



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)

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 and no wheels."

Goal: Classification of unseen instances















Tree?

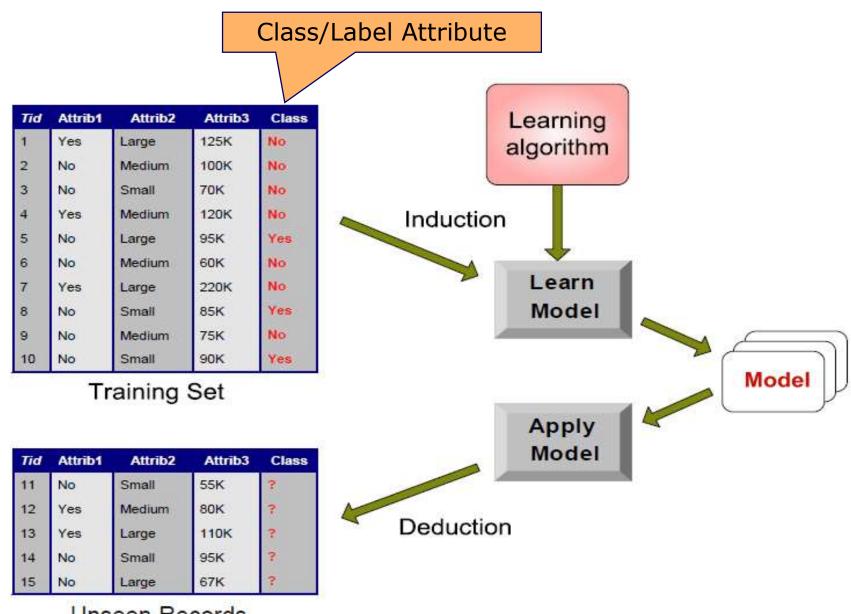
Tree?

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 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?

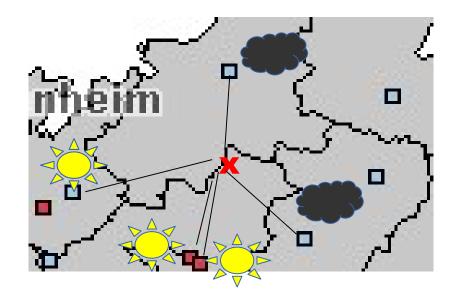






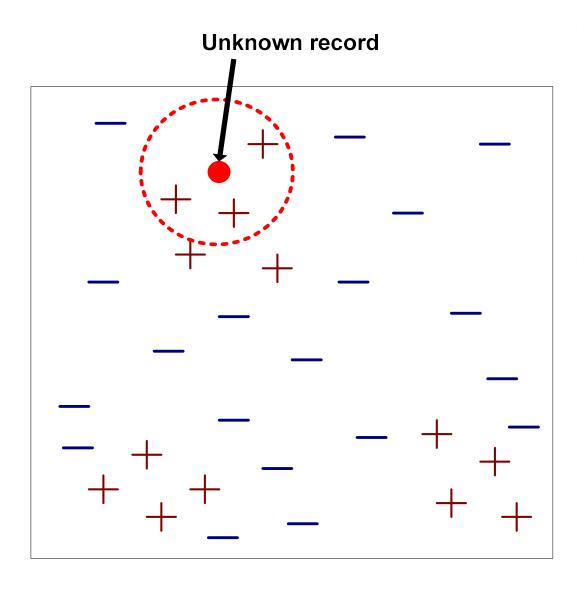
Basic Idea

- 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

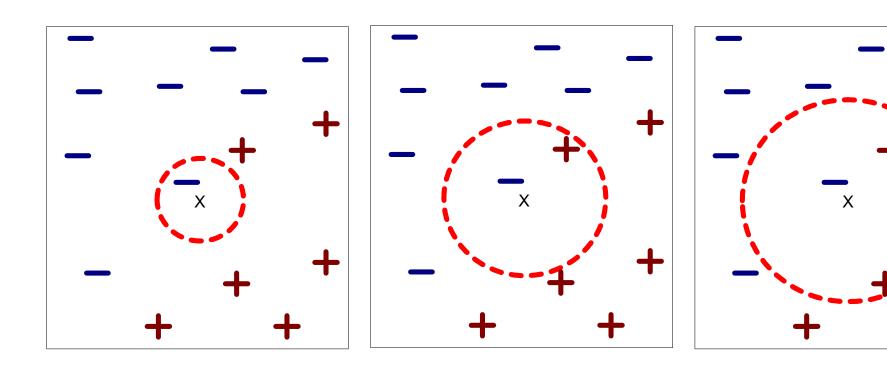


Require three things

- 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
 - 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

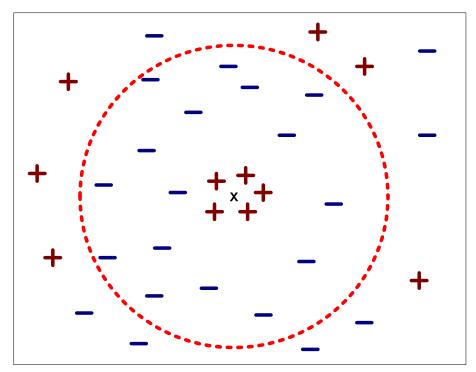
The k-nearest neighbors of a record x are data points that have the k smallest distances to x



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

Choosing a Good Value for K

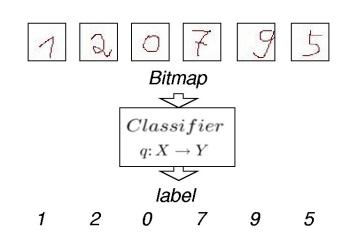
- If k is too small, the result is sensitive to noise points
- If k is too large, the neighborhood may include points from other classes



- Rule of thumb: Test k values between 1 and 20
 - setup: see section on Hyperparameter Selection

