*** Applied Machine Learning Fundamentals ***
Decision Trees and Ensembles

Daniel Wehner

SAP SE

October 30, 2019

Find all slides on GitHub

Agenda October 30, 2019

Section:

Introduction

What we want...

Outlook	Temperature	Humidity	Wind	PlayGolf
sunny	hot	high	weak	**no**
sunny	hot	high	strong	**no**
overcast	hot	high	weak	**yes**
rainy	mild	high	weak	**yes**
rainy	cool	normal	weak	**yes**
rainy	cool	normal	strong	**no**
overcast	cool	normal	strong	**yes**
sunny	mild	high	weak	**no**
sunny	cool	normal	weak	**yes**
rainy	mild	normal	weak	**yes**
sunny	mild	normal	strong	**yes**
overcast	mild	high	strong	**yes**
overcast	hot	normal	weak	**yes**
rainy	mild	high	strong	**no**
rainy	mild	normal	strong	**???**
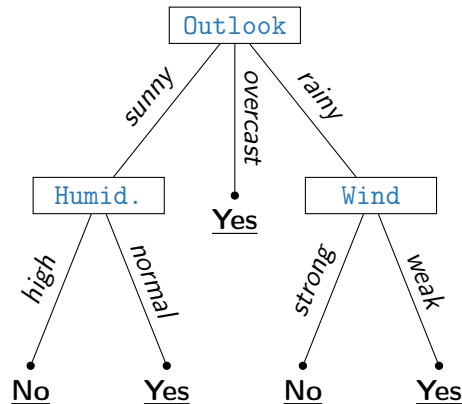
What are Decision Trees?

- Decision trees are induced in a **supervised** fashion

- Originally invented by *Ross Quinlan* (1986)

- Decision trees are grown **recursively** $\rightarrow$ *'divide-and-conquer'*

- A decision tree consists of:

  Nodes   Each node corresponds to an attribute test
  Edges   One edge per possible test outcome
  Leaves   Class label to predict

Classifying new Instances

- Suppose we get a new instance:

  Outlook   rainy
  Temperature   mild
  Humidity   normal
  Wind   strong

- **What is its class?**

- Answer: **No**
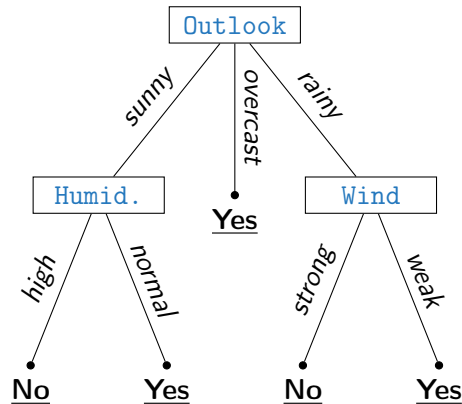
Another Decision Tree...
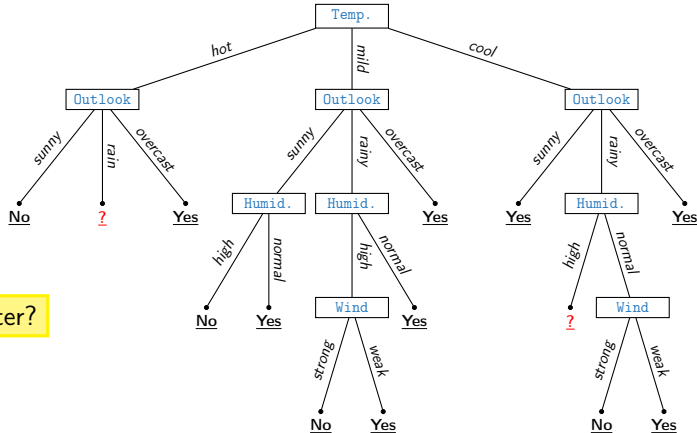
Is this one better?

Section:
Iterative Dichotomizer (ID3)

Introduction
Iterative Dichotomizer (ID3)
Extensions and Variants
Ensemble Methods
Wrap-Up

Inductive Bias
Entropy and Information Gain
ID3 Algorithm

Inductive Bias of Decision Trees

- Complex models tend to **overfit** the data and **do not generalize well**

- Small decision trees are preferred

  > **Occam's razor**:
  > **'More things should not be used than are necessary.'**

- Prefer the simplest hypothesis that fits the data!

Introduction
Iterative Dichotomizer (ID3)
Extensions and Variants
Ensemble Methods
Wrap-Up

Inductive Bias
Entropy and Information Gain
ID3 Algorithm

The Root of all Evil... Which Attribute to choose?

Outlook

sunny / overcast / rainy

- Yes Yes No No No
- Yes Yes Yes Yes
- Yes Yes Yes No No

Temp.

hot / mild / cool

- Yes Yes No No
- Yes Yes Yes No No
- Yes Yes Yes No

Wind

strong / weak

- Yes Yes Yes Yes Yes Yes No No
- Yes Yes Yes No No No

Humid.

high / normal

- Yes Yes Yes No No No No
- Yes Yes Yes Yes Yes Yes No

Introduction
Iterative Dichotomizer (ID3)
Extensions and Variants
Ensemble Methods
Wrap-Up

Inductive Bias
Entropy and Information Gain
ID3 Algorithm

Finding a proper Attribute

- Simple and small trees are preferred
  - Data in successor node should be **as pure as possible**
  - I. e. nodes containing one class only are preferable
- **Question**: How can we express this thought as a mathematical formula?
- **Answer**:
  - Entropy (*Claude E. Shannon*)
  - Originates in the field of **information theory**

Introduction
Iterative Dichotomizer (ID3)
Extensions and Variants
Ensemble Methods
Wrap-Up

Inductive Bias
Entropy and Information Gain
ID3 Algorithm
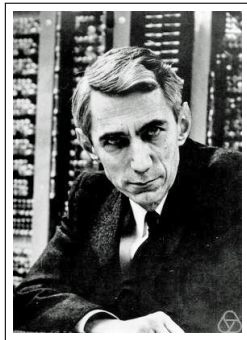
Measure of Impurity: Entropy

- Entropy is a measure of chaos in the data (measured in bits)

- **Example:** Consider two classes A and B ($\mathcal{C} = \{A, B\}$)

$$
\begin{aligned}
E(\{\boldsymbol{A}, \boldsymbol{A}, \boldsymbol{A}, \boldsymbol{A}, \boldsymbol{A}, \boldsymbol{A}, \boldsymbol{A}, \boldsymbol{A}\}) \quad &\rightarrow 0 \quad && Bits \\
E(\{\boldsymbol{A}, \boldsymbol{A}, \boldsymbol{A}, \boldsymbol{A}, \boldsymbol{A}, \boldsymbol{A}, B, B\}) \quad &\rightarrow 0.81 \quad && Bits \\
E(\{\boldsymbol{A}, \boldsymbol{A}, \boldsymbol{A}, \boldsymbol{A}, B, B, B, B\}) \quad &\rightarrow 1 \quad && Bit \\
E(\{\boldsymbol{A}, \boldsymbol{A}, B, B, B, B, B, B\}) \quad &\rightarrow 0.81 \quad && Bits \\
E(\{B, B, B, B, B, B, B, B\}) \quad &\rightarrow 0 \quad && Bits
\end{aligned}
$$

> If both classes are equally distributed, the entropy function E reaches its maximum. Pure data sets have minimal entropy.

