

*** Applied Machine Learning Fundamentals ***

Decision Trees and Ensembles

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SAP SE

October 23, 2019



Agenda October 23, 2019

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② Iterative Dichotomizer (ID3)

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- Regression Trees

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- Boosting
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⑤ Wrap-Up

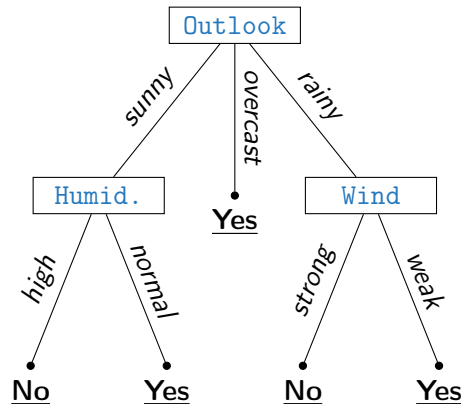
- Summary
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Section:
Introduction



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** → '*divide-and-conquer*'
- A decision tree consists of:

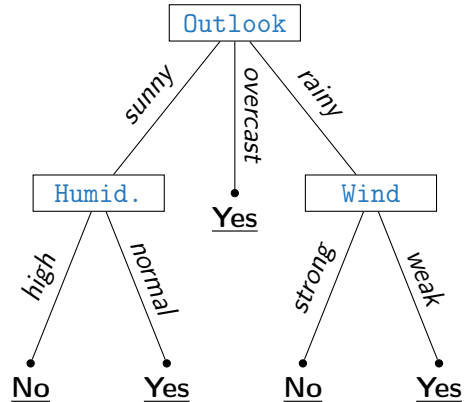
| | |
|---------------|--|
| Nodes | Each node corresponds to an attribute test |
| Edges | One edge per possible test outcome |
| Leaves | Class label to predict |

Classifying new Instances

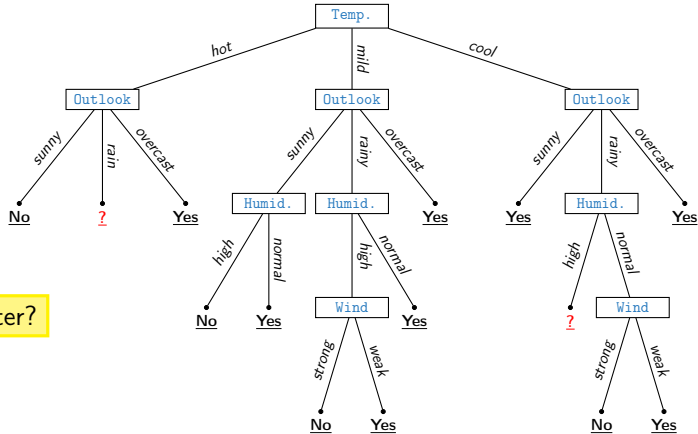
- Suppose we get a new instance:

| | |
|-------------|--------|
| 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)





Inductive Bias of Decision Trees

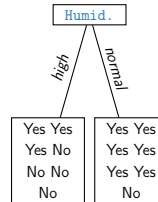
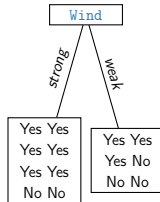
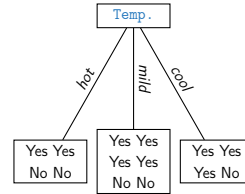
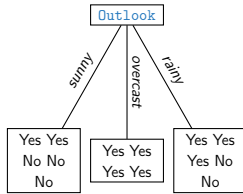
- Complex models tend to **overfit** the data and **do not generalize well**
- Small decision trees are preferred

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



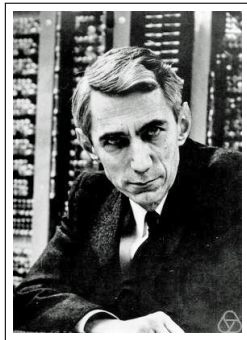
- **Prefer the simplest hypothesis that fits the data!**

