P(B_j) \cdot H(\mathcal{A} \mid B_j),$$

$$\text{where} \quad H(\mathcal{A} \mid B_j) = -\sum_{i=1}^{k} P(A_i \mid B_j) \log_2(P(A_i \mid B_j))$$

The information gain due to experiment $\mathcal{B}$ is defined as follows:

$$H(\mathcal{A}) - H(\mathcal{A} \mid \mathcal{B}) = H(\mathcal{A}) - \sum_{j=1}^{s} P(B_j) \cdot H(\mathcal{A} \mid B_j)$$


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Remarks [Bayes for classification]:

- Information gain is defined as reduction in entropy.
- In the context of decision trees, experiment $\mathcal{A}$ corresponds to classifying feature vector $\mathbf{x}$ with regard to the target concept. A possible question, whose answer will inform us about which event $A_i \in \mathcal{A}$ occurred, is the following: "Does $\mathbf{x}$ belong to class $c_i$?"
  Likewise, experiment $\mathcal{B}$ corresponds to evaluating feature $B$ of feature vector $\mathbf{x}$. A possible question, whose answer will inform us about which event $B_j \in \mathcal{B}$ occurred, is the following: "Does $\mathbf{x}$ have value $b_j$ for feature $B$?"
- Rationale: Typically, the events "target concept class" and "feature value" are statistically dependent. Hence, the entropy of the event $c(\mathbf{x})$ will become smaller if we learn about the value of some feature of $\mathbf{x}$ (recall that the class of $\mathbf{x}$ is unknown). We experience an information gain with regard to the outcome of experiment $\mathcal{A}$, which is rooted in our information about the outcome of experiment $\mathcal{B}$. Under no circumstances the information gain will be negative; the information gain is zero if the involved events are *conditionally independent*:
  $$P(A_i) = P(A_i \mid B_j), \quad i \in \{1, \ldots, k\},\ j \in \{1, \ldots, s\},$$
  which leads to a split as specified as the special case in Lemma 8.


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Remarks (continued):

- Since $H(\mathcal{A})$ is constant, the feature that provides the maximum information gain (= the maximally informative feature) is given by the minimization of $H(\mathcal{A} \mid \mathcal{B})$.
- The expanded form of $H(\mathcal{A} \mid \mathcal{B})$ reads as follows:

$$H(\mathcal{A} \mid \mathcal{B}) = -\sum_{j=1}^{s} P(B_j) \cdot \sum_{i=1}^{k} P(A_i \mid B_j) \log_2(P(A_i \mid B_j))$$


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# Impurity Functions

## Impurity Functions Based on Entropy (continued)

Definition for two classes:

$$\iota_{entropy}(p_1, p_2) = -(p_1 \log_2(p_1) + p_2 \log_2(p_2))$$

$$\iota_{entropy}(D) = -\left(\frac{|\{(\mathbf{x}, c(\mathbf{x})) \in D : c(\mathbf{x}) = c_1\}|}{|D|} \cdot \log_2 \frac{|\{(\mathbf{x}, c(\mathbf{x})) \in D : c(\mathbf{x}) = c_1\}|}{|D|} + \frac{|\{(\mathbf{x}, c(\mathbf{x})) \in D : c(\mathbf{x}) = c_2\}|}{|D|} \cdot \log_2 \frac{|\{(\mathbf{x}, c(\mathbf{x})) \in D : c(\mathbf{x}) = c_2\}|}{|D|}\right)$$


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# Impurity Functions

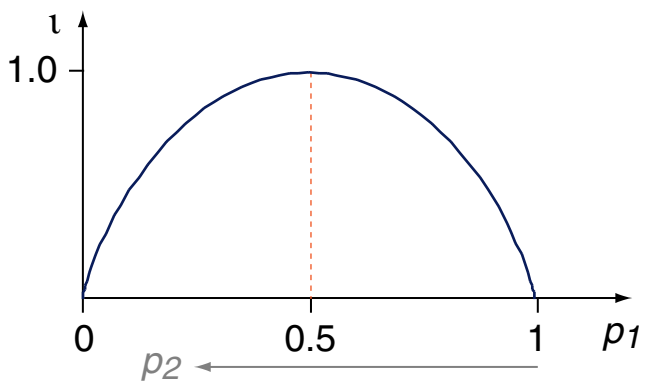
## Impurity Functions Based on Entropy (continued)

Definition for two classes:

$$\iota_{entropy}(p_1, p_2) = -(p_1 \log_2(p_1) + p_2 \log_2(p_2))$$

$$\iota_{entropy}(D) = -\left(\frac{|\{(\mathbf{x}, c(\mathbf{x})) \in D : c(\mathbf{x}) = c_1\}|}{|D|} \cdot \log_2 \frac{|\{(\mathbf{x}, c(\mathbf{x})) \in D : c(\mathbf{x}) = c_1\}|}{|D|} + \frac{|\{(\mathbf{x}, c(\mathbf{x})) \in D : c(\mathbf{x}) = c_2\}|}{|D|} \cdot \log_2 \frac{|\{(\mathbf{x}, c(\mathbf{x})) \in D : c(\mathbf{x}) = c_2\}|}{|D|}\right)$$

Graph of the function $\iota_{entropy}(p_1, 1 - p_1)$:




[Graph: Misclassification, Gini]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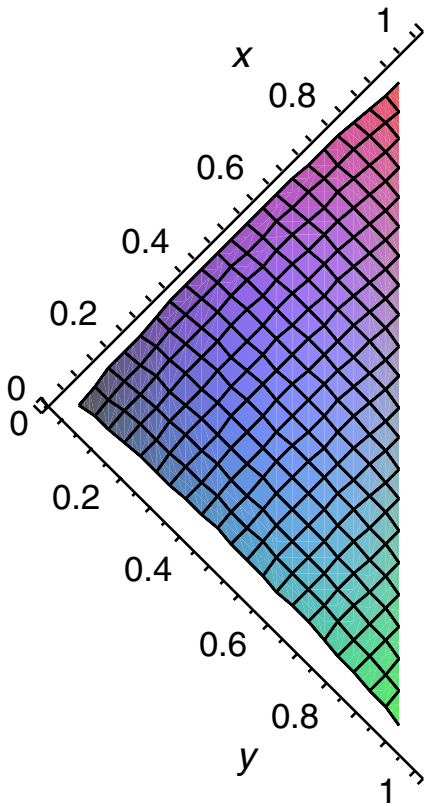
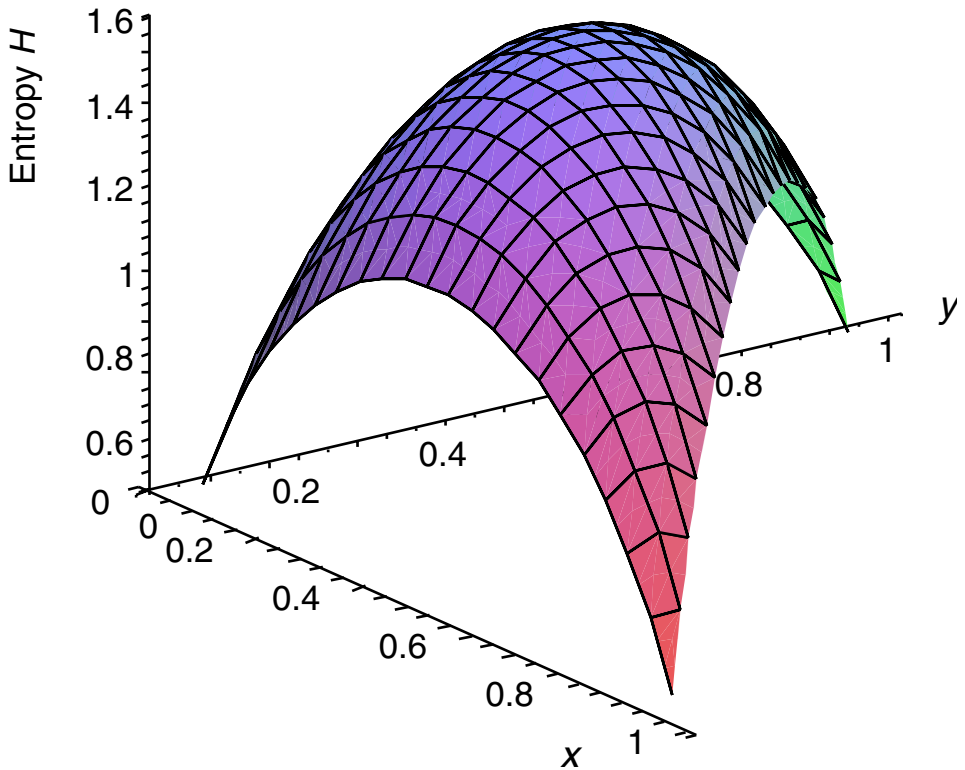
# Impurity Functions

## Impurity Functions Based on Entropy (continued)

Graph of the function $\iota_{entropy}(p_1, p_2, 1 - p_1 - p_2)$ :





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# Impurity Functions

## Impurity Functions Based on Entropy (continued)

Definition for $k$ classes:

$$\iota_{entropy}(p_1, \ldots, p_k) = -\sum_{i=1}^{k} p_i \log_2(p_i)$$

$$\iota_{entropy}(D) = -\sum_{i=1}^{k} \frac{|\{(\mathbf{x}, c(\mathbf{x})) \in D : c(\mathbf{x}) = c_i\}|}{|D|} \cdot \log_2 \frac{|\{(\mathbf{x}, c(\mathbf{x})) \in D : c(\mathbf{x}) = c_i\}|}{|D|}$$


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# Impurity Functions

## Impurity Functions Based on Entropy (continued)

$\underline{\Delta\iota}_{entropy}$ corresponds to the information gain $H(\mathcal{A}) - H(\mathcal{A} \mid \mathcal{B})$:

$$\underline{\Delta\iota}_{entropy} = \underbrace{\iota_{entropy}(D)}_{H(\mathcal{A})} - \underbrace{\sum_{j=1}^{s} \frac{|D_j|}{|D|} \cdot \iota_{entropy}(D_j)}_{H(\mathcal{A}|\mathcal{B})}$$


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# Impurity Functions

## Impurity Functions Based on Entropy (continued)

$\Delta\iota_{entropy}$ corresponds to the information gain $H(\mathcal{A}) - H(\mathcal{A} \mid \mathcal{B})$:

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Legend:

- $\iota_{entropy}(D) = \iota_{entropy}(P(A_1), \ldots, P(A_k))$
- $\iota_{entropy}(D_j) = \iota_{entropy}(P(A_1 \mid B_j), \ldots, P(A_k \mid B_j)),\ j = 1, \ldots, s$
- $\iota_{entropy}(p_1, \ldots, p_k) = -\sum_{i=1}^{k} p_i \cdot \log_2(p_i)$
- $\frac{|D_j|}{|D|} = P(B_j),\ j = 1, \ldots, s$
- $A_i,\ i = 1, \ldots, k$, denotes the event that $\mathbf{x} \in X(t)$ belongs to class $c_i$. The experiment $\mathcal{A}$ corresponds to the classification $c : X(t) \to C$.
- $B_j,\ j = 1, \ldots, s$, denotes the event that $\mathbf{x} \in X(t)$ has value $b_j$ for feature $B$. The experiment $\mathcal{B}$ corresponds to evaluating feature $B$ and entails the following splitting: $X(t) = X(t_1) \cup \ldots \cup X(t_s) = \{\mathbf{x} \in X(t) : \mathbf{x}|_B = b_1\} \cup \ldots \cup \{\mathbf{x} \in X(t) : \mathbf{x}|_B = b_s\}$
- $P(A_i), P(B_j), P(A_i \mid B_j)$ are estimated as relative frequencies based on $D$.


