Data Mining

DECISION TREE
Decision Tree

• It is one of the most widely used classification techniques that allows you to represent a set of classification rules with a tree.

• Tree: hierarchical structure consisting of a set of nodes, correlated by arcs labeled and oriented. There are two types of nodes:
  • Leaf nodes identify classes, while the remaining nodes are labeled based on the attribute that partitions the records. The partitioning criterion represents the label of the arcs

• Each root-leaf path represents a classification rule
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- Tree: hierarchical structure consisting of a set of nodes, correlated by arcs labeled and oriented. There are two types of nodes:
  - Leaf nodes identify classes, while the remaining nodes are labeled based on the attribute that partitions the records. The partitioning criterion represents the label of the arcs.
- Each root-leaf path represents a classification rule.
Decision Tree: an Example

<table>
<thead>
<tr>
<th>Tid</th>
<th>Refund</th>
<th>Marital Status</th>
<th>Taxable Income</th>
<th>Cheat</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Yes</td>
<td>Single</td>
<td>125K</td>
<td>No</td>
</tr>
<tr>
<td>2</td>
<td>No</td>
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<td>No</td>
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<tr>
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<tr>
<td>4</td>
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<td>Married</td>
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<td>No</td>
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<tr>
<td>5</td>
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<tr>
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<td>7</td>
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<td>220K</td>
<td>No</td>
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<tr>
<td>8</td>
<td>No</td>
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<td>85K</td>
<td>Yes</td>
</tr>
<tr>
<td>9</td>
<td>No</td>
<td>Married</td>
<td>75K</td>
<td>No</td>
</tr>
<tr>
<td>10</td>
<td>No</td>
<td>Single</td>
<td>90K</td>
<td>Yes</td>
</tr>
</tbody>
</table>

Training Data

Model: Decision Tree

Split Attribute

Refund

Yes

No

MarSt

Single, Divorced

Married

TaxInc

< 80K

> 80K

NO

YES

NO

NO
**Decision Tree: an Example**

For each dataset several decision tree could be defined

<table>
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</tbody>
</table>
Applying the model

<table>
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<tr>
<th>Tid</th>
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<tr>
<td>1</td>
<td>Yes</td>
<td>Large</td>
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<td>10</td>
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<td>Yes</td>
</tr>
</tbody>
</table>

Test Set

<table>
<thead>
<tr>
<th>Tid</th>
<th>Attrib1</th>
<th>Attrib2</th>
<th>Attrib3</th>
<th>Class</th>
</tr>
</thead>
<tbody>
<tr>
<td>11</td>
<td>No</td>
<td>Small</td>
<td>55K</td>
<td>?</td>
</tr>
<tr>
<td>12</td>
<td>Yes</td>
<td>Medium</td>
<td>80K</td>
<td>?</td>
</tr>
<tr>
<td>13</td>
<td>Yes</td>
<td>Large</td>
<td>110K</td>
<td>?</td>
</tr>
<tr>
<td>14</td>
<td>No</td>
<td>Small</td>
<td>95K</td>
<td>?</td>
</tr>
<tr>
<td>15</td>
<td>No</td>
<td>Large</td>
<td>67K</td>
<td>?</td>
</tr>
</tbody>
</table>

Training Set

Decision Tree

Learn Model

Tree Induction algorithm

Apply Model

Induction

Deduction
Applying the model

Start from the root

Refund

Yes

NO

No

MarSt

Single, Divorced

TaxInc

< 80K

NO

> 80K

YES

NO

Married

Test Data

<table>
<thead>
<tr>
<th>Refund</th>
<th>Marital Status</th>
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<tr>
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Applying the model

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Applicare il modello al data set

Test Data

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</table>

Refund | Marital Status | Taxable Income | Cheat |
--------|----------------|----------------|-------|
NO      | Married        | 80K            | ?     |

Yes | No | MarSt
-----|----|----------------|
NO   | Single, Divorced | Married |

TaxInc | NO | NO | YES
< 80K | > 80K |
Applying the model

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Refund Marital Status Taxable Income Cheat
No Married 80K ?