Introduction
Iterative Dichotomizer (ID3)
Extensions and Variants
Ensemble Methods
Wrap-Up

Inductive Bias
Entropy and Information Gain
ID3 Algorithm

Measure of Impurity: Entropy (Ctd.)

$$E(\mathcal{D}) = -\sum_{c \in \mathcal{C}} p_c \cdot \log_2 p_c$$

Introduction
Iterative Dichotomizer (ID3)
Extensions and Variants
Ensemble Methods
Wrap-Up

Inductive Bias
Entropy and Information Gain
ID3 Algorithm
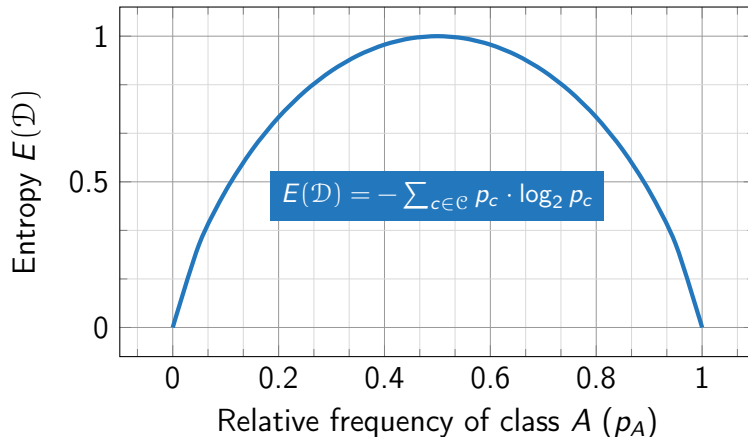
Measure of Impurity: Entropy (Ctd.)

Entropy formula:

$$E(\mathcal{D}) = -\sum_{c \in \mathcal{C}} p_c \cdot \log_2 p_c \qquad (1)$$

- p_c denotes the relative frequency of class $c \in \mathcal{C}$
- **Weather data:**

$$\mathcal{C} = \{yes, no\} \qquad \text{i. e.} \qquad p_{yes} = {}^9\!/_{14} \quad \text{and} \quad p_{no} = {}^5\!/_{14}$$

$$E(\mathcal{D}) = -\sum_{c \in \mathcal{C}} p_c \cdot \log_2 p_c = -({}^9\!/_{14} \cdot \log_2 {}^9\!/_{14} + {}^5\!/_{14} \cdot \log_2 {}^5\!/_{14}) = \mathbf{0.9403}$$

Introduction
Iterative Dichotomizer (ID3)
Extensions and Variants
Ensemble Methods
Wrap-Up

Inductive Bias
Entropy and Information Gain
ID3 Algorithm

Quality of the Split: Average Entropy

- We still don't know which attribute to use for the split

- Calculate the entropy after each potential split

- **Average Entropy** after splitting by attribute `A`:

$$E(\mathcal{D}, \mathtt{A}) = \sum_{v \in \mathrm{dom}(\mathtt{A})} \frac{|\mathcal{D}_{\mathtt{A}=v}|}{|\mathcal{D}|} \cdot E(\mathcal{D}_{\mathtt{A}=v}) \tag{2}$$

- Legend:

`A`	Attribute
$\mathrm{dom}(\mathtt{A})$	Possible values attribute `A` can take (domain of `A`)
$|\mathcal{D}_{\mathtt{A}=v}|$	Number of examples satisfying $\mathtt{A} = v$

Introduction
Iterative Dichotomizer (ID3)
Extensions and Variants
Ensemble Methods
Wrap-Up

Inductive Bias
Entropy and Information Gain
ID3 Algorithm

Quality of the Split: Average Entropy (Ctd.)

Example: Attribute `Outlook`

$$E(\mathcal{D}, \texttt{Outlook}) = \sum_{v \in \text{dom}(\texttt{Outlook})} \frac{|\mathcal{D}_{\texttt{Outlook}=v}|}{|\mathcal{D}|} \cdot E(\mathcal{D}_{\texttt{Outlook}=v})$$

$$= {}^5\!/_{14} \cdot 0.9710 + {}^5\!/_{14} \cdot 0.9710 + {}^4\!/_{14} \cdot 0 \qquad = \mathbf{0.6936}$$

$$E(\mathcal{D}_{\texttt{Outlook}=sunny}) = -({}^2\!/_5 \cdot \log_2({}^2\!/_5) + {}^3\!/_5 \cdot \log_2({}^3\!/_5)) \qquad = 0.9710$$

$$E(\mathcal{D}_{\texttt{Outlook}=rainy}) = -({}^3\!/_5 \cdot \log_2({}^3\!/_5) + {}^2\!/_5 \cdot \log_2({}^2\!/_5)) \qquad = 0.9710$$

$$E(\mathcal{D}_{\texttt{Outlook}=overcast}) = -({}^4\!/_4 \cdot \log_2({}^4\!/_4) + {}^0\!/_4 \cdot \log_2({}^0\!/_4)) \qquad = 0$$

Introduction
Iterative Dichotomizer (ID3)
Extensions and Variants
Ensemble Methods
Wrap-Up

Inductive Bias
Entropy and Information Gain
ID3 Algorithm

Information Gain

- We have calculated the entropy before and after the split
- The difference of both is called the information gain (IG)
- Select the attribute with the highest IG

Attribute	E_{before}	E_{after}	IG
`Outlook`	0.9403	0.6936	0.2464
`Temperature`	0.9403	0.9111	0.0292
`Humidity`	0.9403	0.7885	0.1518
`Wind`	0.9403	0.8922	0.0481

- Attribute `Outlook` maximizes IG
- After the split: Remove attribute `Outlook`

Introduction
Iterative Dichotomizer (ID3)
Extensions and Variants
Ensemble Methods
Wrap-Up

Inductive Bias
Entropy and Information Gain
ID3 Algorithm

Training Data after the Split by Attribute `Outlook`

~~Outlook~~	Temperature	Humidity	Wind	PlayGolf
~~sunny~~	hot	high	weak	no
~~sunny~~	hot	high	strong	no
~~sunny~~	mild	high	weak	no
~~sunny~~	cool	normal	weak	yes
~~sunny~~	mild	normal	strong	yes
~~rainy~~	mild	high	weak	yes
~~rainy~~	cool	normal	weak	yes
~~rainy~~	cool	normal	strong	no
~~rainy~~	mild	normal	weak	yes
~~rainy~~	mild	high	strong	no
~~overcast~~	cool	normal	strong	yes
~~overcast~~	hot	high	weak	yes
~~overcast~~	mild	high	strong	yes
~~overcast~~	hot	normal	weak	yes

- Data set $\mathcal{D}$ after the split

- We obtain three subsets (one per attribute value)

- Attribute `Outlook` is removed

Introduction
Iterative Dichotomizer (ID3)
Extensions and Variants
Ensemble Methods
Wrap-Up

Inductive Bias
Entropy and Information Gain
ID3 Algorithm

Important

How to proceed?

