

Data Mining

Classification

- Part 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)



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**

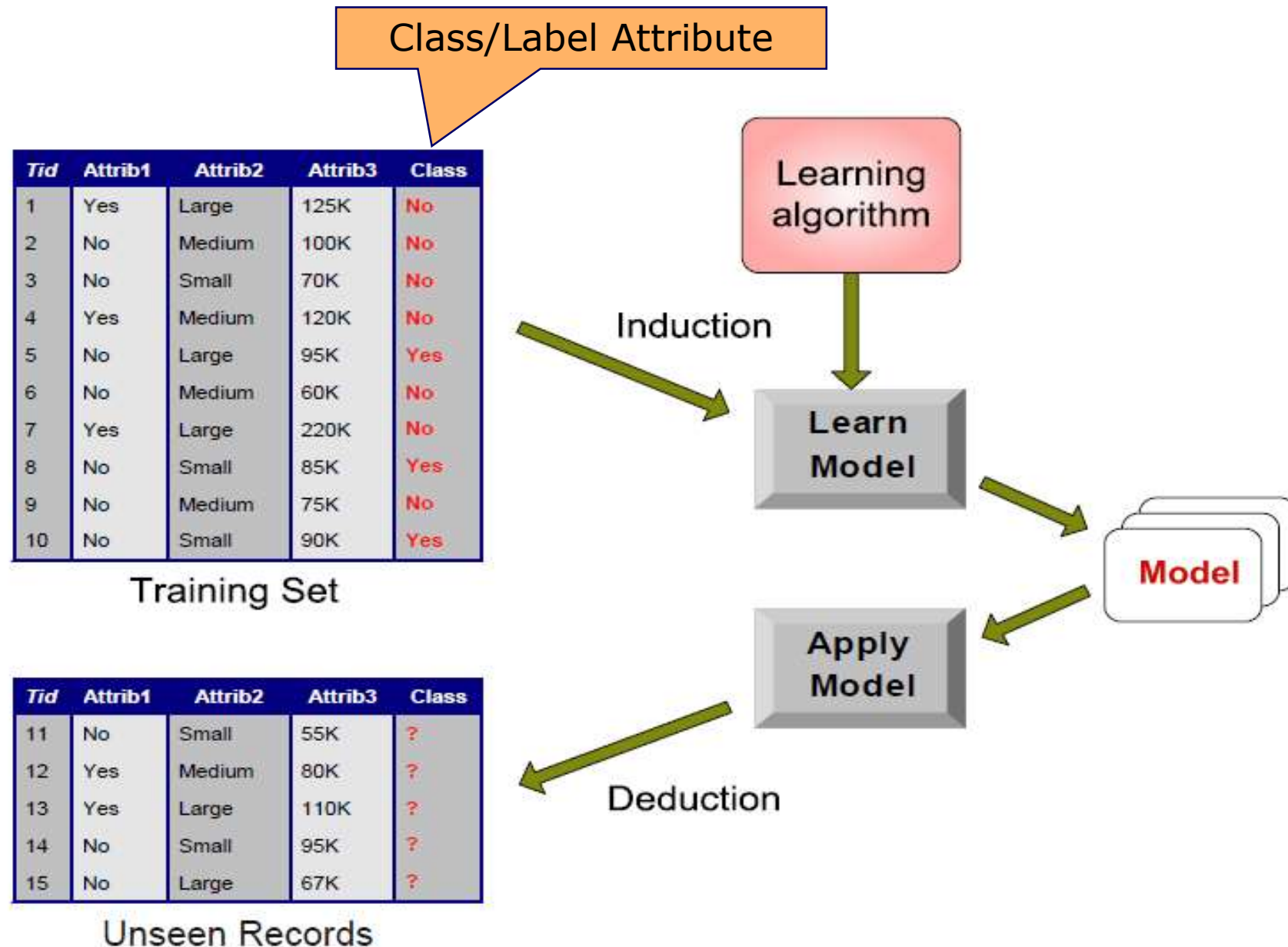


Tree?

Tree?

Warning:
Models are only
approximating examples!
Not guaranteed to be
correct or complete!

