

Outline

- 1. What is Classification?
- 2. K-Nearest-Neighbors
- 3. Decision Trees
- 4. Model Evaluation
- 5. Rule Learning
- 6. Naïve Bayes
- 7. Artificial Neural Networks
- 8. Support Vector Machines
- 9. Parameter Tuning

1. What is Classification?

 Goal: Previously unseen records should be assigned a class from a given set of classes as accurately as possible.



– Approach:

- Given a collection of records (training set)
 - each record contains a set of attributes
 - one of the attributes is the class (label) that should be predicted.
- Learn a model for the class attribute as a function of the values of other attributes.

Variants:

- single-class problems (class labels e.g. true/false or fraud/no fraud)
- multi-class problems (class labels e.g. low, medium, high)

Introduction to Classification

A Couple of Questions:

- What is this?
- Why do you know?
- How have you come to that knowledge?



Introduction to Classification

- Goal: Learn a model for recognizing a concept, e.g. trees
- Training data:



"tree"



"tree"



"tree"



"not a tree"



"not a tree"



"not a tree"

Introduction to Classification

 We (or the learning algorithm) look at positive and negative examples (training data)

... and derive a model

e.g., "Trees are big, green plants that have a trunk."

Goal: Classification of unseen instances















Tree?

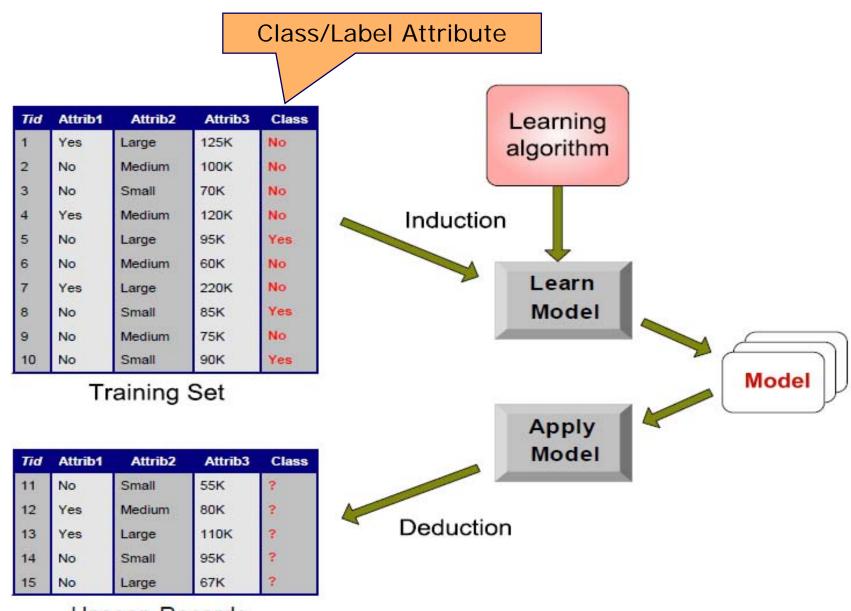
Tree?

Warning:

Models are only
approximating examples!

Not guaranteed to be
correct or complete!

Model Learning and Model Application Process



Unseen Records

Classification Examples

Credit Risk Assessment

- Attributes: your age, income, debts, ...
- Class: Are you getting credit by your bank?

Marketing

- Attributes: previously bought products, browsing behaviour
- Class: Are you a target customer for a new product?

Tax Fraud

- Attributes: the values in your tax declaration
- Class: Are you trying to cheat?

SPAM Detection

- Attributes: words and header fields of an e-mail
- Class: Is it a spam e-mail?

Classification Techniques

- 1. K-Nearest-Neighbors
- 2. Decision Trees
- 3. Rule Learning
- 4. Naïve Bayes
- 5. Support Vector Machines
- 6. Artificial Neural Networks
- 7. Deep Neural Networks
- 8. Many others ...

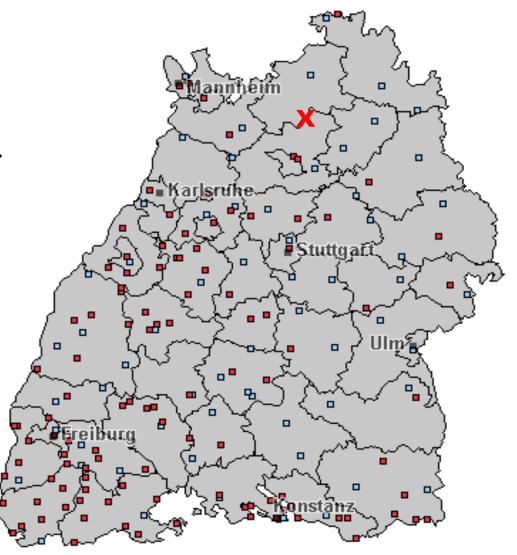
2. K-Nearest-Neighbors

Example Problem

Predict what the current weather is in a certain place

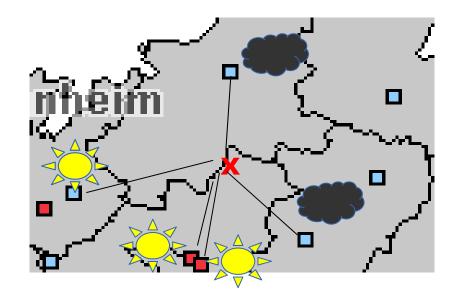
where there is no weather station.

– How could you do that?



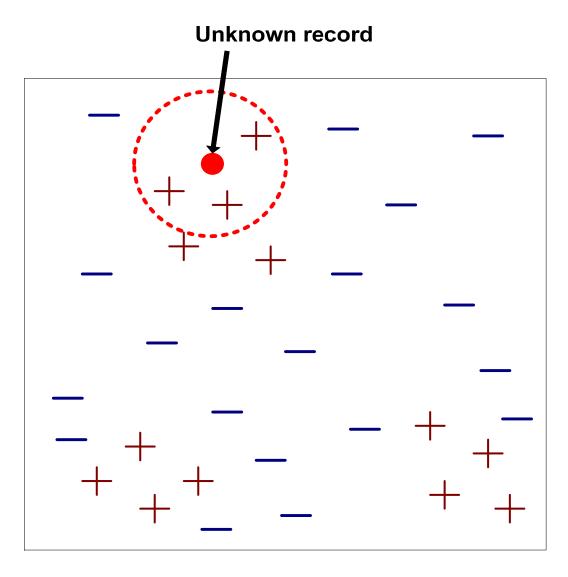
Basic Idea

- Use the average of the nearest stations
- Example:
 - 3x sunny
 - 2x cloudy
 - result = sunny



- This approach is called K-Nearest-Neighbors
 - where k is the number of neighbors to consider
 - in the example: k=5
 - in the example: "near" denotes geographical proximity

K-Nearest-Neighbors Classifiers

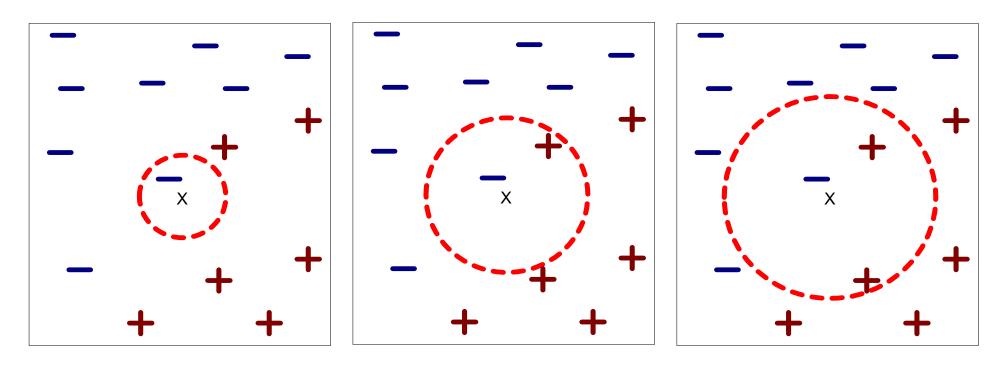


Require three things

- The set of stored records
- A distance measure to compute distance between records
- The value of k, the number of nearest neighbors to consider
- To classify an unknown record:
 - Compute distance to each training record
 - 2. Identify k-nearest neighbors
 - 3. Use class labels of nearest neighbors to determine the class label of unknown record
 - by taking majority vote or
 - by weighing the vote according to distance

Examples of K-Nearest Neighbors

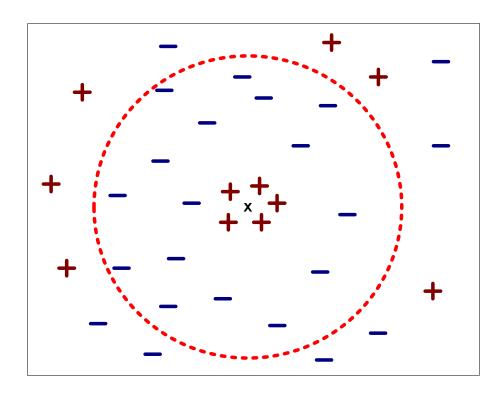
The k-nearest neighbors of a record x are data points that have the k smallest distances to x.