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



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**



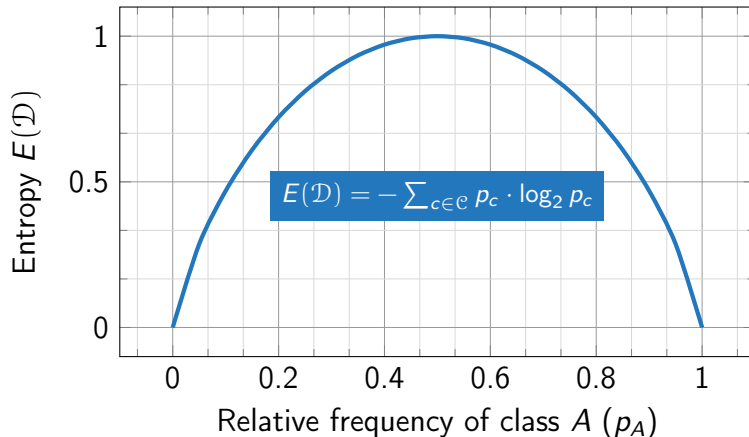
Measure of Impurity: Entropy

- Entropy is a measure of chaos in the data (measured in bits)
- Example:** Consider two classes A and B ($\mathcal{C} = \{A, B\}$)

| | | |
|---------------------------------|--------------------|-------------|
| $E(\{A, A, A, A, A, A, A, A\})$ | $\rightarrow 0$ | <i>Bits</i> |
| $E(\{A, A, A, A, A, A, B, B\})$ | $\rightarrow 0.81$ | <i>Bits</i> |
| $E(\{A, A, A, A, B, B, B, B\})$ | $\rightarrow 1$ | <i>Bit</i> |
| $E(\{A, A, B, B, B, B, B, B\})$ | $\rightarrow 0.81$ | <i>Bits</i> |
| $E(\{B, B, B, B, B, B, B, B\})$ | $\rightarrow 0$ | <i>Bits</i> |

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

Measure of Impurity: Entropy (Ctd.)



Measure of Impurity: Entropy (Ctd.)

Entropy formula:

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

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

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

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

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:

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

- Legend:

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

Quality of the Split: Average Entropy (Ctd.)

Example: Attribute Outlook

$$\begin{aligned}
 E(\mathcal{D}, \text{Outlook}) &= \sum_{v \in \text{dom}(\text{Outlook})} \frac{|\mathcal{D}_{\text{Outlook}=v}|}{|\mathcal{D}|} \cdot E(\mathcal{D}_{\text{Outlook}=v}) \\
 &= 5/14 \cdot 0.9710 + 5/14 \cdot 0.9710 + 4/14 \cdot 0 = \mathbf{0.6936}
 \end{aligned}$$

$$E(\mathcal{D}_{\text{Outlook}=\text{sunny}}) = -(2/5 \cdot \log_2(2/5) + 3/5 \cdot \log_2(3/5)) = 0.9710$$

$$E(\mathcal{D}_{\text{Outlook}=\text{rainy}}) = -(3/5 \cdot \log_2(3/5) + 2/5 \cdot \log_2(2/5)) = 0.9710$$

$$E(\mathcal{D}_{\text{Outlook}=\text{overcast}}) = -(4/4 \cdot \log_2(4/4) + 0/4 \cdot \log_2(0/4)) = 0$$

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

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 |

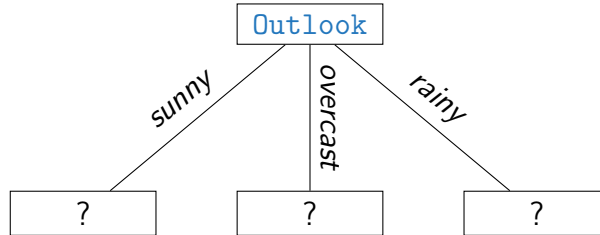
- Data set \mathcal{D} after the split
- We obtain three subsets (one per attribute value)
- Attribute Outlook is removed



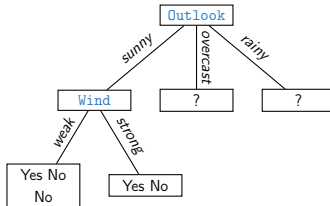
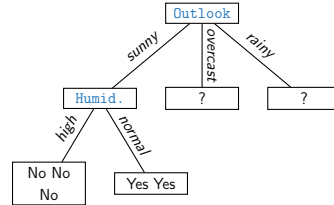
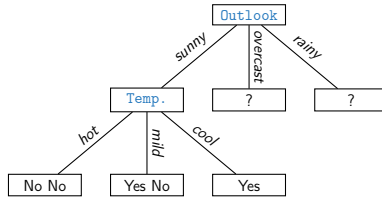
How to proceed?

