

# **Data Mining**

# Classification - Part 1 -

University of Mannheim – Prof. Bizer: Data Mining

Slide 1

### Outline

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

# 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 attribute (label)* that should be predicted
  - Learn a model for the class attribute as a function of the values of other attributes
- Variants:
  - Binary classification (e.g. fraud/no fraud or true/false)
  - Multi-class classification (e.g. low, medium, high)
  - Multi-label classification (more than one class per record, e.g. user interests)





A Couple of Questions:

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

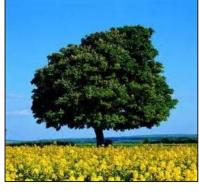


### **Introduction to Classification**

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



"tree"



"tree"



"tree"



"not a tree"



"not a tree"

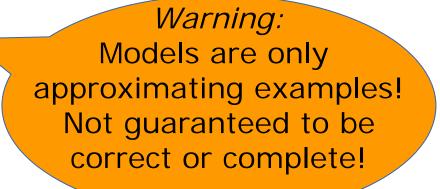


"not a tree"

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# 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 and no wheels."
- Goal: Classification of unseen instances





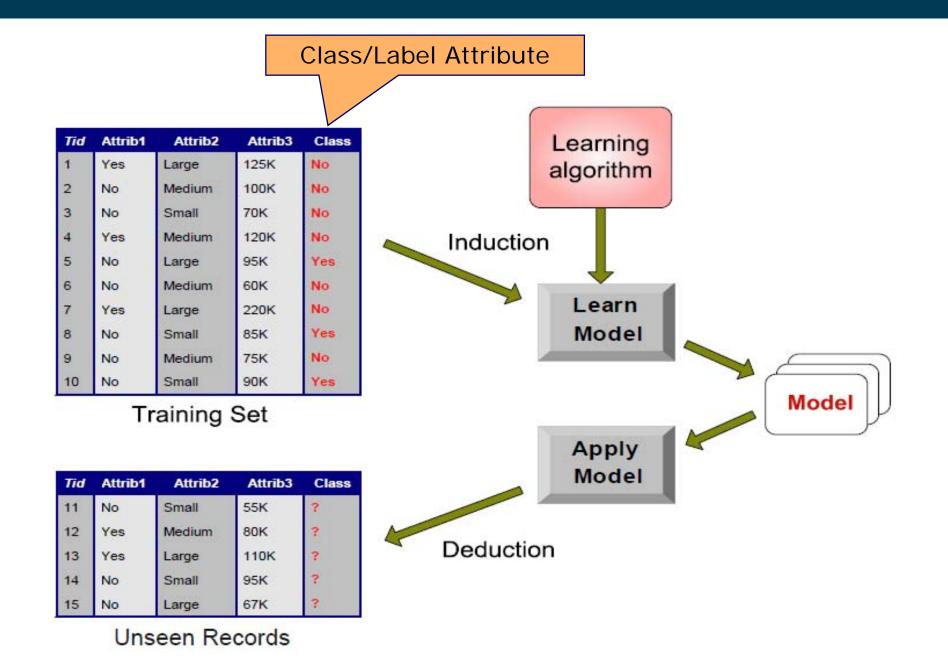




Tree?

Tree?

### **Model Learning and Model Application Process**



### **Classification Examples**

- Credit Risk Assessment
  - Attributes: your age, income, debts, ...
  - Class: are you getting credit by your bank?
- Marketing
  - Attributes: previously bought products, browsing behavior
  - Class: are you a target customer for a new product?
- SPAM Detection
  - Attributes: words and header fields of an e-mail
  - Class: regular e-mail or spam e-mail?
- Identifying Tumor Cells
  - Attributes: features extracted from x-rays or MRI scans
  - Class: malignant or benign cells

### **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**

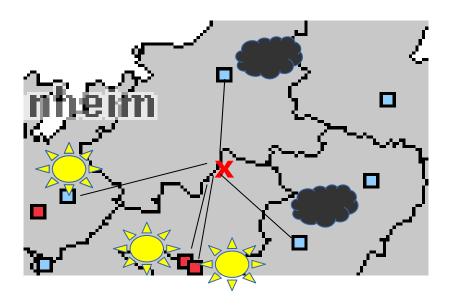
- Predict the current weather in a certain place
- where there is no weather station
- How could you do that?





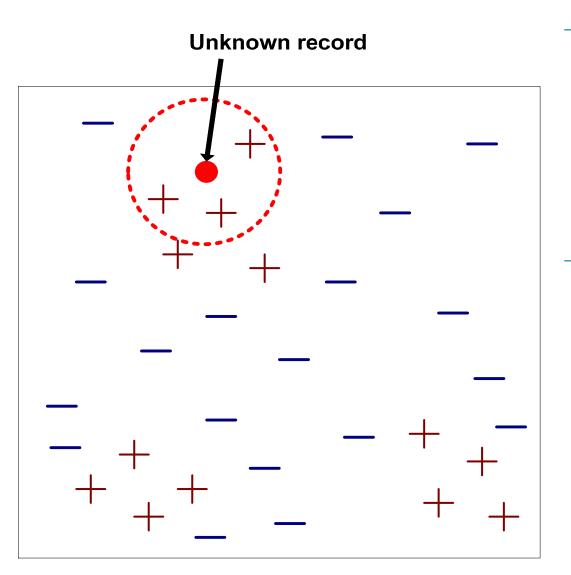
### **Basic Idea**

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



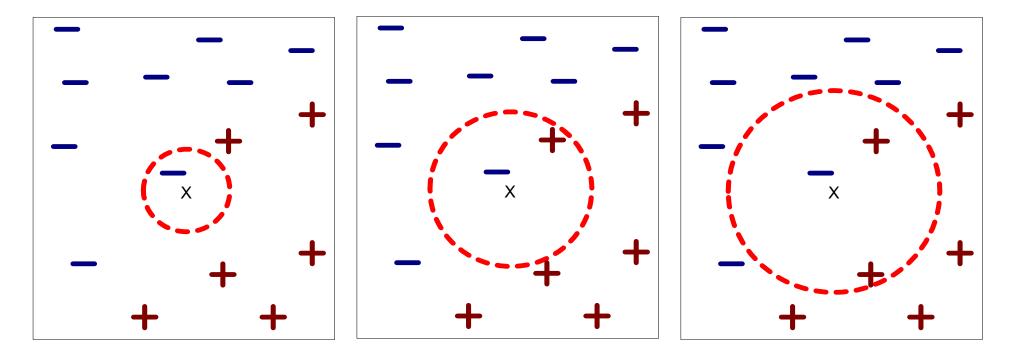
- This approach is called K-Nearest-Neighbors
  - where k is the number of neighbors to consider
  - in the example: k=5
  - in the example: "near" denotes geographical proximity

### **K-Nearest-Neighbors Classifiers**



- Require three things
  - A 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:
  - 1. Compute distance to each training record
  - 2. Identify k-nearest neighbors
  - 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