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# Impurity Functions

## Impurity Functions Based on the Gini Index

Definition for two classes:

$$\iota_{Gini}(p_1, p_2) = 1 - ({p_1}^2 + {p_2}^2) = 2 \cdot p_1 \cdot p_2$$

$$\iota_{Gini}(D) = 2 \cdot \frac{|\{(\mathbf{x}, c(\mathbf{x})) \in D : c(\mathbf{x}) = c_1\}|}{|D|} \cdot \frac{|\{(\mathbf{x}, c(\mathbf{x})) \in D : c(\mathbf{x}) = c_2\}|}{|D|}$$


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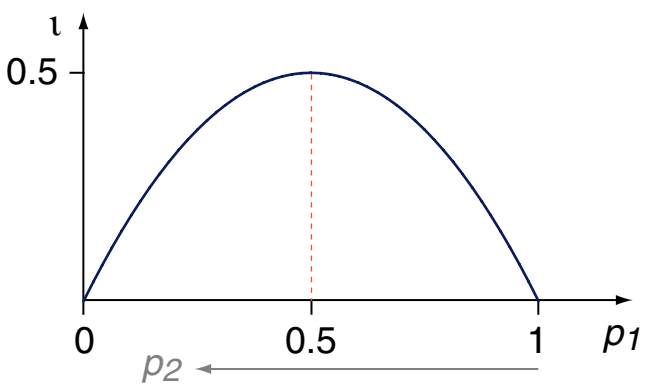
Graph of the function $\iota_{Gini}(p_1, 1 - p_1)$:




[Graph: Misclassification, Entropy]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# Impurity Functions

## Impurity Functions Based on the Gini Index (continued)

Definition for $k$ classes:

$$\iota_{Gini}(p_1, \ldots, p_k) = 1 - \sum_{i=1}^{k} (p_i)^2$$

$$\iota_{Gini}(D) = \left( \sum_{i=1}^{k} \frac{|\{(\mathbf{x}, c(\mathbf{x})) \in D : c(\mathbf{x}) = c_i\}|}{|D|} \right)^2 - \sum_{i=1}^{k} \left( \frac{|\{(\mathbf{x}, c(\mathbf{x})) \in D : c(\mathbf{x}) = c_i\}|}{|D|} \right)^2$$

$$= 1 - \sum_{i=1}^{k} \left( \frac{|\{(\mathbf{x}, c(\mathbf{x})) \in D : c(\mathbf{x}) = c_i\}|}{|D|} \right)^2$$


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# Chapter ML:III

## III. Decision Trees

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


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# 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 $c$.


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# 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.


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# Decision Tree Algorithms

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

ID3(D, Attributes, Target)

- Create a node t for the tree.
- 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 "–".
- Label t with the most common value of Target in D.
- If Attributes is empty, return the single-node tree t.
- Otherwise:
  - Let A* be the attribute from Attributes that best classifies examples in D.
  - Assign t the decision attribute A*.
  - 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).
- Return t.


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# Decision Tree Algorithms

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

*ID3*$(D, \textit{Attributes}, \textit{Target})$

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


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# Decision Tree Algorithms

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

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

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


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# Decision Tree Algorithms

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

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

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


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# Decision Tree Algorithms

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

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

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


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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 be comprised of multiple (more than two) classes.
- Step 2 of of the ID3 algorithm checks the purity of $D$ and, given this case, assigns the unique class $c$, $c \in \mathit{dom}(\mathit{Target})$, as label to the respective node.


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# 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 |


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# 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:

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


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# Decision Tree Algorithms

## ID3 Algorithm: Example (continued)

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

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| | toxic | eatable |
|---|---|---|
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$\Rightarrow \quad |D_{\text{red}}| = 2,\ |D_{\text{brown}}| = 2,\ |D_{\text{green}}| = 1$

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:

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

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


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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 is maximum for the two features “color” and “points”.


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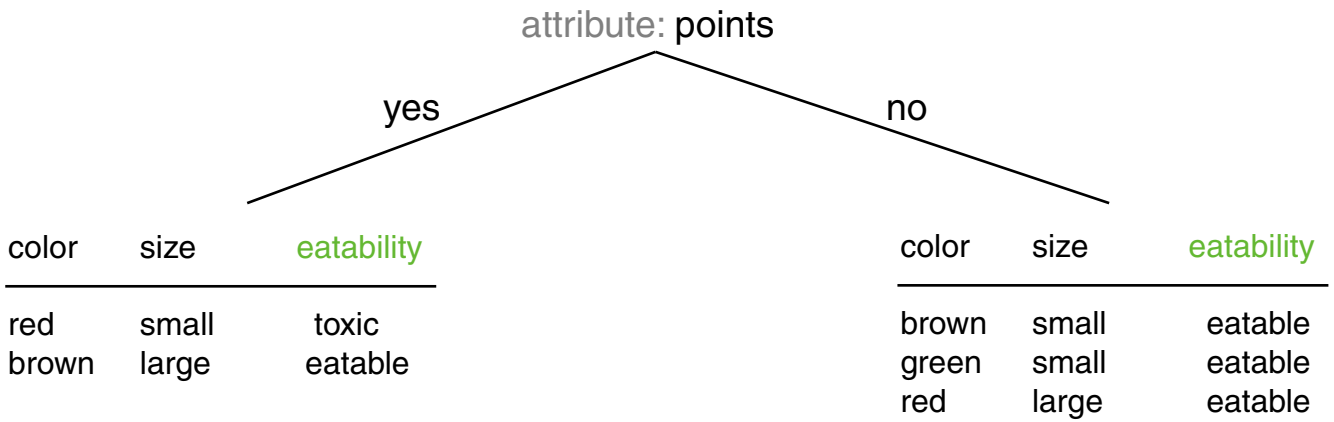
# Decision Tree Algorithms