Model Learning and Model Application Process



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

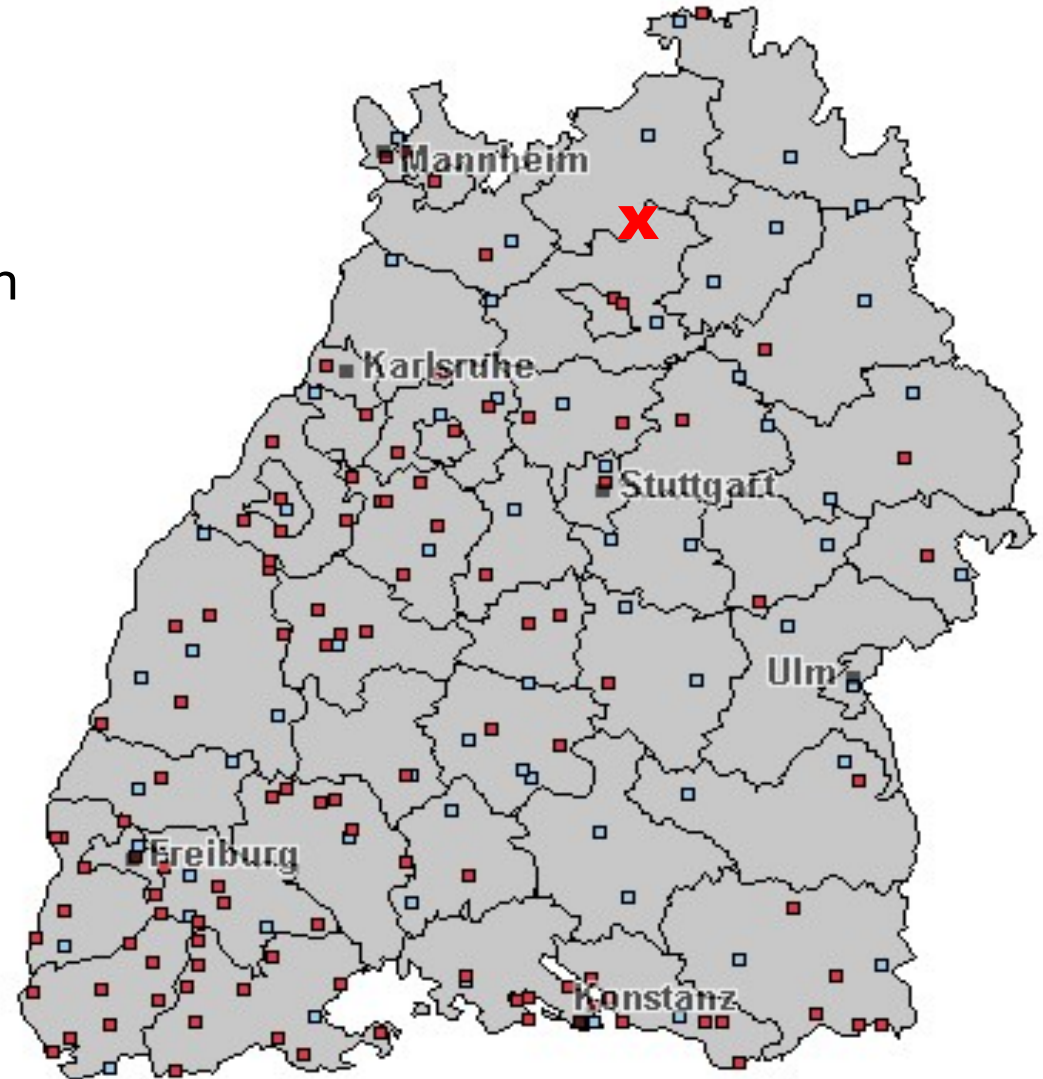
Classification Techniques

1. K-Nearest-Neighbors
2. Decision Trees / Random Forests
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?

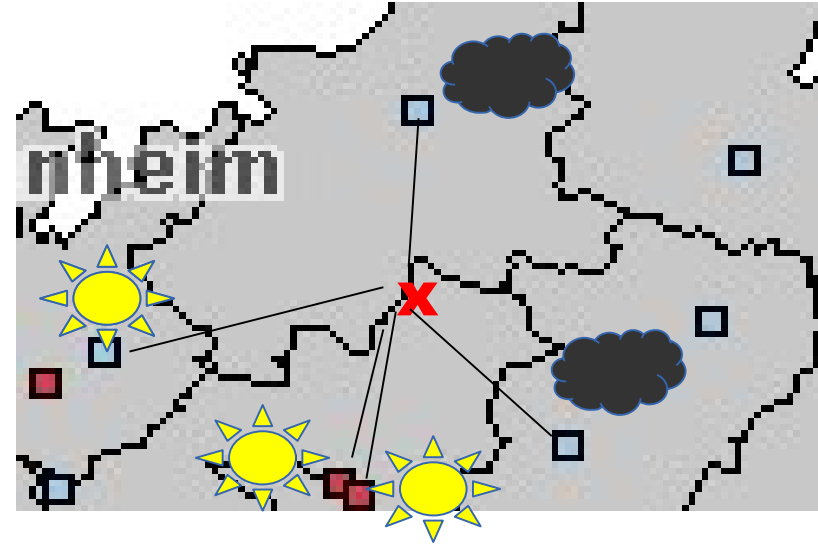


Basic Idea

- Use the **average forecast of the nearest stations**

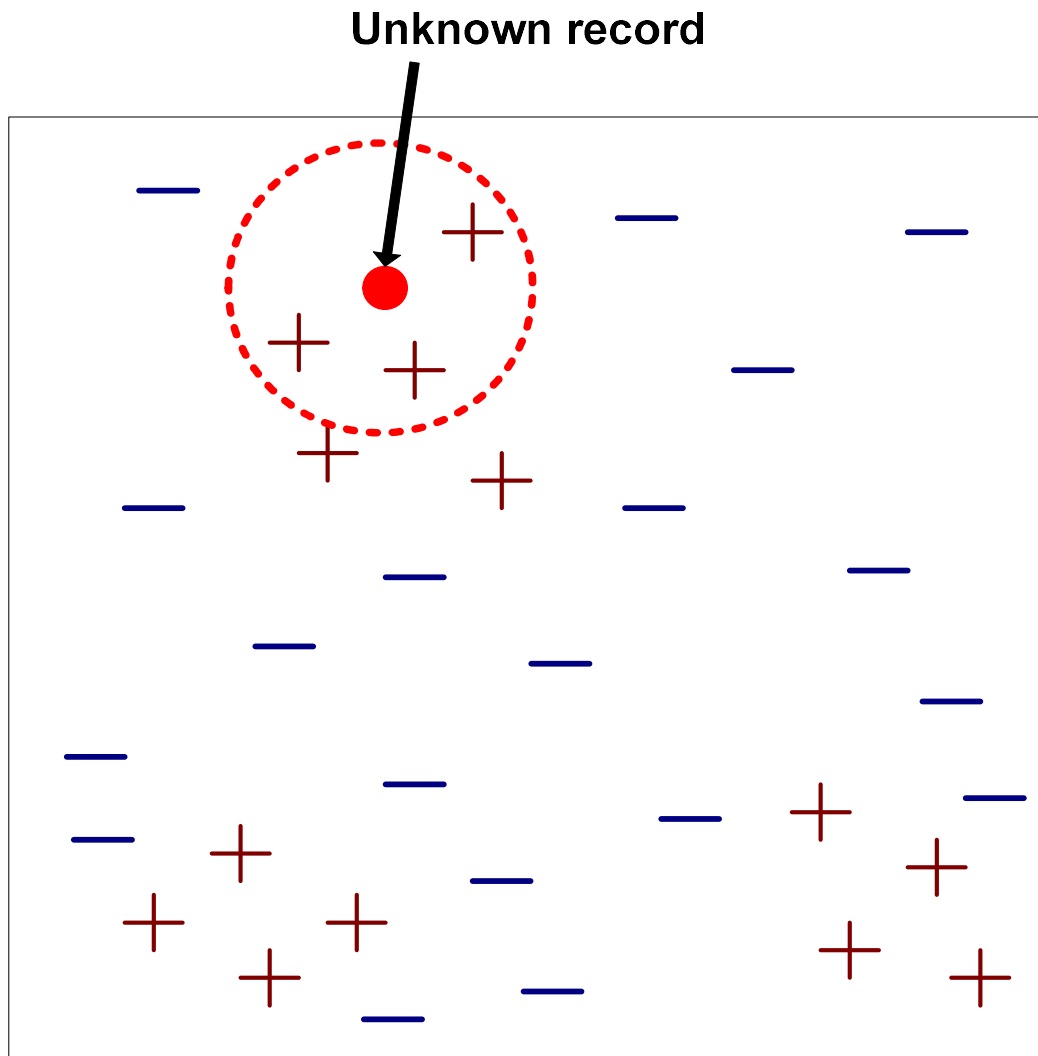
- Example:

- 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

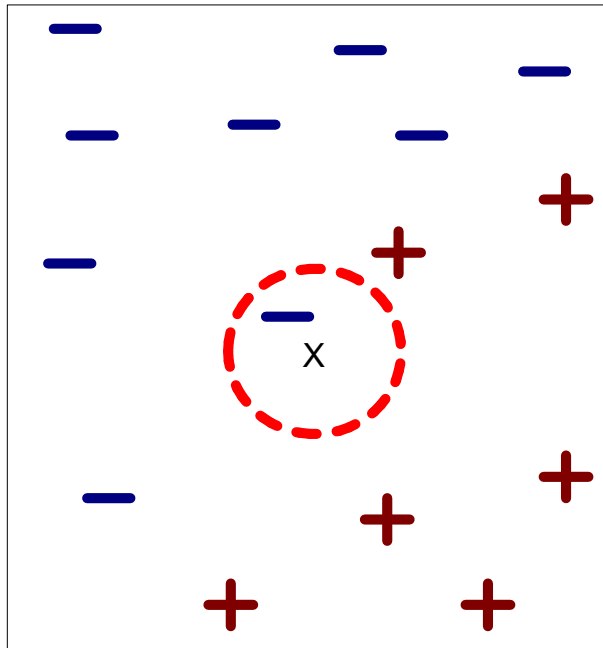
K-Nearest-Neighbors Classifiers



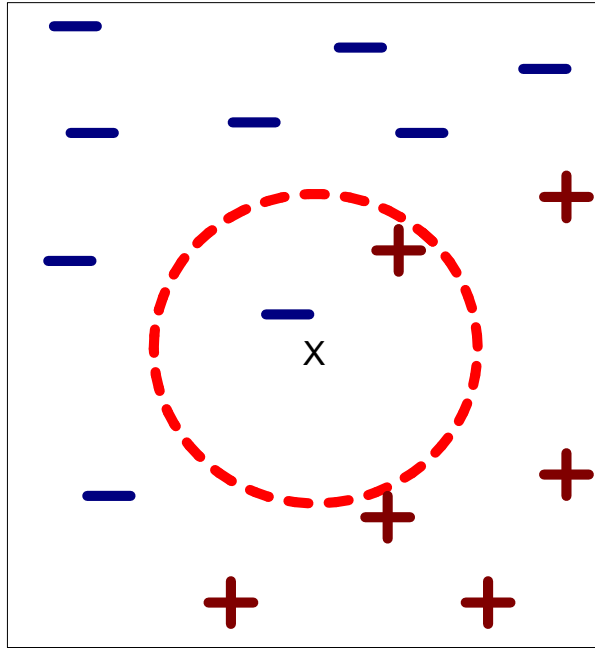
- Require three things
 - A **set of stored records**
 - A **distance measure** to compute distance between records
 - The **value of k**, the number of nearest neighbors to consider
- To classify an unknown record:
 1. Compute distance to each training record
 2. Identify k-nearest neighbors
 3. Use 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

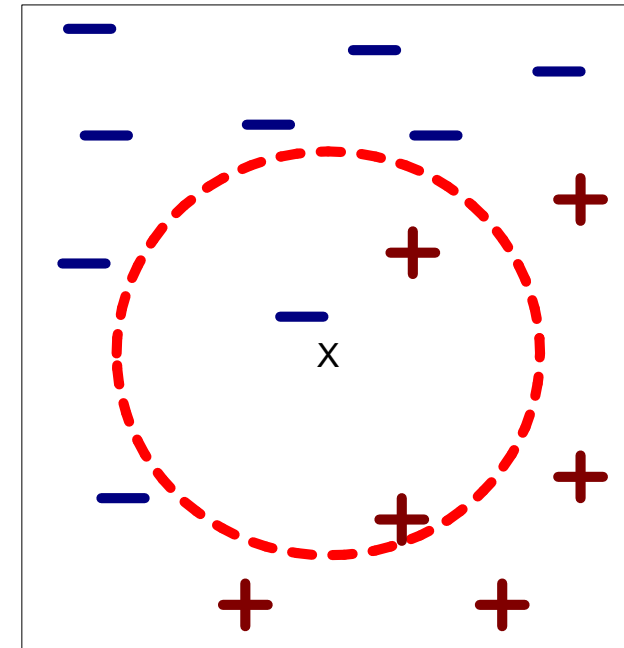
The k -nearest neighbors of a record x are data points that have the k smallest distances to x



(a) 1-nearest neighbor



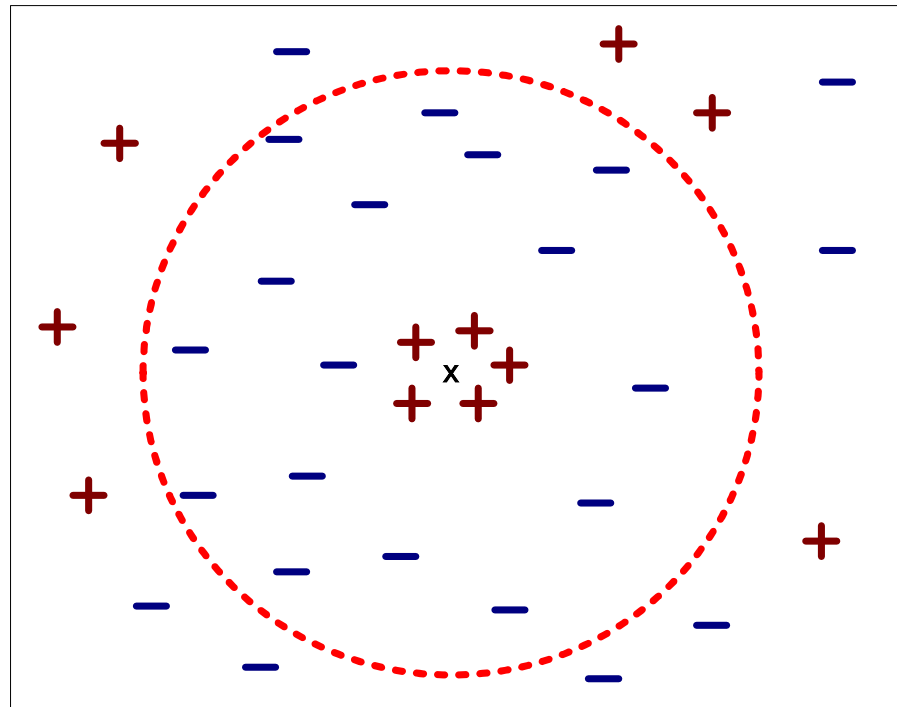
(b) 2-nearest neighbor



(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)