- The algorithm is recursively applied to the resulting subsets
  1. Calculate entropy (before and after the split)
  2. Calculate information gain for each attribute
  3. Choose the attribute with max. information gain for the split
  4. In the current branch: Do not consider the attribute any more
  5. **Recursion** ↺ (`Go to 1`)
- Recursion stops as soon as the subset is pure
- In the example above the subset $\mathcal{D}_{\texttt{Outlook}=overcast}$ is already pure
- This algorithm is referred to as **ID3 (Iterative Dichotomizer)**

Introduction
Iterative Dichotomizer (ID3)
Extensions and Variants
Ensemble Methods
Wrap-Up

Inductive Bias
Entropy and Information Gain
ID3 Algorithm

Step by Step: Construction of the Tree

Introduction
Iterative Dichotomizer (ID3)
Extensions and Variants
Ensemble Methods
Wrap-Up

Inductive Bias
Entropy and Information Gain
ID3 Algorithm
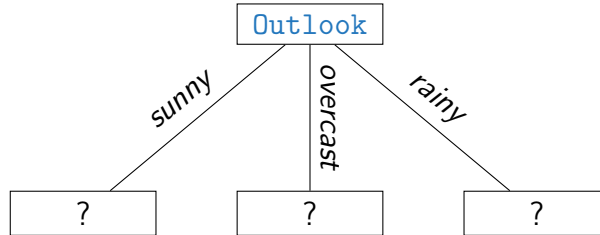
Step by Step: Construction of the Tree (Ctd.)
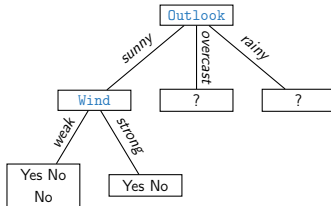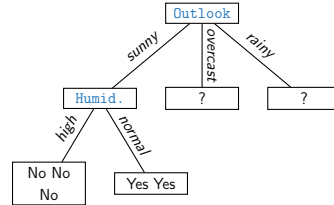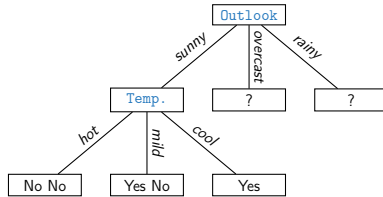
- $IG(\texttt{Temperature}) = 0.571$

- $IG(\texttt{Humidity}) = \mathbf{0.971}$

- $IG(\texttt{Wind}) = 0.020$

Introduction
Iterative Dichotomizer (ID3)
Extensions and Variants
Ensemble Methods
Wrap-Up

Inductive Bias
Entropy and Information Gain
ID3 Algorithm

Step by Step: Construction of the Tree (Ctd.)

Introduction
Iterative Dichotomizer (ID3)
Extensions and Variants
Ensemble Methods
Wrap-Up

Inductive Bias
Entropy and Information Gain
ID3 Algorithm

Step by Step: Construction of the Tree (Ctd.)

Introduction
Iterative Dichotomizer (ID3)
Extensions and Variants
Ensemble Methods
Wrap-Up

Inductive Bias
Entropy and Information Gain
ID3 Algorithm
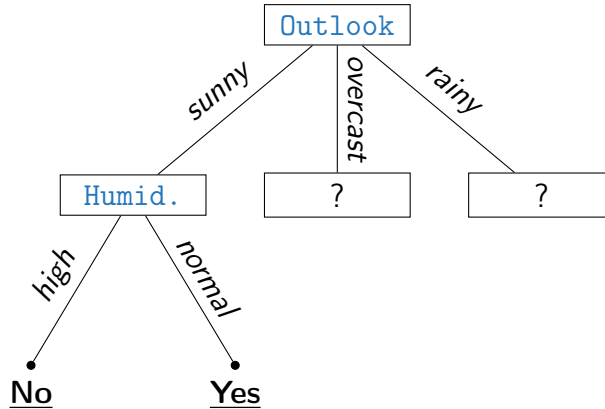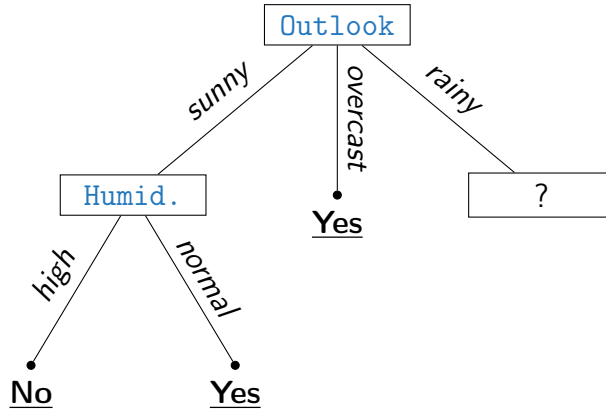
Step by Step: Construction of the Tree (Ctd.)
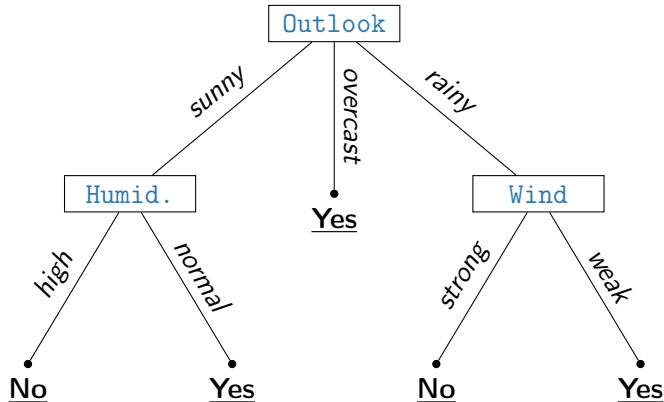
Algorithm 1: ID3 Algorithm (Iterative Dichotomizer)