- (a) 1-nearest neighbor
- (b) 2-nearest neighbor
- (c) 3-nearest neighbor

Choosing a Good Value for K

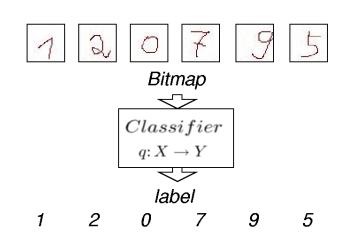
- If k is too small, the result is sensitive to noise points
- If k is too large, the neighborhood may include points from other classes



Rule of thumb: Test k values between 1 and 10.

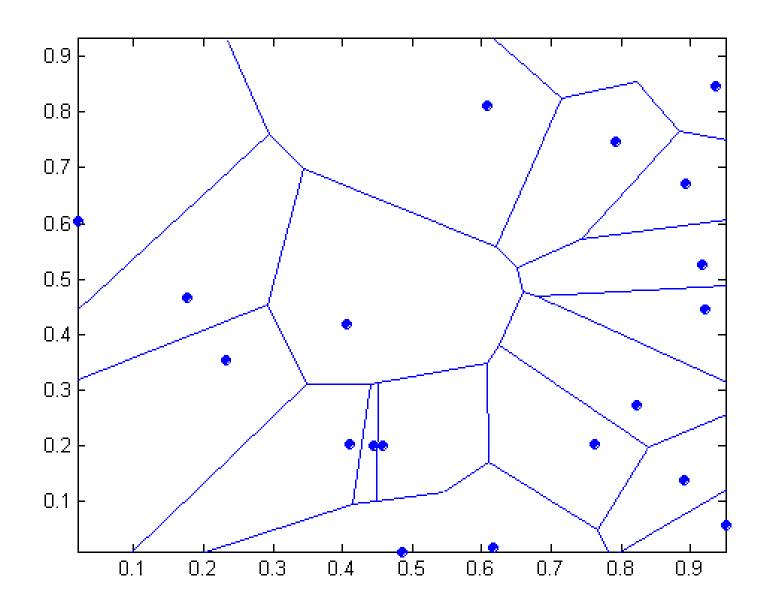
Discussion of K-Nearest-Neighbor Classification

- Often very accurate
 - for instance for optical character recognition (OCR)
- ... but slow
 - as training data needs to be searched

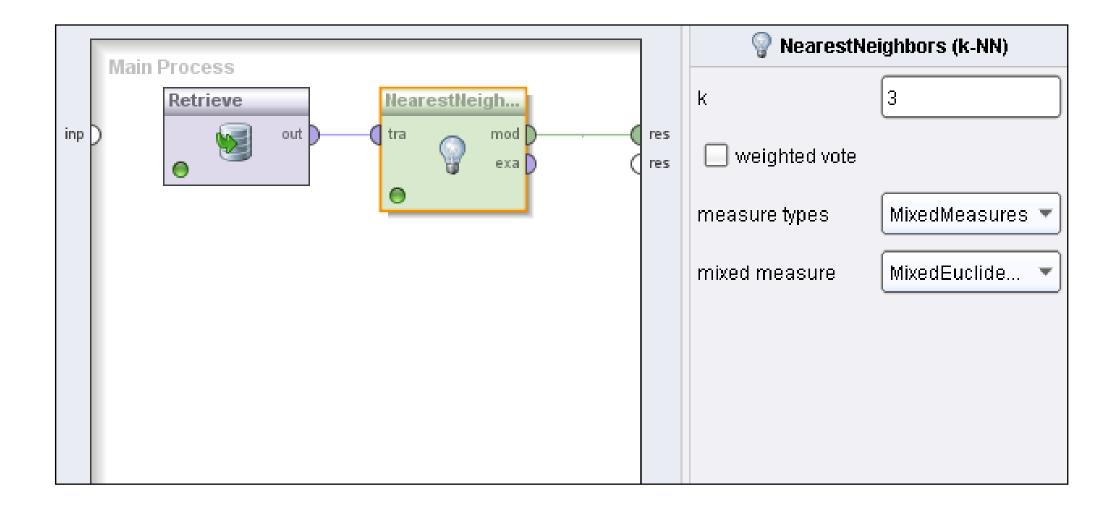


- Assumes that all attributes are equally important
 - remedy: attribute selection or attribute weights
- Can handle decision boundaries which are not parallel to the axes (unlike decision trees)

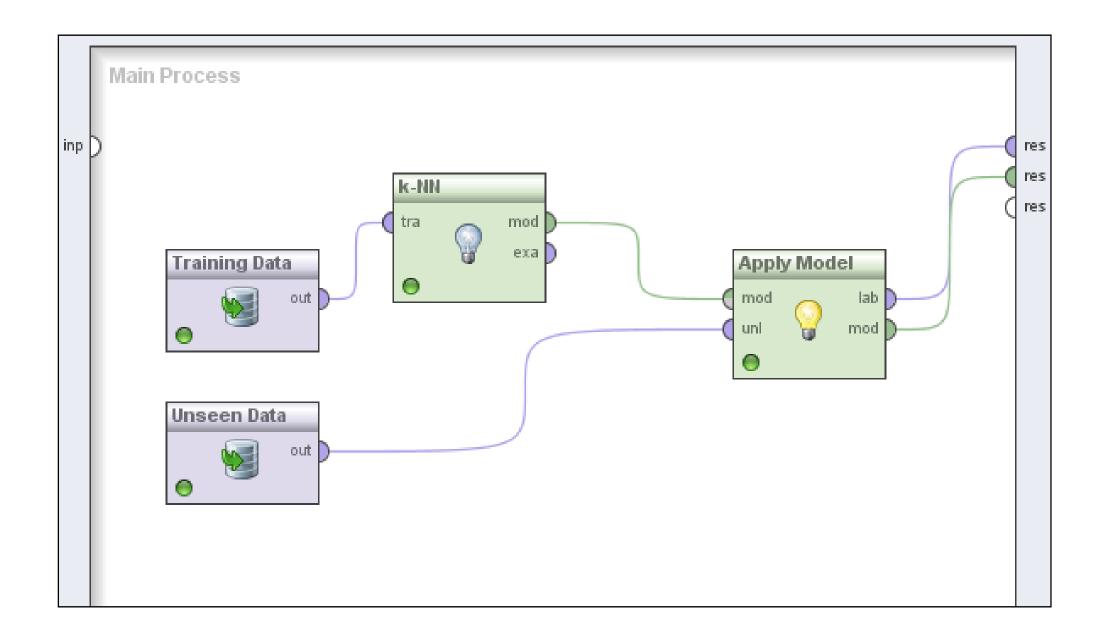
Decision Boundaries of a 1-NN Classifier