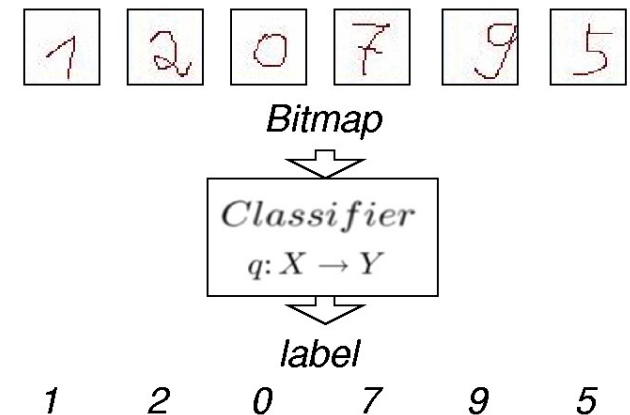
- ... but slow

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

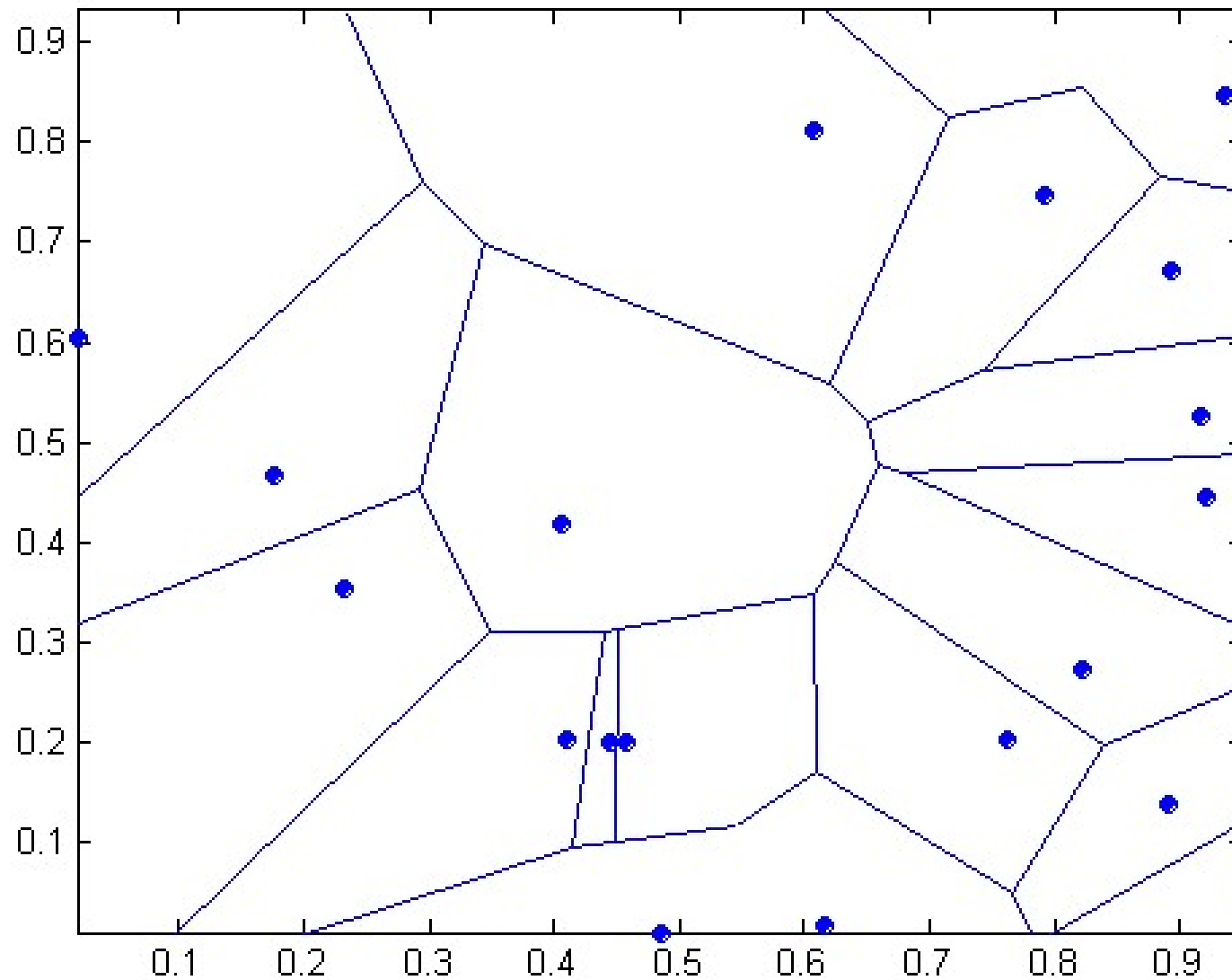
- Results depend on choosing a good proximity measure

- 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

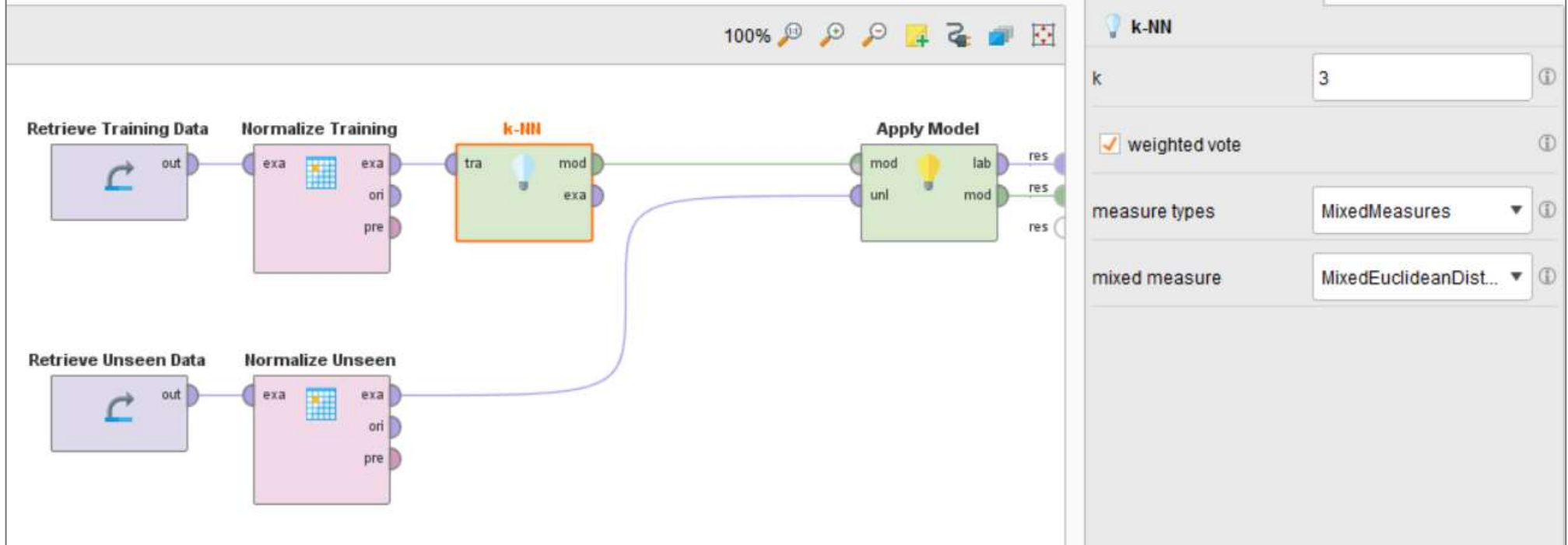
Python

```
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)
```

RapidMiner



Resulting Dataset

Prediction

Confidence scores

| Result History | | KNNClassification (k-NN) | | ExampleSet (Applied Model) | | | | | |
|----------------|------|--------------------------|----------------|----------------------------|----------|--------------------------------|----------|-------|--|
| Open in | | Turbo Prep | Auto Model | | | Filter (14 / 14 examples): all | | | |
| Row No. | Play | prediction(Play) | confidence(no) | confidence(yes) | Outlook | Temperature | Humidity | Wind | |
| 1 | yes | yes | 0.451 | 0.549 | sunny | 85 | 85 | false | |
| 2 | no | no | 0.630 | 0.370 | overcast | 80 | 90 | true | |
| 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 | |
| 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 | |
| 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 versus Eager Learning