Refund

Refund

Yes

NO

No

MarSt

Married

NO

Single, Divorced

TaxInc

< 80K

NO

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YES
Applying the model

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Single, Divorced

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NO

> 80K

NO

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Applying the model

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Set Cheat = “No”
Learning the model

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Learning the model

The decision tree number grows exponentially with the number of attributes. Algorithms generally use greedy techniques that locally make the "best" choice.

Many algorithms are available:
- Hunt's Algorithm
- CART
- ID3, C4.5
- Sliq, SPRINT

Different issues have to be addressed:
- Choice of the split policy
- Choice of the stop policy
- Underfitting/Overfitting
- Data Fragmentation
- Search Criteria
- Expression
- Replication of trees
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The Hunt’s Algorithm

Recursive approach that progressively subdivides a set of \( D_t \) records into purely pure record sets

Let \( D_t \) be the set of records of the training set corresponding to node \( t \) and \( y_t = \{y_1, ..., y_k\} \) the possible class labels

Overall procedure:
- If \( D_t \) contains records belonging to the \( y_j \) class only, then \( t \) is a leaf node with label \( y_j \)
- If \( D_t \) is an empty set, then \( t \) is a leaf node to which a parent node class is assigned
- If \( D_t \) contains records belonging to several classes, you choose an attribute and a split policy to partition the records into multiple subsets.
- Apply recursively the current procedure for each subset

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</table>
Pseudocode

// Let E be the training set and F the attributes

result = PostPrune(TreeGrowth(E, F));

TreeGrowth(E, F)
    if StoppingCond(E, F) = TRUE then
        leaf = CreateNode();
        leaf.label = Classify(E);
        return leaf;
    else
        root = CreateNode();
        root.test_cond = FindBestSplit(E, F);
        let V = {v | v is a possible outcome of root.test_cond}
        for each v ∈ V do
            E_v = {e | root.test_cond(e) = v and e ∈ E}
            child = TreeGrowth(E_v, F);
            add child as descendants of root and label edge (root→child) as v
        end for
    end if
end;
Further Remarks...

Finding an optimal decision tree is a NP-Complete problem, but many heuristic algorithms are available and very efficient

• Most approaches run a top down recursive partition based on greedy criteria

Classification using a decision tree is extremely fast and provides easy interpretation of the criteria

• The worst case is $O(w)$ where $w$ is the depth of the tree

Decision trees are robust enough to strongly correlated attributes

• One of the two attributes will not be considered
• It is also possible to try to discard one of the preprocessing attributes through appropriate feature selection techniques
Further Remarks...

Decision tree expressivity is limited to the possibility of performing search space partitions with conditions that involve only one attribute at a time

- Decision boundary parallel to the axes

This split is not feasible with traditional decision trees
Characteristic features

Starting from the basic logic to completely define an algorithm for building decision trees it is necessary to define:

• **The split condition**
  • The criterion defining the best split
  • The criterion for interrupting splitting
  • Methods for evaluating the goodness of a decision tree
Defining the Split Condition

Depends on the type of attribute
• Nominal
• Ordinal
• Continuous

Depends on the number of splits applicable to attribute values
• Binary splits
• N-ary splits
Splitting Nominal Attributes

**N-ary Split:** Creates as many partitions as the attribute values are.

```
CarType
  /   \
Family  Luxury
  /     \
Sports
```

**Binary Split:** Creates two partitions only. The attribute value optimally split the dataset must be found.

```
CarType
  /   \ OR
{Sports, Luxury}  {Family}
  /     \
{Family}  
```

```
CarType
  /   \ OR
{Family, Luxury}  {Sports}
  /     \
{Sports}
```
Splitting Ordinal Attributes

- Partitioning should not violate order sorting.

**N-ary Split:** Creates as many partitions as the attribute values are

```
Size
  /   \
Small  Medium  Large
```

**Binary Split:** Creates two partitions only. The attribute value optimally split the dataset must be found.

```
Size
  /   \  {Medium, Large}
Small   Large
```

OR

```
Size
  /   \  {Small}
Small   Medium
```

```
Size
  /   \  {Large}
Small   Medium
```

```
Size
  /   \  {Small, Medium}
Small   Large
```

Splitting Continuous Attributes

- **N-ary Split**: The split condition can be expressed as a Boolean test that results in multiple ranges of values. The algorithm must consider all possible range of values as possible split points.