## ID3 Algorithm: Example (continued)

Decision tree before the first recursion step:




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

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

The feature “points” was chosen in Step 5 of the ID3 algorithm.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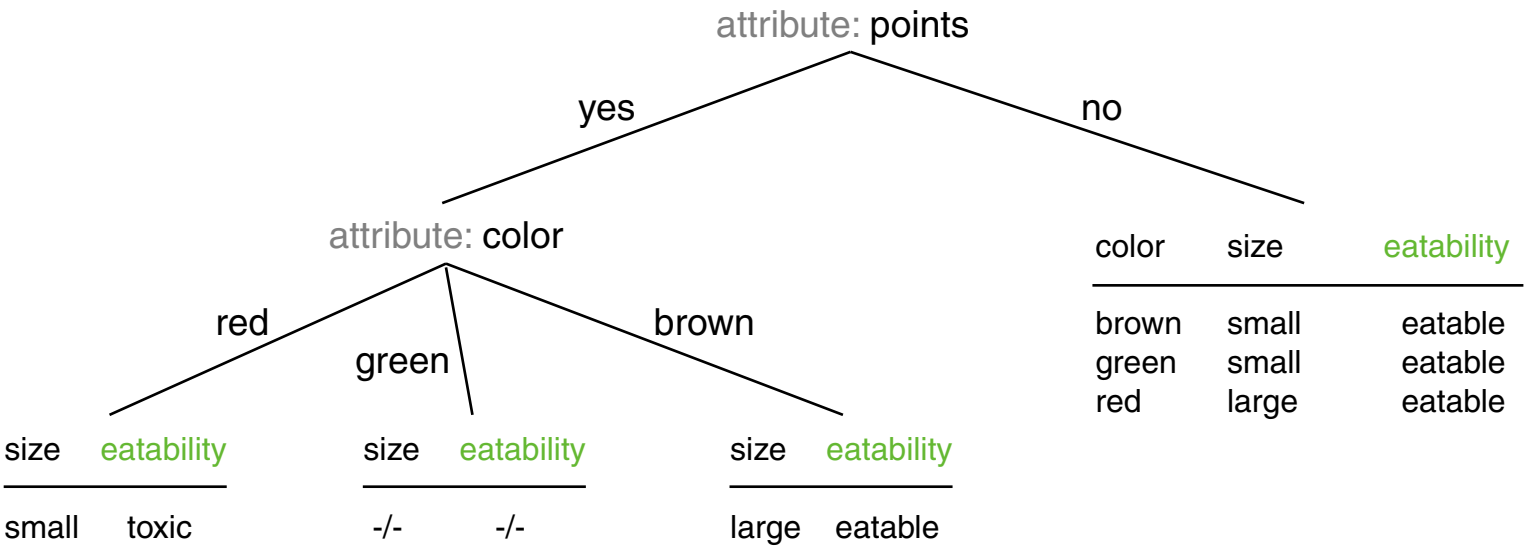
# Decision Tree Algorithms

## ID3 Algorithm: Example (continued)

Decision tree before the second recursion step:




The feature “color” was chosen in Step 5 of the ID3 algorithm.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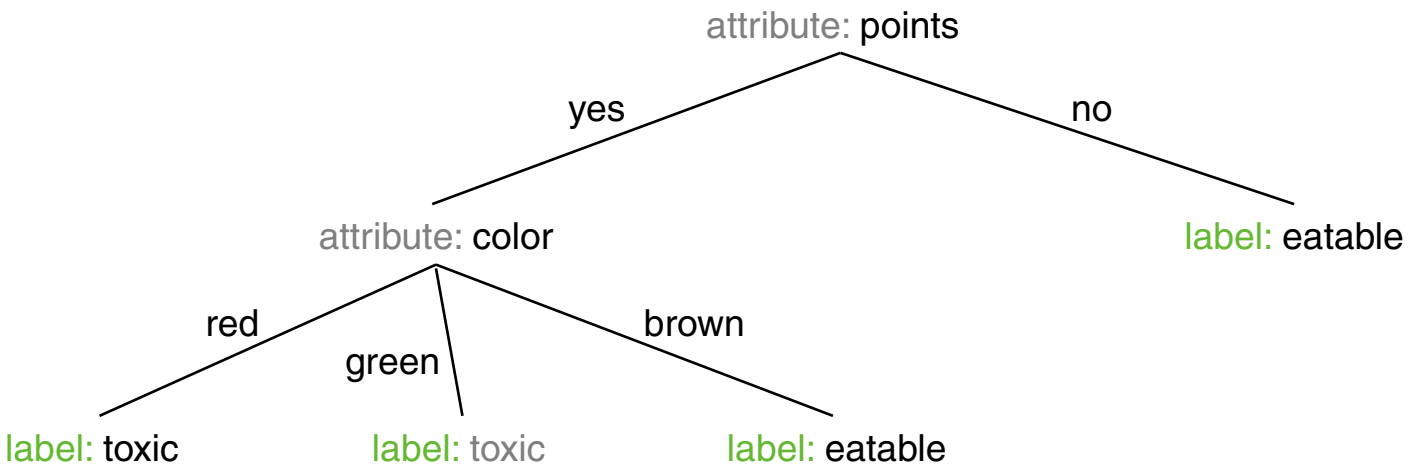
# Decision Tree Algorithms