Input: Training set $\mathcal{D}$, Attribute list *Attr_List*

1 Create a node N
2 **if** *all tuples in $\mathcal{D}$ have class c* **then**
3   **return** N as leaf node labeled with class c
4 **if** $|Attr\_List| = 0$ **then**
5   **return** N as leaf node labeled with majority class in $\mathcal{D}$
6 Find best split attribute $\mathtt{A}^*$ and label node N with $\mathtt{A}^*$
7 *Attr_List* $\longleftarrow$ *Attr_List* $\setminus \{\mathtt{A}^*\}$
8 **forall** $v \in dom(\mathtt{A}^*)$ **do**
9   Let $\mathcal{D}_{\mathtt{A}^*=v}$ be the set of tuples in $\mathcal{D}$ that satisfy $\mathtt{A}^* = v$
10   **if** $|\mathcal{D}_{\mathtt{A}^*=v}| = 0$ **then**
11   Attach leaf labeled with majority class in $\mathcal{D}$ to node N
12   **else**
13   Attach node returned by *ID3*($\mathcal{D}_{\mathtt{A}^*=v}$, *Attr_List*)
14 **return** N

Section:

Extensions and Variants

Introduction
Iterative Dichotomizer (ID3)
Extensions and Variants
Ensemble Methods
Wrap-Up

Other Measures of Impurity
Highly-branching Attributes
Numeric Attributes
Regression Trees

An Alternative to Information Gain: Gini Index

Gini index:

$$Gini(\mathcal{D}) = \sum_{c \in \mathcal{C}} p_c \cdot (1 - p_c) = 1 - \sum_{c \in \mathcal{C}} p_c^2 \tag{3}$$

- Used e. g. in **CART (Classification and Regression Trees)**
- **Gini gain** could be defined analogously to IG
  (usually not done)

Introduction
Iterative Dichotomizer (ID3)
Extensions and Variants
Ensemble Methods
Wrap-Up

Other Measures of Impurity
Highly-branching Attributes
Numeric Attributes
Regression Trees

Why not use the Error as a splitting Criterion?

- The bias towards pure leaves is **not strong enough**
- **Example:**

Split 1

| 40 of A | 60 of A |
| 60 of A | 40 of B |

Split 2

Error without splitting:
20 %

Error after splitting:
20 %

Both splits don't improve the error.
But together they give a perfect split!

Introduction
Iterative Dichotomizer (ID3)
Extensions and Variants
Ensemble Methods
Wrap-Up

Other Measures of Impurity
Highly-branching Attributes
Numeric Attributes
Regression Trees

Summary: Impurity Measures

Introduction
Iterative Dichotomizer (ID3)
Extensions and Variants
Ensemble Methods
Wrap-Up

Other Measures of Impurity
Highly-branching Attributes
Numeric Attributes
Regression Trees
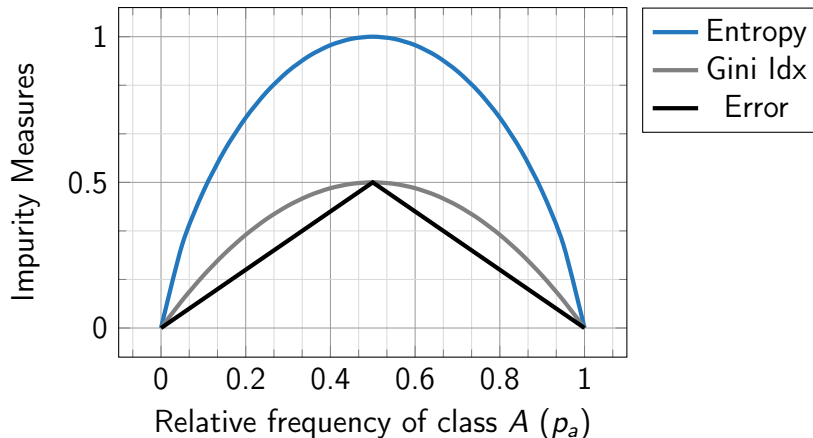
Highly-branching Attributes

Attributes with a large number of values are problematic, since the leaves are not 'backed' with sufficient data examples.

In extreme cases only one example per node (e. g. IDs)

This may lead to:

- **Overfitting** (Selection of attributes which are not optimal for prediction)
- **Fragmentation** (Data is fragmented into (too) many small sets)

Introduction
Iterative Dichotomizer (ID3)
Extensions and Variants
Ensemble Methods
Wrap-Up

Other Measures of Impurity
Highly-branching Attributes
Numeric Attributes
Regression Trees

Highly-branching Attributes (Ctd.)
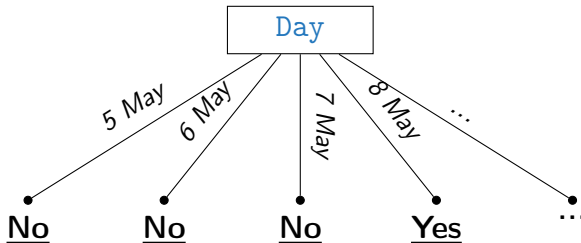
- Entropy before was 0.9403, Entropy after split is 0
- IG($\mathcal{D}$, Day) = 0.9403
- Attribute Day would be chosen for the split $\Rightarrow$ **Bad for prediction** ☠

Introduction
Iterative Dichotomizer (ID3)
Extensions and Variants
Ensemble Methods
Wrap-Up

Other Measures of Impurity
Highly-branching Attributes
Numeric Attributes
Regression Trees

Highly-branching Attributes (Ctd.)

- Calculate the **intrinsic information (IntI)**:

$$IntI(\mathcal{D}, \mathtt{A}) = -\sum_{v \in \mathsf{dom}(\mathtt{A})} \frac{|\mathcal{D}_{\mathtt{A}=v}|}{|\mathcal{D}|} \cdot \log_2 \frac{|\mathcal{D}_{\mathtt{A}=v}|}{|\mathcal{D}|} \tag{4}$$

- Attributes with high *IntI* are **less useful** (high fragmentation)
- New splitting heuristic **Gain ratio (GR)**:

$$GR(\mathcal{D}, \mathtt{A}) = \frac{IG(\mathcal{D}, \mathtt{A})}{IntI(\mathcal{D}, \mathtt{A})} \tag{5}$$

Introduction
Iterative Dichotomizer (ID3)
Extensions and Variants
Ensemble Methods
Wrap-Up

Other Measures of Impurity
Highly-branching Attributes
Numeric Attributes
Regression Trees

Highly-branching Attributes (Ctd.)