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



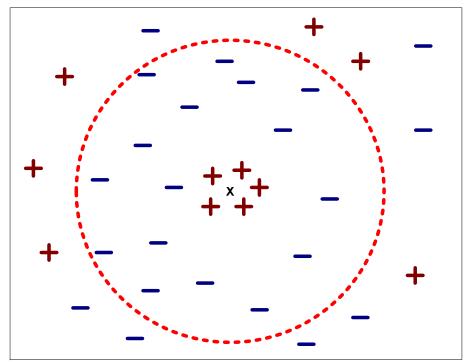
(a) 1-nearest neighbor

(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 20
  - setup: see section on Hyperparameter Selection

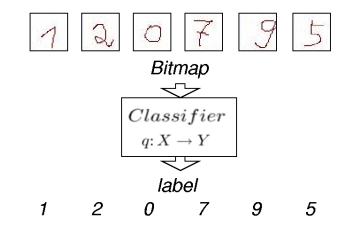
### **Discussion of K-Nearest-Neighbor Classification**

### - Often very accurate

 for instance for optical character recognition (OCR)

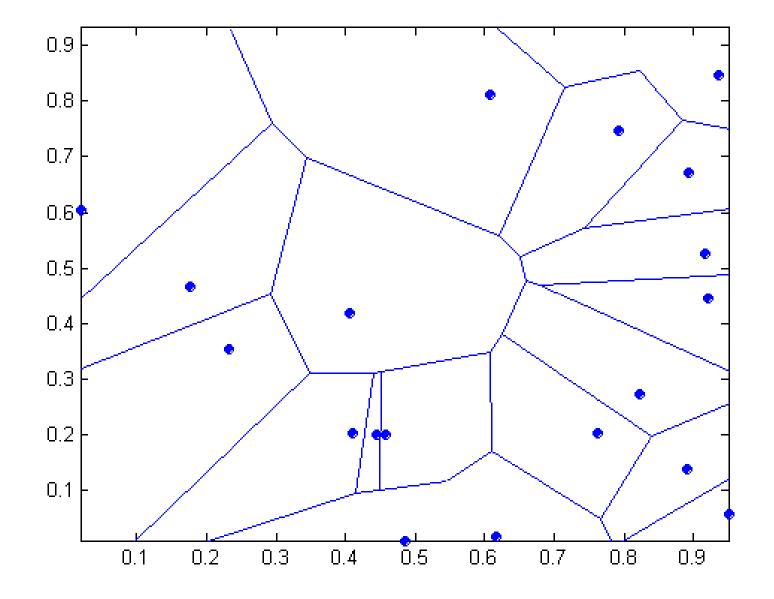
### – … but slow

• as unseen record needs to be compared to all training examples

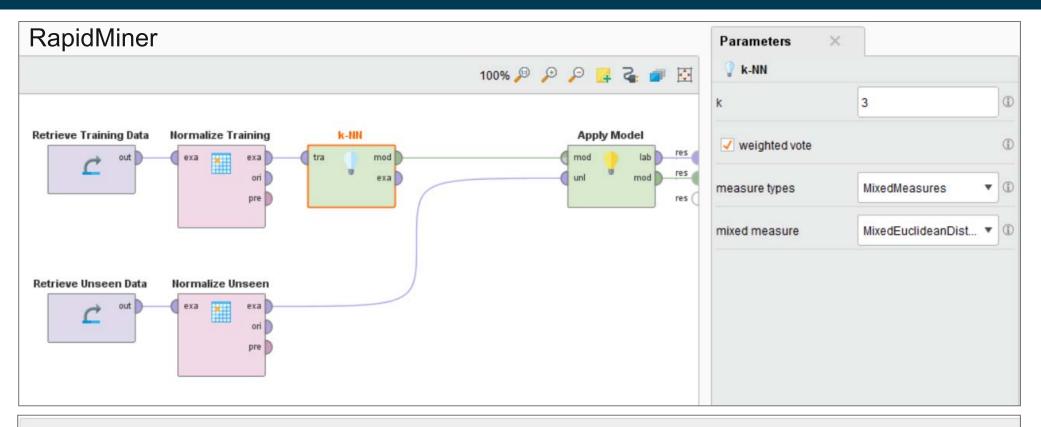


- Results depend on choosing a good proximity measure
  - attribute weights, asymmetric binary attributes, ...
  - see slide set Cluster Analysis
- KNN can handle decision boundaries which are not parallel to the axes (unlike decision trees)

### **Decision Boundaries of a 1-NN Classifier**



### KNN Classification in RapidMiner and Python



#### Python

from sklearn.neighbors import KNeighborsClassifier

#### # Train classifier

knn\_estimator = KNeighborsClassifier(n\_neighbors=3)
knn\_estimator.fit(preprocessed\_training\_data, training\_labels)

#### # Use classifier to predict labels

prediction = knn\_estimator.predict(preprocessed\_unseen\_data)

### **Resulting Dataset**

	Prediction			(	Confidence scores				
Result History	Vector     KNNClassification (k-NI     ExampleSet (Apple Set (Ap								
Data	Row No.	Play	prediction(Play)	confidence(no)	confidence(yes)	Outlook	Temperature	Humidity	Wind
	1	yes	yes	0.451	0.549	sunny	85	85	false
Σ	2	no	no	0.630	0.370	overcast	80	90	true
Statistics	3	yes	yes	0.190	0.810	overcast	83	78	false
	4	yes	no	0.544	0.456	rain	70	96	false
	5	yes	yes	0.394	0.606	rain	68	80	true
Visualizations	6	no	yes	0.250	0.750	rain	65	70	true
	7	yes	yes	0.218	0.782	overcast	64	65	true
	8	no	no	0.559	0.441	sunny	72	95	false
	9	yes	yes	0.212	0.788	sunny	69	70	false
Annotations	10	no	yes	0.213	0.787	sunny	75	80	false
	11	yes	yes	0.222	0.778	sunny	68	70	true
	12	yes	no	0.554	0.446	overcast	72	90	true
	13	no	yes	0.164	0.836	overcast	81	75	true
	14	yes	yes	0.250	0.750	rain	71	80	true