## ID3 Algorithm: Example (continued)

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.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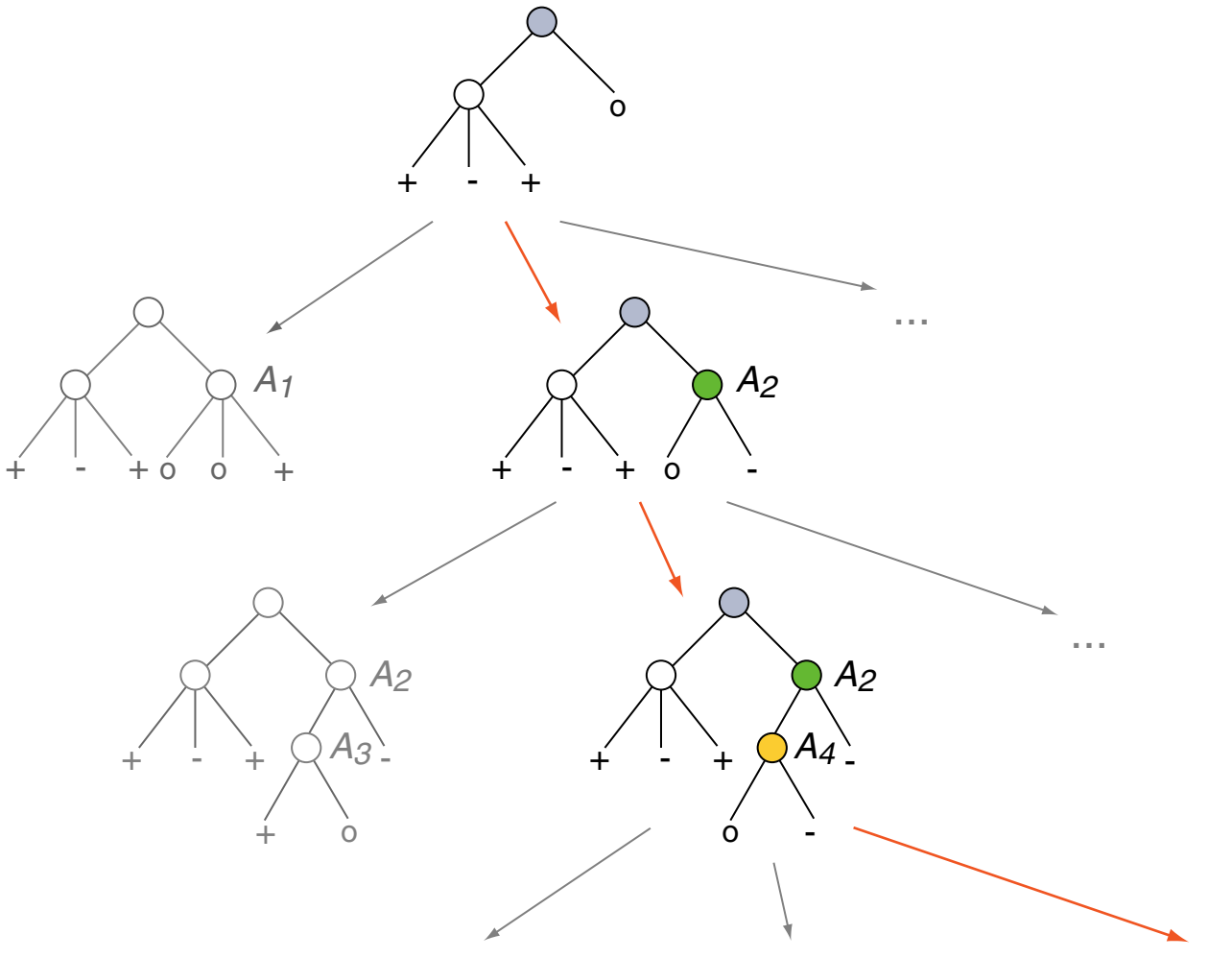
# Decision Tree Algorithms

## ID3 Algorithm: Hypothesis Space





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# 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.


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# Decision Tree Algorithms

## ID3 Algorithm: Inductive Bias

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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


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# 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:

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

Is this justified?


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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 $h,\ h : \mathbf{A}_1 \times \ldots \times \mathbf{A}_p \rightarrow C$. 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 with respect to noise.


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# 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 measurement scales of the features.
- $C$ 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 $c$.


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# Decision Tree Algorithms

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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.


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# 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 $D$.


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# Decision Tree Algorithms

## CART Algorithm (continued)

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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 $t$.


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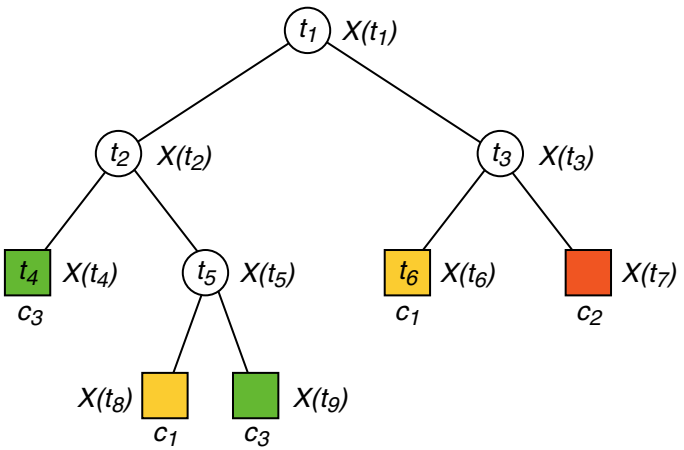
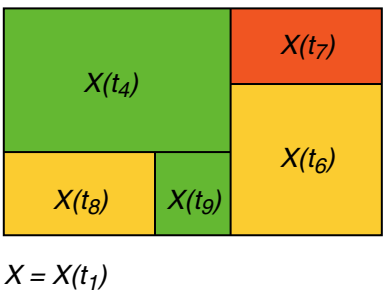
# Decision Tree Algorithms