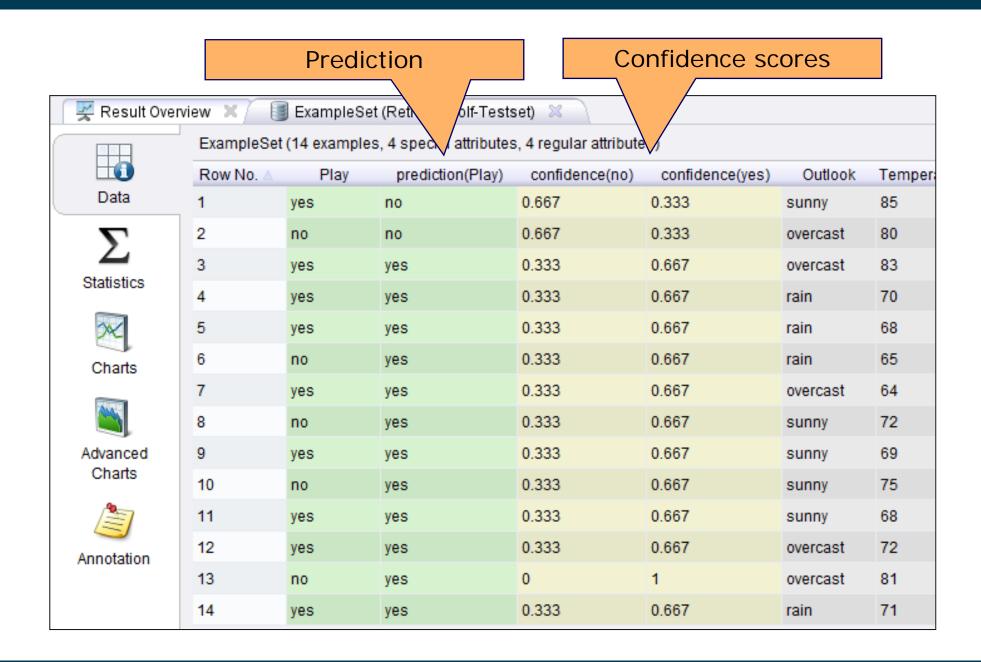
KNN in RapidMiner



Applying the Model



Resulting Dataset



Lazy versus Eager Learning

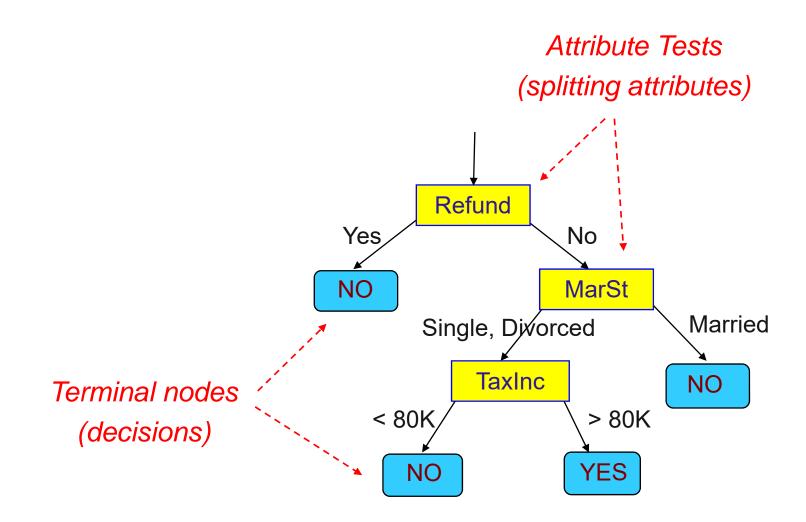
Lazy Learning

- Instance-based learning approaches, like KNN, are also called lazy learning as no explicit knowledge (model) is learned
- Single goal: Classify unseen records as accurately as possible

Eager Learning

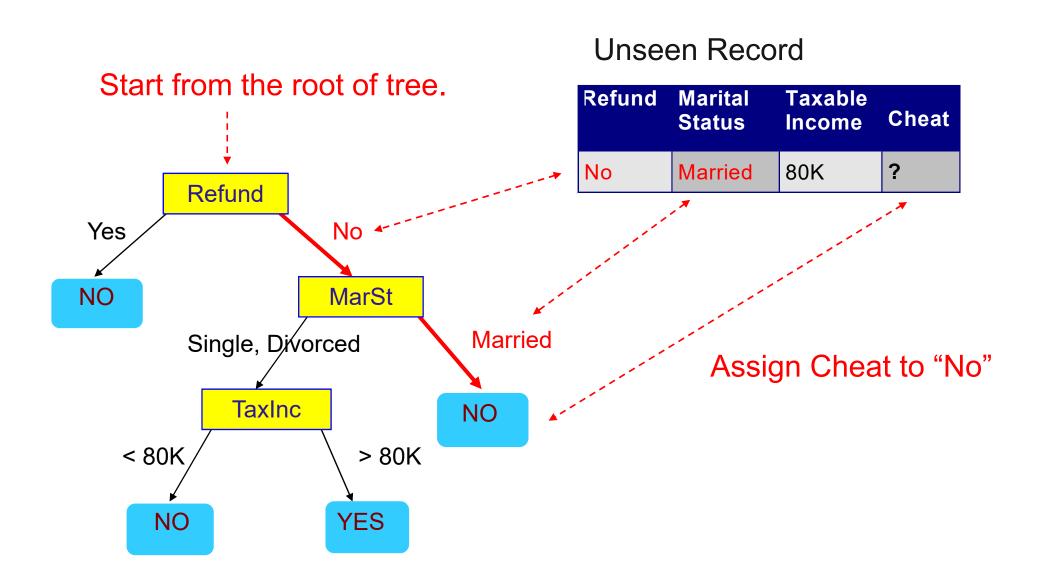
- but actually, we might have two goals
 - 1. classify unseen records
 - 2. understand the application domain as a human
- Eager learning approaches generate models that are (might be) interpretable by humans
- Examples of eager techniques: Decision Tree Learning, Rule Learning

3. Decision Tree Classifiers

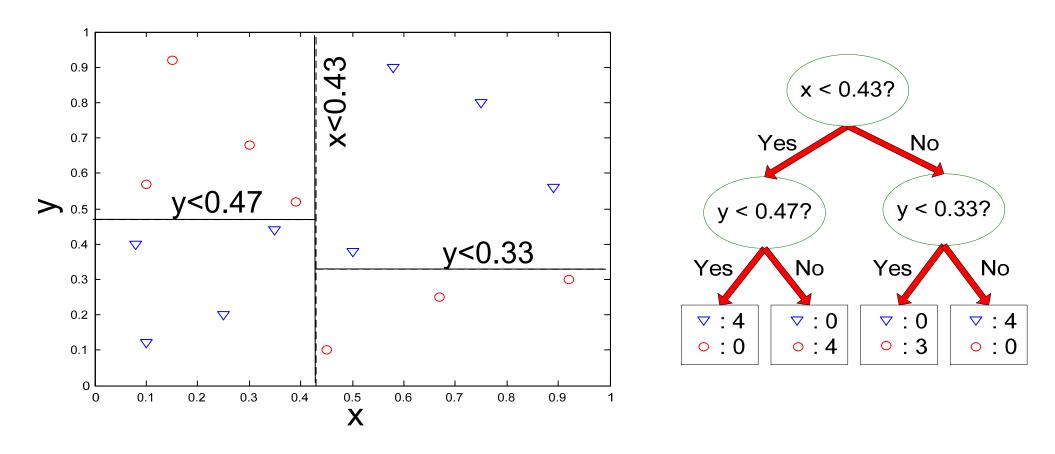


Decision trees encode a procedure for taking a classification decision.