- Intrinsic information for attribute Day:

$$IntI(\mathcal{D}, \text{Day}) = 14 \cdot (-1/14 \cdot \log_2(1/14)) = \mathbf{3.807} \tag{6}$$

- Gain ratio for attribute Day:

$$GR(\mathcal{D}, \text{Day}) = \frac{0.9403}{3.807} = \mathbf{0.246} \tag{7}$$

> In this case the attribute Day would still be chosen. Be careful what features to include into the training data set! **(Feature engineering is important!)**

Introduction
Iterative Dichotomizer (ID3)
Extensions and Variants
Ensemble Methods
Wrap-Up

Other Measures of Impurity
Highly-branching Attributes
Numeric Attributes
Regression Trees

Handling numeric Attributes

- Usually, only **binary splits** are considered, e. g.:
  - $\texttt{Temperature} < 48$
  - $\texttt{CPU} > 24$
  - **Not:** $24 \leqslant \texttt{Temperature} \leqslant 31$
- To support multiple splits, the attribute is **not removed**

  (the same attribute can be used again for another split)
- **Problem:** There is an **infinite number** of possible splits!
- **Solution:** Discretize range (fixed step size, ...)
- Splitting on numeric attributes is computationally demanding!

Introduction
Iterative Dichotomizer (ID3)
Extensions and Variants
Ensemble Methods
Wrap-Up

Other Measures of Impurity
Highly-branching Attributes
Numeric Attributes
Regression Trees

Handling numeric Attributes (Ctd.)

- Consider the attribute `Temperature`:
  Use **numerical values** instead of discrete values like *cool*, *mild*, *hot*:

64	65	68	69	70	71	72	72	75	75	80	81	83	85
Yes	No	Yes	Yes	Yes	No	No	Yes	Yes	Yes	No	Yes	Yes	No

- `Temperature` < 71.5

  yes: 4 | no: 2

- `Temperature` $\geqslant 71.5$

  yes: 5 | no: 3

$$E(\mathcal{D}, \texttt{Temp.}) = \text{\textonesuperior}/\text{\tiny 14} \cdot E(\texttt{Temp.} < 71.5) + \text{\tiny 8}/\text{\tiny 14} \cdot E(\texttt{Temp.} \geqslant 71.5) = \mathbf{0.939}$$

Introduction
Iterative Dichotomizer (ID3)
Extensions and Variants
Ensemble Methods
Wrap-Up

Other Measures of Impurity
Highly-branching Attributes
Numeric Attributes
Regression Trees

Handling numeric Attributes (Ctd.)

Sorted Values									
No	No	No	Yes	Yes	Yes	No	No	No	No
Taxable Income									
60	70	75	85	90	95	100	120	125	220

Split	55		65		72		80		87		92		97		110		122		172		230	
	⩽	>	⩽	>	⩽	>	⩽	>	⩽	>	⩽	>	⩽	>	⩽	>	⩽	>	⩽	>	⩽	>
Yes	0	3	0	3	0	3	0	3	1	2	2	1	3	0	3	0	3	0	3	0	3	0
No	0	7	1	6	2	5	3	4	3	4	3	4	3	4	4	3	5	2	6	1	7	0
Gini	0.420		0.400		0.375		0.343		0.417		0.400		0.300		0.343		0.375		0.400		0.420	

Introduction
Iterative Dichotomizer (ID3)
Extensions and Variants
Ensemble Methods
Wrap-Up

Other Measures of Impurity
Highly-branching Attributes
Numeric Attributes
Regression Trees

Regression Trees

- Prediction of continuous variables
- Predict average value of all examples in the leaf
- Split the data such that variance in the leaves is minimized
- **Termination criterion is important, otherwise single point per leaf!**

Standard deviation reduction (SDR):

$$SDR(\mathcal{D}, \mathtt{A}) = SD(\mathcal{D}) - \sum_{v \in dom(\mathtt{A})} \frac{|\mathcal{D}_{\mathtt{A}=v}|}{|\mathcal{D}|} \cdot SD(\mathcal{D}_{\mathtt{A}=v}) \qquad (8)$$

Section:
Ensemble Methods

Introduction
Iterative Dichotomizer (ID3)
Extensions and Variants
Ensemble Methods
Wrap-Up

Introduction to Ensembles
Bagging and Randomization
Boosting
Stacking
Error-correcting Output Codes

Introduction Ensemble Methods

- **Key Idea**: Don't learn a single classifier but a **set of classifiers**
- Combine the predictions of the single classifiers to obtain the final prediction

Problem: How can we induce multiple classifiers from a single data set without getting the same classifier over and over again? **We want to have diverse classifiers, otherwise the ensemble is useless!**

- Basic techniques:
  - Bagging
  - Boosting
  - Stacking

Introduction
Iterative Dichotomizer (ID3)
Extensions and Variants
Ensemble Methods
Wrap-Up

Introduction to Ensembles
Bagging and Randomization
Boosting
Stacking
Error-correcting Output Codes

What is the Advantage?

- Consider the following:
  - There are 25 **independent** base classifiers
  - Independence assumption: Probability of misclassification **does not** depend on other classifiers in the ensemble
  - Usually, this assumption does not fully hold in practice
  - Each classifier has an error rate of $\varepsilon = 0.35$
- The ensemble makes a wrong prediction **if the majority is wrong** ($\Rightarrow$ i.e. at least 13)

$$\varepsilon_{ensemble} = \sum_{u=13}^{25} \binom{25}{u} \cdot \varepsilon^u \cdot (1-\varepsilon)^{25-u} \approx \mathbf{0.06} \ll \varepsilon \qquad (9)$$

Introduction
Iterative Dichotomizer (ID3)
Extensions and Variants
Ensemble Methods
Wrap-Up

Introduction to Ensembles
Bagging and Randomization
Boosting
Stacking
Error-correcting Output Codes

Bagging: General Approach

Bagging $\widehat{=}$ **B**ootstrap **Agg**regat**ing**

Introduction
Iterative Dichotomizer (ID3)
Extensions and Variants
Ensemble Methods
Wrap-Up

Introduction to Ensembles
Bagging and Randomization
Boosting
Stacking
Error-correcting Output Codes
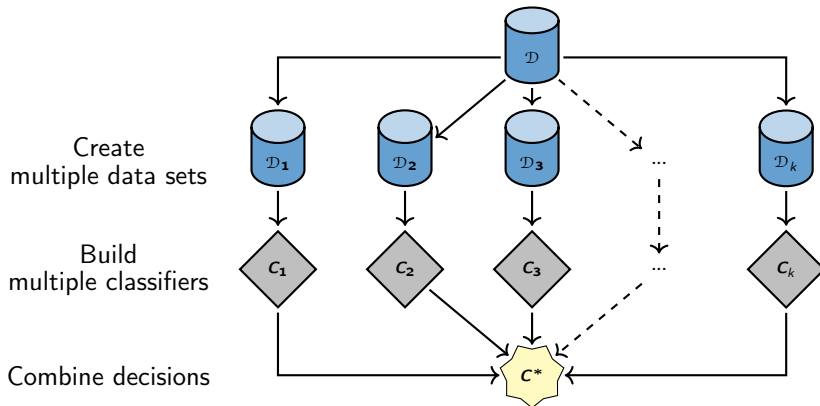
Creating the Bootstrap Samples

- How to generate multiple data sets which are different?