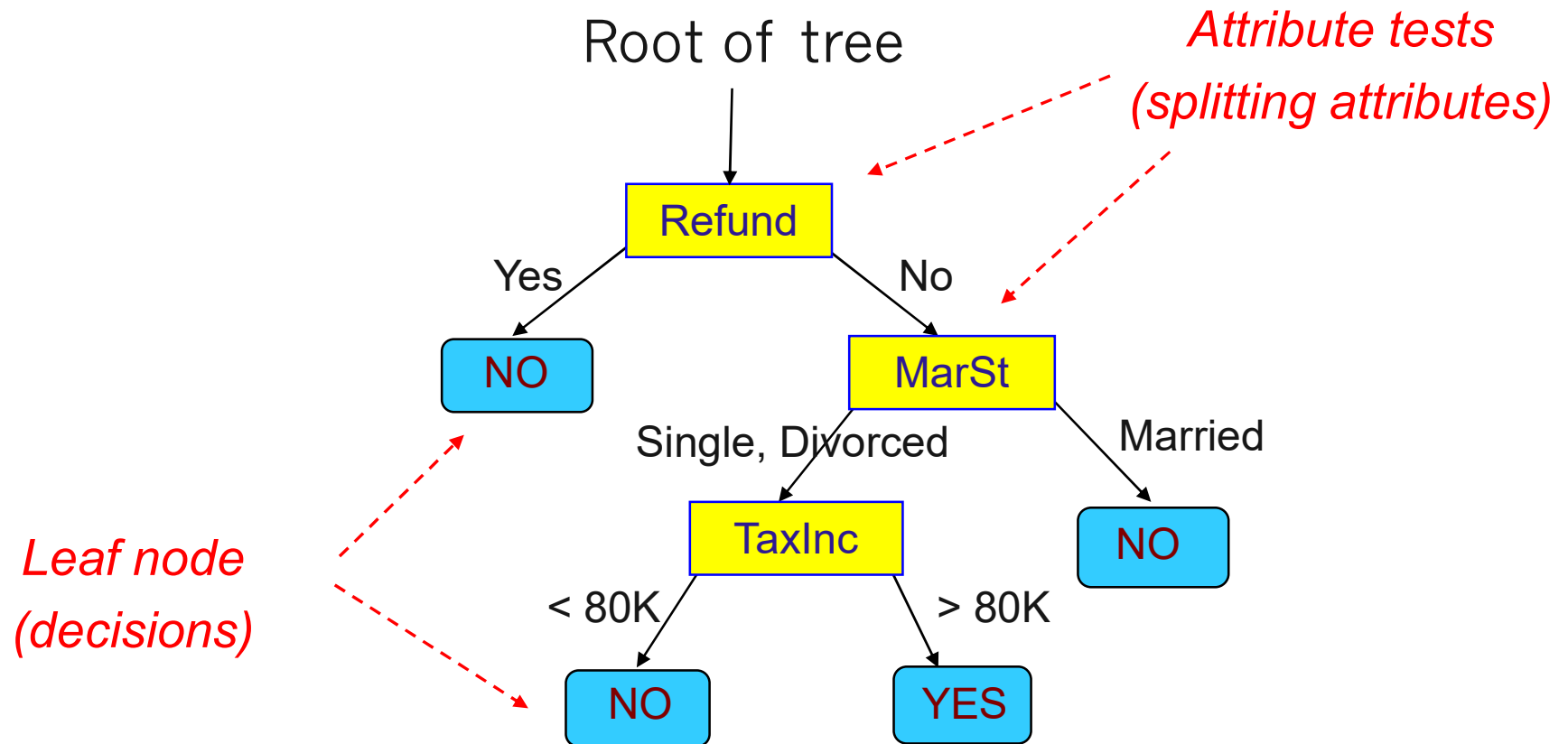
– Lazy Learning

- 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

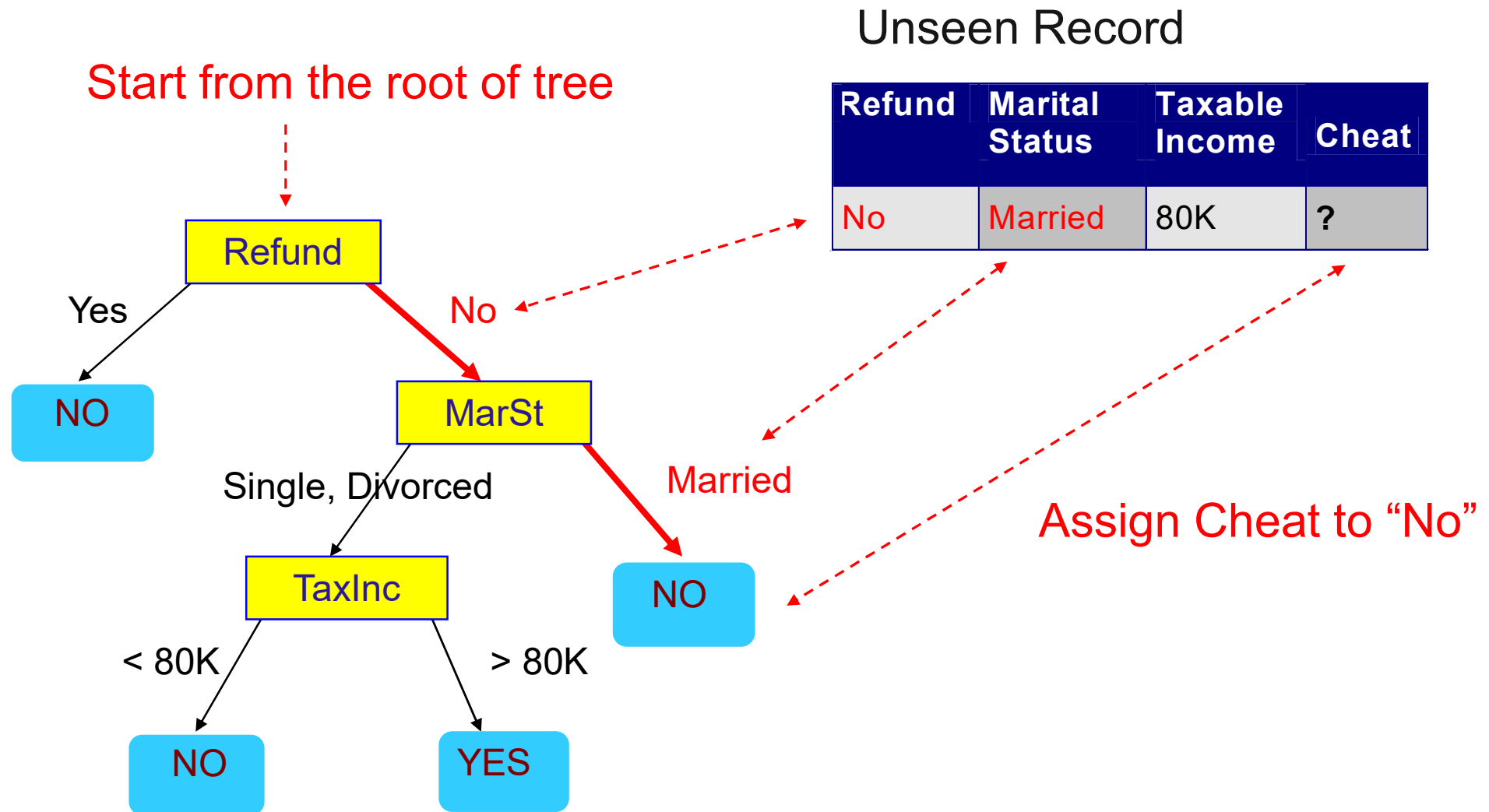
- but actually, we might have two goals
 1. classify unseen records
 2. understand the application domain as a human
- Eager learning approaches generate models that are (might be) interpretable by humans
- Examples of eager techniques: decision tree learning, rule learning