Applying a Decision Tree to Unseen Data



Decision Boundary

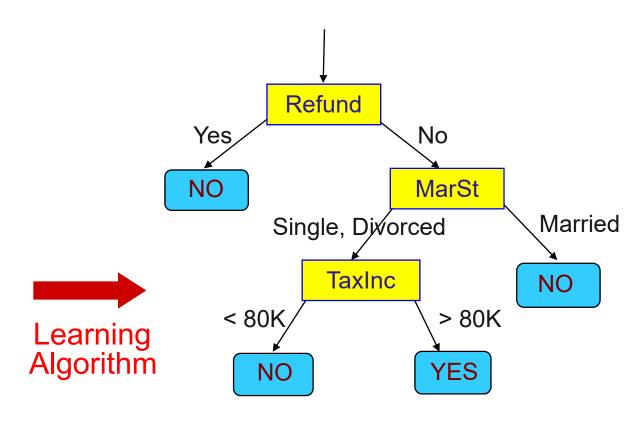


The decision boundaries are parallel to the axes because the test condition involves a single attribute at-a-time.

Decision Tree Induction

categorical continuous

Tid	Refund	Marital Status	Taxable Income	Cheat
1	Yes	Single	125K	No
2	No	Married	100K	No
3	No	Single	70K	No
4	Yes	Married	120K	No
5	No	Divorced	95K	Yes
6	No	Married	60K	No
7	Yes	Divorced	220K	No
8	No	Single	85K	Yes
9	No	Married	75K	No
10	No	Single	90K	Yes



Model: Decision Tree

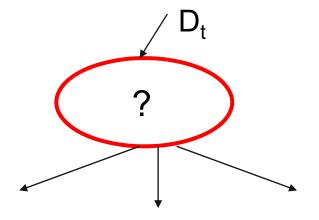
Training Data

Decision Tree Induction

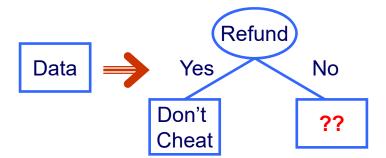
- How to learn a decision tree from training data?
- Finding an optimal decision tree is NP-hard.
- Tree building algorithms thus use a greedy, top-down, recursive partitioning strategy to induce a reasonable solution.
- Many different algorithms have been proposed:
 - Hunt's Algorithm
 - ID3
 - C4.5
 - CHAID

Hunt's Algorithm

- Let D_t be the set of training records that reach a node t
- General procedure:
 - If D_t only contains records that belong to the same class y_t, then t is a leaf node labeled as y_t
 - If D_t contains records that belong to more than one class, use an attribute test to split the data into subsets having a higher purity.
 - Recursively apply the procedure to each subset.



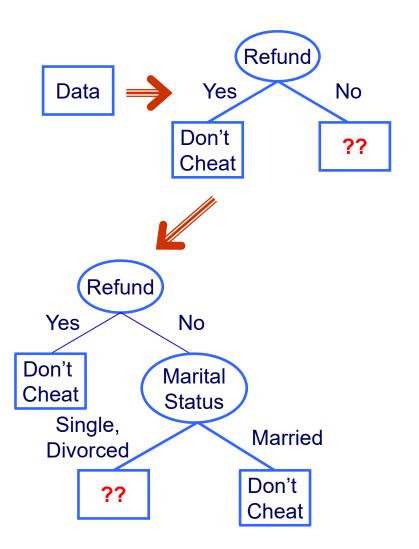
Hunt's Algorithm – Step 1



- We test all possible splits and measure the purity of the resulting subsets
- 2. We find the split on Refund to produce the purest subsets

Tid	Refund	Marital Status	Taxable Income	Cheat
1	Yes	Single	125K	No
2	No	Married	100K	No
3	No	Single	70K	No
4	Yes	Married	120K	No
5	No	Divorced	95K	Yes
6	No	Married	60K	No
7	Yes	Divorced	220K	No
8	No	Single	85K	Yes
9	No	Married	75K	No
10	No	Single	90K	Yes

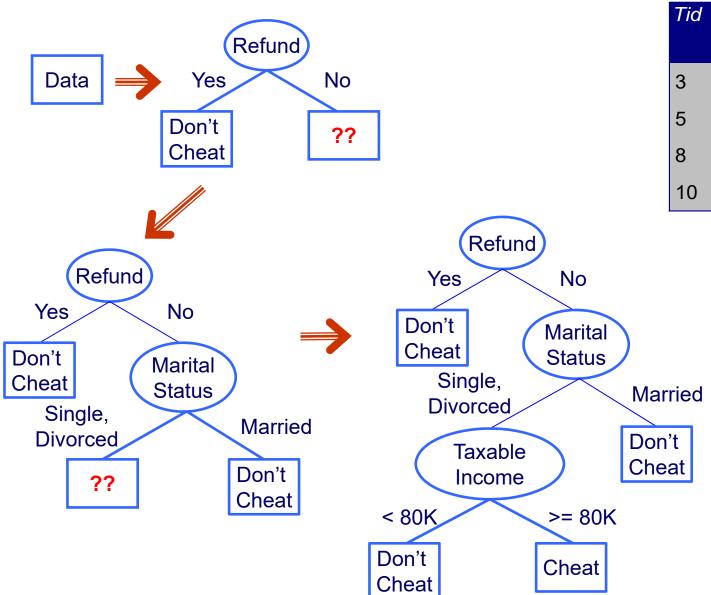
Hunt's Algorithm – Step 2



Tid	Refund	Marital Status	Taxable Income	Cheat
2	No	Married	100K	No
3	No	Single	70K	No
5	No	Divorced	95K	Yes
6	No	Married	60K	No
8	No	Single	85K	Yes
9	No	Married	75K	No
10	No	Single	90K	Yes

- We further examine the Refund=No records
- 2. Again, we test all possible splits
- 3. We find the split on Marital Status to produce the purest subsets

Hunt's Algorithm – Step 3



Tid	Refund	Marital Status	Taxable Income	Cheat
3	No	Single	70K	No
5	No	Divorced	95K	Yes
8	No	Single	85K	Yes
10	No	Single	90K	Yes

- We further examine the Marital Status=Single or =Divorced records
- We find a split on Taxable Income to produce pure subsets

Tree Induction Issues

- 1. Determine how to split the records
 - How to specify the attribute test condition?
 - How to determine the best split?
- 2. Determine when to stop splitting

3.1 How to Specify the Attribute Test Condition?

- 1. Depends on attribute types
 - Nominal
 - Ordinal
 - Continuous
- 2. Depends on number of ways to split
 - 2-way split
 - Multi-way split

Splitting Based on Nominal Attributes

Multi-way split: Use as many partitions as distinct values.

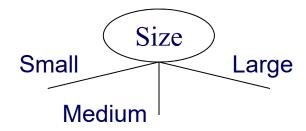


Binary split: Divides values into two subsets.
 Need to find optimal partitioning.



Splitting Based on Ordinal Attributes

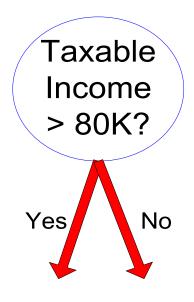
Multi-way split: Use as many partitions as distinct values.



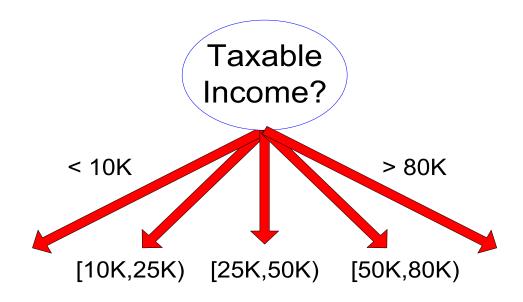
 Binary split: Divides values into two subsets while keeping the order.
 Need to find optimal partitioning.



