VI. Decision Trees

- Decision Trees Basics
- Impurity Functions
- Decision Tree Algorithms
- Decision Tree Pruning
Decision Trees Basics
Classification Problems with Nominal Features

Setting:
- $X$ is a multiset of feature vectors.
- $C$ is a set of classes.
- $D = \{(x_1, c_1), \ldots, (x_n, c_n)\} \subseteq X \times C$ is a multiset of examples.

Learning task:
- Fit $D$ using a decision tree $T$. 
Decision Trees Basics
Decision Tree for the Concept “EnjoySurfing” [concept learning]

<table>
<thead>
<tr>
<th>Example</th>
<th>Sky</th>
<th>Temperature</th>
<th>Humidity</th>
<th>Wind</th>
<th>Water</th>
<th>Forecast</th>
<th>EnjoySurfing</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>sunny</td>
<td>warm</td>
<td>normal</td>
<td>strong</td>
<td>warm</td>
<td>same</td>
<td>yes</td>
</tr>
<tr>
<td>2</td>
<td>sunny</td>
<td>warm</td>
<td>high</td>
<td>strong</td>
<td>warm</td>
<td>same</td>
<td>yes</td>
</tr>
<tr>
<td>3</td>
<td>rainy</td>
<td>cold</td>
<td>high</td>
<td>strong</td>
<td>warm</td>
<td>change</td>
<td>no</td>
</tr>
</tbody>
</table>

```
feature: Sky
  sunny
  cloudy
  rainy

feature: Temperature
  cold
  warm

label: yes

feature: Wind
  strong
  light

label: no

label: yes
```

ML:VI-3 Decision Trees © STEIN/LETTMANN 2024
Decision Trees Basics

Decision Tree for the Concept “EnjoySurfing”  

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Splitting of $X$ at the root node:

$$X = \{ x \in X : x_{\text{Sky}} = \text{sunny} \} \cup \{ x \in X : x_{\text{Sky}} = \text{cloudy} \} \cup \{ x \in X : x_{\text{Sky}} = \text{rainy} \}$$
**Definition 1 (Splitting, Induced Splitting)**

Let $X$ be a multiset of feature vectors and $D$ a multiset of examples. A splitting of $X$ is a decomposition of $X$ into mutually exclusive subsets $X_1, \ldots, X_m$. I.e., $X = X_1 \cup \ldots \cup X_m$ with $X_l \neq \emptyset$ and $X_l \cap X_{l'} = \emptyset$, where $l, l' \in \{1, \ldots, m\}, l \neq l'$.

A splitting $X_1, \ldots, X_m$ of feature vectors $X$ induces a splitting $D_1, \ldots, D_m$ of examples $D$, where $D_l$, $l = 1, \ldots, m$, is defined as $\{(x, c) \in D \mid x \in X_l\}$. 
**Decision Trees Basics**

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A splitting of $X$ depends on the *measurement scale* of a feature $A$:

$$
\begin{align*}
\mathbf{x} &= \begin{pmatrix}
  x_1 \\
  x_2 \\
  \vdots \\
  x_3 \\
  \vdots \\
  x_p \\
\end{pmatrix} \\
A \leftrightsquigarrow \{a_1, a_2, a_3, \ldots, a_m\} \\
\mathbf{x} \mid_A &= x_3
\end{align*}
$$
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A splitting of $X$ depends on the measurement scale of a feature $A$:

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

   $dom(A) = \{a_1, \ldots, a_m\}$ : $X = \{x \in X : x|_A = a_1\} \cup \ldots \cup \{x \in X : x|_A = a_m\}$
Decision Trees Basics

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A splitting of $X$ depends on the **measurement scale** of a feature $A$:

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2. **Binary splitting** induced by a (nominal) feature $A$:
   
   $V \subset dom(A)$: $X = \{x \in X : x|_A \in V\} \cup \{x \in X : x|_A \notin V\}$
Decision Trees Basics

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A splitting of $X$ depends on the [measurement scale](#) of a feature $A$:

1. **$m$-ary splitting induced by a (nominal) feature $A$ with finite domain:**
   
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   $V \subset \text{dom}(A) : \quad X = \{x \in X : x|_A \in V\} \cup \{x \in X : x|_A \notin V\}$

3. **Binary splitting induced by an ordinal feature $A$:**
   
   $v \in \text{dom}(A) : \quad X = \{x \in X : x|_A \geq v\} \cup \{x \in X : x|_A < v\}$
Remarks:

- $x_A$ denotes the projection operator, which returns that vector component (dimension) of $x$, $x = (x_1, \ldots, x_p)$, that is associated with the feature $A$. 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 $X$. Such kinds of splittings are called “monothetic splittings”.