- 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 $\mathcal{D}_{\text{outlook}=\text{overcast}}$ is already pure
- This algorithm is referred to as **ID3 (Iterative Dichotomizer)**

Step by Step: Construction of the Tree

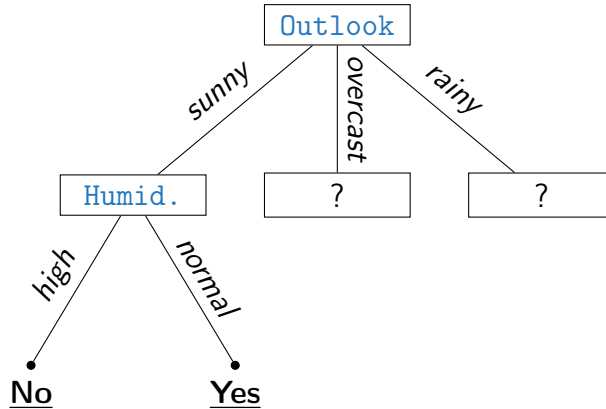


Step by Step: Construction of the Tree (Ctd.)

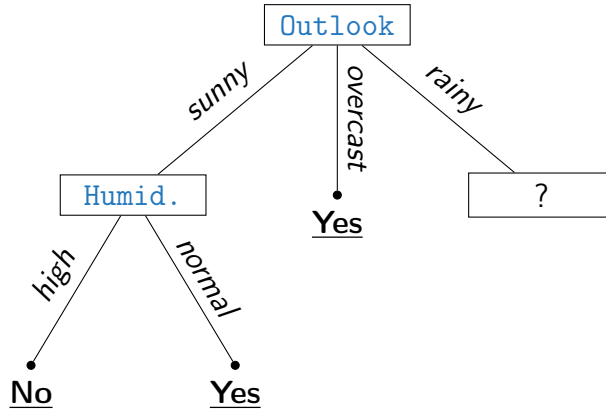


- $IG(\text{Temperature}) = 0.571$
- $IG(\text{Humidity}) = \mathbf{0.971}$
- $IG(\text{Wind}) = 0.020$

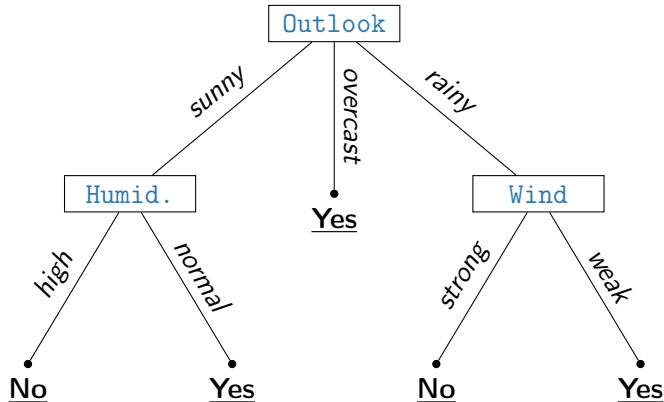
Step by Step: Construction of the Tree (Ctd.)