- **Solution**: Use sampling with replacement

Original Data	1	2	3	4	5	6	7	8	9	10
Bagging (Round 1)	7	8	10	8	2	5	10	10	5	9
Bagging (Round 2)	1	4	9	1	2	3	2	7	3	2
Bagging (Round 3)	1	8	5	10	5	5	9	6	3	7

- Some examples may appear **in more than one set**

- Some examples may appear **more than once** in one set

- Some examples may **not appear at all**

Algorithm 2: Bagging Algorithm

Input: Training set $\mathcal{D}$, number of base classifiers k

1 **Training:**

2 **forall** $u \in \{1, 2, \ldots, k\}$ **do**

3   Draw a bootstrap sample $\mathcal{D}_u$ with replacement from $\mathcal{D}$

4   Learn a classifier C_u from $\mathcal{D}_u$

5   Add classifier C_u to the ensemble

6 **Prediction:**

7 **forall** *unlabeled instances* **do**

8   Get predictions from all classifiers C_u

9 **return** *Class which receives the majority of votes (combined classifier C^*)*

Introduction
Iterative Dichotomizer (ID3)
Extensions and Variants
Ensemble Methods
Wrap-Up

Introduction to Ensembles
Bagging and Randomization
Boosting
Stacking
Error-correcting Output Codes

Bagging Variations

- The bootstrap samples had equal size and were drawn with replacement
- Also conceivable:
  1. **Varying the size** of the bootstrap samples
  2. Sampling **without replacement** $\Rightarrow$ **Pasting**
  3. **Sampling of features**, not instances
     - Not all features are available in all bootstrap samples
     - This is how **random forests** work
  4. Creating **heterogeneous ensembles**
     (Neural networks, decision trees, support vector machines, ...)

Introduction
Iterative Dichotomizer (ID3)
Extensions and Variants
Ensemble Methods
Wrap-Up

Introduction to Ensembles
Bagging and Randomization
Boosting
Stacking
Error-correcting Output Codes

Bagged Decision Trees
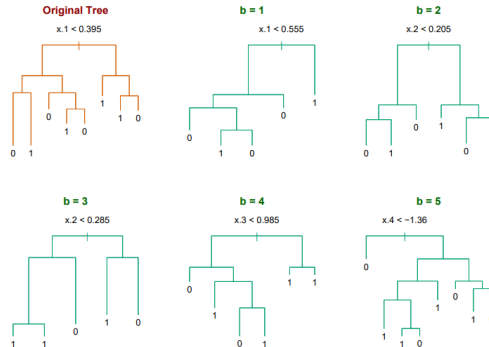
Figure: Bagged decision trees; cf. Hastie 2008, page 284

Introduction
Iterative Dichotomizer (ID3)
Extensions and Variants
Ensemble Methods
Wrap-Up

Introduction to Ensembles
Bagging and Randomization
Boosting
Stacking
Error-correcting Output Codes

Randomization

- Why not **randomizing the algorithm** instead of the data?
- Some algorithms already do that: E. g. neural networks (random initialization of weights)
- Especially greedy algorithms can be randomized:
  - Pick from the options **randomly** instead of picking the best one
  - E. g. decision trees: Do not choose attribute with highest information gain

A random forest combines randomization and bagging.

Introduction
Iterative Dichotomizer (ID3)
Extensions and Variants
Ensemble Methods
Wrap-Up

Introduction to Ensembles
Bagging and Randomization
Boosting
Stacking
Error-correcting Output Codes

Random Forest Algorithm

- Ensemble of decision trees
- Combines **bagging** and **random attribute subset selection**
- Build decision tree from a bootstrap sample
- Select best split attribute among a random subset of f attributes

A random forest selects the best splitting attributes from the set of features available, but the globally best features **may not** be available.
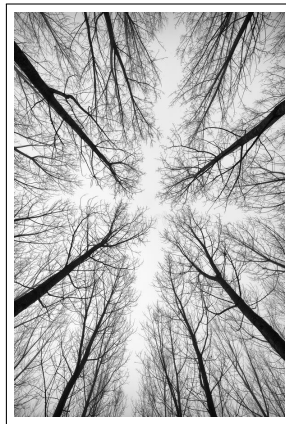
Algorithm 3: Random Forest Algorithm

Input: Training set $\mathcal{D}$, number of base classifiers k

1 **Training:**

2 **for** $u \in \{1, 2, \ldots, k\}$ **do**

3   Create a bootstrap sample from $\mathcal{D}$ (e. g. with replacement) $\Rightarrow$ **Bagging**

4   **begin**

5   Grow the tree

6   At every node: Randomly choose f attributes to be considered for the split

7          $\Rightarrow$ **Randomization**

8   Do not prune tree C_u

9   Add tree C_u to the ensemble

10 **Prediction:**

11 **forall** *unlabeled instances* **do**

12   Get predictions from all classifiers C_u

13 **return** *Class which receives the majority of votes (combined classifier C^*)*

Introduction
Iterative Dichotomizer (ID3)
Extensions and Variants
Ensemble Methods
Wrap-Up

Introduction to Ensembles
Bagging and Randomization
Boosting
Stacking
Error-correcting Output Codes

ExtraTrees (Randomization 2.0)

- One more step of randomization ⇒ **Ext**remely **Ra**ndomized **Trees**

- The general approach is the same as for random forests
  But:
  - Instead of choosing the optimal split point...
  - ...it is selected randomly
  - The decision tree is grown without having to calculate entropy

- It is **much faster** (due to less computation)

The large number of classifiers compensates for suboptimal splits

Introduction
Iterative Dichotomizer (ID3)
Extensions and Variants
Ensemble Methods
Wrap-Up

Introduction to Ensembles
Bagging and Randomization
Boosting
Stacking
Error-correcting Output Codes

Boosting Overview

- **Key Idea**:
  - New classifiers focus on examples misclassified by others
  - Assign a weight to each classifier (depending on their error)
- **How to**: *(Unlike bagging, boosting **cannot** be parallelized!)*
  1. Initialize example weights with $1/n$
  2. Train a model using the example weights, calculate error and model weight
  3. Update example weights according to model weight
  4. Train the next model using the updated example weights
  5. Combine predictions according to model weights

Algorithm 4: AdaBoost Algorithm

Input: Training set $\mathcal{D}$, number of base classifiers k

1 Training:

2 Initialize example weights $w_i \longleftarrow \frac{1}{n}$

3 forall $u \in \{1, 2, \ldots, k\}$ **do**

4   Learn a classifier C_u using the current example weights

5   Compute weighted error estimate of the model: $\varepsilon_u \longleftarrow \sum_{i=1}^{n} w_i \cdot \mathbb{1}\{y_{pred} \neq y^{(i)}\}$