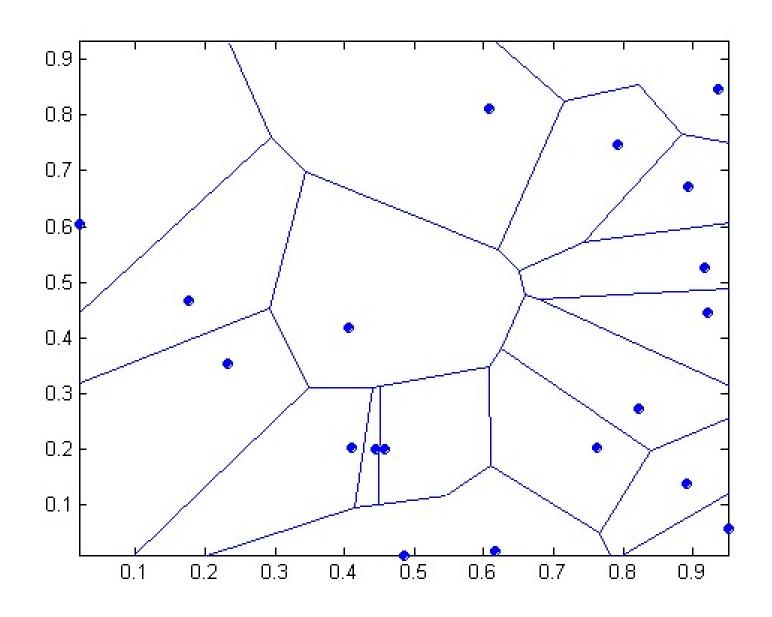
Discussion of K-Nearest-Neighbor Classification

- Often very accurate
 - for instance for optical character recognition (OCR)
- ... but slow
 - as unseen record needs to be compared to all training examples

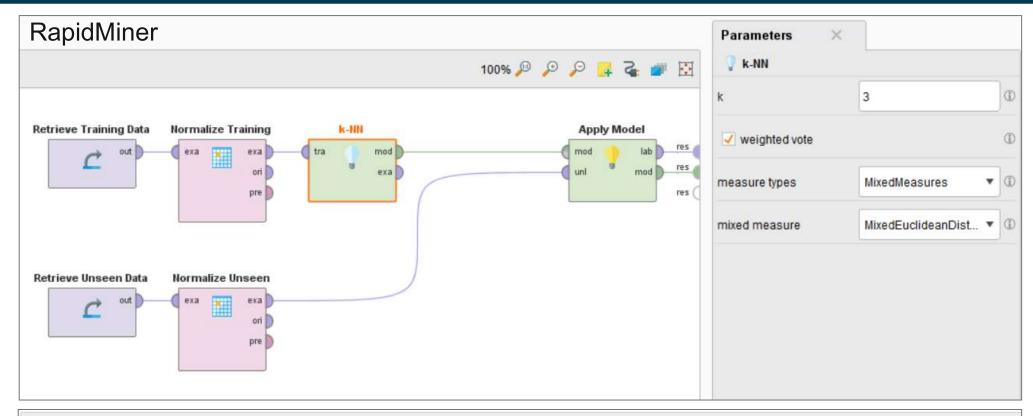


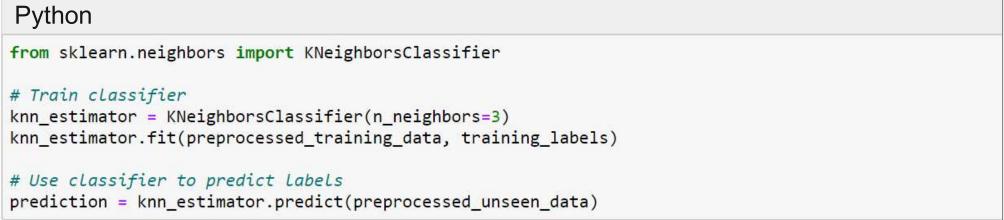
- Results depend on choosing a good proximity measure
 - attribute weights, asymmetric binary attributes, ...
 - see slide set Cluster Analysis
- KNN can handle decision boundaries which are not parallel to the axes (unlike decision trees)