- **Binary Split**: The split condition can be expressed as a binary comparison test. The algorithm must consider all values as possible split points.

### Example

(i) **Binary split**
- **Taxable Income > 80K?**
  - Yes
  - No

(ii) **Multi-way split**
- **Taxable Income?**
  - < 10K
  - [10K,25K)
  - [25K,50K)
  - [50K,80K)
  - > 80K
Splitting Continuous Attributes

A discretization technique can be used to manage the complexity of the search for optimal split points

- **Static:** discretization takes place only once before applying the algorithm
- **Dynamic:** discretization takes place at each recursion step by exploiting information about the distribution of input data to the Dt node.
Characteristic features

Starting from the basic logic to completely define an algorithm for building decision trees it is necessary to define:

• The split condition
• The criterion defining the best split
• The criterion for interrupting splitting
• Methods for evaluating the goodness of a decision tree
How to determine the best split value?

- Before splitting a single class with 10 records in C0 class and 10 records in C1 class

- The split criterion must allow you to determine more pure classes. It needs a measure of purity
  - Gini index
  - Entropy
  - Misclassification error
How to determine the best split value?

Before Splitting:

<table>
<thead>
<tr>
<th></th>
<th>C0</th>
<th>C1</th>
</tr>
</thead>
<tbody>
<tr>
<td>A?</td>
<td>N10</td>
<td>N11</td>
</tr>
<tr>
<td></td>
<td>N20</td>
<td>N21</td>
</tr>
<tr>
<td></td>
<td>N30</td>
<td>N31</td>
</tr>
<tr>
<td></td>
<td>N40</td>
<td>N41</td>
</tr>
</tbody>
</table>

Gain = M0 – M12 vs M0 – M34
Impurity Measures

- Given a node \( p \) with records belonging to \( k \) classes and its partitioning in \( n \) child nodes
  - \( M = \) record number in father node \( p \)
  - \( M_i = \) number of records in son node \( i \)

**ATTENTION** do not confuse the number of classes \( (k) \) and that of child nodes \( (n) \)

- Several index can be adopted
  - Gini index: adopted in CART, SLIQ, SPRINT.
  - Entropy adopted in ID3 e C4.5
  - Misclassification Error

- The total impurity of the split is given by the following formula where \( \text{meas}(\cdot) \) is one of the measures introduced so far

\[
\text{Impurity}_{\text{split}} = \sum_{i=1}^{n} \frac{m_i}{m} \text{meas}(i)
\]
Comparing Impurity Measures

- Impurity measures behavior for a two-class problem
Computing Gini for Binary Attributes

\[
\text{Gini(N3) = } 1 - \left(\frac{5}{7}\right)^2 - \left(\frac{2}{7}\right)^2 = 0.408
\]

Gini(N4) = 1 – (1/5)^2 – (4/5)^2 = 0.320

Impurity = \[\frac{7}{12} * 0.408 + \frac{5}{12} * 0.320 = 0.371\]
Computing Gini for Categorical Attributes

It is usually more efficient to create a "count matrix" for each distinct value of the classification attribute and then perform calculations using that matrix.

N-ary split

<table>
<thead>
<tr>
<th>CarType</th>
<th>Family</th>
<th>Sports</th>
<th>Luxury</th>
</tr>
</thead>
<tbody>
<tr>
<td>C1</td>
<td>1</td>
<td>2</td>
<td>1</td>
</tr>
<tr>
<td>C2</td>
<td>4</td>
<td>1</td>
<td>1</td>
</tr>
<tr>
<td>Gini</td>
<td>0.393</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Binary split

<table>
<thead>
<tr>
<th>CarType</th>
<th>{Sports, Luxury}</th>
<th>{Family}</th>
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<th>{Family, Luxury}</th>
</tr>
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<tbody>
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<td>5</td>
</tr>
<tr>
<td>Gini</td>
<td>0.419</td>
<td></td>
</tr>
</tbody>
</table>
Computing Gini for Continuous Attributes

It requires to define the split point using a binary condition. The number of possible conditions is equal to the number of distinct values of the attribute.