## 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.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# Chapter ML:III

## III. Decision Trees

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


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# Decision Tree Pruning

## Overfitting

### Definition 10 (Overfitting)

Let $D$ be a set of examples and let $H$ be a hypothesis space. The hypothesis $h \in H$ is considered to overfit $D$ if an $h' \in H$ with the following property exists:

$$\mathit{Err}(h, D) < \mathit{Err}(h', D) \quad \text{and} \quad \mathit{Err}^*(h) > \mathit{Err}^*(h'),$$

where $\mathit{Err}^*(h)$ denotes the true misclassification rate of $h$, while $\mathit{Err}(h, D)$ denotes the error of $h$ on the example set $D$.


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# Decision Tree Pruning

## Overfitting

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where $\mathit{Err}^*(h)$ denotes the true misclassification rate of $h$, while $\mathit{Err}(h, D)$ denotes the error of $h$ on the example set $D$.

Reasons for overfitting are often rooted in the example set $D$ :

- $D$ is noisy
- $D$ is biased and hence non-representative
- $D$ is too small and hence pretends unrealistic data properties


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# Decision Tree Pruning

## Overfitting (continued)

Let $D_{tr} \subset D$ be the training set. Then $\mathit{Err}^*(h)$ can be estimated with a test set $D_{ts} \subset D$ where $D_{ts} \cap D_{tr} = \emptyset$ (holdout estimation). The hypothesis $h \in H$ is considered to overfit $D$ if an $h' \in H$ with the following property exists:

$$\mathit{Err}(h, D_{tr}) < \mathit{Err}(h', D_{tr}) \quad \text{and} \quad \mathit{Err}(h, D_{ts}) > \mathit{Err}(h', D_{ts})$$


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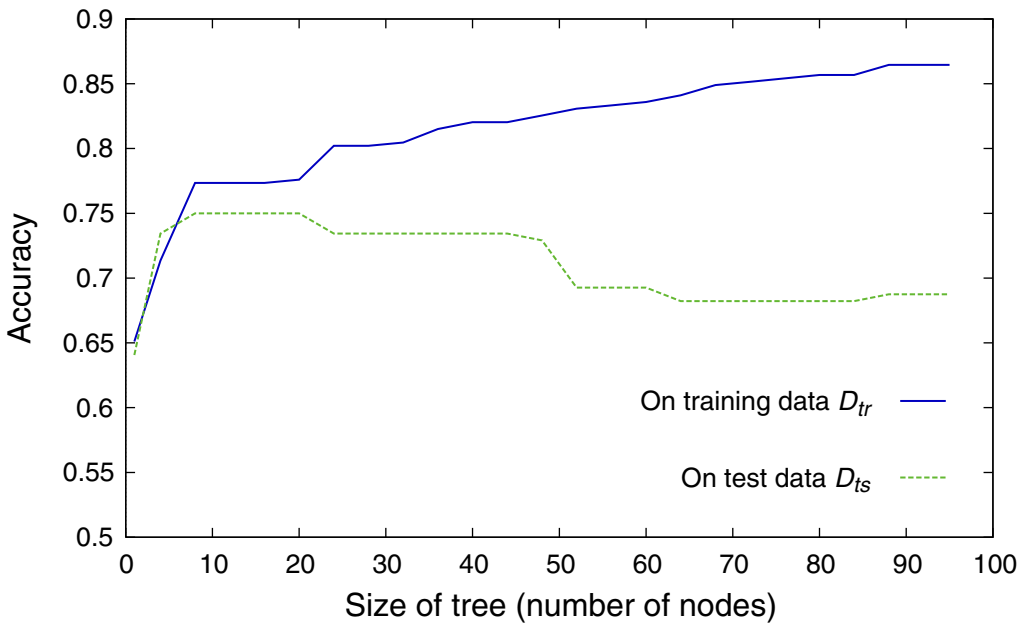
# Decision Tree Pruning

## Overfitting (continued)

Let $D_{tr} \subset D$ be the training set. Then $Err^*(h)$ can be estimated with a test set $D_{ts} \subset D$ where $D_{ts} \cap D_{tr} = \emptyset$ (holdout estimation). The hypothesis $h \in H$ is considered to overfit $D$ if an $h' \in H$ with the following property exists:

$$Err(h, D_{tr}) < Err(h', D_{tr}) \quad \text{and} \quad Err(h, D_{ts}) > Err(h', D_{ts})$$




[Mitchell 1997]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Remarks:

- Accuracy is the percentage of correctly classified examples.
- When does $\mathit{Err}(T, D_{tr})$ of a decision tree $T$ become zero?
- The training error $\mathit{Err}(T, D_{tr})$ of a decision tree $T$ is a monotonically decreasing function in the size of $T$. See the following Lemma.


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# Decision Tree Pruning

## Overfitting (continued)

### Lemma 10

Let $t$ be a node in a decision tree $T$. Then, for each induced splitting $D(t_1), \ldots, D(t_s)$ of a set of examples $D(t)$ holds:

$$\underline{Err_{cost}(t, D(t))} \geq \sum_{i \in \{1,\ldots,s\}} Err_{cost}(t_i, D(t_i))$$

The equality is given in the case that all nodes $t, t_1, \ldots, t_s$ represent the same class.