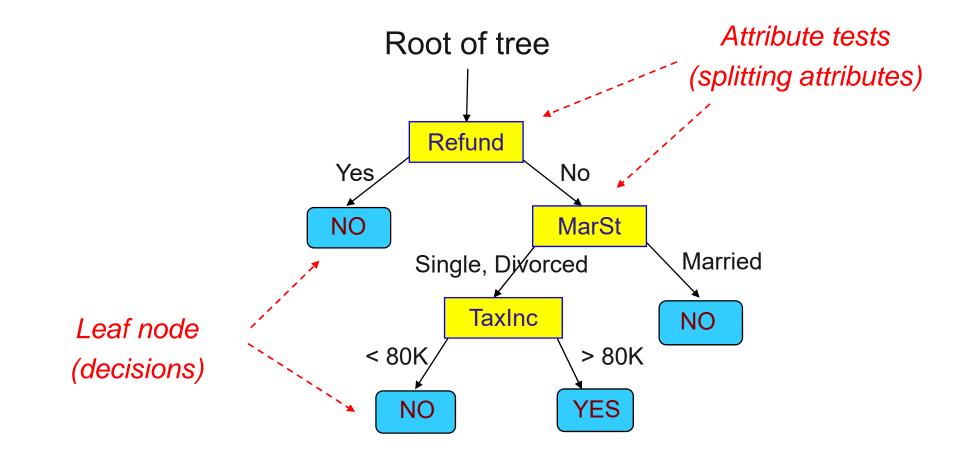
### Lazy Learning

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

### Eager Learning

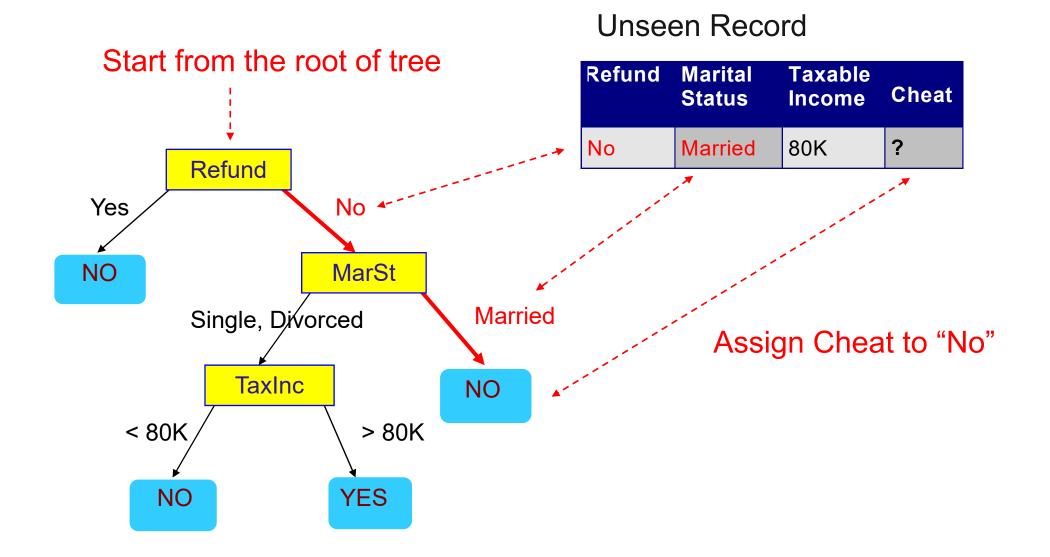
- but actually, we might have <u>two goals</u>
  - 1. classify unseen records
  - 2. understand the application domain as a human
- Eager learning approaches generate models that are (might be) interpretable by humans
- Examples of eager techniques: decision tree learning, rule learning

### 3. Decision Tree Classifiers

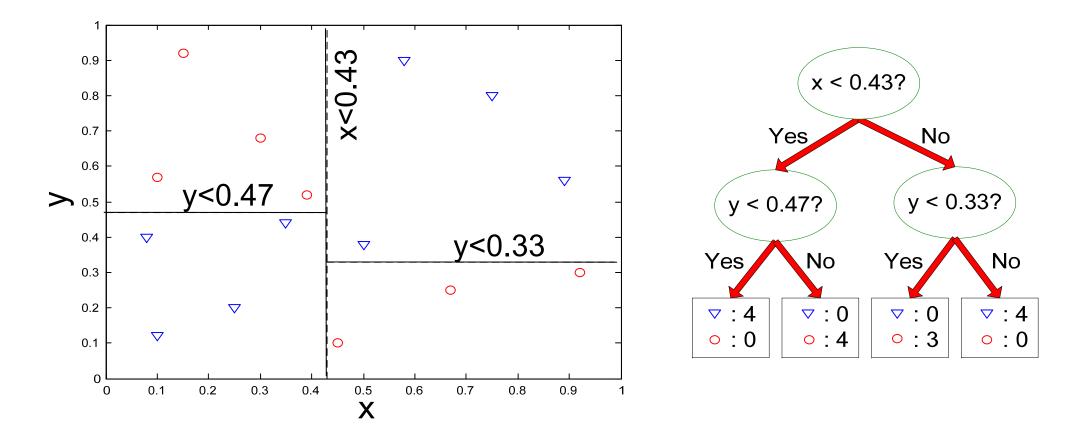


Decision trees encode a procedure for taking a classification decision

### **Applying a Decision Tree to Unseen Data**



### **Decision Boundary**

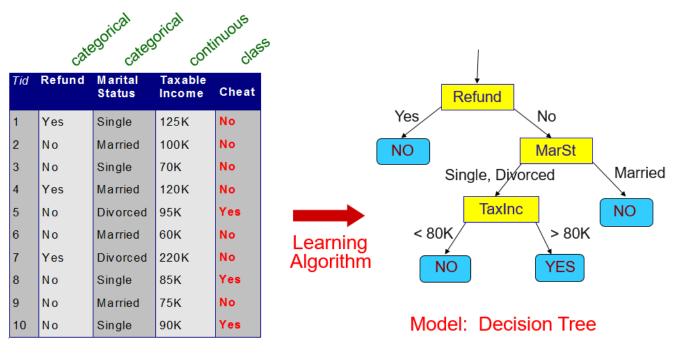


The decision boundaries are parallel to the axes because the test condition involves a single attribute at-a-time

### Learning a Decision Tree

#### – How to learn a decision tree from training data?

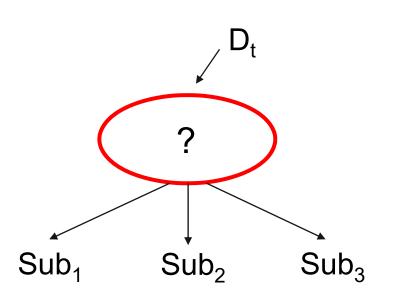
- finding an optimal decision tree is NP-hard
- tree building algorithms thus use a greedy, top-down, recursive partitioning strategy to induce a reasonable solution
- Many different algorithms have been proposed:
  - Hunt's Algorithm
  - ID3
  - C4.5
  - CHAID



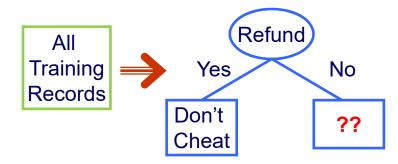
#### Training Data

# Hunt's Algorithm

- Let  $D_t$  be the set of training records that reach a node t
- Generate leaf node or attribute test:
  - if D<sub>t</sub> only contains records that belong to the same class y<sub>t</sub>, then t is a leaf node labeled as y<sub>t</sub>
  - if D<sub>t</sub> contains records that belong to more than one class, use an attribute test to split the data into subsets having a higher purity.
    - for all possible tests: calculate purity of the resulting subsets
    - choose test resulting in highest purity
- Recursively apply this procedure to each subset



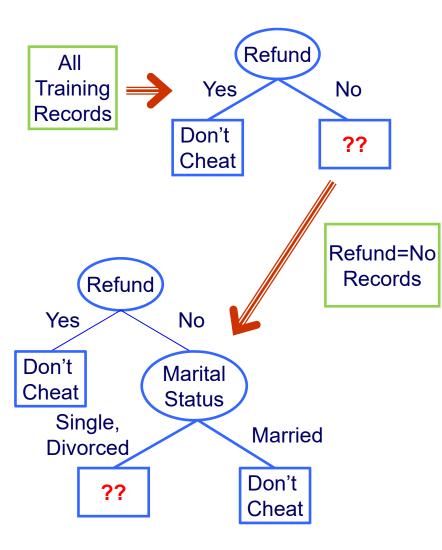
### Hunt's Algorithm – Step 1



- 1. We calculate the purity of the resulting subsets for all possible splits
  - Purity of split on Refund
  - Purity of split on Marital Status
  - Purity of split on Taxable Income
- 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