You can calculate a matrix count for each split value. The array will count the elements of each class for attribute values greater than or less than the split value.

A naive approach:
• For each split v value, read the DB (with N records) to build the count matrix and calculate the Gini index
• Computationally inefficient - O (N^2) – since:
  • Scan DB O (N)
  • Repeat for each value of v O (N)
Computing Gini for Continuous Attributes

A more efficient solution is to:

- Sort records by attribute value
- Read the values sorted and update the count matrix, then calculate the Gini index
- Choose as the split point the value that minimizes the index

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<th>Yes</th>
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<th>No</th>
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<td>0.343</td>
<td>0.375</td>
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</table>

Sono possibili ulteriori ottimizzazioni?
Gain-based Split

Using class impurity measures such as Gini and Entropy requires choosing the split value that maximizes the "gain" in terms of reducing the impurity of the classes after the split. For example, considering entropy, the gain of partitioning of a node in child nodes is:

\[
GAIN_{\text{split}} = \text{Entropy}(p) - \left( \sum_{i=1}^{m} \frac{m_i}{m} \text{Entropy}(i) \right)
\]

Selecting the split value that maximizes GAIN tends to determine split criteria that generate a very large number of very pure classes but with few records.

- Partitioning students according to their enrollment guarantees that all classes (formed by only one student) are totally pure!!
Split based on split info

To avoid the problem of spraying classes, it is preferable to maximize the Gain Ratio:

- \( N \) = number of child nodes
- \( M \) = record number in father \( p \)
- \( M_i \) = number of records in child node \( i \)

The higher the number of children, the greater the value of \( \text{SplitINFO} \) with a consequent reduction in the GainRatio.

For example, assuming that each child node contains the same number of records, \( \text{SplitINFO} = \log n \).

C4.5 uses the \( \text{SplitINFO} \)-based criterion.

\[
\text{GainRATIO}_{\text{split}} = \frac{\text{GAIN}_{\text{split}}}{\text{SplitINFO}}
\]

\[
\text{SplitINFO} = -\sum_{i=1}^{n} \frac{m_i}{m} \log \frac{m_i}{m}
\]
To avoid the problem of spraying classes, it is preferable to maximize the Gain Ratio:

\[ n = da \ 2 \ a \ 64 \]
\[ m = 100 \]
\[ mi = m/n \]
Compute Gini index and information gain for the following binary problem and comment on the results.

<table>
<thead>
<tr>
<th>A</th>
<th>B</th>
<th>Classe</th>
</tr>
</thead>
<tbody>
<tr>
<td>T</td>
<td>F</td>
<td>+</td>
</tr>
<tr>
<td>T</td>
<td>T</td>
<td>+</td>
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<td>-</td>
</tr>
<tr>
<td>T</td>
<td>F</td>
<td>-</td>
</tr>
</tbody>
</table>
Characteristic features

Starting from the basic logic to completely define an algorithm for building decision trees it is necessary to define:

• The split condition
• The criterion defining the best split
• **The criterion for stopping the split**
• Methods for evaluating the goodness of a decision tree
Stop Criteria for Decision Tree Induction

Stop splitting a node when all its records belong to the same class

Stop splitting a node when all its records have similar values on all attributes

• Classification would be unimportant and dependent on small fluctuations in values

Stop splitting when the number of records in the node is below a certain threshold (data fragmentation)

• The selected criterion would not be statistically relevant
Characteristic features

Starting from the basic logic to completely define an algorithm for building decision trees it is necessary to define:

• The split condition
• The criterion defining the best split
• The criterion for stopping the split
• **Methods for evaluating the goodness of a decision tree**
Starting from the basic logic to completely define an algorithm for building decision trees it is necessary to define:

- The split condition
- The criterion defining the best split
- The criterion for stopping the split
- Methods for evaluating the goodness of a decision tree
Metrics for model evaluation

The Confusion Matrix evaluates the ability of a classifier based on the following indicators:

- **TP (true positive):** records correctly classified as Yes class
- **FN (false negative):** Incorrectly classified records as class No
- **FP (false positive):** Incorrectly classified records as class Yes
- **TN (true negative):** records correctly classified as class No

If the classification uses $n$ classes, the confusion matrix will be $n \times n$
Accuracy

Accuracy is the most widely used metric to synthesize the information of a confusion matrix

\[
\text{Accuracy} = \frac{TP + TN}{TP + TN + FP + FN}
\]

Equally, the frequency of the error could be used

\[
\text{Error rate} = \frac{FP + FN}{TP + TN + FP + FN}
\]
Accuracy Limitations

Accuracy is not an appropriate metric if the classes contain a very different number of records. Consider a binary classification problem in which

• # Record of class 0 = 9990
• # Record of class 1 = 10

A model that always returns class 0 will have an accuracy of 9990/10000 = 99.9%

In the case of binary classification problems, the class "rare" is also called a "positive class", while the class that includes most of the records is called a "negative class".
Precision and Recall are two metrics used in applications where the correct classification of positive class records is more important. **Precision** measures the fraction of record results actually positive among all those who were classified as such:
- High values indicate that few negative class records were incorrectly classified as positive.

**Recall** measures the fraction of positive records correctly classified:
- High values indicate that few records of the positive class were incorrectly classified as negatives.

\[
\text{Precision, } p = \frac{TP}{TP + FP}
\]

\[
\text{Recall, } r = \frac{TP}{TP + FN}
\]
Precision and Recall

Precision = 1 if all the positive records were actually detected

Recall = 1 if there are no false negatives

If both are valid 1, the predetermined classes coincide with the real ones
F-measure

A metric that summarizes precision and recall is called F-measure

$$F\text{-measure, } F = \frac{2rp}{r + p} = \frac{2 \times TP}{2 \times TP + FP + FN}$$

F-measure represents the harmonic mean of precision and recall

- The harmonic average between two x and y numbers tends to be close to the smallest of the two numbers. So if the harmonic average is high, it means both precision and recall are.
  - ... so there have been no false negative or false positives
Cost-Based Evaluation

Accuracy, Precision-Recall and F-measure classify an instance as positive if \( P(+,i) > P(-,i) \).

- They assume that FN and FP have the same weight, thus they are Cost-Insensitive.
- In many domains this is not true!
  - For a cancer screening test, for example, we may be prepared to put up with a relatively high false positive rate in order to get a high true positive, it is most important to identify possible cancer sufferers.
  - For a follow-up test after treatment, however, a different threshold might be more desirable, since we want to minimize false negatives, we don’t want to tell a patient they’re clear if this is not actually the case.

![Graph showing True Positives and True Negatives compared to False Positives and False Negatives.](image)
The Cost Matrix

The cost matrix encodes the penalty that a classifier incurs in classifying a record in a different class. A negative penalty indicates the "prize" that is obtained for a correct classification.

\[
C(M) = TP \times C(+) + FP \times C(+|-) + FN \times C(-|+) + TN \times C(-|-)
\]

A model constructed by structuring, as a purity function, a cost matrix will tend to provide a model with a minimum cost over the specified weights.
Computing the Cost

<table>
<thead>
<tr>
<th>Cost Matrix</th>
<th>PREDICTED CLASS</th>
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<tbody>
<tr>
<td>ACTUAL CLASS</td>
<td>C(ij)</td>
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<tr>
<td></td>
<td>+</td>
</tr>
<tr>
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<td>-</td>
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</table>

Accuracy = 80%
Cost = 3910

<table>
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<tr>
<th>Model M₁</th>
<th>PREDICTED CLASS</th>
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</thead>
<tbody>
<tr>
<td>ACTUAL CLASS</td>
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</tr>
<tr>
<td>+</td>
<td>150</td>
</tr>
<tr>
<td>-</td>
<td>60</td>
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</table>