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



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  $A^*$  and label node  $N$  with  $A^*$ 
7  $Attr\_List \leftarrow Attr\_List \setminus \{A^*\}$ 
8 forall  $v \in dom(A^*)$  do
9   Let  $\mathcal{D}_{A^*=v}$  be the set of tuples in  $\mathcal{D}$  that satisfy  $A^* = v$ 
10  if  $|\mathcal{D}_{A^*=v}| = 0$  then
11    Attach leaf labeled with majority class in  $\mathcal{D}$  to node  $N$ 
12  else
13    Attach node returned by  $ID3(\mathcal{D}_{A^*=v}, Attr\_List)$ 
14 return  $N$ 
```

Section:
Extensions and Variants



An Alternative to Information Gain: Gini Index

Gini index:

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

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

Why not use the Error as a splitting Criterion?

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

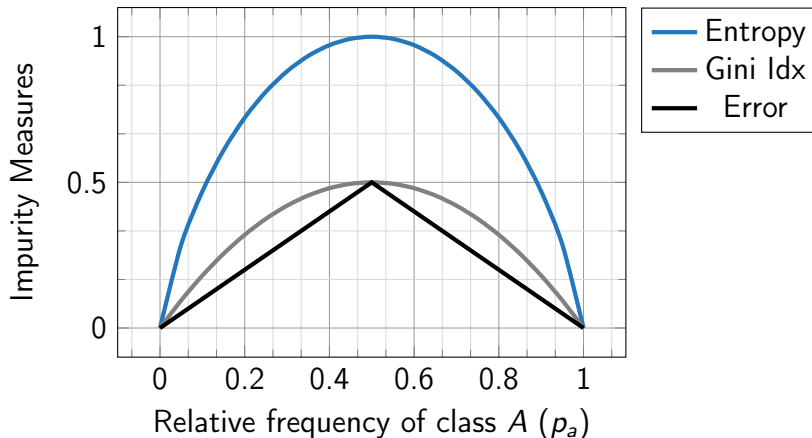
| | | |
|---------|---------|---------|
| Split 1 | 40 of A | 60 of A |
| | 60 of A | 40 of B |
| | | Split 2 |

Error without splitting:
20 %

Error after splitting:
20 %

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

Summary: Impurity Measures



Highly-branching Attributes

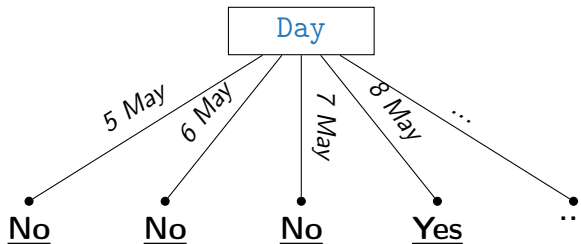
Attributes with a large number of values are problematic, since the leaves are not 'backed' with sufficient data examples.

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)

Highly-branching Attributes (Ctd.)



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

Highly-branching Attributes (Ctd.)

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

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

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

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

Highly-branching Attributes (Ctd.)

- Intrinsic information for attribute Day:

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

- Gain ratio for attribute Day:

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

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!)**

Handling numeric Attributes

- Usually, only **binary splits** are considered, e. g.:
 - Temperature < 48
 - CPU > 24
 - **Not:** $24 \leq \text{Temperature} \leq 31$
- 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!**

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 ≥ 71.5

yes: 5 | no: 3

$$E(\mathcal{D}, \text{Temp.}) = \frac{6}{14} \cdot E(\text{Temp.} < 71.5) + \frac{8}{14} \cdot E(\text{Temp.} \geq 71.5) = \mathbf{0.939}$$

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 | | <u>0.300</u> | | 0.343 | | 0.375 | | 0.400 | | 0.420 | |