6   Compute model weight: $\alpha_u \longleftarrow 1/2 \cdot \ln\left(\frac{1-\varepsilon_u}{\varepsilon_u}\right)$

7   For all correctly classified examples: $w_i \longleftarrow w_i \cdot \exp\{-\alpha_u\}$

8   For all incorrectly classified examples: $w_i \longleftarrow w_i \cdot \exp\{\alpha_u\}$

9   Normalize the weights w_i (such that they sum up to one): $\frac{w_i}{\sum_{i=1}^{n} w_i}$

10 Prediction:

11 forall *unlabeled instances* **do**

12   Get predictions from all classifiers C_u

13 return *Class which receives the the highest sum of weights* α_u *(combined classifier C^*)*

Introduction
Iterative Dichotomizer (ID3)
Extensions and Variants
Ensemble Methods
Wrap-Up

Introduction to Ensembles
Bagging and Randomization
Boosting
Stacking
Error-correcting Output Codes

AdaBoost: Illustration of Weights

Model weights α_u
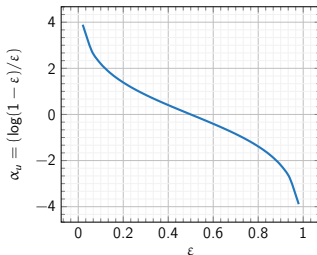
Example weights w_i
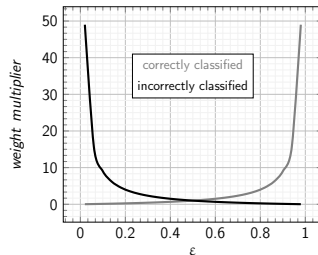
- Classifier weights α_u grow exponentially

- Classifier weight is 0 if error is $\frac{1}{2}$ (model cannot be trusted, random guessing)

- For high errors $\Rightarrow$ **Do the opposite of what the classifiers predicts**

Introduction
Iterative Dichotomizer (ID3)
Extensions and Variants
Ensemble Methods
Wrap-Up

Introduction to Ensembles
Bagging and Randomization
Boosting
Stacking
Error-correcting Output Codes

AdaBoost: Two Classes

- With two classes, $-\mathbf{1}$ and $+\mathbf{1}$, the final classifier C^* can be written as:

$$H(\boldsymbol{x}) = sign\left(\sum_{u=1}^{k} \alpha_u h_u(\boldsymbol{x})\right) \tag{10}$$

- α_u is defined as above

- The weight update for the examples is given by:

$$w_i^{new} = \frac{w_i^{old} \cdot \exp\{-\alpha_u y^{(i)} h_i(\boldsymbol{x}^{(i)})\}}{\sum_{i=1}^{n} w_i} \tag{11}$$

Introduction
Iterative Dichotomizer (ID3)
Extensions and Variants
Ensemble Methods
Wrap-Up

Introduction to Ensembles
Bagging and Randomization
Boosting
Stacking
Error-correcting Output Codes

Boosting Example

- Ensemble of **decision stumps** ($\widehat{=}$ tree with a single split only)
- 10 examples (5 from class $+\mathbf{1}$ and 5 from class $-\mathbf{1}$)
- Each example is initially weighted with a factor of $^1/_{10}$

Introduction
Iterative Dichotomizer (ID3)
Extensions and Variants
Ensemble Methods
Wrap-Up

Introduction to Ensembles
Bagging and Randomization
Boosting
Stacking
Error-correcting Output Codes
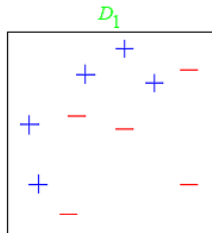
Boosting Example (Ctd.)

1st Iteration

$\varepsilon_1 = 0.30$

$\alpha_1 = 0.42$

Introduction
Iterative Dichotomizer (ID3)
Extensions and Variants
Ensemble Methods
Wrap-Up

Introduction to Ensembles
Bagging and Randomization
Boosting
Stacking
Error-correcting Output Codes
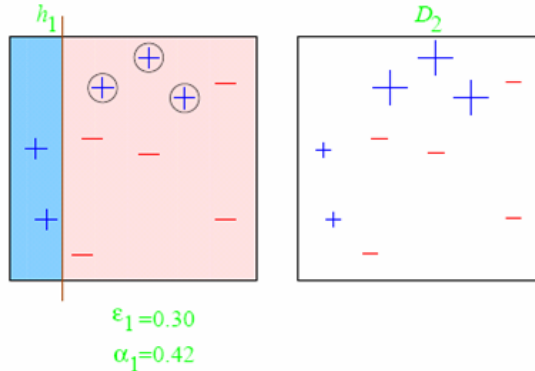
Boosting Example (Ctd.)
2nd Iteration

$\varepsilon_2 = 0.21$
$\alpha_2 = 0.65$

Introduction
Iterative Dichotomizer (ID3)
Extensions and Variants
Ensemble Methods
Wrap-Up

Introduction to Ensembles
Bagging and Randomization
Boosting
Stacking
Error-correcting Output Codes
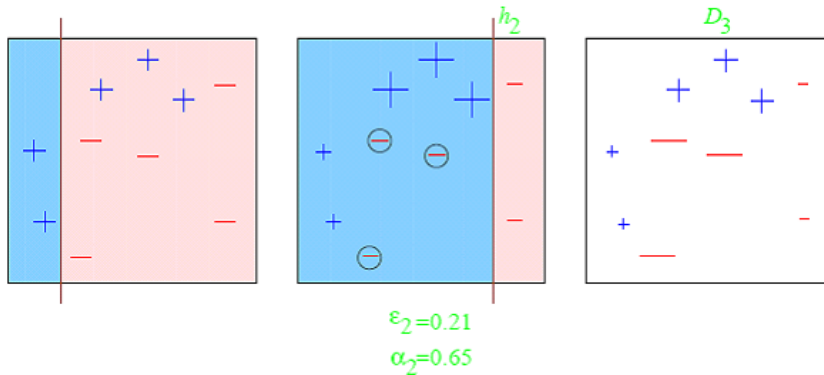
Boosting Example (Ctd.)
3rd Iteration

$\varepsilon_3 = 0.14$

$\alpha_3 = 0.92$

Introduction
Iterative Dichotomizer (ID3)
Extensions and Variants
Ensemble Methods
Wrap-Up

Introduction to Ensembles
Bagging and Randomization
Boosting
Stacking
Error-correcting Output Codes
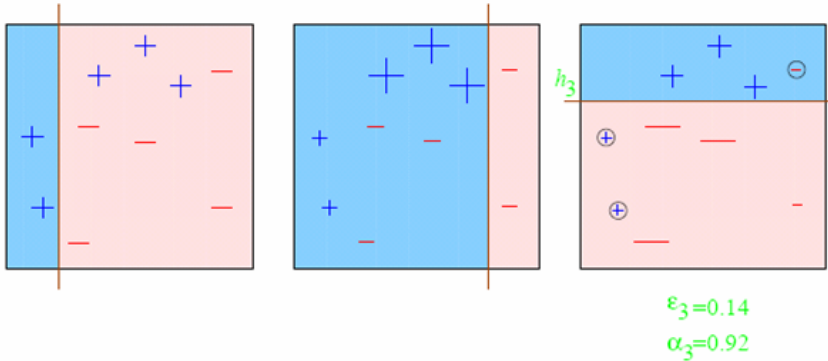
Boosting Example (Ctd.)
Prediction