Decision Boundaries of a 1-NN Classifier

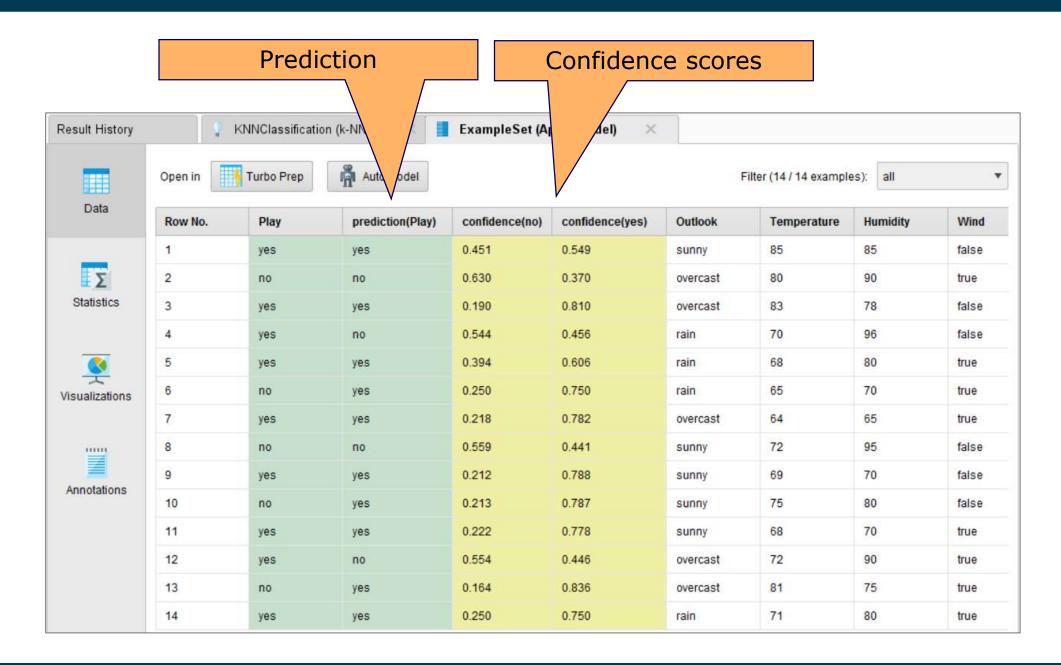


KNN Classification in RapidMiner and Python





Resulting Dataset



Lazy versus Eager Learning

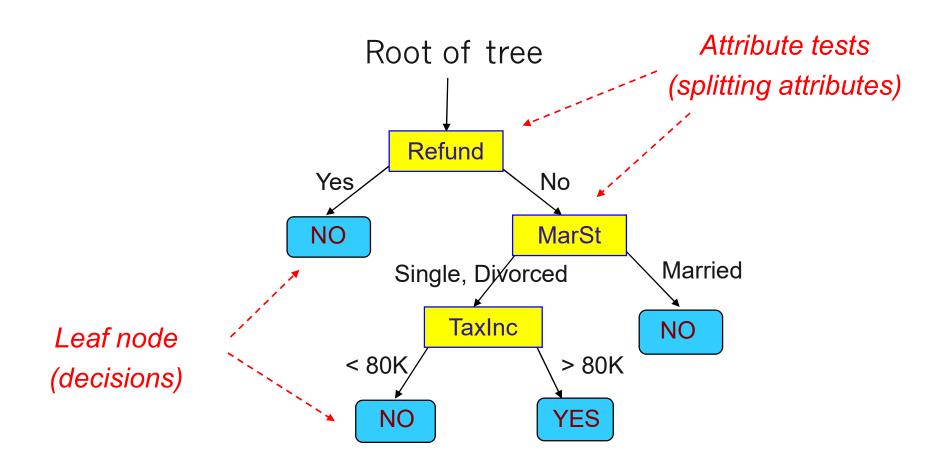
Lazy Learning

- 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

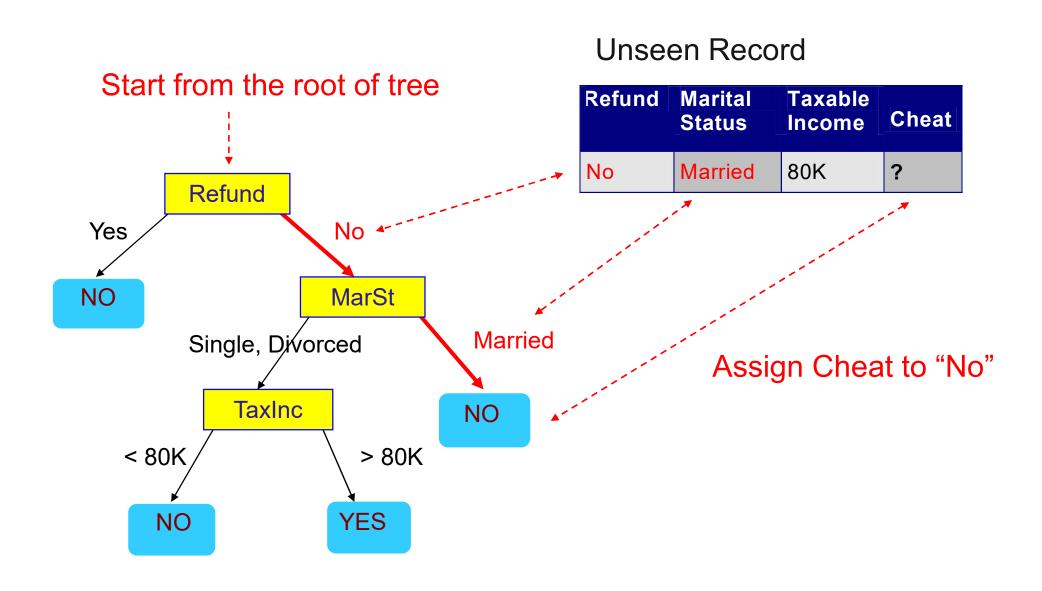
- but actually, we might have two goals
 - 1. classify unseen records
 - 2. understand the application domain as a human
- Eager learning approaches generate models that are (might be) interpretable by humans
- Examples of eager techniques: decision tree learning, rule learning