3. Decision Tree Classifiers

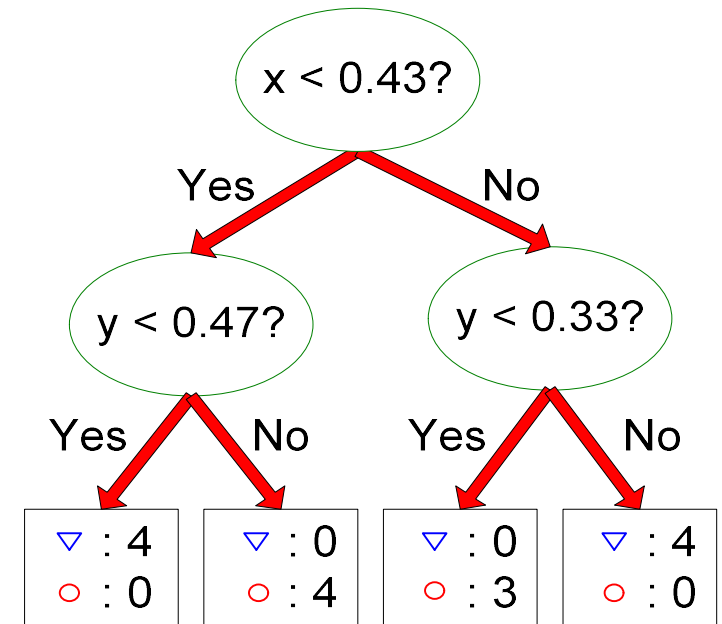
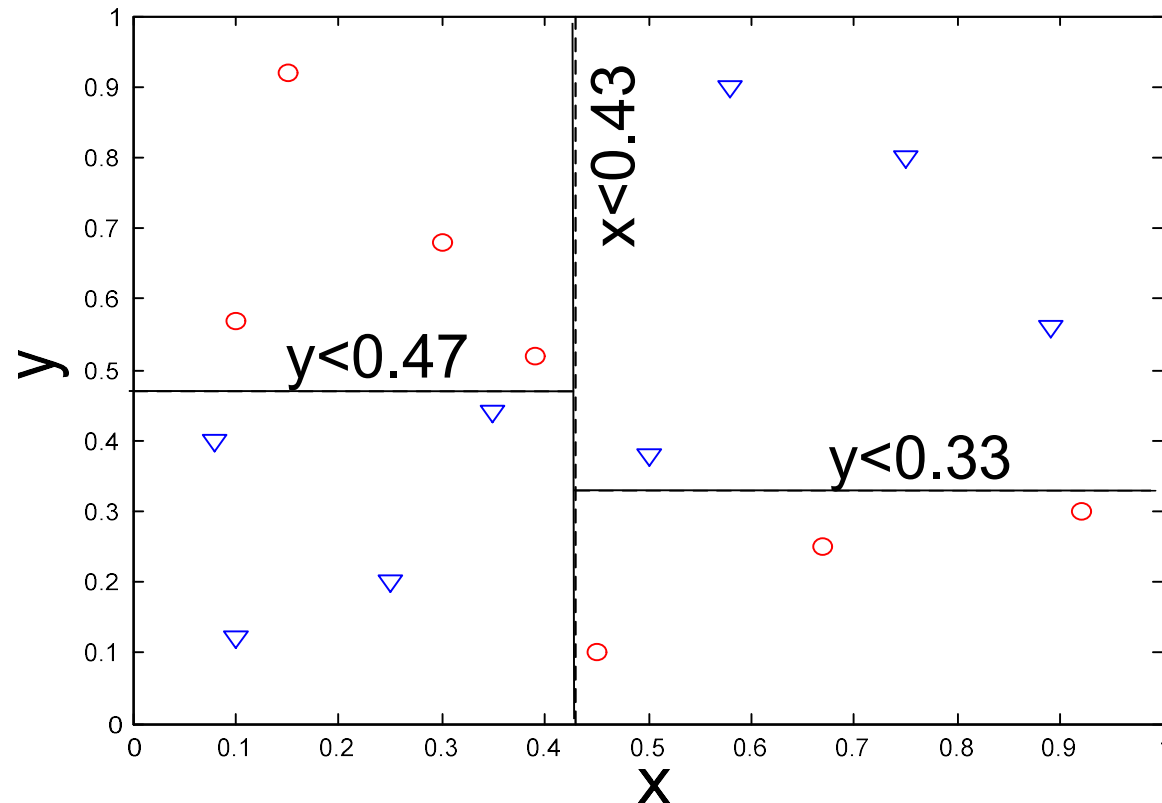


Decision trees encode a procedure for taking a classification decision

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

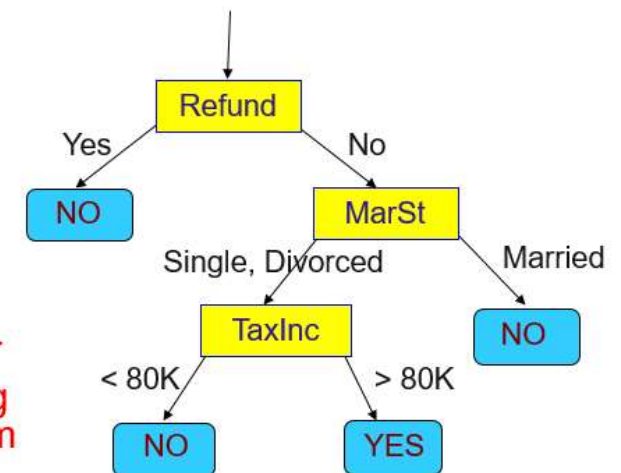
Learning a Decision Tree

- 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

| | categorical | | categorical | continuous | class |
|-----|-------------|----------------|----------------|------------|-------|
| 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 | |