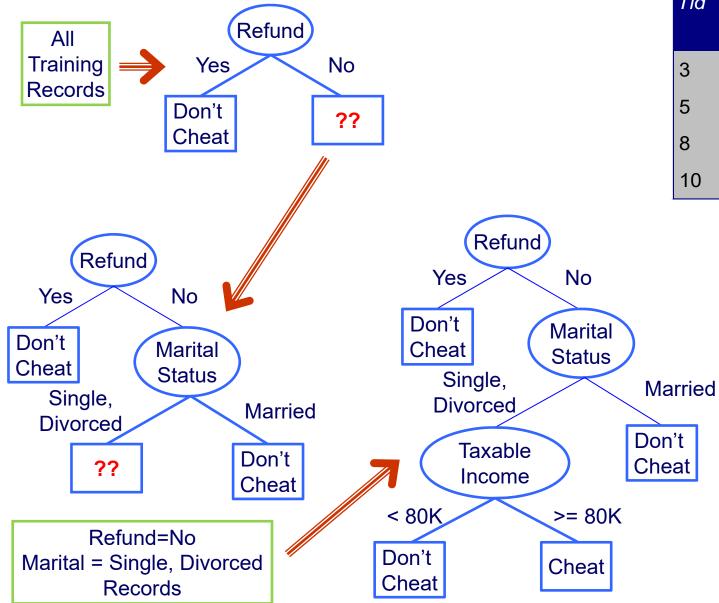
### Hunt's Algorithm – Step 2



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

- 1. 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 onTaxable Incometo produce pure subsets
- 3. We stop splitting as no sets containing different classes are left

#### 1. How should training records be split?

- How to specify the attribute test condition?
  - Depends on number of ways to split: 2-way split, multi-way split
  - Depends on attribute data type: nominal, ordinal, continuous
- How to determine the best split?
  - Different purity measures can be used

#### 2. When should the splitting procedure stop?

- Shallow trees might generalize better to unseen records
- Fully grown trees might overfit training data

### **Splitting Based on Nominal Attributes**

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

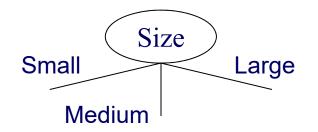


- Binary split: Divides values into two subsets



### **Splitting Based on Ordinal Attributes**

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

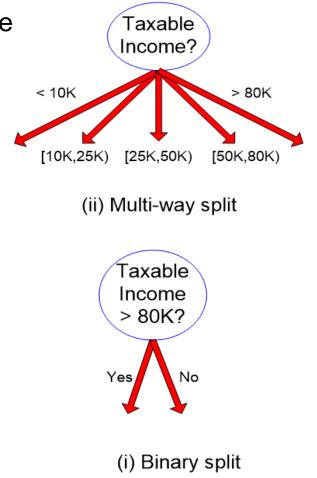


 Binary split: Divides values into two subsets while keeping the order



### **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  $(A \ge v)$ 
    - 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

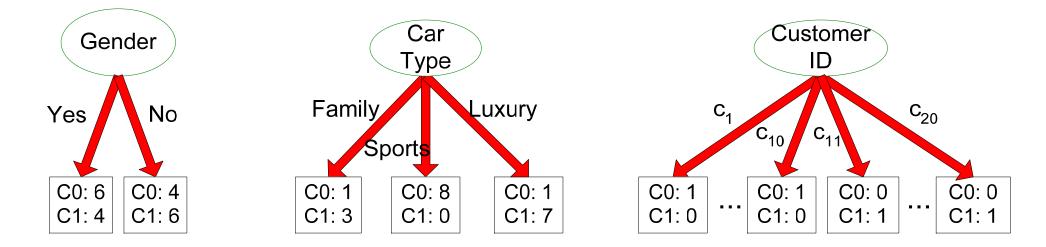
### **3.2 How to Find the Best Split?**

Before splitting the dataset contains:

- 10 records of class C0 and
- 10 records of class C1

#### Which attribute test is the best?

Customer Id	Gender	Car Type	Shirt Size	Class
1	Μ	Family	Small	C0
2	Μ	Sports	Medium	C0
3	Μ	Sports	Medium	C0
4	Μ	Sports	Large	C0
5	Μ	Sports	Extra Large	C0
6	Μ	Sports	Extra Large	C0
7	$\mathbf{F}$	Sports	Small	C0
8	$\mathbf{F}$	Sports	Small	C0
9	$\mathbf{F}$	Sports	Medium	C0
10	$\mathbf{F}$	Luxury	Large	C0
11	Μ	Family	Large	C1
12	Μ	Family	Extra Large	C1
13	Μ	Family	Medium	C1
14	Μ	Luxury	Extra Large	C1
15	$\mathbf{F}$	Luxury	Small	C1
16	$\mathbf{F}$	Luxury	Small	C1
17	$\mathbf{F}$	Luxury	Medium	C1
18	$\mathbf{F}$	Luxury	Medium	C1
19	$\mathbf{F}$	Luxury	Medium	C1
20	$\mathbf{F}$	Luxury	Large	C1



### 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 node impurity C0: 9 C1: 1

Homogeneous Low degree of node impurity

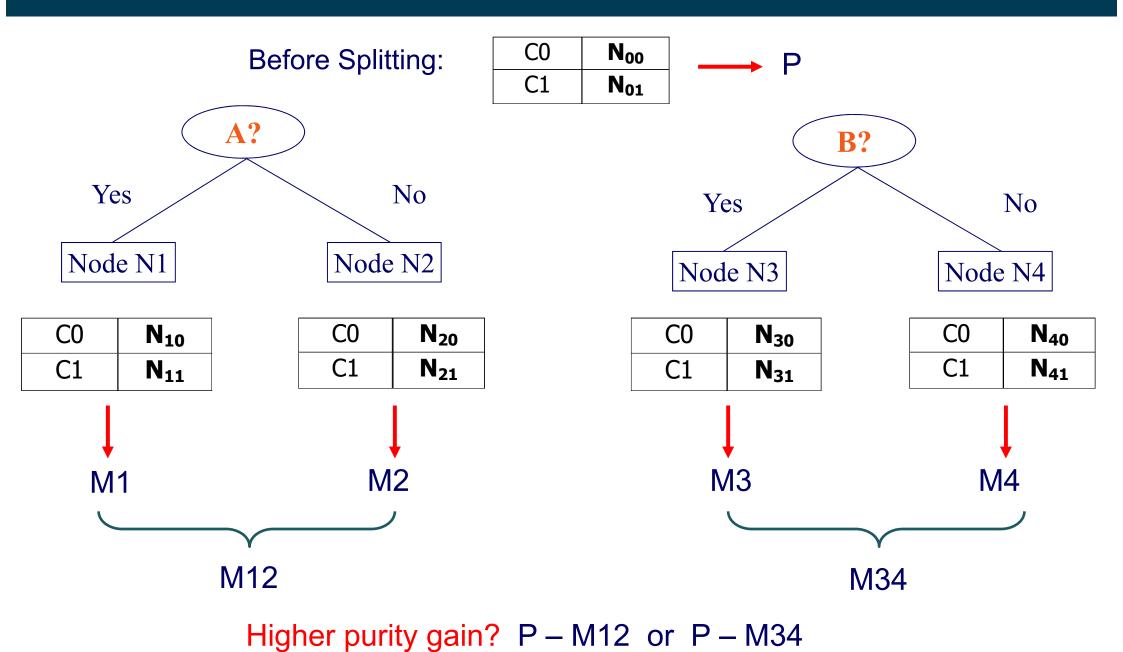
- Common measures of node impurity:
  - 1. GINI Index
  - 2. Entropy