Splitting Based on Continuous Attributes



(i) Binary split



(ii) Multi-way split

Splitting Based on Continuous Attributes

- Different ways of handling continuous attributes
 - Discretization to form an ordinal categorical attribute
 - equal-interval binning
 - equal-frequency binning
 - binning based on user-provided boundaries
 - Binary Decision: (A < v) or (A ≥ v)
 - usually sufficient in practice
 - find the best splitting border v based on a purity measure (see below)
 - can be compute intensive

Discretization Example

- Values of the attribute, e.g., age of a person:
 - 0, 4, 12, 16, 16, 18, 24, 26, 28
- Equal-interval binning for bin width of e.g., 10:
 - Bin 1: 0, 4

[-,10) bin

• Bin 2: 12, 16, 16, 18 [10,20] bin

• Bin 3: 24, 26, 28

[20,+) bin

- denote negative infinity, + positive infinity
- Equal-frequency binning for bin density of e.g., 3:
 - Bin 1: 0, 4, 12

[-, 14) bin

• Bin 2: 16, 16, 18

[14, 21) bin

• Bin 3: 24, 26, 28

[21,+] bin

3.2 How to Find the Best Split?

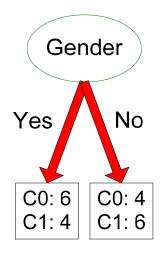
Before splitting the dataset contains:

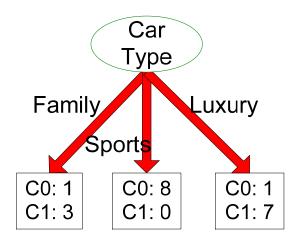
- 10 records of class 0 and
- 10 records of class 1

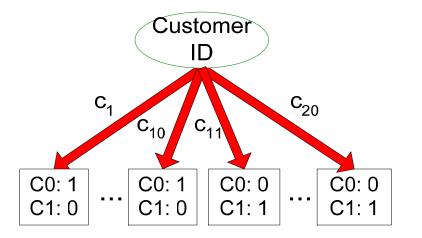
1	M	Family	Small	C0
2	M	Sports	Medium	C0
3	M	Sports	Medium	C0
4	\mathbf{M}	Sports	Large	C0
5	$_{ m M}$	Sports	Extra Large	C0
6	\mathbf{M}	Sports	Extra Large	C0
7	F	Sports	Small	C0
8	F	Sports	Small	C0
9	F	Sports	Medium	C0
10	F	Luxury	Large	C0
11	\mathbf{M}	Family	Large	C1
12	\mathbf{M}	Family	Extra Large	C1
13	M	Family	Medium	C1
14	\mathbf{M}	Luxury	Extra Large	C1
15	F	Luxury	Small	C1
16	F	Luxury	Small	C1
17	F	Luxury	Medium	C1
18	F	Luxury	Medium	C1
19	F	Luxury	Medium	C1
20	F	Luxury	Large	C1
				-

Car Type

Shirt Size







Customer Id

Gender

Which test condition is the best?

How to Find the Best Split?

- Greedy approach: Test all possible splits and use the one that results in the most homogeneous (= pure) nodes.
- Need a measure of node impurity:

C0: 5

C1: 5

Non-homogeneous,

High degree of impurity

C0: 9

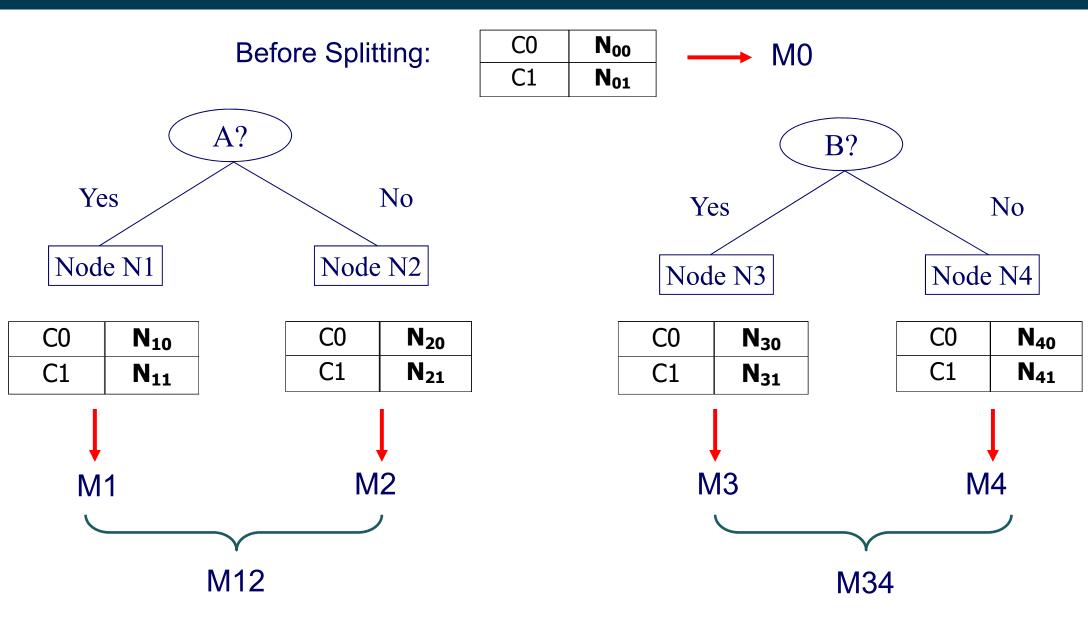
C1: 1

Homogeneous,

Low degree of impurity

- Common measures of node impurity:
 - GINI Index
 - 2. Entropy
 - 3. GainRATIO

Comparing different Splits



Largest purity gain? M0 – M12 versus M0 – M34

3.2.1 Measure of Impurity: GINI Index

GINI Index for a given node t :

$$GINI(t) = 1 - \sum_{j} [p(j|t)]^{2}$$

 $p(j \mid t)$ is the relative frequency of class j at node t.

- Minimum (0.0) when all records belong to one class
- Maximum (1 1/n_c) when records are equally distributed among all classes. n_c = number of classes

C1	0
C2	6
Gini=	0.000

C1	1
C2	5
Gini=	0.278

C1	2
C2	4
Gini=	0.444

C1	3
C2	3
Gini=	0.500

Examples for computing GINI

$$GINI(t) = 1 - \sum_{j} [p(j|t)]^{2}$$

$$P(C1) = 0/6 = 0$$
 $P(C2) = 6/6 = 1$

Gini =
$$1 - P(C1)^2 - P(C2)^2 = 1 - 0 - 1 = 0$$

$$P(C1) = 1/6$$
 $P(C2) = 5/6$

Gini =
$$1 - (1/6)^2 - (5/6)^2 = 0.278$$

$$P(C1) = 2/6$$
 $P(C2) = 4/6$

Gini =
$$1 - (2/6)^2 - (4/6)^2 = 0.444$$

Splitting Based on GINI

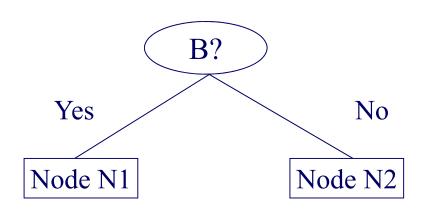
- When a node p is split into k partitions (children),
 the GINI index of each partition is weighted according to the partition's size.
- The quality of the overall split is computed as:

$$GINI_{split} = \sum_{i=1}^{k} \frac{n_i}{n} GINI(i)$$

where: n_i = number of records at child i n = number of records at node p

Example: Calculating the Purity Gain of a Possible Split

Split into two partitions



	Parent
C1	6
C2	6
Gini	= 0.500

GINI(N1)

$$= 1 - (5/7)^2 - (2/7)^2$$

= 0.408

GINI(N2)

$$= 1 - (1/5)^2 - (4/5)^2$$

= 0.32

	N1	N2
C1	5	1
C2	2	4
Gin	i=0.3	71

$\mathsf{GINI}_{\mathsf{Split}}$

= 7/12 * 0.408 +

5/12 * 0.32

= 0.371

Purity Gain = 0.5 - 0.371 = 0.129

Categorical Attributes: Computing Gini Index

For each distinct attribute value, gather counts for each class.