Accuracy = 90%
Cost = 4255

<table>
<thead>
<tr>
<th>Model M₂</th>
<th>PREDICTED CLASS</th>
</tr>
</thead>
<tbody>
<tr>
<td>ACTUAL CLASS</td>
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</tr>
<tr>
<td>+</td>
<td>250</td>
</tr>
<tr>
<td>-</td>
<td>5</td>
</tr>
</tbody>
</table>
ROC Space

ROC graphs are two-dimensional graphs that depict relative tradeoffs between benefits (true positive) and costs (false positive) induced by a classifier. We distinguish between:

- **Probabilistic classifiers** return a score that is not necessarily a *sensu stricto* probability but represents the degree to which an object is a member of one particular class rather than another one (e.g. Decision tree, Naive Bayes)
  - In a decision tree an instance in a leaf is associated to the class + if the number positive training instances in the leaf (*pos*) is greater than the number of negative instances (*neg*). The ratio *pos*/(*pos*+*neg*) can be used as a score showing the likelihood of an instance to be of class + or -

- **Discrete classifier** predicts only the classes to which a test object belongs (e.g. SVM)

ROC curve characterizes a probabilistic classifier, and each point of this curve corresponds to a discrete classifier.
A ROC graph for a probabilistic classifier is obtained varying the threshold (or the probability if available) used to assign an instance \( i \) to a class (+/-).

- Instead of \( P(+,i) > P(-,i) \) than \( i \) is +
- We have if \( P(+,i) > x \) than \( i \) is + \( x \in [0,..,1] \)

Each \( x \) value determines different TPR and FPR

The ROC curve shape depends both on the classifier capabilities and on the dataset features.
A good classifier tends to have performance close to the higher-left corner of the ROC graph that is: High TPR and Low FPR.

The **Area Under the Curve** – AUC provides an overall rating of the classifier, while segments of the curve provide a rating in specific TPR – FPR settings.

The larger the overlap between + and – instances distributions, the harder for the classifier to distinguish between positive and negative instances.

A dummy classifier performs on the ROC graph diagonal: the TPR is equal to the FPR since the classifier answers are random.
Comparison of Classifier via ROC curve

A classifier comparison based on ROC curves or AUC values can be either graphical or numerical.

• A ROC curve running above another is an indicator of better classifier performance, and by the same token, the bigger the AUC, the better the overall performance of the test.

• However, this reasoning is meaningful only if the two ROC curves do not cross at any point. If they do, then it makes intuitive sense to point out the region in which one classifier outperforms the other, but the comparison of the complete AUC values is not very informative.
  • DALI is better than SW when a low FP rate is needed
  • BLAST is always worse than DALI & SW
ROC space properties

ROC curves are insensitive to changes in class distribution. If the proportion of positive to negative instances changes in a test set, the ROC curves will not change.

The class distribution is the relationship of the left (P) column to the right (N) column. Any performance metric that uses values from both columns will be inherently sensitive to class skews. Metrics such as accuracy, precision and F score use values from both columns of the confusion matrix. As a class distribution changes these measures will change as well, even if the fundamental classifier performance does not.

ROC graphs are based upon TPR and FPR, in which each dimension is a strict columnar ratio, so do not depend on class distributions.

\[
\text{fp rate} = \frac{FP}{N} \quad \text{tp rate} = \frac{TP}{P} \\
\text{precision} = \frac{TP}{TP + FP} \quad \text{recall} = \frac{TP}{P} \\
\text{accuracy} = \frac{TP + TN}{P + N} \\
\text{F-measure} = \frac{2}{\frac{1}{\text{precision}} + \frac{1}{\text{recall}}} 
\]
Where do ROC curves come from?

ROC stands for *Receiver Operator Characteristic*. The term has its roots in World War II. ROC curves were originally developed by the British as part of the “Chain Home” radar system. ROC analysis was used to analyze radar data to differentiate between enemy aircraft and signal noise (e.g. flocks of geese).

Radar Operators were human classifiers!
Classification Errors

**Training error:** are mistakes that are made on the training set.

**Generalization error:** errors are made on the test set (i.e. records that have not been trained on the system).

**Underfitting:** The model is too simple and does not allow a good classification or set training set or test set.

**Overfitting:** The model is too complex, it allows a good classification of the training set, but a poor classification of the test set.