- 1. Compute impurity measure (P) before splitting
- 2. Compute impurity measure (M) after splitting for all possible splits
  - compute impurity measure of each child node
  - M is the weighted impurity of children
- 3. Choose the attribute test condition (split) that produces the highest purity gain

$$Gain = P - M$$

or equivalently, lowest impurity measure after splitting (M)

### **Comparing Two Splits by Purity Gain**



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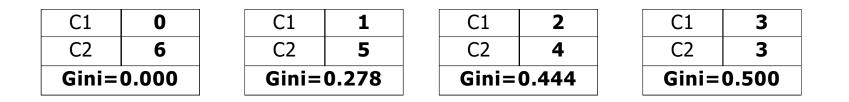
#### **3.2.1 Impurity Measure: GINI Index**

– GINI Index for a given node t :

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

p(j | 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



#### **Examples for computing GINI**

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

C1	0
C2	6

P(C1) = 0/6 = 0 P(C2) = 6/6 = 1Gini = 1 -  $P(C1)^2 - P(C2)^2 = 1 - 0 - 1 = 0$ 

C1	1
C2	5

P(C1) = 1/6 P(C2) = 5/6Gini = 1 - (1/6)<sup>2</sup> - (5/6)<sup>2</sup> = 0.278

C1	2
C2	4

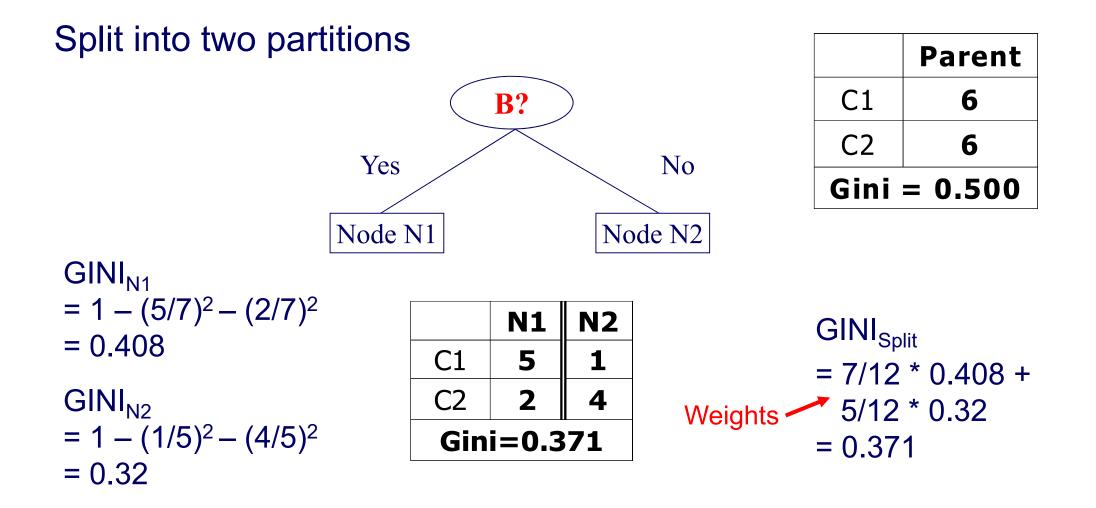
P(C1) = 2/6 P(C2) = 4/6Gini = 1 - (2/6)<sup>2</sup> - (4/6)<sup>2</sup> = 0.444

- When a node p is split into k partitions (subsets), 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 Split**



**Purity Gain** = 0.5 – 0.371 = 0.129

For each distinct attribute value, gather counts for each class

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

Multi-way split

#### Two-way split (find best partition of values)

	CarT	уре		CarType				
	{Sports, Luxury}	{Family}		{Sports}	{Family, Luxury}			
C1	3	1	C1	2	2			
C2	2	4	C2	1	5			
Gini	0.4	00	Gini	0.4	19			

### **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

		Taxable Income																					
Sorted Values		(	60		70	)	7	5	85	5	9(	)	9	5	10	00	12	20	12	25		220	
Split Positions		5	5	6	5	7	2	8	0	8	7	9	2	9	7	11	0	12	22	17	2	23	0
	F	<=	>	<=	>	<=	>	<=	>	<=	>	<=	>	<=	>	<=	>	<=	>	<=	>	<=	>
	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	20	0.4	00	0.3	575	0.3	343	0.4	17	0.4	00	<u>0.3</u>	<u>800</u>	0.3	43	0.3	575	0.4	00	0.4	120



#### **3.2.2 Alternative Impurity Measure: Information Gain**

- 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 | 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<sub>2</sub> n<sub>c</sub>) 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	$_{2}0 - 1 \log_{2} 1 = -0 - 0 = 0$

C1	1
C2	5

P(C1) = 1/6 P(C2) = 5/6Entropy = - (1/6)  $\log_2 (1/6) - (5/6) \log_2 (5/6) = 0.65$ 

C1	2
C2	4

P(C1) = 2/6 P(C2) = 4/6Entropy = - (2/6)  $\log_2 (2/6) - (4/6) \log_2 (4/6) = 0.92$  – 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 <sub>split</sub> = 
$$\frac{GAIN_{split}}{SplitINFO}$$
 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

- We want to learn models that are good at classifying unseen records
- Overfitting: Learned models can fit the training data too closely and thus work poorly on unseen data
- Model perfectly fitting the training data:

"Trees are big, green plants that have a trunk and no wheels"

- Unseen example:





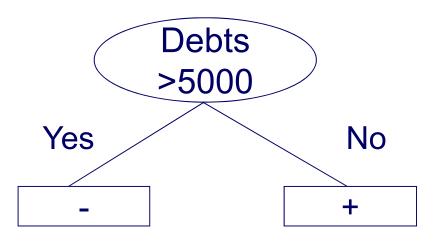




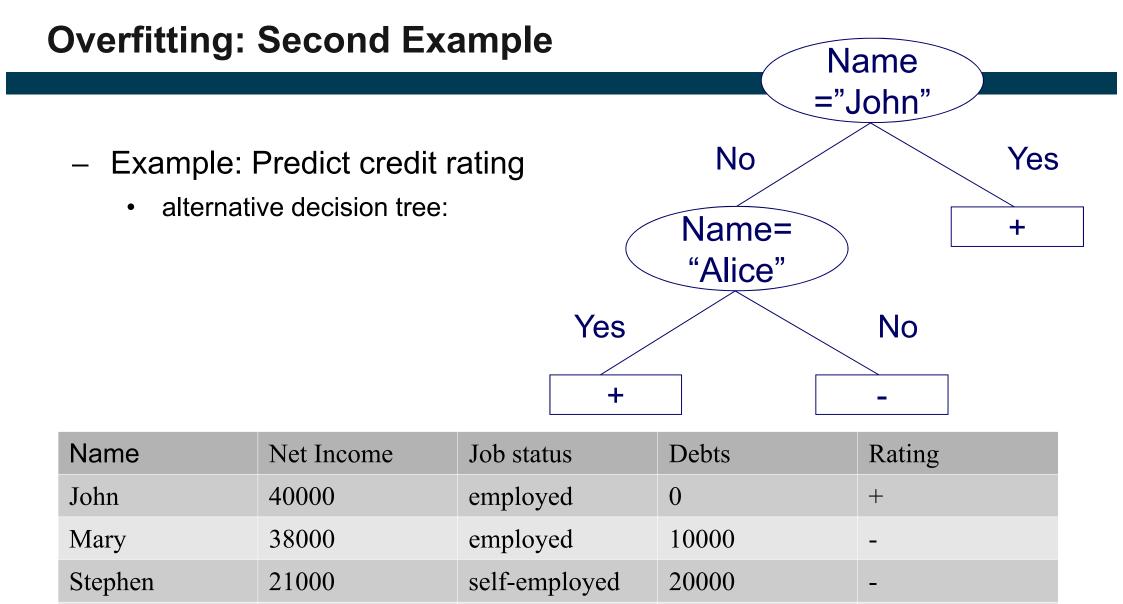
 Goal: Find good compromise between specificness and generality of the learned model

#### **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	+



student

employed

10000

4000

2000

35000

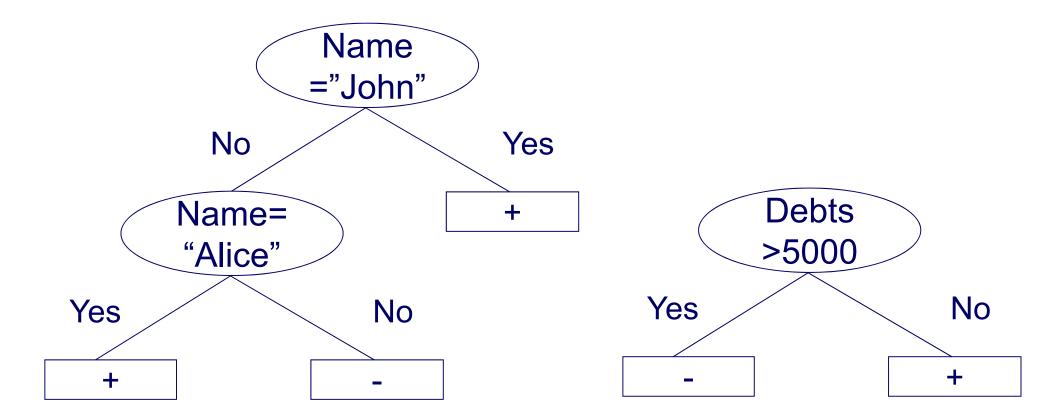
Eric

Alice

+

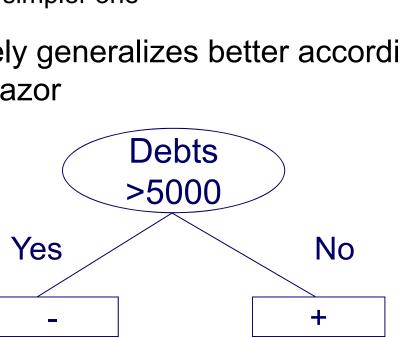
#### **Overfitting: Second Example**

- 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
- Tree that likely generalizes better according to Occam's razor



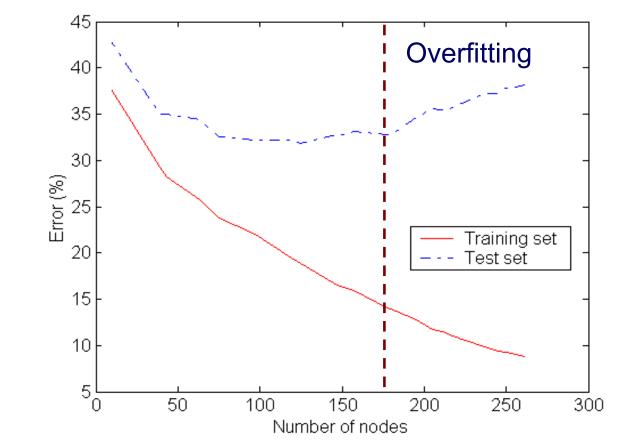


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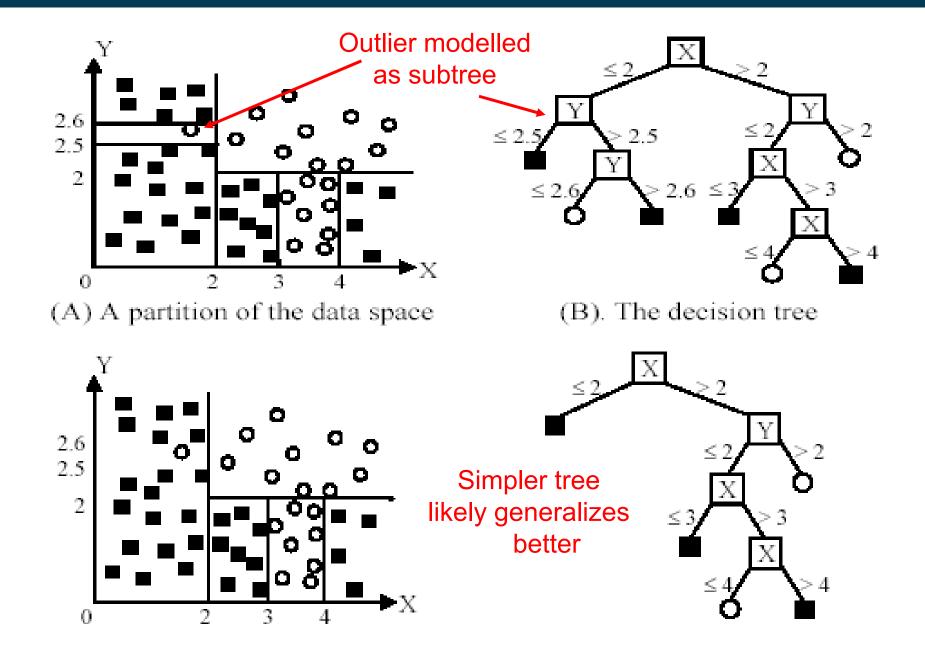
#### **Overfitting: Symptoms and Causes**