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):

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

Section:
Ensemble Methods



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

What is the Advantage?

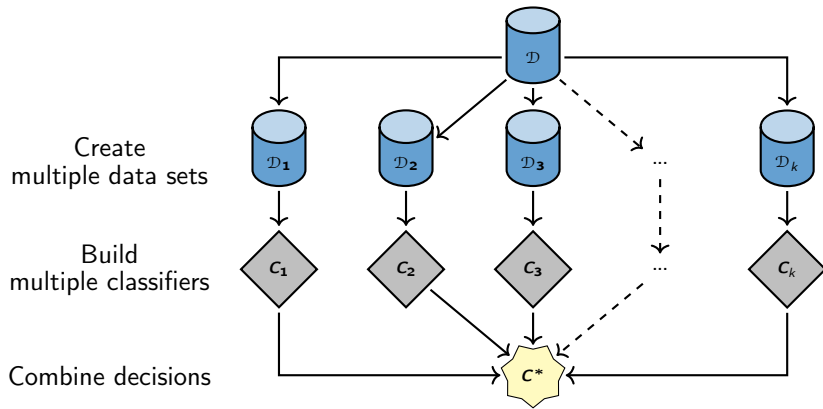
- Consider the following:
 - There are 25 **independent** base classifiers
 - **Independence assumption**: Probability of misclassification **does not** depend on other classifiers in the ensemble
 - Usually, this assumption does not fully hold in practice
 - Each classifier has an error rate of $\varepsilon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

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



Bagging: General Approach

Bagging $\hat{=}$ Bootstrap Aggregating



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** $u \in \{1, 2, \dots, k\}$ **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^*)*

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, ...)

Bagged Decision Trees

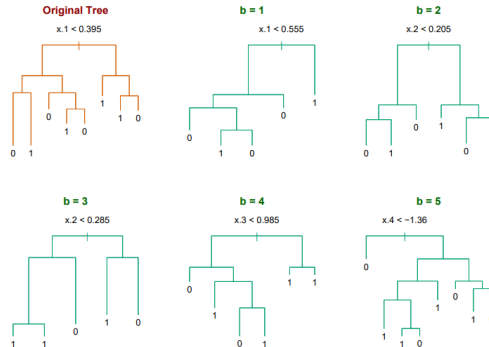


Figure: Bagged decision trees; cf. Hastie 2008, page 284

Randomization

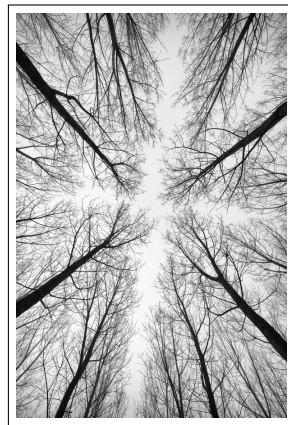
- Why not **randomizing the algorithm** instead of the data?
- Some algorithms already do that: E. g. neural networks (random initialization of weights)
- Especially greedy algorithms can be randomized:
 - Pick from the options **randomly** instead of picking the best one
 - E. g. decision trees: Do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

A random forest combines randomization and bagging.

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** $u \in \{1, 2, \dots, k\}$ **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^*)*

ExtraTrees (Randomization 2.0)

- One more step of randomization \Rightarrow **Extremely Randomized 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



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 $w_i \leftarrow \frac{1}{n}$

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

4 Learn a classifier C_u using the current example weights

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

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

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

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

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**

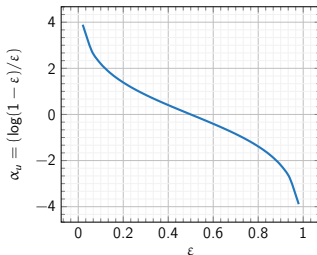
12 Get predictions from all classifiers C_u

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

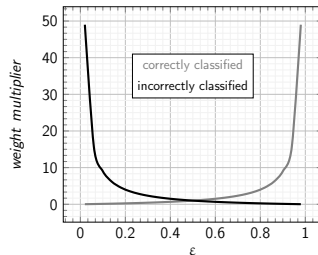


AdaBoost: Illustration of Weights

Model weights α_u



Example weights w_i



- Classifier weights α_u grow exponentially