  By contrast, a polythetic splitting considers several features at the same time.
Decision Trees Basics

**Definition 2 (Decision Tree)**

Let $X$ be a set of features and $C$ 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.

A leaf node of $T$ has assigned a class from $C$. $X(t) = X$ iff $t$ is root node.
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How to classify some $x \in X$ given a decision tree $T$:

1. Find the root node $t$ of $T$.
2. If $t$ is a non-leaf node, find among its successors that node $t'$ whose subset of the splitting of $X(t)$ contains $x$. Repeat Step 2 with $t = t'$.
3. If $t$ is a leaf node, label $x$ with the associated class.
Decision Trees Basics

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

[hypothesis space: LMS, Find-S, log. regression]
Remarks:

- The classification of an \( x \in X \) 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 \( x \) 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:

  \[
  \text{IF Sky=rainy AND Wind=light THEN EnjoySurfing=yes}
  \]

  If all tests in \( T \) are of the kind shown in the example, namely, an equality test regarding a feature value, all feature domains must be finite.

- Since at all non-leaf nodes of \( T \) 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 Ross Quinlan.

- Recap. The string “Iff” or “iff” is an abbreviation for “If and only if”.
Decision Trees Basics

Notation

Let $T$ be a 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 $X$ that is represented by $t$. [decision tree definition (1)]
- $D(t)$ denotes the subset of the example set $D$ that is represented by $t$, i.e.,
  $$D(t) = \{(x, c) \in D \mid x \in X(t)\}.$$ [splitting definition]

Illustration (colors correspond to classes):

```
  t1  D(t1)
   / \          / \
  t2  D(t2)  t3  D(t3)
 / \        /  \
 t4  D(t4) t5  D(t5) t6  D(t6)
  \     \   \     \  
   c3    c1  c3    c1
```

```
D(t1)  
D(t2)  D(t3)  
D(t4)  D(t5)  D(t6)  
  
```
Remarks:

- The set $X(t)$ consists of those members $x$ of $X$ that are filtered by a path from the root node of $T$ to the node $t$.
- $\text{leaves}(T)$ denotes the set of all leaf nodes of $T$.
- Each 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 $x$, 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:

$$t, T : X \to C$$  (instead of $y_t, y_T : X \to C$)
Algorithm: \textit{DT-construct} \hspace{1em} Decision Tree Construction

Input: \hspace{1em} \(D\) \hspace{1em} Multiset of examples.

Output: \hspace{1em} \(t\) \hspace{1em} Root node of a decision tree.

\textit{DT-construct}(D)

1. \(t = \text{createNode}()\)
   \hspace{1em} \text{label}(t) = \text{representativeClass}(D)

2. IF \(\text{impure}(D)\)
   THEN \(\text{criterion} = \text{splitCriterion}(D)\)
   ELSE \(\text{return}(t)\)

3. \(\{D_1, \ldots, D_m\} = \text{decompose}(D, \text{criterion})\)

4. \textbf{FOREACH} \(D'\) \textbf{IN} \(\{D_1, \ldots, D_m\}\) \textbf{DO}
   \hspace{1em} \text{addSuccessor}(t, \textit{DT-construct}(D'))
   \textbf{ENDDO}

5. \(\text{return}(t)\)
Algorithm: \( DT\text{-}construct \)  
Decision Tree Construction

Input: \( D \)  
Multiset of examples.

Output: \( t \)  
Root node of a decision tree.

\[
\text{\( DT\text{-}construct(D) \)}
\]

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4. FOREACH \( D' \) IN \( \{D_1, \ldots, D_m\} \) DO
   \( \text{addSuccessor}(t, DT\text{-}construct(D')) \)
   ENDDO

5. \( \text{return}(t) \)
Algorithm: $DT$-construct Decision Tree Construction

Input: $D$ Multiset of examples.

Output: $t$ Root node of a decision tree.