- The model fails to generalize because it is based on the specific peculiarities of the training set that are not found in the test set (e.g. noise present in the training set)
Underfitting and Overfitting

• 500 circles and 500 triangles
• Circular points: $0.5 \leq \sqrt{x_1^2+x_2^2} \leq 1$
• Triangular points: $\sqrt{x_1^2+x_2^2} > 0.5$ or $\sqrt{x_1^2+x_2^2} < 1$
Overfitting Due to Noise

The boundaries of the areas are distorted due to noise
Overfitting due to the reduced size of the training set

Lack of points at the bottom of the chart makes it difficult to find a proper classification for that portion of the region.
How to handle the Overfitting: pre-pruning (Early stopping rule)

Stop splitting before you reach a deep tree

A node can not be split further if:
- Node does not contain instances
- All instances belong to the same class
- All attributes have the same values

More restrictive conditions potentially applicable are:
- Stop splitting if the number of instances in the node is less than a fixed amount
- Stop splitting if distribution of instances between classes is independent of attribute values
- Stop splitting if you do not improve the purity measure (e.g. Gini or information gain).
How to handle the Overfitting: post-pruning (Reduced Error Pruning)

Run all possible splits
Examine the decision tree nodes obtained with a bottom-up logic
Collate a sub tree in a leaf node if this allows to reduce the generalization error (i.e. on the validation set)
• Choose to collapse the sub tree that determines the maximum error reduction (N.B. greedy choice)

Instances in the new leaf can be tagged
• Based on the label that appears most frequently in the sub-tree
• According to the label that occurs most frequently in the instances of the training set that belong to the sub-tree

Post-pruning is more effective but involves more computational cost. It is based on the evidence of the result of a complete tree
Notes on Overfitting

Overfitting results in more complex decision-making trees than necessary.

The classification error done on the training set does not provide accurate estimates about tree behavior on unknown records.

It requires new techniques to estimate generalization errors.
Estimate generalization errors

A decision tree should minimize the error on the real data set, unfortunately during construction, only the training set is available. Then the real time data error must be estimated.

- **Re-substitution error:** number of errors in the training set
- **Generalization error:** number of errors in the real data set

The methods for estimating the generalization error are:

- **Optimistic approach:** $e'(t) = e(t)$
- **Pessimistic approach**
- **Minimum Description Length (MDL)**
- **Using the test set:** The generalization error is equal to the error on the test set.
  - Normally the test set is obtained by extracting from the initial training set 1/3 of the records
  - It offers good results but the risk is to work with a too small training set
Occam’s Razor

Give two models with a similar generalization error always choose the simplest one

- For complex models, it is more likely that errors are caused by accidental data conditions

It is therefore useful to consider the complexity of the model when evaluating the goodness of a decision tree

Note: The methodological principle has been expressed in the 14th century by the English Franciscan philosopher and friar William of Ockham
Minimum Description Length

Give two models choose the one that minimizes the cost to describe a classification
To describe the model I can:
   A) Sequentially send class O (n)
   B) Build a classifier, and send the description along with a detailed description of the mistakes it makes

\[
\text{Cost(model, data)} = \text{Cost(model)} + \text{Cost(data | model)}
\]

<table>
<thead>
<tr>
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<th>y</th>
</tr>
</thead>
<tbody>
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<tr>
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<tr>
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<td>...</td>
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</table>

<table>
<thead>
<tr>
<th>X</th>
<th>y</th>
</tr>
</thead>
<tbody>
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<td>...</td>
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<tr>
<td>Xn</td>
<td>?</td>
</tr>
</tbody>
</table>
Datasets with n records described by 16 binary attributes and 3 class values

- Each inner node is modeled with the ID of the used attribute $\rightarrow \log_2(16)=4$ bit
- Each leaf is modeled with the ID of the class $\rightarrow \log_2(3)=2$ bit
- Each error is modeled with its position in the training set considering n record $\rightarrow \log_2(n)$