3. Decision Tree Classifiers

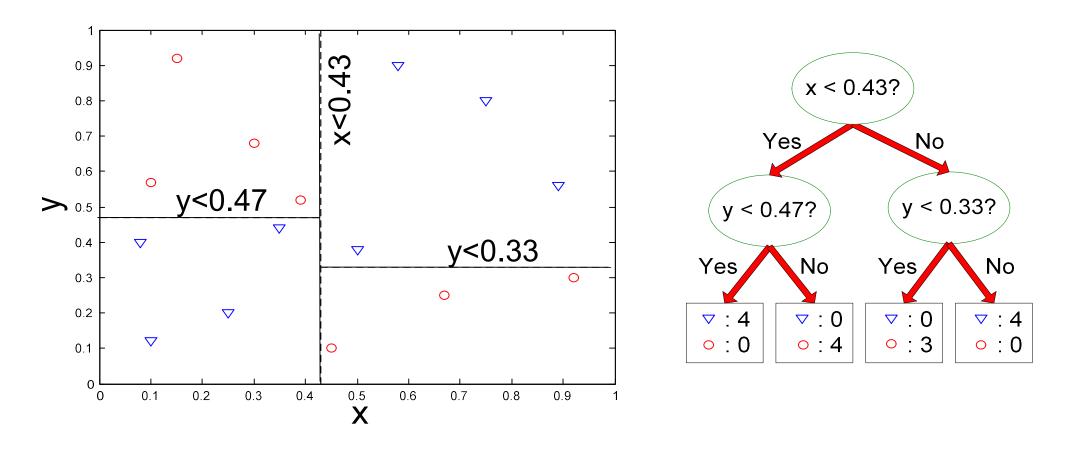


Decision trees encode a procedure for taking a classification decision

Applying a Decision Tree to Unseen Data



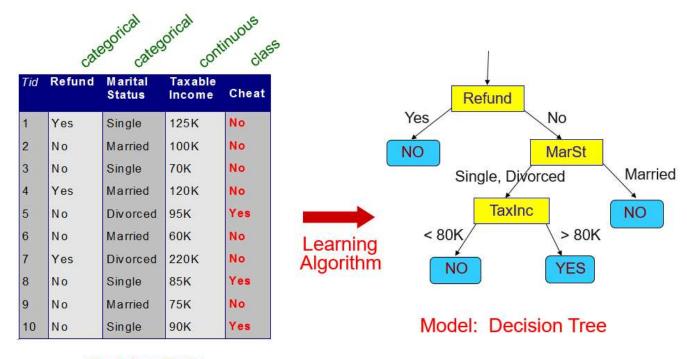
Decision Boundary



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

Learning a Decision Tree

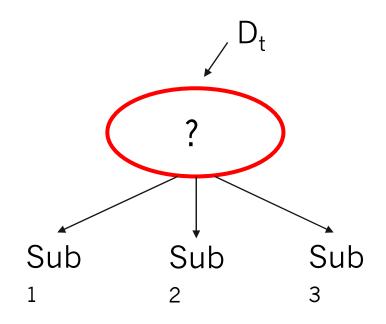
- How to learn a decision tree from training data?
 - finding an optimal decision tree is NP-hard
 - tree building algorithms thus use a greedy, top-down, recursive partitioning strategy to induce a reasonable solution
- Many different algorithms have been proposed:
 - Hunt's Algorithm
 - ID3
 - C4.5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



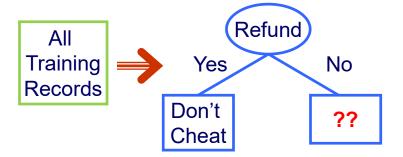
Training Data

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_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.
 - for all possible tests: calculate purity of the resulting subsets
 - choose test resulting in highest purity
- Recursively apply this procedure to each subset



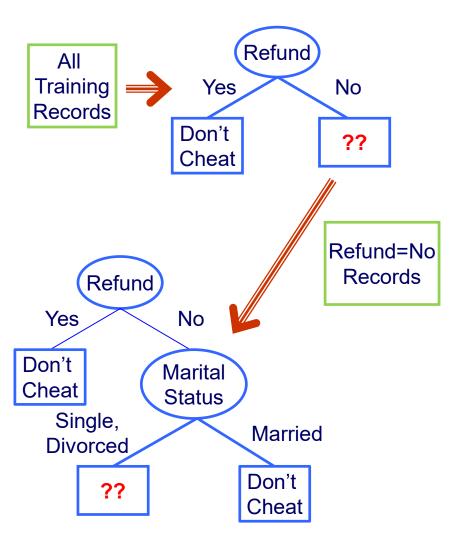
Hunt's Algorithm – Step 1



- 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	

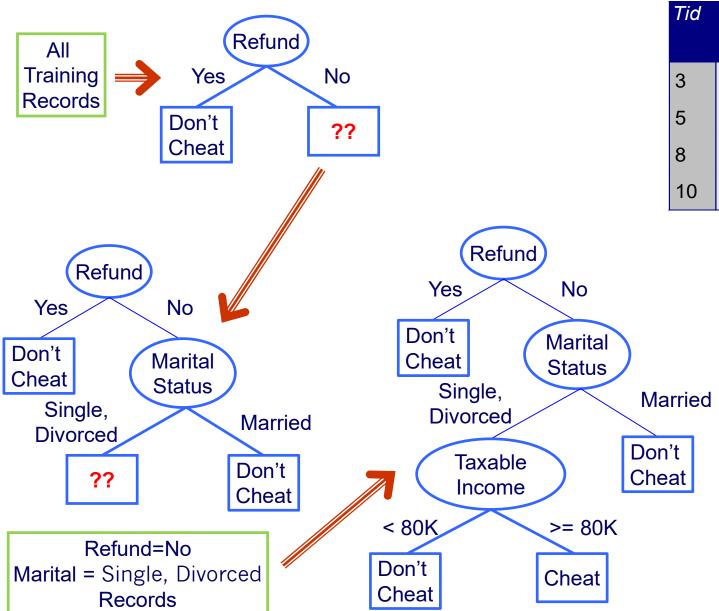
Hunt's Algorithm – Step 2



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 on
 Taxable Income
 to produce pure subsets
- 3. We stop splitting as no sets containing different classes are left

Design Issues for Learning Decision Trees

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

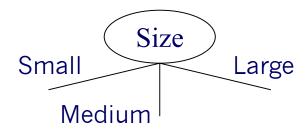


Binary split: Divides values into two subsets



Splitting Based on Ordinal Attributes

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

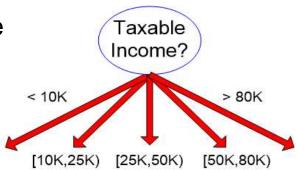


 Binary split: Divides values into two subsets while keeping the order



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 ≥ v)
 - usually sufficient in practice
 - find the best splitting border v based on a purity measure (see below)
 - can be compute intensive



(ii) Multi-way split



(i) Binary split

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

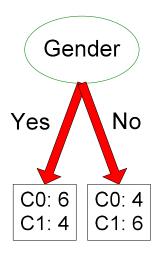
- [-, 14) bin
- Bin 2: 16, 16, 18
- [14, 21) bin
- Bin 3: 24, 26, 28
- [21,+] bin

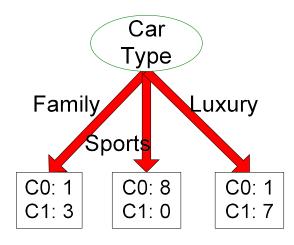
3.2 How to Find the Best Split?