Introduction
Iterative Dichotomizer (ID3)
Extensions and Variants
Ensemble Methods
Wrap-Up

Introduction to Ensembles
Bagging and Randomization
Boosting
Stacking
Error-correcting Output Codes
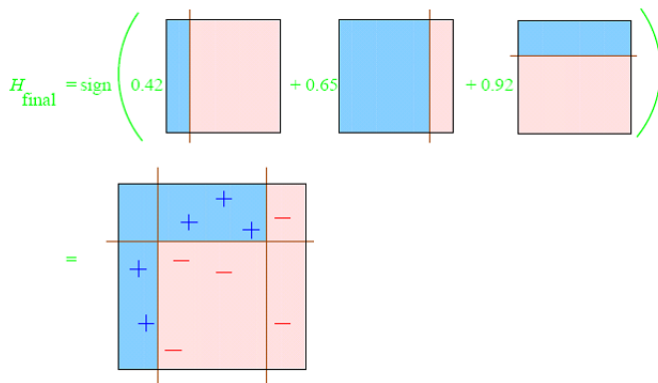
Combining Predictions

① **Voting** ✓
- Each classifier votes for one of the classes
- Each classifier has the same (model) weight
- This is **Bagging**

② **Weighted Voting** ✓
- Weight the individual predictions with model weight
- This is **Boosting**

③ **Stacking**
- Use a **meta classifier** to combine the predictions
- See next slides…

Algorithm 5: Stacking Algorithm

Input: Training set $\mathcal{D}$, number of base classifiers k

1 Train k base classifiers $C_1, C_2, \ldots, C_k$

2 Let all base classifiers predict the labels for the training set

3 Create the meta data set (*)

4 Train a meta classifier M on the meta data set

(*) Meta data set:

- **Labels**:
  Use the same labels as in the original data set

- **Attributes**:
  One attribute for each base classifier (k attributes)
  The attribute values are the predictions of the corresponding classifiers

Introduction
Iterative Dichotomizer (ID3)
Extensions and Variants
Ensemble Methods
Wrap-Up

Introduction to Ensembles
Bagging and Randomization
Boosting
Stacking
Error-correcting Output Codes

Stacking Example

Attributes			Class
$x_1^{(1)}$	$\dots$	$x_m^{(1)}$	true
$x_1^{(2)}$	$\dots$	$x_m^{(2)}$	false
$\dots$	$\dots$	$\dots$	$\dots$
$x_1^{(n)}$	$\dots$	$x_m^{(n)}$	true

Table: Original training set

C_1	C_2	$\dots$	C_k
true	true	$\dots$	false
false	true	$\dots$	true
$\dots$	$\dots$	$\dots$	$\dots$
false	false	$\dots$	true

Table: Predictions base classifiers

C_1	C_2	$\dots$	C_k	Class
true	true	$\dots$	false	true
false	true	$\dots$	true	false
$\dots$	$\dots$	$\dots$	$\dots$	$\dots$
false	false	$\dots$	true	true

Table: Meta data set

Introduction
Iterative Dichotomizer (ID3)
Extensions and Variants
Ensemble Methods
Wrap-Up

Introduction to Ensembles
Bagging and Randomization
Boosting
Stacking
Error-correcting Output Codes

Multi-Class-Problems

- Usually, a **class binarization** technique is needed
- One-vs-Rest (one classifier for each class)
- Each class is encoded in a **bit-string**

Class	Class Vector			
a	1	0	0	0
b	0	1	0	0
c	0	0	1	0
d	0	0	0	1

What would you do if the result were **1100**? It is not clear if the new instance belongs to class **a** or class **b**.
Solution: Use error-correcting output codes instead!

Introduction
Iterative Dichotomizer (ID3)
Extensions and Variants
Ensemble Methods
Wrap-Up

Introduction to Ensembles
Bagging and Randomization
Boosting
Stacking
Error-correcting Output Codes

Error-Correcting Output Codes (ECOCs)

- Use code words that have a high pairwise Hamming distance d

- Can correct up to $(d-1)/2$ single bit-errors

- In this case: Use seven classifiers

Class	Class Vector						
a	1	1	1	1	1	1	1
b	0	0	0	0	1	1	1
c	0	0	1	1	0	0	1
d	0	1	0	1	0	1	0

- Predicted code-word: 1011111 $\Rightarrow$ What is the true class???
  *Probably class **a**, the second classifier made a mistake...*

Introduction
Iterative Dichotomizer (ID3)
Extensions and Variants
Ensemble Methods
Wrap-Up

Introduction to Ensembles
Bagging and Randomization
Boosting
Stacking
Error-correcting Output Codes

ECOCs: How to encode the classes?

- Criteria for the code words
  - **Row separation** guarantees that errors can be corrected
  - **Column separation** (identical columns $\Rightarrow$ Classifier makes same error several times)

- **Exhaustive Codes**
  - **Class 1:** Code word consists of 1s only
  - **Class 2:** 2^{k-2} 0s followed by $2^{k-2} - 1$ 1s ($k \mathrel{\widehat{=}} \#$ classes)
  - **Class i:** Alternating runs of 2^{k-i} 0s and 1s
    (Last run is one bit shorter than the others)

Section:

Wrap-Up

Introduction
Iterative Dichotomizer (ID3)
Extensions and Variants
Ensemble Methods
Wrap-Up

Summary
Lecture Overview
Self-Test Questions
Recommended Literature and further Reading

Summary

Introduction
Iterative Dichotomizer (ID3)
Extensions and Variants
Ensemble Methods
Wrap-Up

Summary
Lecture Overview
Self-Test Questions
Recommended Literature and further Reading

Lecture Overview

Unit I: Machine Learning Introduction

Introduction
Iterative Dichotomizer (ID3)
Extensions and Variants
Ensemble Methods
Wrap-Up

Summary
Lecture Overview
Self-Test Questions
Recommended Literature and further Reading

Self-Test Questions

Introduction
Iterative Dichotomizer (ID3)
Extensions and Variants
Ensemble Methods
Wrap-Up

Summary
Lecture Overview
Self-Test Questions
Recommended Literature and further Reading

Recommended Literature and further Reading

Thank you very much for the attention!

Topic: *** Applied Machine Learning Fundamentals *** Decision Trees and Ensembles
Date: October 30, 2019

Contact:
Daniel Wehner (D062271)
SAP SE
daniel.wehner@sap.com

Do you have any questions?