Training Data

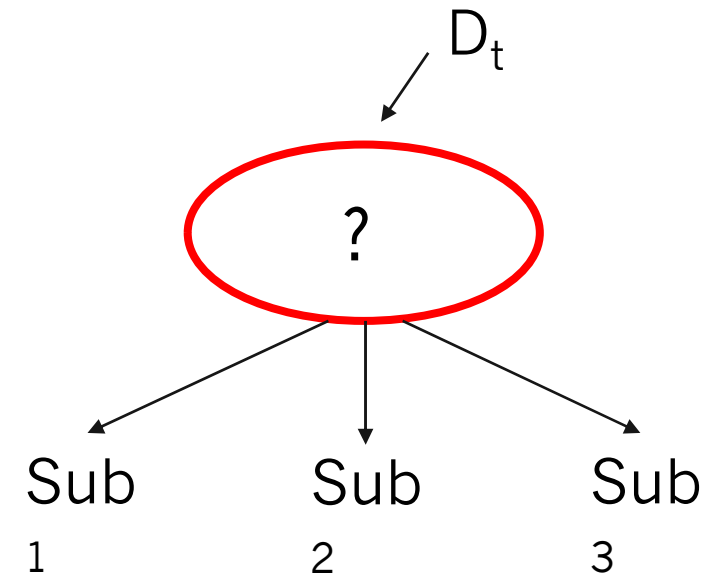
Learning Algorithm



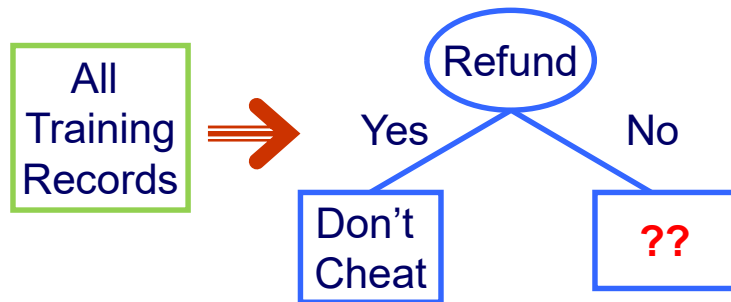
Model: Decision Tree

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



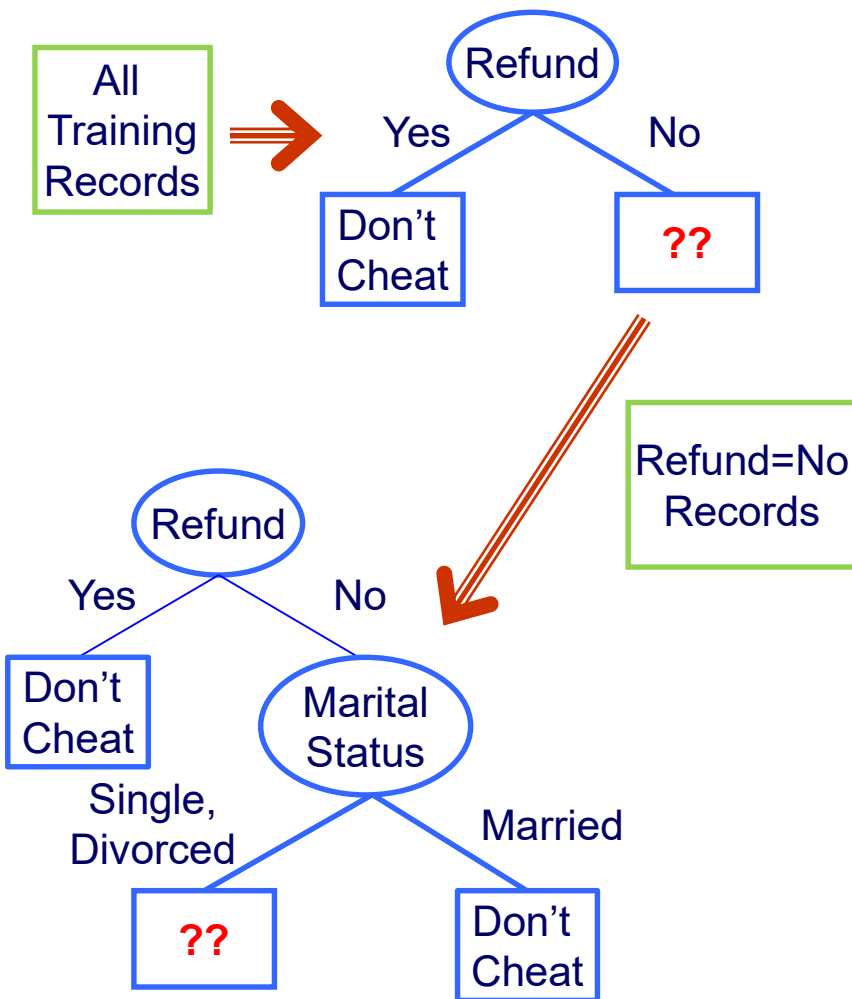
Hunt's Algorithm – Step 1



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

| <i>Tid</i> | 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 |
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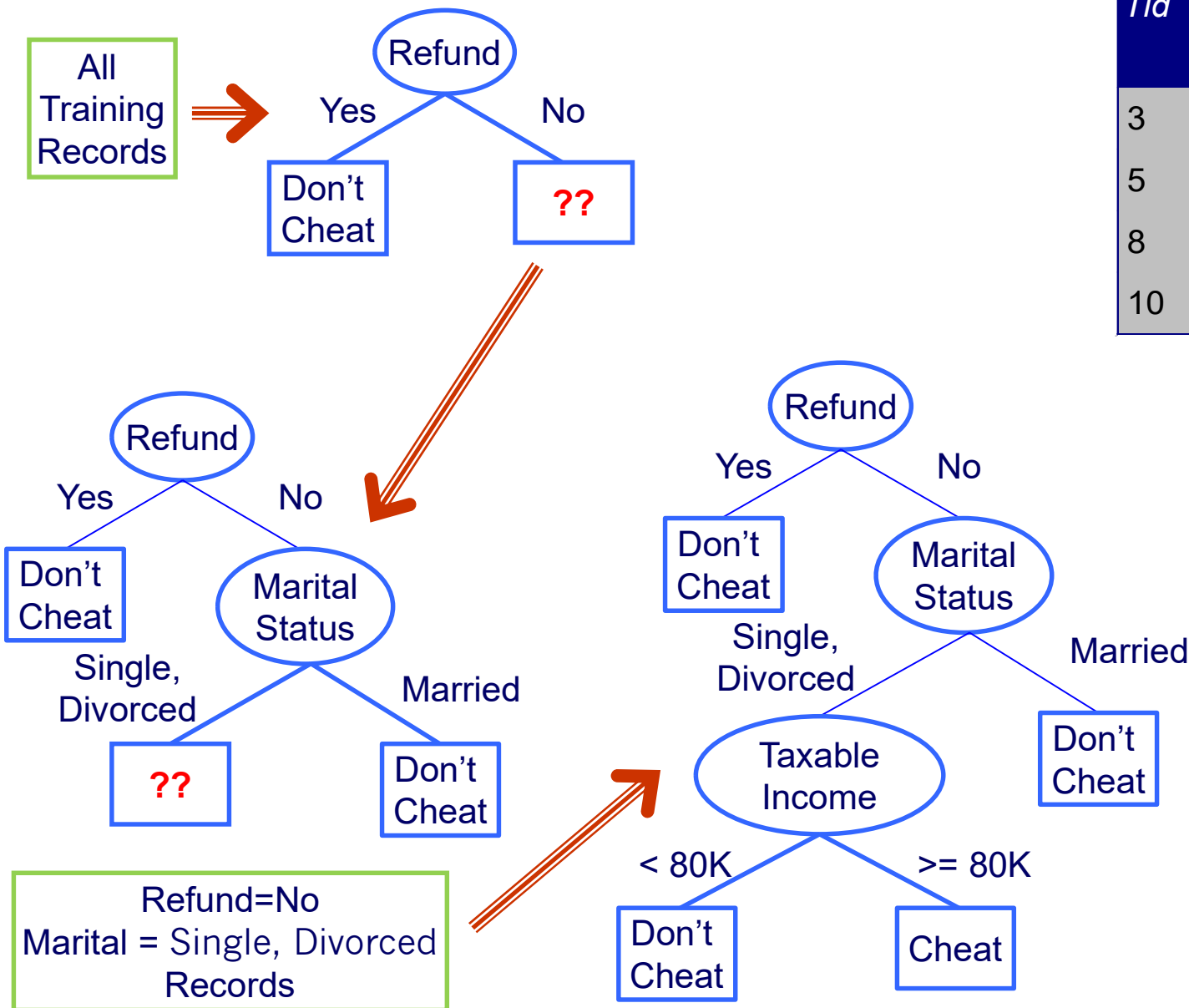
Hunt's Algorithm – Step 2