Multi-way split

		CarType								
	Family Sports Luxury									
C1	1	2	1							
C2	4	1	1							
Gini	0.393									

Two-way split (find best partition of values)

	CarType						
	{Sports, Luxury}	{Family}					
C1	3	1					
C2	2	4					
Gini	0.4	00					

	CarType							
	{Sports}	{Family, Luxury}						
C1	2	2						
C2	1	5						
Gini	0.419							

Continuous Attributes: Computing Gini Index

- How to find the best binary split for a continuous attribute?
- Efficient computation:
 - 1. Sort the attribute on values
 - 2. Linearly scan these values, each time updating the count matrix and computing the gini index
 - 3. Choose the split position that has the smalest gini index

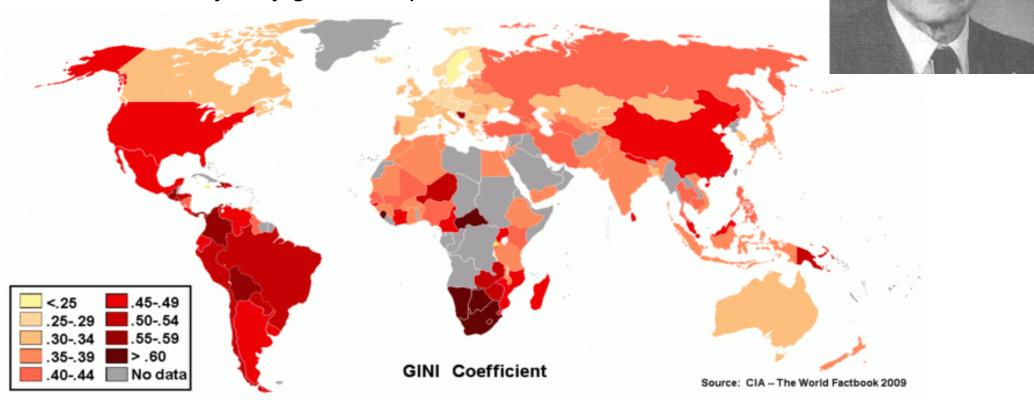


Sorted	Values
Split Po	sitions

	Taxable Income																																									
	60 70 75 85		90 9			9	5 100		0 120		125		220																													
	→ 55		55		55		55		55		55		55		55		55		55		→ 55		6	5	7	2	8	0	8	7	9	2	9	7	11	10	12	22	17	72	23	80
	<=	>	<=	>	<=	>	<=	>	<=	>	<=	>	<=	>	<=	>	<=	>	<=	>	<=	>																				
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	0.4	0.420		0.400 <u>0.300</u>			00 0.343			0.375 0.4			00 0.420																													

Gini Index

- Named after Corrado Gini (1885-1965)
- Used to measure the distribution of income
 - 1: somebody gets everything
 - 0: everybody gets an equal share



3.2.2 Alternative Splitting Criterion: Information Gain

- Calculating the information gain relies on the entropy of each node.
- Entropy of a given node t:

Entropy
$$(t) = -\sum_{j} p(j|t) \log_2 p(j|t)$$

 $p(j \mid t)$ is the relative frequency of class j at node t

- Entropy measures homogeneity of a node
 - Minimum (0.0) when all records belong to one class.
 - Maximum (log n_c) when records are equally distributed among all classes.

Examples for Computing Entropy

Entropy
$$(t) = -\sum_{j} p(j|t) \log_2 p(j|t)$$

C1	0
C2	6

$$P(C1) = 0/6 = 0$$
 $P(C2) = 6/6 = 1$

Entropy =
$$-0 \log_2 0 - 1 \log_2 1 = -0 - 0 = 0$$

$$P(C1) = 1/6$$
 $P(C2) = 5/6$

Entropy =
$$-(1/6) \log_2 (1/6) - (5/6) \log_2 (5/6) = 0.65$$

$$P(C1) = 2/6$$
 $P(C2) = 4/6$

Entropy =
$$-(2/6) \log_2 (2/6) - (4/6) \log_2 (4/6) = 0.92$$

Splitting Based on Information Gain

Information Gain:

$$GAIN_{split} = Entropy(p) - \left(\sum_{i=1}^{k} \frac{n_{i}}{n} Entropy(i)\right)$$

Parent Node p is split into k partitions; n_i is number of records in partition i

- Information gain measures the entropy reduction of a split.
- We choose the split with the largest reduction (maximal GAIN)
- Disadvantage: Tends to prefer splits that result in large number of partitions, each being small but pure (split by ID attribute?)

3.2.3 Alternative Splitting Criterion: GainRATIO

- GainRATIO is designed to overcome the tendency to generate a large number of small partitions.
- GainRATIO adjusts information gain by the entropy of the partitioning (SplitINFO).
- Higher entropy of the partitioning (large number of small partitions) is penalized!

GainRATIO
$$_{split} = \frac{GAIN_{Split}}{SplitINFO}$$
 $SplitINFO = -\sum_{i=1}^{k} \frac{n_{i}}{n} \log \frac{n_{i}}{n}$

Parent Node p is split into k partitions n_i is the number of records in partition i

3.3 Overfitting

- Problem: Learned models can fit the training data too closely and thus work poorly on unseen data.
- Possible model fitting the training data:
 - "Trees are big, green plants that have a trunk and no wheels."
- Unseen instance:



Training data









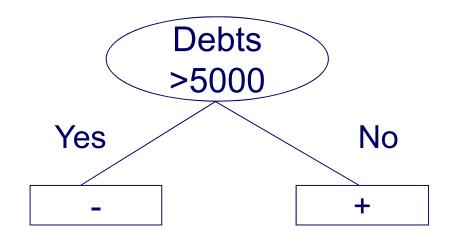




 Goal: Find good compromise between specificness and generality of a model.

Overfitting: Second Example

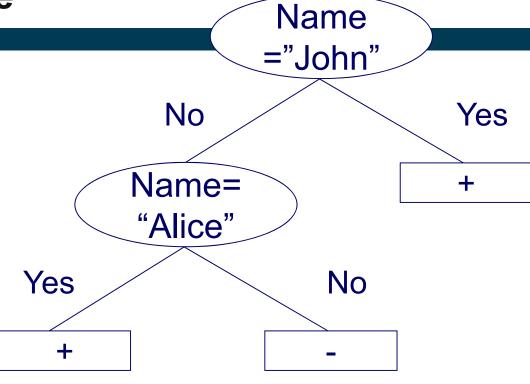
- Example: Predict credit rating
 - possible decision tree:



Name	Net Income	Job status	Debts	Rating
John	40000	employed	0	+
Mary	38000	employed	10000	-
Stephen	21000	self-employed	20000	-
Eric	2000	student	10000	-
Alice	35000	employed	4000	+

Overfitting: Second Example

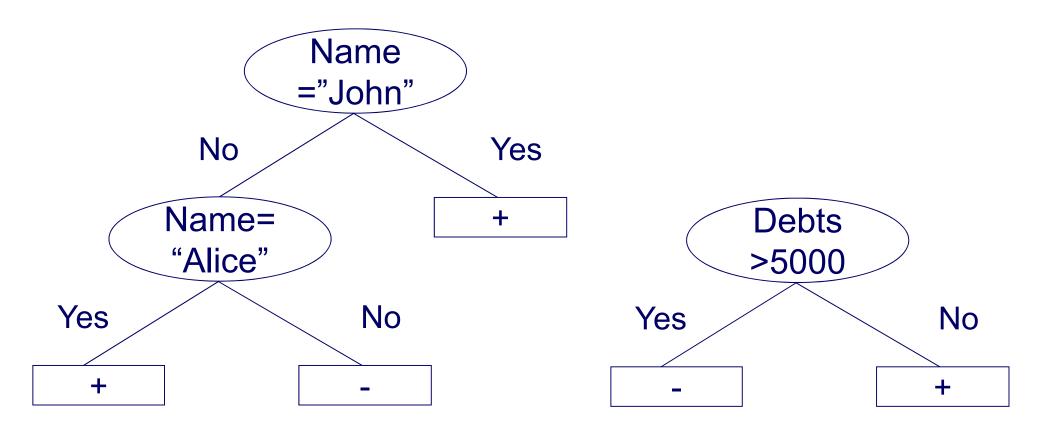
- Example: Predict credit rating
 - alternative decision tree:



Name	Net Income	Job status	Debts	Rating
John	40000	employed	0	+
Mary	38000	employed	10000	-
Stephen	21000	self-employed	20000	-
Eric	2000	student	10000	-
Alice	35000	employed	4000	+

Overfitting: Second Example

- Both trees seem equally good
 - as they classify all instances in the training set correctly
 - Which one do you prefer?