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# Decision Tree Pruning

## Overfitting (continued)

### Proof (sketch)

$$
\begin{aligned}
\mathit{Err}_{\mathit{cost}}(t, D(t)) &= \min_{c' \in C} \sum_{c \in C} p(c \mid t) \cdot p(t) \cdot \mathit{cost}(c' \mid c) \\
&= \sum_{c \in C} p(c, t) \cdot \mathit{cost}(\mathit{label}(t) \mid c) \\
&= \sum_{c \in C} (p(c, t_1) + \ldots + p(c, t_{k_s})) \cdot \mathit{cost}(\mathit{label}(t) \mid c) \\
&= \sum_{i \in \{1,\ldots,k_s\}} \sum_{c \in C} (p(c, t_i) \cdot \mathit{cost}(\mathit{label}(t) \mid c)
\end{aligned}
$$

$$
\mathit{Err}_{\mathit{cost}}(t, D(t)) - \textstyle\sum_{i \in \{1,\ldots,k_s\}} \mathit{Err}_{\mathit{cost}}(t_i, D(t_i)) =
$$

$$
\sum_{i \in \{1,\ldots,k_s\}} \left( \sum_{c \in C} p(c, t_i) \cdot \mathit{cost}(\mathit{label}(t) \mid c) \; - \min_{c' \in C} \sum_{c \in C} p(c, t_i) \cdot \mathit{cost}(c' \mid c) \right)
$$

The summands on the right equation side are greater than or equal to zero.


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Remarks:

- The lemma does also hold if the misclassification rate is used as performance measure.
- The algorithm template for the construction of decision trees, *DT-construct*, prefers larger trees, entailing a more fine-grained partitioning of $D$. A consequence of this behavior is a tendency to overfitting.


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# Decision Tree Pruning

## Overfitting (continued)

Approaches to counter overfitting:

1. Stopping of the decision tree construction process *during training*.
2. Pruning of a decision tree *after training*:
   - Partitioning of $D$ into three sets for training, validation, and test:
     (a) reduced error pruning
     (b) minimal cost complexity pruning
     (c) rule post pruning
   - statistical tests such as $\chi^2$ to assess generalization capability
   - heuristic pruning


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# Decision Tree Pruning

## Stopping

Possible criteria for stopping [splitting criteria]:

1. Size of $D(t)$.
   $D(t)$ will not be partitioned further if the number of examples, $|D(t)|$, is below a certain threshold.

2. Purity of $D(t)$.
   $D(t)$ will not be partitioned further if all induced splittings yield no significant impurity reduction $\Delta\iota$.

Problems:

ad 1) A threshold that is too small results in oversized decision trees.

ad 1) A threshold that is too large omits useful splittings.

ad 2) $\Delta\iota$ cannot be extrapolated with regard to the tree height.


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# Decision Tree Pruning

## Pruning

The pruning principle:

1. Construct a sufficiently large decision tree $T_{\text{max}}$.
2. Prune $T_{\text{max}}$, starting from the leaf nodes towards the tree root.

Each leaf node $t$ of $T_{\text{max}}$ fulfills one or more of the following conditions:

- $D(t)$ is sufficiently small. Typically, $|D(t)| \leq 5$.
- $D(t)$ is comprised of examples of only one class.
- $D(t)$ is comprised of examples with identical feature vectors.


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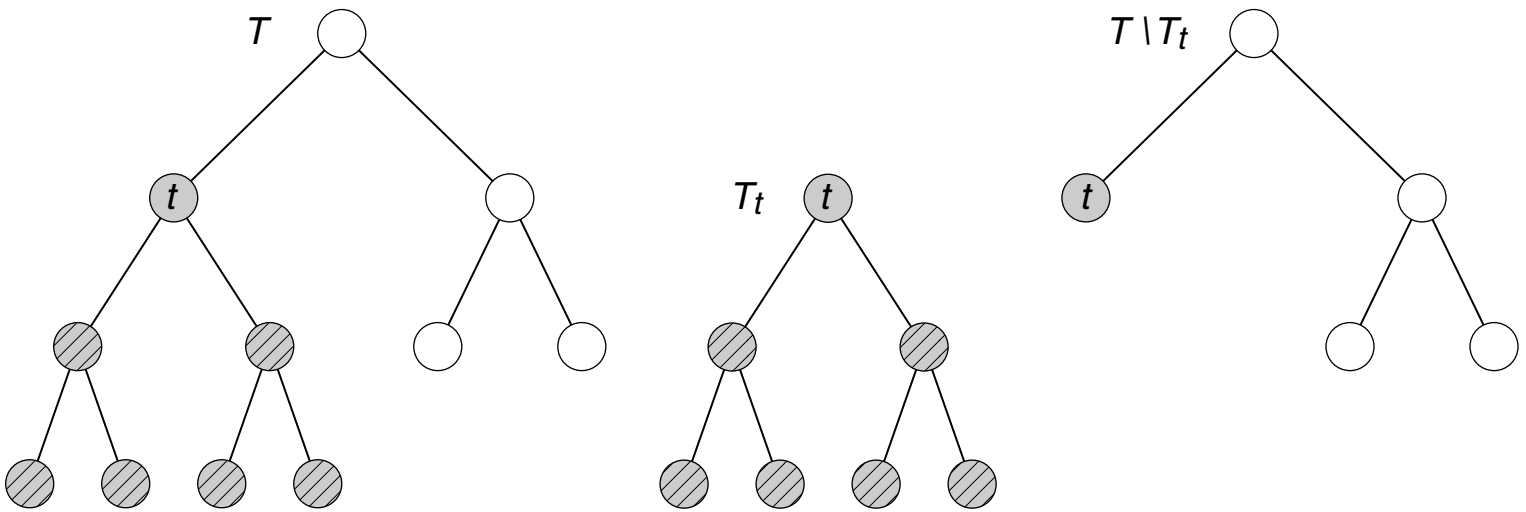
# Decision Tree Pruning

## Pruning (continued)

**Definition 11 (Decision Tree Pruning)**

Given a decision tree $T$ and an inner (non-root, non-leaf) node $t$. Then pruning of $T$ wrt. $t$ is the deletion of all successor nodes of $t$ in $T$. The pruned tree is denoted as $T \setminus T_t$. The node $t$ becomes a leaf node in $T \setminus T_t$.