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

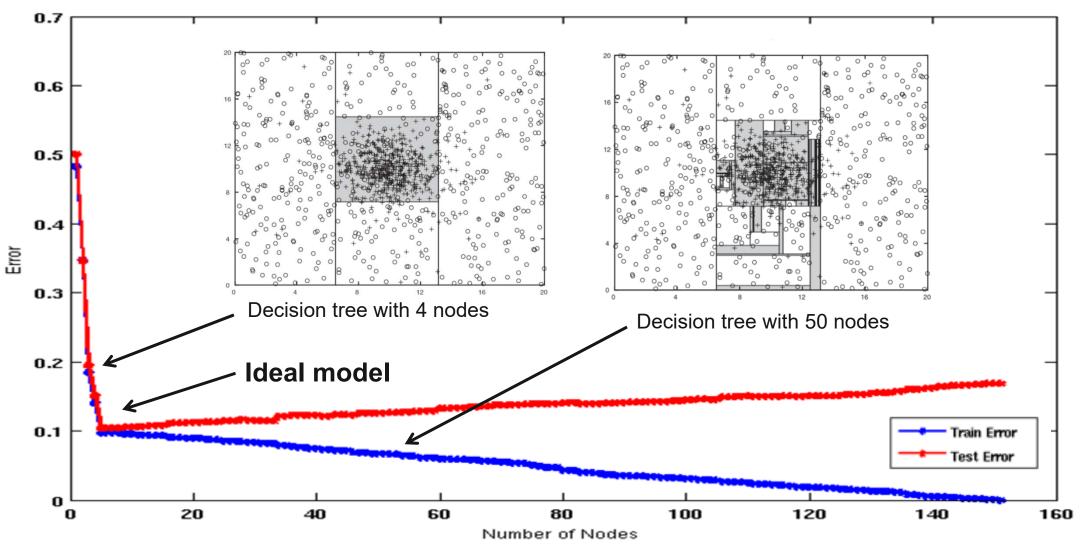
An overfitted model does not generalize well to unseen data.



#### **Example of an Outlier causing Overfitting**

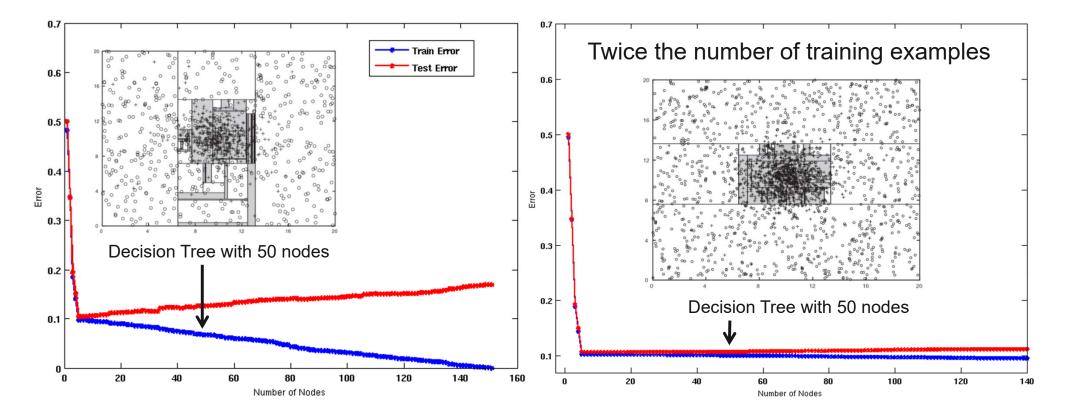


#### **Underfitting versus Overfitting**



**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 Prevent Overfitting 1: Use More Training Data



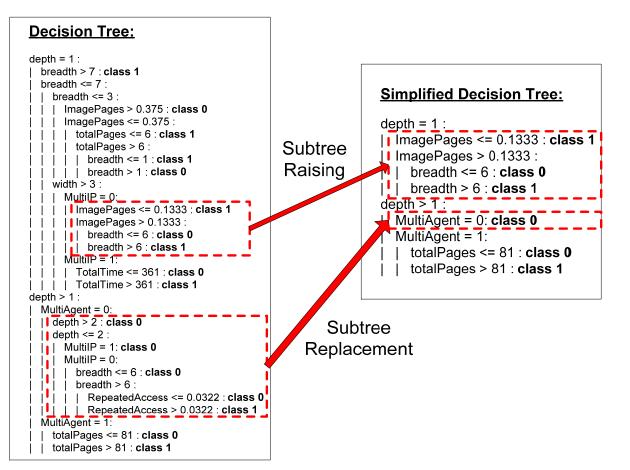
- If training data is under-representative, training errors decrease but testing errors increase on increasing number of nodes
- Increasing the size of training set reduces the difference between training and testing errors at a given number of nodes

#### **How to Prevent Overfitting 2: Pre-Pruning**

- Stop the algorithm before tree becomes fully-grown
  - shallower tree potentially generalizes better (Occam's razor)
- 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)

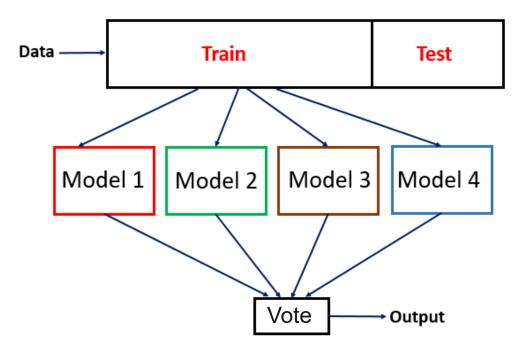
## **How to Prevent Overfitting 3: Post-Pruning**

- 1. Grow decision tree to its entirety
- 2. Trim the nodes of the decision tree in a bottom-up fashion
- 3. Estimate generalization error before and after trimming
  - using a validation set
- 4. If generalization error improves after trimming
  - replace sub-tree by a leaf node or
  - replace subtree by most frequently used branch



#### **How to Prevent Overfitting 4: Ensembles**

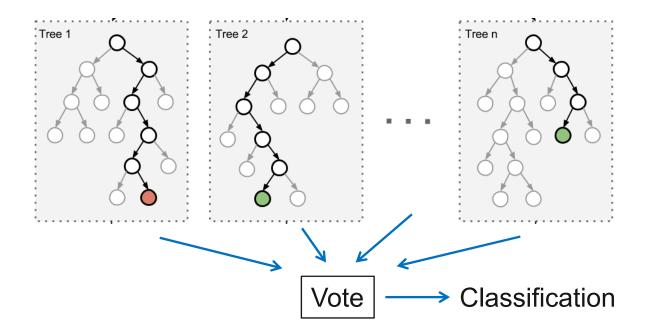
- Lean different models (base learners)
- Have them vote on the final classification decision



- Idea: Wisdom of the crowds applied to classification
  - A single classifier might focus too much on one aspect
  - Multiple classifiers can focus on different aspects