Before splitting the dataset contains:

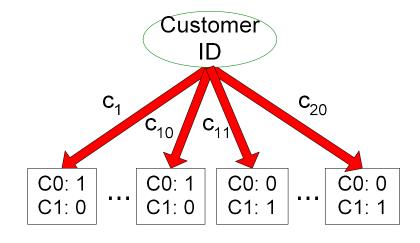
- 10 records of class C0 and
- 10 records of class C1

Which attribute test is the best?





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

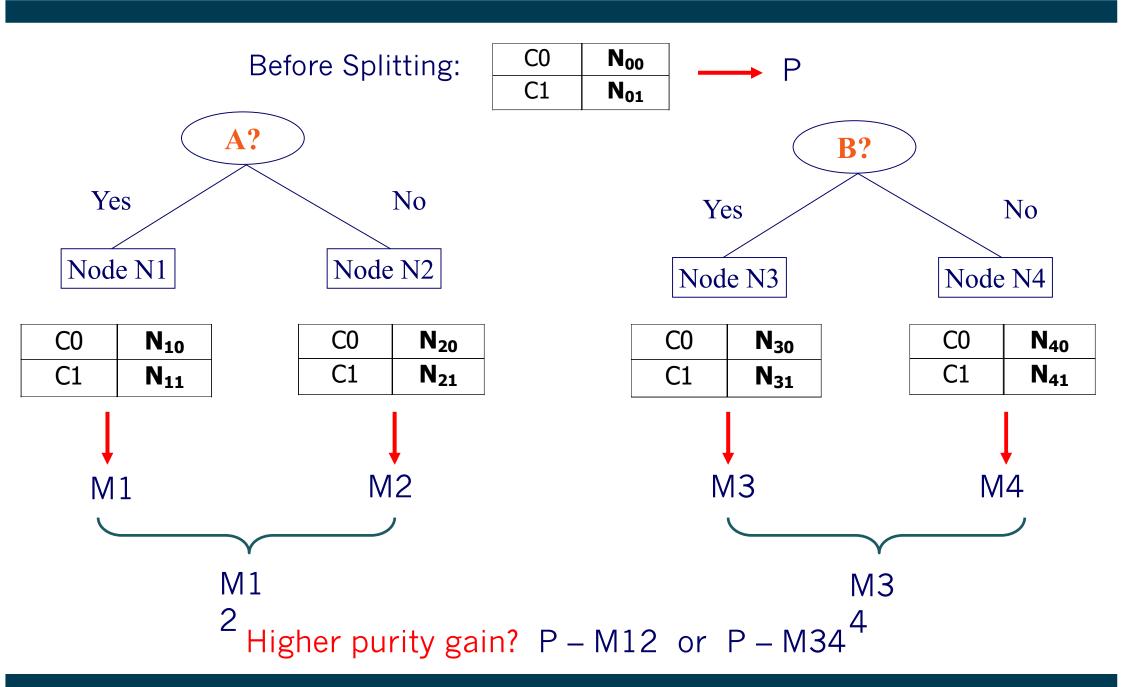
How to Find the Best Split?

- 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



3.2.1 Impurity Measure: GINI Index

GINI Index for a given node t :

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

 $p(j \mid t)$ 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

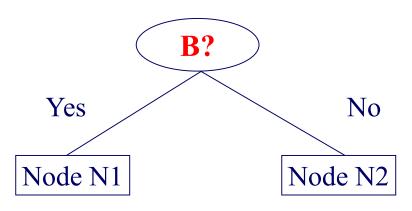
- When a node p is split into k partitions (subsets),
 the GINI index of each partition is weighted according to the partition's size
- The quality of the overall split is computed as:

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

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

Example: Calculating the Purity Gain of a Split

Split into two partitions



	Parent
C1	6
C2	6
Gini	= 0.500

$$GINI_{N1}$$

= 1 - (5/7)² - (2/7)²
= 0.408

$$GINI_{N2} = 1 - (1/5)^2 - (4/5)^2$$

	N1	N2					
C1	5	1					
C2	2	4					
Gini=0.371							

$$GINI_{Split}$$
= 7/12 * 0.408 + Weights 5/12 * 0.32 = 0.371

 \overline{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	0.400								

	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



0 1 1 1 1 1			Taxable Income																				
Sorted Values			60		70		7	5	85	5	90		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	72	23	0
		<=	>	<=	>	<=	>	\=	>	<=	>	<=	>	<=	>	<=	>	"	>	<=	>	<=	>
	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	75	0.3	343	0.4	17	0.4	00	<u>0.3</u>	<u>800</u>	0.3	43	0.3	75	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:

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

 $p(j \mid t)$ 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 (log₂ n_c) when records are equally distributed among all classes

Examples for Computing Entropy

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

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

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

- 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:



Training data









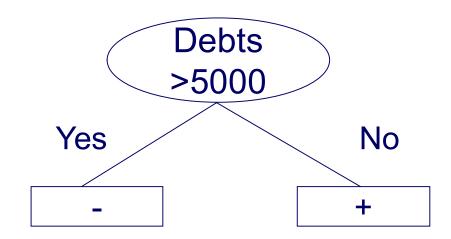




 Goal: Find good compromise between specificness and generality of the learned model

Overfitting: Second Example

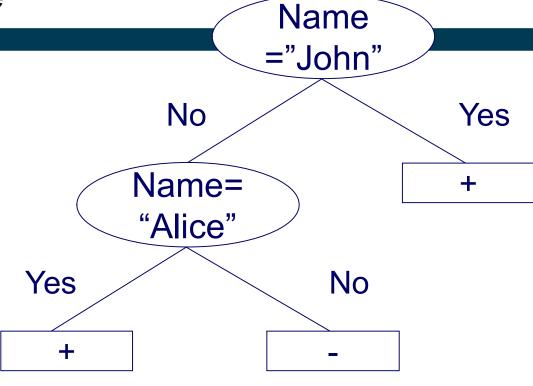
- Example: Predict credit rating
 - possible decision tree:



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	+

Overfitting: Second Example

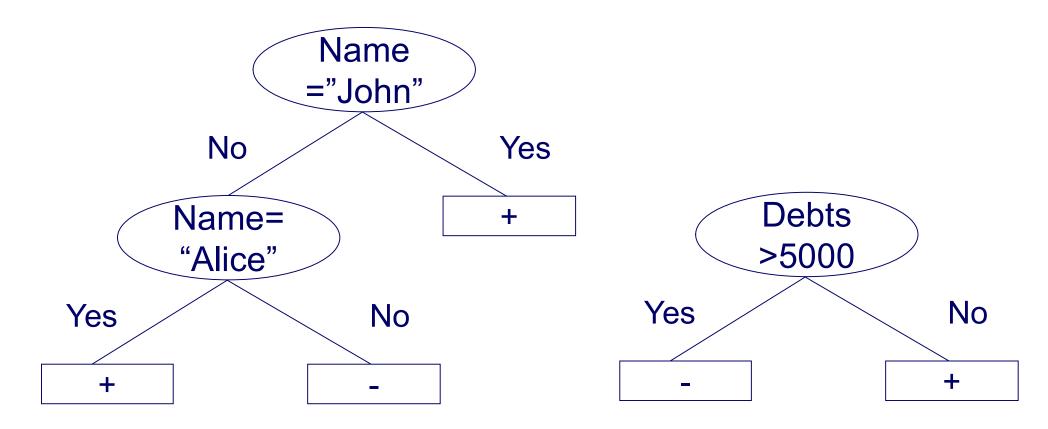
- Example: Predict credit rating
 - alternative decision tree:



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	+

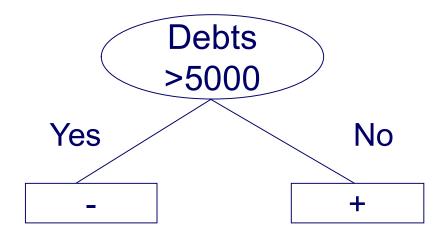
Overfitting: Second Example

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



Occam's Razor

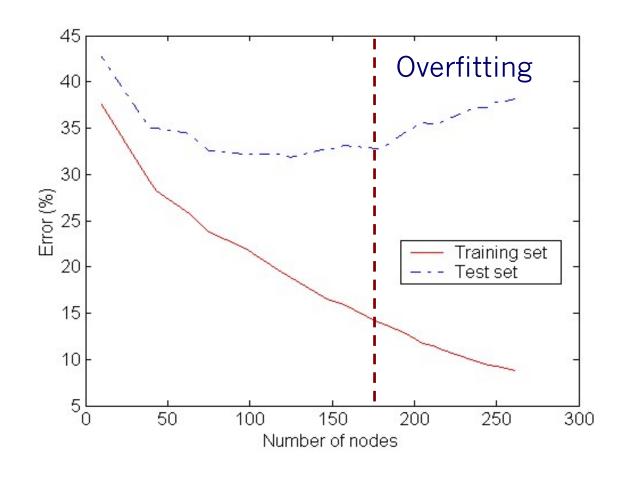
- Named after William of Ockham (1287-1347)
- A fundamental principle of science
 - if you have two theories
 - that explain a phenomenon equally well
 - choose the simpler one
- Tree that likely generalizes better according to Occam's razor