$DT$-construct$(D)$

1. $t = \text{createNode}()$
   
   \hspace{1cm} $\text{label}(t) = \text{representativeClass}(D)$

2. IF $\text{impure}(D)$
   
   THEN $\text{criterion} = \text{splitCriterion}(D)$

   ELSE $\text{return}(t)$

3. $\{D_1, \ldots, D_m\} = \text{decompose}(D, \text{criterion})$

4. FOREACH $D'$ IN $\{D_1, \ldots, D_m\}$ DO

   \hspace{1cm} $\text{addSuccessor}(t, DT$-construct$(D'))$

   ENDDO

5. $\text{return}(t)$
Remarks:

- **Functions of** $DT$-$construct()$:
  - $createNode()$
    Returns the data structure for a node according to the definition.
  - $representativeClass(D)$
    Returns a representative class for the example set $D$. Note that, due to pruning, each node may become a leaf node.
  - $impure(D)$
    Assesses the (im)purity of a set $D$ of examples.
  - $splitCriterion(D)$
    Returns a split criterion for $X(t)$ based on the examples in $D(t)$.
  - $decompose(D, criterion)$
    Returns a splitting of $D$ according to $criterion$.
  - $addSuccessor(t, t')$
    Inserts the successor $t'$ for node $t$.

- 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.
Decision Trees Basics
Algorithm Template: Classification

Algorithm: \( DT\text{-classify} \) Decision Tree Classification

Input: \( x \) Feature vector.
\( t \) Root node of a decision tree.

Output: \( y(x) \) Class of feature vector \( x \) in the decision tree below \( t \).

\( DT\text{-classify}(x, t) \)

1. IF \( \text{isLeafNode}(t) \) THEN \( \text{return}(\text{label}(t)) \)
   ELSE \( \text{return}(DT\text{-classify}(x, \text{splitSuccessor}(t, x))) \)
Remarks:

Functions of $DT\text{-classify}()$:

- $isLeafNode(t)$
  Tests whether $t$ is a leaf node.

- $splitSuccessor(t, x)$
  Returns the (unique) successor $t'$ of $t$ for which $x \in X(t')$ holds.
Decision Trees Basics

When to Use Decision Trees

Problem characteristics that 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 can be represented in disjunctive normal form.  
  Example:
  \[ \alpha = (\text{Sky}=\text{sunny} \land \text{Temperature}=\text{warm}) \lor \text{Sky}=\text{cloudy} \lor (\text{Sky}=\text{rainy} \land \text{Wind}=\text{light}) \]
- the training set contains noise
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Exemplary fields of application:

- medical diagnosis
- fault detection in technical systems
- risk analysis in financial applications
- scheduling tasks such as calendar management
- classification of design flaws and patterns in software engineering
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 assess decision tree performance?
Decision Trees Basics
Assessment 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 $x$ 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.
1. **Size**

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2. **Classification error**

Quantifies the rigor according to which a class label is assigned to \( x \) in a leaf node of \( T \), based on the examples in \( D \). [Illustration]

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.
Decision Trees Basics
Assessment of Decision Trees: Size

- **Leaf node number**
  The leaf node number corresponds to the 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 with each length value weighted by the number of examples in $D$ that are classified by this path.
Decision Trees Basics
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Decision Trees Basics
Assessment of Decision Trees: Size (continued)

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

<table>
<thead>
<tr>
<th>Color</th>
<th>Size</th>
<th>Points</th>
<th>Edibility</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>red</td>
<td>small</td>
<td>yes</td>
</tr>
<tr>
<td>2</td>
<td>brown</td>
<td>small</td>
<td>no</td>
</tr>
<tr>
<td>3</td>
<td>brown</td>
<td>large</td>
<td>yes</td>
</tr>
<tr>
<td>4</td>
<td>green</td>
<td>small</td>
<td>no</td>
</tr>
<tr>
<td>5</td>
<td>red</td>
<td>large</td>
<td>no</td>
</tr>
</tbody>
</table>
The following trees correctly classify all examples in $D$:

(a) Feature: Color
   - Red
   - Green
   - Brown

   Feature: Size
   - Small
   - Large

   Feature: Points
   - Yes
   - No

(b) Feature: Size
   - Small
   - Large

   Feature: Points
   - Yes
   - No

Criterion | (a) | (b) |
----------|-----|-----|
Leaf node number | 4   | 3   |
Tree height       | 2   | 2   |
External path length | 6   | 5   |
Decision Trees Basics
Assessment of Decision Trees: Size (continued)

The following trees correctly classify all examples in $D$:

(a) Feature: Color
   - red
     - Feature: Size
       - small
         - Label: toxic 1x
       - large
         - Label: edible 1x
   - green
     - Feature: Size
       - small
         - Label: toxic 1x
       - large
         - Label: edible 1x
   - brown
     - Feature: Size
       - small
         - Label: toxic 1x
       - large
         - Label: edible 2x