Cost(Tree1) = $4 \times 2 + 2 \times 3 + 7 \times \log_2(n) = 14 + 7 \times \log_2(n)$
Cost(Tree2) = $4 \times 4 + 2 \times 5 + 4 \times \log_2(n) = 26 + 4 \times \log_2(n)$
Cost(Tree1) < Cost(Tree2) if $n < 16$
Pessimistic approach

- The generalization error is estimated by adding to the error on the training set a penalty related to the complexity of the model.
- $e(t_i)$: classification errors on leaf $i$
  - $\Omega(t_i)$: leaf-related penalty $i$
  - $n(t_i)$: number of record in the training set belonging to leaf $i$

$$E(T) = \frac{\sum_{i=1}^{k} e(t_i) + \Omega(t_i)}{\sum_{i=1}^{k} n(t_i)}$$

- For binary trees a penalty equal to 0.5 implies that a node should always be expanded in the two child nodes if it improves the classification of at least one record.
Post Pruning: an example

Class = Yes 20
Class = No 10
Error = 10/30

Training error (before split) = 10/30
Pessimistic error = (10 + 0.5) / 30 = 10.5 / 30
Training error (after split) = 9/30
Pessimistic error (After splitting) = (9 + 4 \times 0.5)/30 = 11/30

PRUNE!
Post Pruning: an example

Optimistic error?
- Do not cut in any of the cases

Pessimistic error (penalty 0.5)?
- Do not cut in case 1, cut in case 2

Pessimistic error (penalty 1)?

Case 1:

- C0: 11
- C1: 3
- C0: 2
- C1: 4

Case 2:

- C0: 14
- C1: 3
- C0: 2
- C1: 2
Building the Test Set

**Holdout**
- Use 2/3 of training records and 1/3 for validation
- Disadvantages:
  - It works with a reduced set of training
  - The result depends on the composition of the training set and test set

**Random subsampling**
- It consists of a repeated execution of the holdout method in which the training dataset is randomly selected
Building the Test Set

**Cross validation**
- Partition the records into separate $k$ subdivisions
- Run the training on $k-1$ partitions and test the remainder
- Repeat the test $k$ times and calculate the average accuracy
- CAUTION: cross validation creates $k$ different classifiers. Thus, validation indicates how much the type of classifier and its parameters are appropriate for the specific problem
- Built decision trees can have different split attributes and conditions depending on the character of the $k$-th training set

**Bootstrap ...**
Bootstrap

Unlike previous approaches, the extracted records are replaced. If the initial dataset consists of N records, you can create a N record set in which each record has approximately 63.2% probability of appearing (with N sufficiently large)

$$1 - (1 - 1 / N)^N = 1 - e^{-1} = 0.632$$

- Records that are not used even once in the current training set form the validation set

The procedure is repeated b times. Commonly, the model's accuracy is calculated as:

$$Acc_{boot} = \frac{1}{b} \sum_{i=1}^{b} 0.632 \times Acc_i + 0.368 \times Acc_s$$

where Acc$_i$ is the accuracy of the i-th bootstrap, while Acc$_s$ is the accuracy of the complete dataset

The bootstrap does not create a (new) dataset with more information, but it can stabilize the obtained results of the available dataset. It is therefore particularly useful for small datasets.
C4.5

Widely used Decision Tree algorithm. It extends ID3 and Hunt Algorithm.

**Features:**
- Use GainRatio as a criterion for determining the split attribute
- It manages the continuous attributes by determining a split point dividing the range of values into two
- It manages data with missing values. Missing attributes are not considered to calculate GainRatio.
- It can handle attributes that are associated with different weights
- Run post Pruning of the created tree

**The tree construction stops when:**
- The node contains records belonging to a single class
- No attribute allows to determine a positive GainRatio
- Node does not contain records.
Exercise

Using the classification error as a measure, identify which attribute should be chosen first and which one per second

- Compute contingency matrices
- Compute the information gain

How do the results change if you use the worst attribute as the split attribute?
Comment on the result

<table>
<thead>
<tr>
<th></th>
<th>A</th>
<th>B</th>
<th>C</th>
<th># instances</th>
</tr>
</thead>
<tbody>
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<td>+</td>
<td>-</td>
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</tr>
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