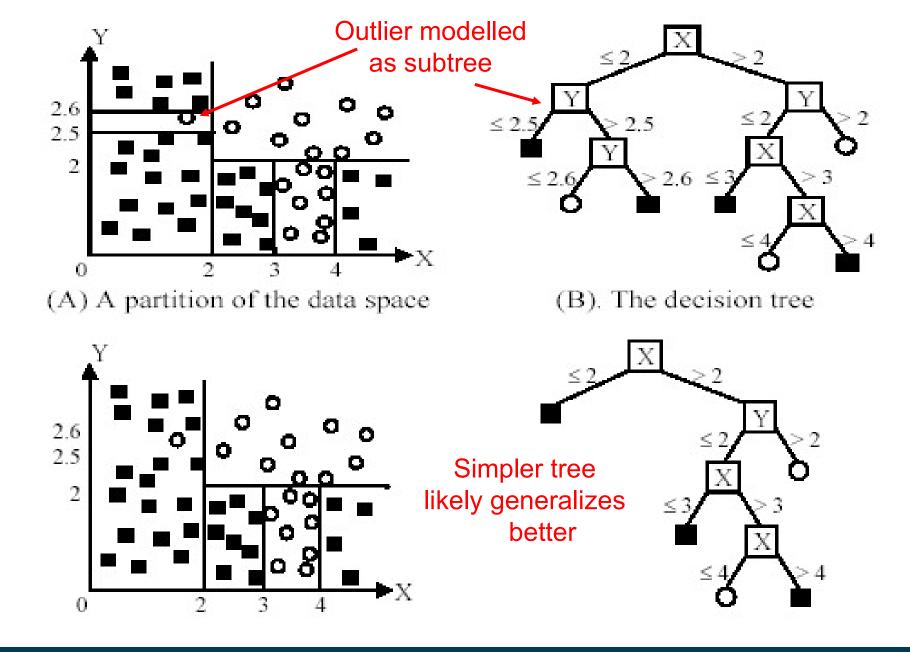
Overfitting: Symptoms and Causes

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

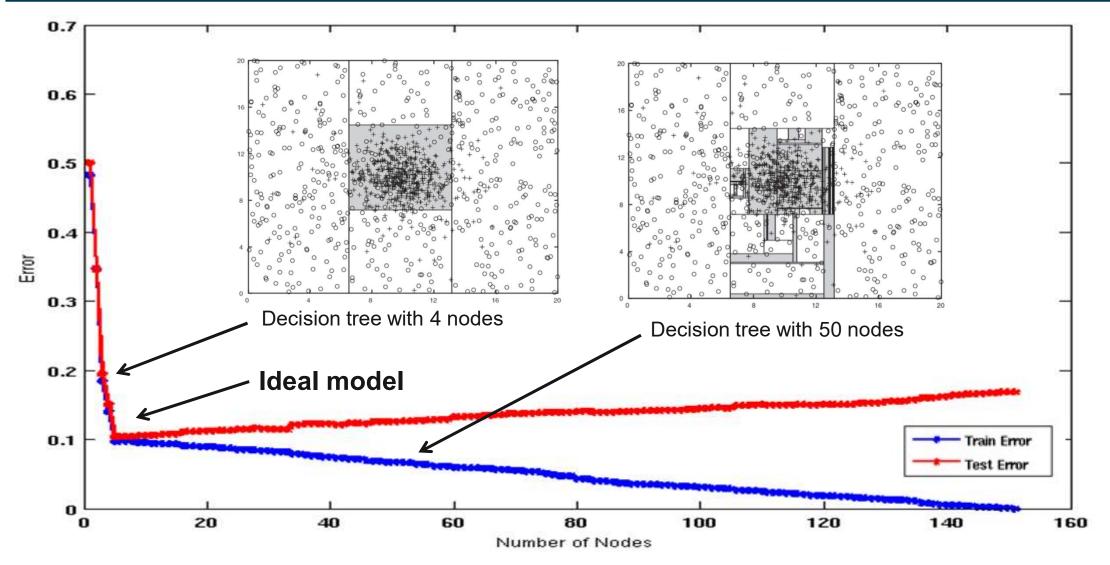


An overfitted model does not generalize well to unseen data.

Example of an Outlier causing Overfitting

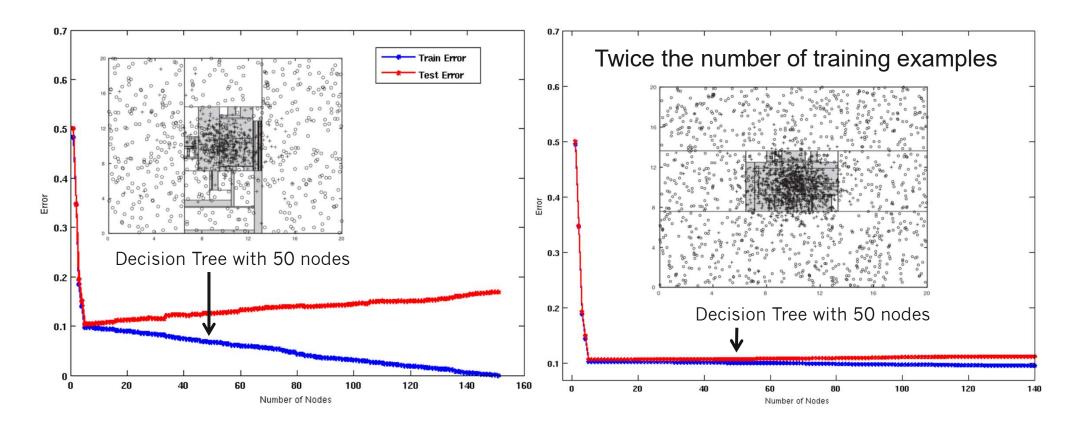


Underfitting versus Overfitting



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



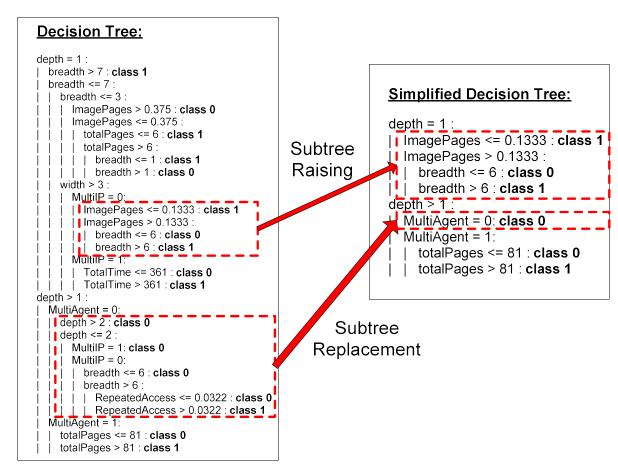
- If training data is under-representative, training errors decrease but testing errors increase on increasing number of nodes
- Increasing the size of training set reduces the difference between training and testing errors at a given number of nodes

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)

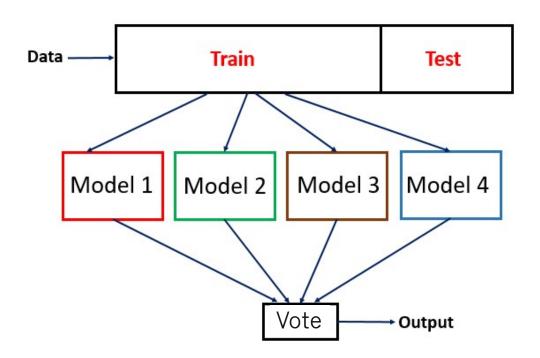
How to Prevent Overfitting 3: Post-Pruning

- 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
- 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

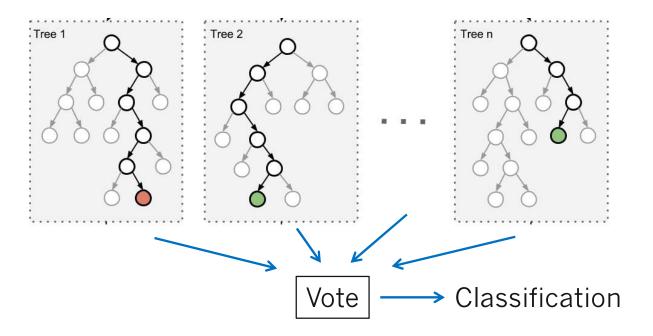
- Lean different models (base learners)
- Have them vote on the final classification decision