(b) Feature: Size
   - small
     - Feature: Points
       - yes
         - Label: toxic 1x
       - no
         - Label: edible 2x
   - large
     - Feature: Points
       - yes
         - Label: toxic 1x
       - no
         - Label: edible 2x

<table>
<thead>
<tr>
<th>Criterion</th>
<th>(a)</th>
<th>(b)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Leaf node number</td>
<td>4</td>
<td>3</td>
</tr>
<tr>
<td>Tree height</td>
<td>2</td>
<td>2</td>
</tr>
<tr>
<td>External path length</td>
<td>6</td>
<td>5</td>
</tr>
<tr>
<td>Weighted external path length</td>
<td>7</td>
<td>8</td>
</tr>
</tbody>
</table>
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.
Decision Trees Basics
Assessment 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 $t$, $\text{label}(t)$, is defined as follows:

$$\text{label}(t) = \arg\max_{c \in C} |\{(x, c) \in D(t)\}|$$
Decision Trees Basics
Assessment 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:

\[
label(t) = \arg\max_{c \in C} |\{(x, c) \in D(t)\}|
\]

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

\[
Err(t, D(t)) = \frac{|\{(x, c) \in D(t) : label(t) \neq c\}|}{|D(t)|}
\]
Decision Trees Basics
Assessment 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 $t$, $\text{label}(t)$, is defined as follows:

$$\text{label}(t) = \arg\max_{c \in C} |\{(x, c) \in D(t)\}|$$

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

$$\text{Err}(t, D(t)) = \frac{|\{(x, c) \in D(t) : \text{label}(t) \neq c\}|}{|D(t)|} = 1 - \max_{c \in C} \frac{|\{(x, c) \in D(t)\}|}{|D(t)|}$$
Decision Trees Basics
Assessment 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 $t$, $\text{label}(t)$, is defined as follows:

$$\text{label}(t) = \arg\max_{c \in C} \left| \{(x, c) \in D(t)\} \right|$$

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

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

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

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

- The classifiers \( t \) and \( T \) may not have been constructed using \( D(t) \) as training data. I.e., the example set \( D(t) \) is in the role of a test set and \( \text{Err}(T, D) \) denotes the holdout error.

- If \( D \) has been used as training set, a reliable interpretation of the (training) error \( \text{Err}(T, D) \) in terms of \( \text{Err}^*(T) \) requires the Inductive Learning Hypothesis to hold.

- Observe the difference between \( \max f() \) and \( \arg\max f() \). Both expressions maximize \( f() \), but the former returns the maximum \( f() \)-value (the image) while the latter returns the argument (the preimage) for which \( f() \) becomes maximum:

\[
\begin{align*}
\max_{c \in C} f(c) &= \max \{f(c) \mid c \in C\} \\
\arg\max_{c \in C} f(c) &= c^* \Rightarrow f(c^*) = \max_{c \in C} f(c)
\end{align*}
\]

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

\[
\text{label}(t) = \arg\max_{c \in C} P(C=c \mid D=X(t)),
\]

where \( C \) denotes a random variable with range \( C \), the set of classes. \( D=X(t) \) is a data event where \( D \) denotes a set of random vectors with realization \( X(t) \).
Remarks (misclassification costs):

- The assessment of decision trees can also be based on **misclassification costs**:

\[
\text{label}(t) = \arg\min_{c' \in C} \sum_{c \in C} |\{(x, c) \in D(t)\}| \cdot \text{cost}(c', c)
\]

\[
\text{Err}_{\text{cost}}(t, D(t)) = \frac{1}{|D(t)|} \cdot \sum_{(x, c) \in D(t)} \text{cost}(\text{label}(t), c) = \min_{c' \in C} \sum_{c \in C} \frac{|\{(x, c) \in D(t)\}|}{|D(t)|} \cdot \text{cost}(c', c)
\]

\[
\text{Err}_{\text{cost}}(T, D) = \sum_{t \in \text{leaves}(T)} \frac{|D(t)|}{|D|} \cdot \text{Err}_{\text{cost}}(t, D(t))
\]

- As before, observe the difference between \(\min f()\) and \(\arg\min f()\). Both expressions minimize \(f()\), but the former returns the minimum \(f()\)-value (the image) while the latter returns the argument (the preimage) for which \(f()\) becomes minimum.