Illustration:





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# Decision Tree Pruning

## Pruning (continued)

### Definition 12 (Pruning-Induced Ordering)

Let $T'$ and $T$ be two decision trees. Then $T' \preceq T$ denotes the fact that $T'$ is the result of a (possibly repeated) pruning applied to $T$. The relation $\preceq$ forms a partial ordering on the set of all trees.


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# Decision Tree Pruning

## Pruning (continued)

**Definition 12 (Pruning-Induced Ordering)**

Let $T'$ and $T$ be two decision trees. Then $T' \preceq T$ denotes the fact that $T'$ is the result of a (possibly repeated) pruning applied to $T$. The relation $\preceq$ forms a partial ordering on the set of all trees.

Problems when assessing pruning candidates:

- Pruned decision trees may not stand in the $\preceq$-relation.
- Starting with $T_{\text{max}}$, promising candidates may not result from locally optimum pruning decisions (greedy strategy).
- Its monotony disqualifies $\mathit{Err}(T, D_{tr})$ as an estimator for $\mathit{Err}^*(T)$. [Lemma]


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# Decision Tree Pruning

## Pruning (continued)

**Definition 12 (Pruning-Induced Ordering)**

Let $T'$ and $T$ be two decision trees. Then $T' \preceq T$ denotes the fact that $T'$ is the result of a (possibly repeated) pruning applied to $T$. The relation $\preceq$ forms a partial ordering on the set of all trees.

Problems when assessing pruning candidates:

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Control pruning with validation set $D_{vd}$, where $D_{vd} \cap D_{tr} = \emptyset$, $D_{vd} \cap D_{ts} = \emptyset$:

1. $D_{tr} \subset D$ for decision tree construction.
2. $D_{vd} \subset D$ for overfitting analysis *during* pruning.
3. $D_{ts} \subset D$ for decision tree evaluation *after* pruning.


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# Decision Tree Pruning

## Pruning: Reduced Error Pruning

Reduced error pruning for decision tree $T_{\text{max}}$ and validation set $D_{vd}$ :

1. $T = T_{\text{max}}$
2. Choose an inner node $t$ in $T$.
3. Tentative pruning of $T$ wrt. $t$ : $T' = T \setminus T_t$.
   Based on $D(t)$ assign class to $t$. [*DT-construct*]
4. If $\mathit{Err}(T', D_{vd}) \leq \mathit{Err}(T, D_{vd})$ then accept pruning: $T = T'$.
5. Continue with Step 2 until all inner nodes of $T$ are tested.


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# Decision Tree Pruning

## Pruning: Reduced Error Pruning

Reduced error pruning for decision tree $T_{\text{max}}$ and validation set $D_{vd}$ :

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4. If *Err*$(T', D_{vd}) \leq$ *Err*$(T, D_{vd})$ then accept pruning: $T = T'$.
5. Continue with Step 2 until all inner nodes of $T$ are tested.

Problem:

If $D$ is small, its partitioning into three sets for training, validation, and test will discard valuable information for decision tree construction.

Improvement: rule post pruning


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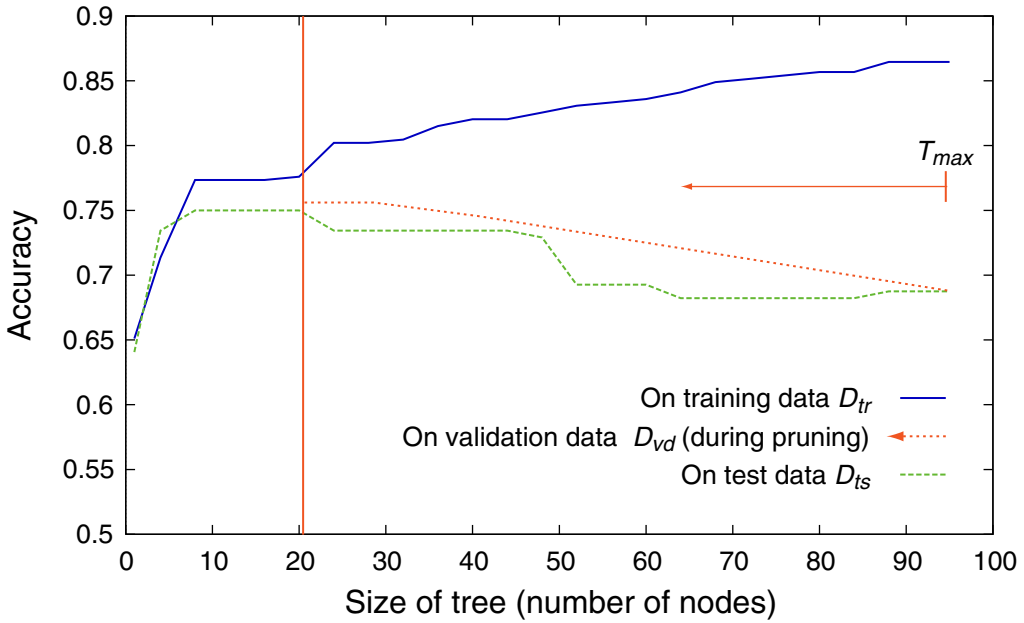
# Decision Tree Pruning

## Pruning: Reduced Error Pruning (continued)




[Mitchell 1997]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# Decision Tree Pruning

## Extensions

- consideration of the misclassification cost introduced by a splitting
- “surrogate splittings” for insufficiently covered feature domains
- splittings based on (linear) combinations of features
- regression trees


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