- Classifier weight is 0 if error is $1/2$ (model cannot be trusted, random guessing)
- For high errors \Rightarrow **Do the opposite of what the classifiers predicts**

AdaBoost: Two Classes

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

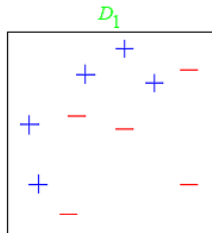
$$H(\mathbf{x}) = \text{sign} \left(\sum_{u=1}^k \alpha_u h_u(\mathbf{x}) \right) \quad (10)$$

- α_u is defined as above
- The weight update for the examples is given by:

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

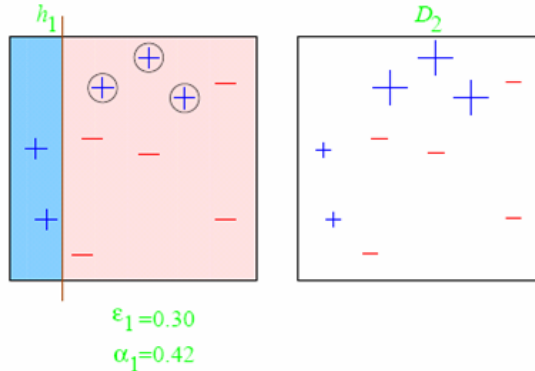
Boosting Example

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



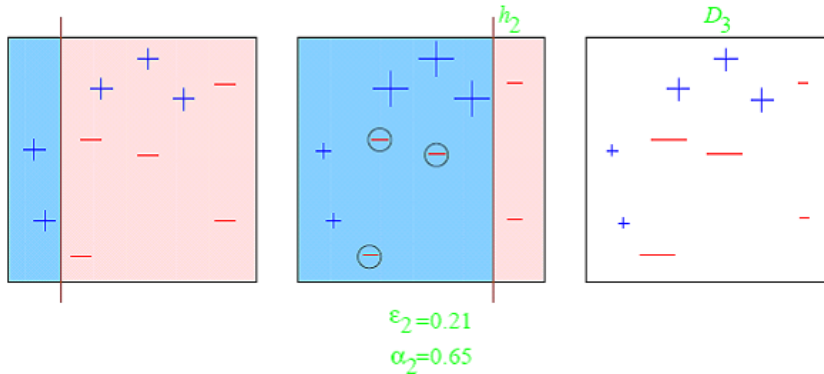
Boosting Example (Ctd.)

1st Iteration



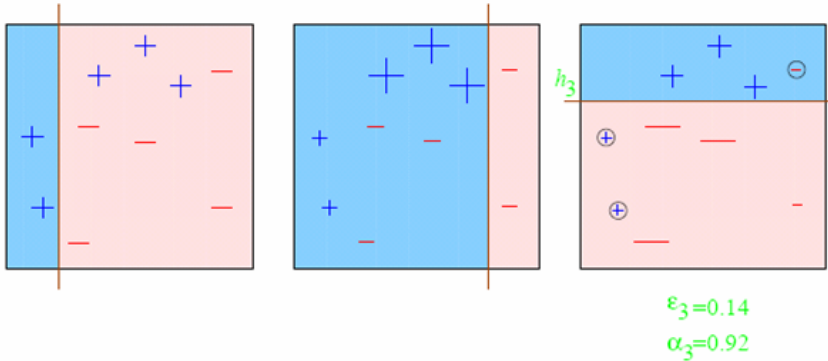
Boosting Example (Ctd.)

2nd Iteration



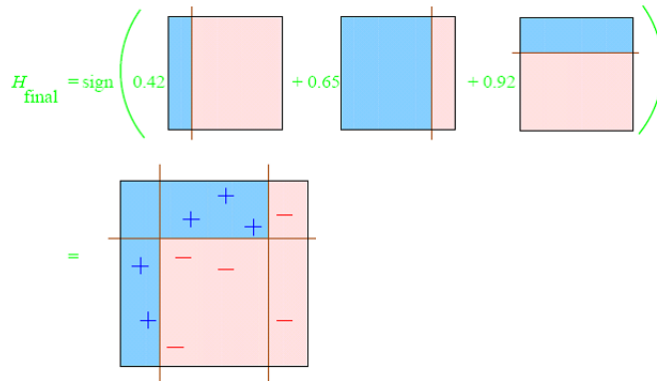
Boosting Example (Ctd.)

3rd Iteration



Boosting Example (Ctd.)

Prediction



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, \dots, 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

Stacking Example

| <i>Attributes</i> | | | <i>Class</i> |
|-------------------|-----|-------------|--------------|
| $x_1^{(1)}$ | ... | $x_m^{(1)}$ | <i>true</i> |
| $x_1^{(2)}$ | ... | $x_m^{(2)}$ | <i>false</i> |
| ... | ... | ... | ... |
| $x_1^{(n)}$ | ... | $x_m^{(n)}$ | <i>true</i> |

Table: Original training set

| C_1 | C_2 | ... | C_k |
|--------------|--------------|-----|--------------|
| <i>true</i> | <i>true</i> | ... | <i>false</i> |
| <i>false</i> | <i>true</i> | ... | <i>true</i> |
| ... | ... | ... | ... |
| <i>false</i> | <i>false</i> | ... | <i>true</i> |

Table: Predictions base classifiers

| C_1 | C_2 | ... | C_k | <i>Class</i> |
|--------------|--------------|-----|--------------|--------------|
| <i>true</i> | <i>true</i> | ... | <i>false</i> | <i>true</i> |
| <i>false</i> | <i>true</i> | ... | <i>true</i> | <i>false</i> |
| ... | ... | ... | ... | ... |
| <i>false</i> | <i>false</i> | ... | <i>true</i> | <i>true</i> |

Table: Meta data set

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!

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...

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 ($k \hat{=}$ # classes)
 - **Class i:** Alternating runs of 2^{k-i} 0s and 1s
(Last run is one bit shorter than the others)

Section:
Wrap-Up



Summary

Lecture Overview

Unit I: Machine Learning Introduction

Self-Test Questions

Recommended Literature and further Reading

Thank you very much for the attention!

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

Date: October 23, 2019

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Do you have any questions?