Occam's Razor

- Named after William of Ockham (1287-1347)
- A fundamental principle of science
 - if you have two theories
 - that explain a phenomenon equally well
 - choose the simpler one

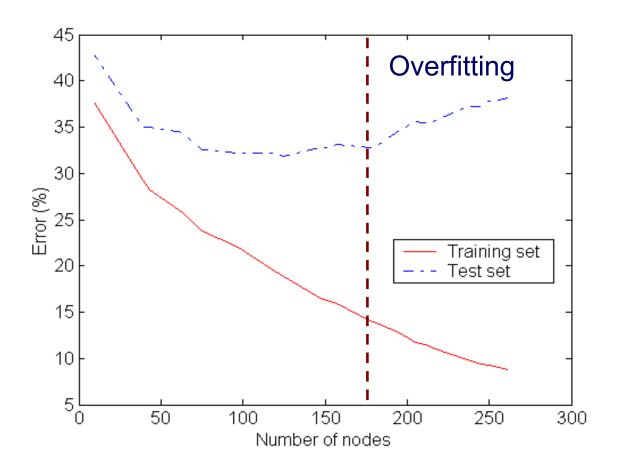


- phenomenon: the street is wet
- theory 1: it has rained
- theory 2: a beer truck has had an accident, and beer has spilled.
 The truck has been towed, and magpies picked the glass pieces, so only the beer remains



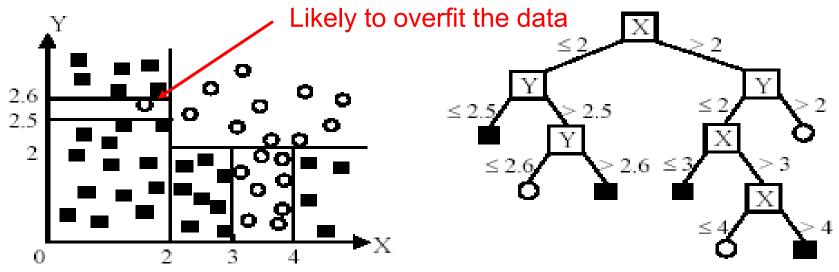
Overfitting: Symptoms and Causes

- Symptoms:
 - 1. decision tree too deep and
 - 2. too many branches
 - model works well on training set but performs bad on test set
- Typical causes of overfitting
 - 1. noise / outliers
 - 2. too little training data
 - 3. poor learning algorithm

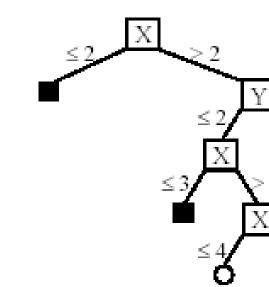


An overfitted model likely does not generalize well to unseen data.

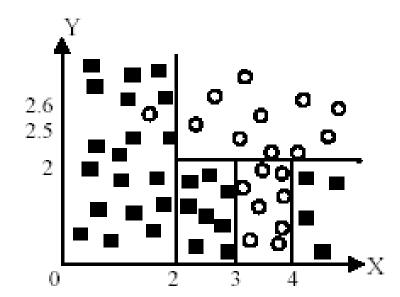
Example of an Outlier causing Overfitting



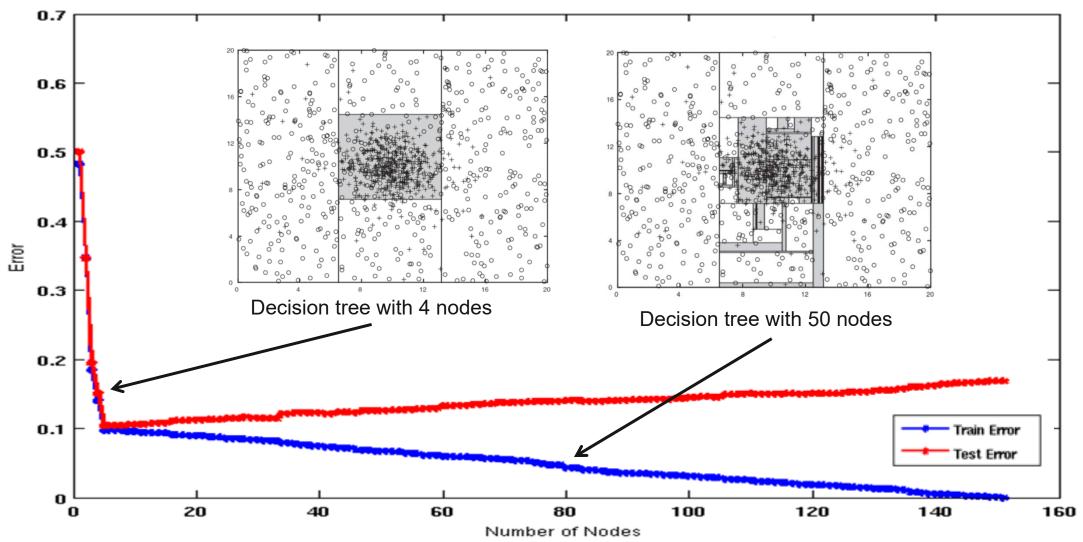
(A) A partition of the data space



(B). The decision tree



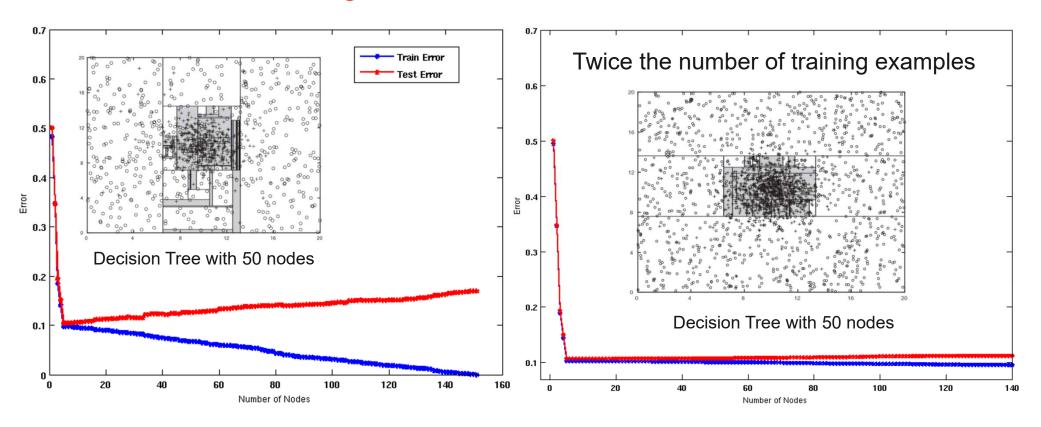
Underfitting versus Overfitting Model



Underfitting: when model is too simple, both training and test errors are large **Overfitting:** when model is too complex, training error is small but test error is large

How to Address Overfitting?

Add more training data!



- If training data is under-representative, testing errors increase and training errors decrease on increasing number of nodes
- Increasing the size of training data reduces the difference between training and testing errors at a given number of nodes

How to Address Overfitting?

- Pre-Pruning (Early Stopping)
 - Stop the algorithm before tree becomes fully-grown
 - Normal stopping conditions for a node (no pruning):
 - Stop if all instances belong to the same class
 - Stop if all the attribute values are the same
 - Early stopping conditions (pre-pruning):
 - Stop if number of instances within a leaf node is less than some user-specified threshold (e.g. leaf size < 4)
 - Stop if expanding the current node only slightly improves the impurity measure (e.g. gain < 0.01)

How to Address Overfitting?