- 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

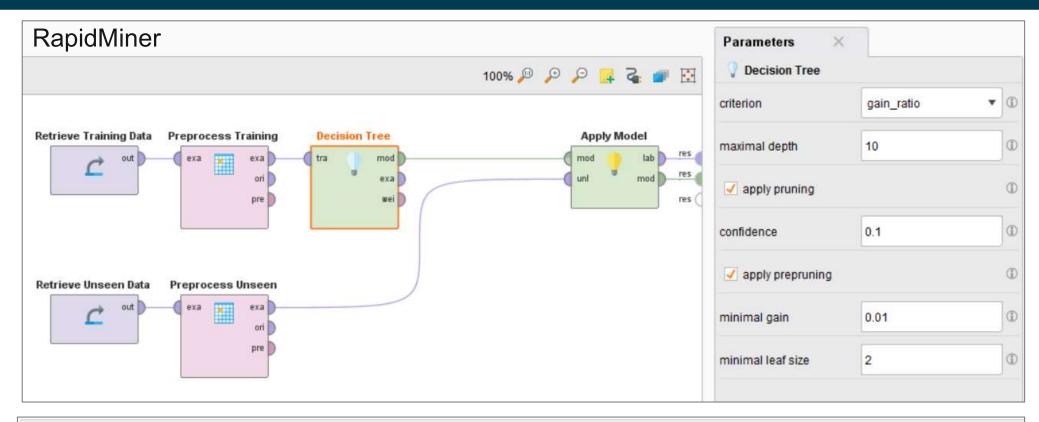
Random Forest

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



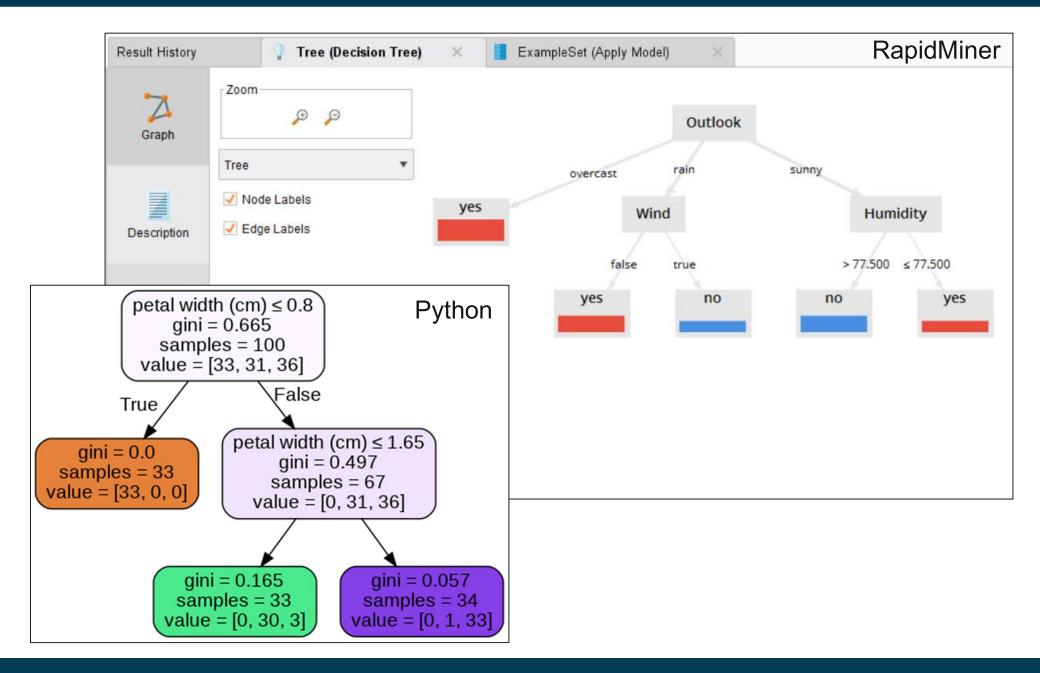
```
Python

from sklearn.tree import DecisionTreeClassifier

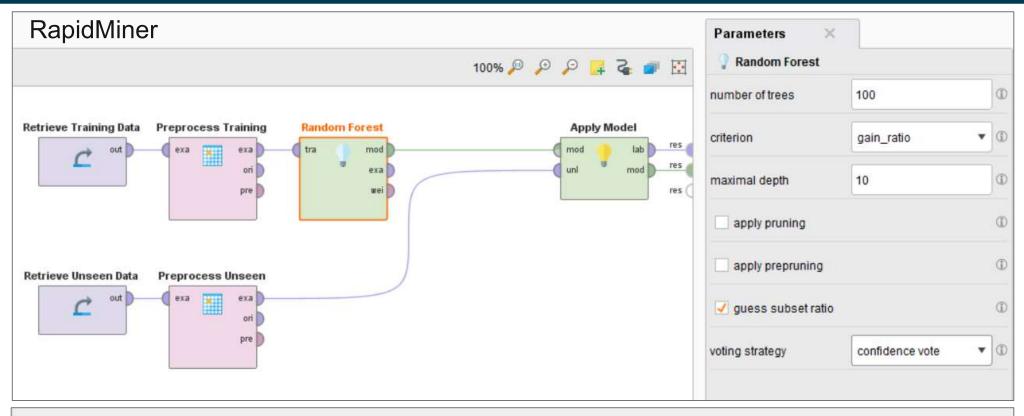
# Train classifier
dt_learner = DecisionTreeClassifier(criterion='gini', max_depth=10)
dt_learner.fit(preprocessed_training_data, training_labels)

# Use classifier to predict labels
prediction = dt_learner.predict(preprocessed_unseen_data)
```

Examples of Learned Decision Trees



Random Forests in RapidMiner and Python



from sklearn.ensemble import RandomForestClassifier # Train classifier forest_estimator = RandomForestClassifier(n_estimators=100, criterion='gini', max_depth=None) forest_estimator.fit(preprocessed_training_data, training_labels) # Use classifier to predict labels prediction = forest_estimator.predict(preprocessed_unseen_data)

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 (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

Literature for this Slideset

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