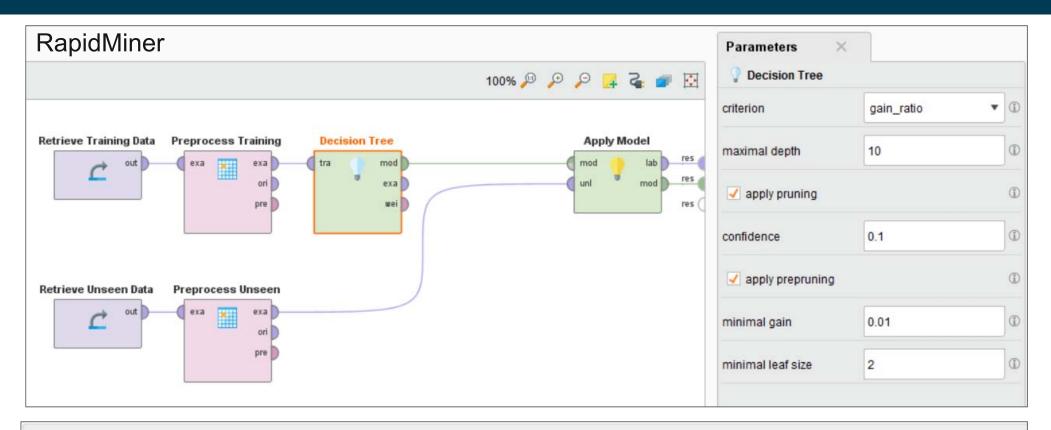
#### **Random Forest**

Ensemble consisting of a large number of different decision trees



- Independence of trees achieved by introducing randomness into the learning process
  - only use an random subset of the attributes at each split
  - learn on different random subsets of the data (bagging)
- Random forests usually outperform single decision trees

# **Decision Tree Classification in RapidMiner and Python**



#### Python

from sklearn.tree import DecisionTreeClassifier

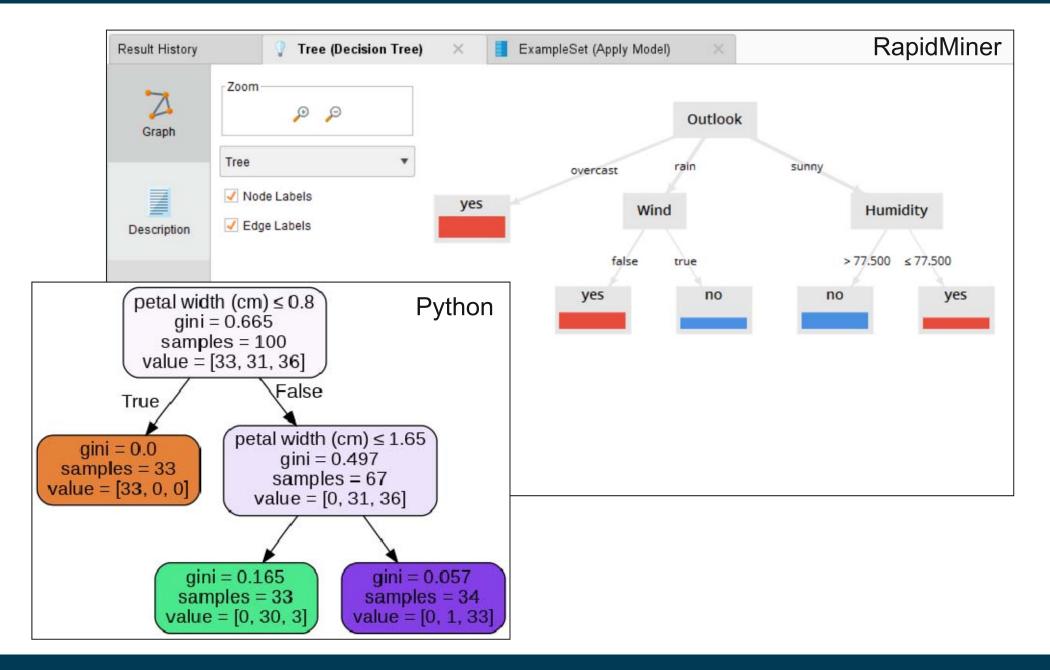
#### # Train classifier

```
dt_learner = DecisionTreeClassifier(criterion='gini', max_depth=10)
dt_learner.fit(preprocessed_training_data, training_labels)
```

#### # Use classifier to predict labels

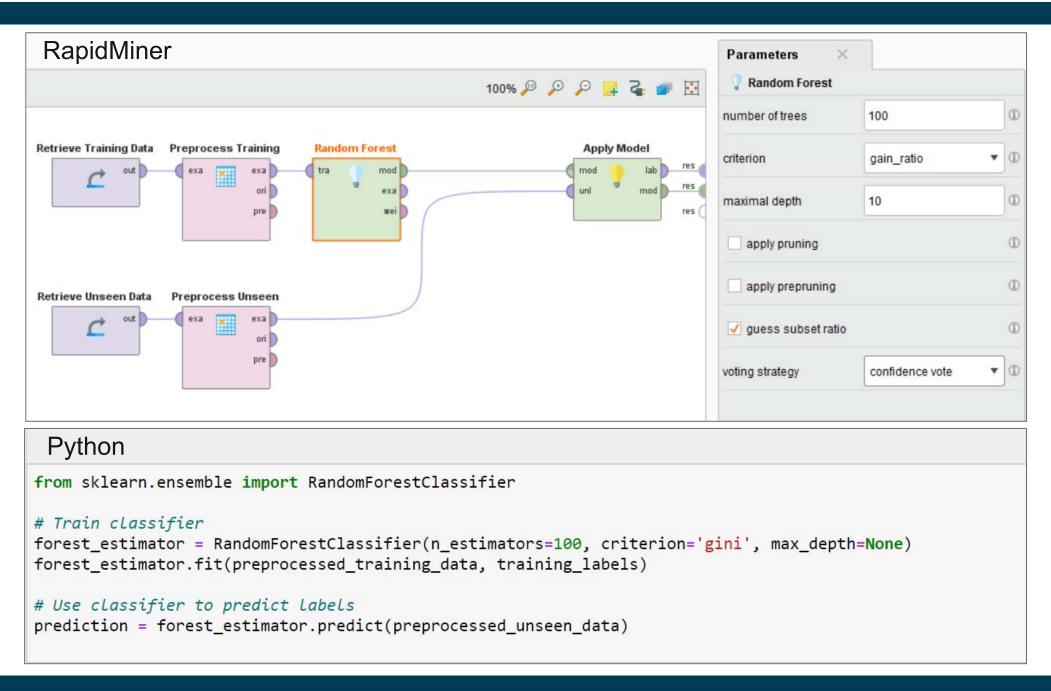
prediction = dt\_learner.predict(preprocessed\_unseen\_data)

#### **Examples of Learned Decision Trees**



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#### **Random Forests in RapidMiner and Python**



#### - 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 (not texts and images)

#### Disadvantages

- Space of possible decision trees is exponentially large. Greedy approaches are often unable to find the best tree
- Trees do not take into account interactions between attributes

Pang-Ning Tan, Michael Steinbach, Anuj Karpatne, Vipin Kumar: Introduction to Data Mining. 2nd Edition. Pearson.

**Chapter 3: Classification** 

**Chapter 6.3: Nearest Neighbor Classifiers** 

**Chapter 3.3: Decision Tree Classifier** 

Chapter 3.4: Overfitting

**Chapter 6.10.6: Random Forests** 