Post-Pruning

Grow decision tree to its entirety

Subtree Replacement

- 1. Trim the nodes of the decision tree in a bottom-up fashion
- 2. Estimate generalization error before and after trimming
 - using a validation set (see in two slides)
 - or by putting a penalty on model complexity (see in two slides)
- 3. If generalization error improves after trimming, replace subtree by a leaf node. Class label of leaf node is determined from majority class of instances in the sub-tree

Subtree Raising

Replace subtree with most frequently used branch

Examples of Post-Pruning

```
Decision Tree:
depth = 1:
  breadth > 7 : class 1
  breadth <= 7:
    breadth <= 3:
      ImagePages > 0.375 : class 0
       ImagePages <= 0.375:
         totalPages <= 6 : class 1
         totalPages > 6:
           breadth <= 1 : class 1
           breadth > 1 : class 0
    width > 3:
       MultilP = 0:
      | ImagePages <= 0.1333 : class 1
      | ImagePages > 0.1333 :
           breadth <= 6 : class 0
          breadth > 6 : class 1
       MultiTP = 1
         TotalTime <= 361 : class 0
        TotalTime > 361 : class 1
depth > 1:
  MultiAgent = 0:
  | depth > 2 : class 0
  | depth <= 2 :
      MultiIP = 1: class 0
      MultiIP = 0:
        breadth <= 6 : class 0
         breadth > 6:
           RepeatedAccess <= 0.0322 : class 0
           RepeatedAccess > 0.0322 : class 1
  MultiAgent = 1:
    totalPages <= 81 : class 0
    totalPages > 81 : class 1
```

```
Simplified Decision Tree:
              depth = 1:
               ImagePages <= 0.1333 : class 1
Subtree
               I ImagePages > 0.1333 :
Raising
                   breadth <= 6 : class 0
                   breadth > 6 : class 1
              depth > 1:
                MultiAgent = 0: class 0
                MultiAgent = 1:
                   totalPages <= 81 : class 0
                   totalPages > 81 : class 1
      Subtree
   Replacement
```

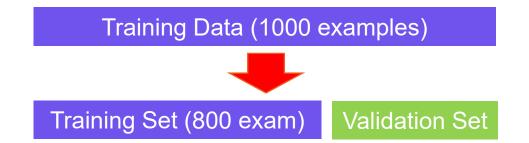
Validation Set versus Penalty on Model Complexity

Validation Set

- Divide <u>training</u> data into two parts:
 - Training set:
 - use for model building
 - Validation set:
 - use for estimating generalization error
 - Note: validation set is not the same as test set (see Model Evaluation later)
- Drawback: Less data available for training

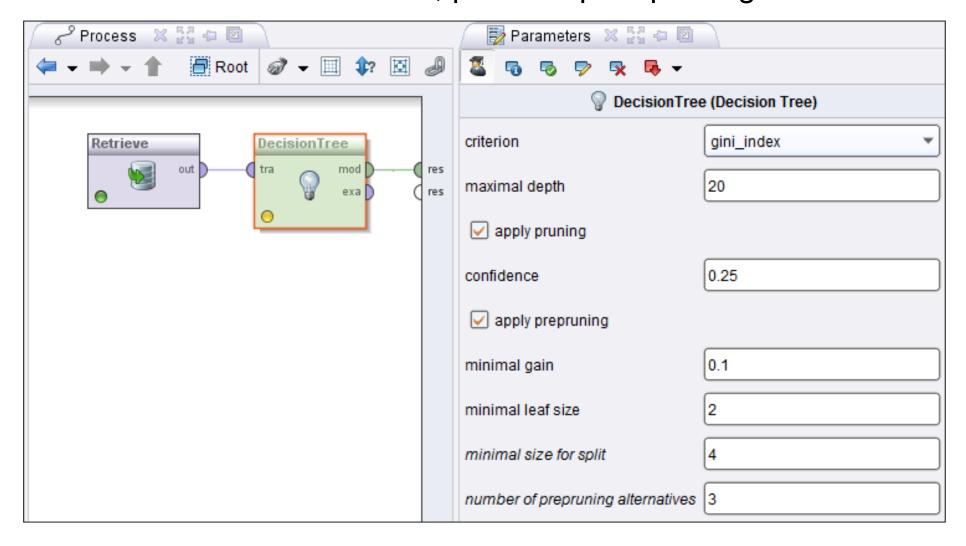
Penalty on Model Complexity

- Gen. Error(Model) = Train. Error(Model, Train. Data) + Complexity(Model)
- Complexity(Model) = α * number of leaf nodes
- User-provided penalty factor: e.g. α = 0.01
- Advantage: All data available for training
- Drawlback: Unclear how to estimate α

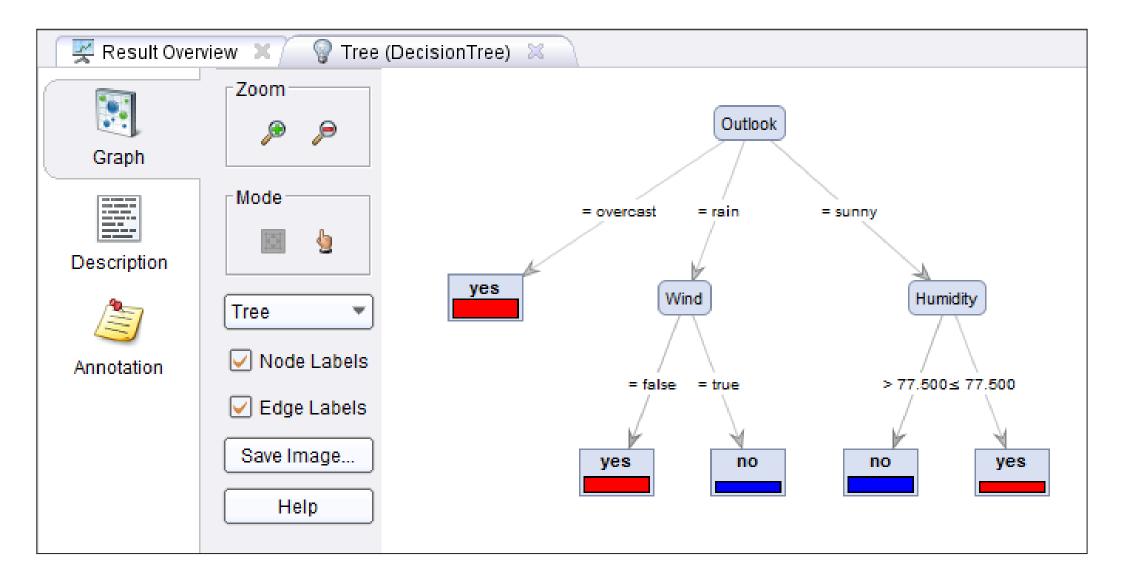


Decision Trees in RapidMiner

The Decision Tree operator implements flexible learning algorithm which includes discretization, pre- and post-pruning.



Learned Decision Tree



3.4 Discussion of Decision Trees

Advantages

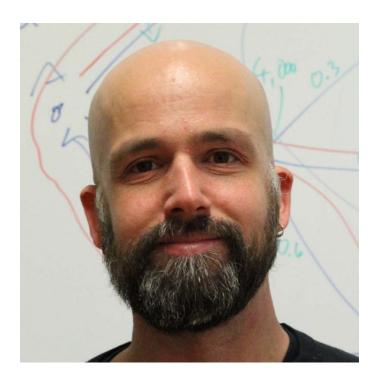
- Inexpensive to construct
- Extremely fast at classifying unknown records
- Easy to interpret by humans for small-sized trees (eager learning)
- Can easily handle redundant or irrelevant attributes
- Accuracy is comparable to other classification techniques for many low dimensional data sets

Disadvantages

- Space of possible decision trees is exponentially large.
 Greedy approaches are often unable to find the best tree.
- Can only represent decision boundaries parallel to the axes

Next week: Heiko Paulheim will give the Lecture.

- 1. What is Classification?
- 2. K-Nearest-Neighbors
- 3. Decision Trees
- 4. Model Evaluation
- 5. Rule Learning
- 6. Naïve Bayes
- 7. Artificial Neural Networks
- 8. Support Vector Machines
- 9. Parameter Tuning



Prof. Dr. Heiko Paulheim