| <i>Tid</i> | 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 |

1. We further examine the Marital Status=Single or =Divorced records
2. 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?

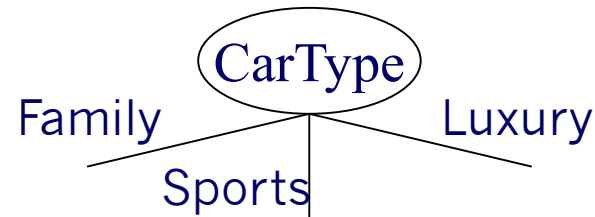
- How to specify the attribute test condition?
 - Depends on number of ways to split: 2-way split, multi-way split
 - Depends on attribute data type: nominal, ordinal, continuous
- How to determine the best split?
 - Different purity measures can be used

2. When should the splitting procedure stop?

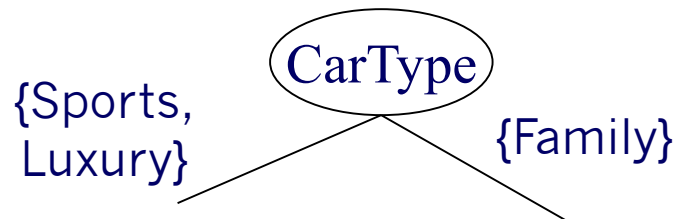
- Shallow trees might generalize better to unseen records
- Fully grown trees might overfit training data

Splitting Based on Nominal Attributes

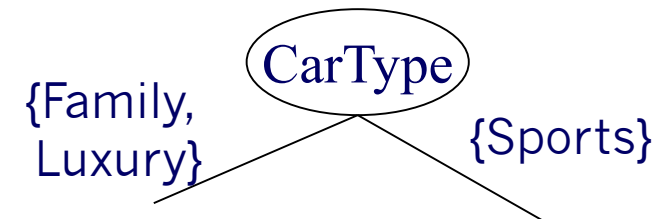
- **Multi-way split:** Use as many partitions as distinct values



- **Binary split:** Divides values into two subsets

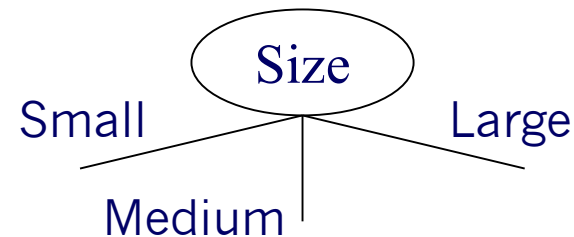


OR

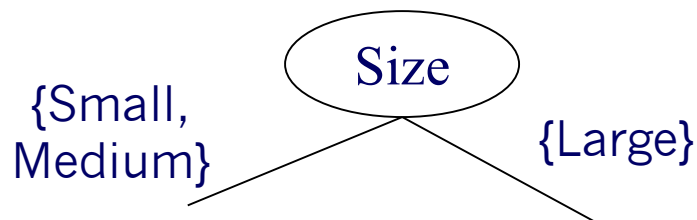


Splitting Based on Ordinal Attributes

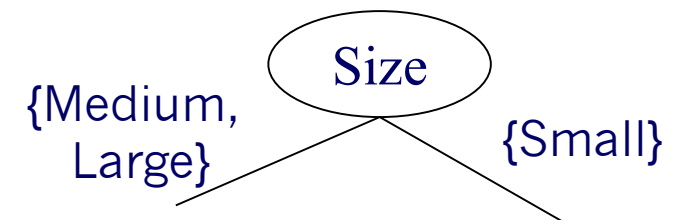
- **Multi-way split:** Use as many partitions as distinct values



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



OR

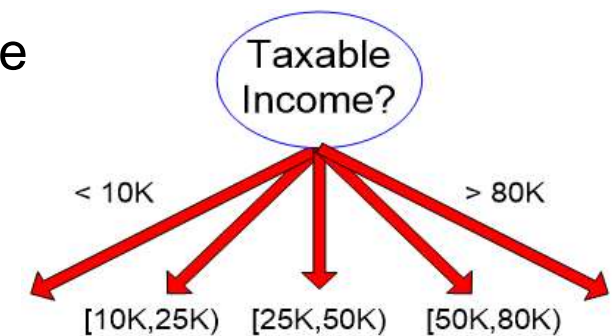


Splitting Based on Continuous Attributes

– 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



(ii) Multi-way split

- **Binary Decision:** $(A < v)$ or $(A \geq v)$

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



(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



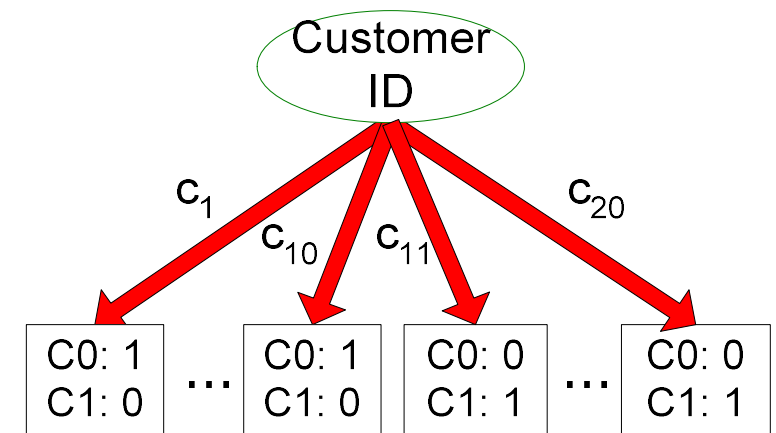
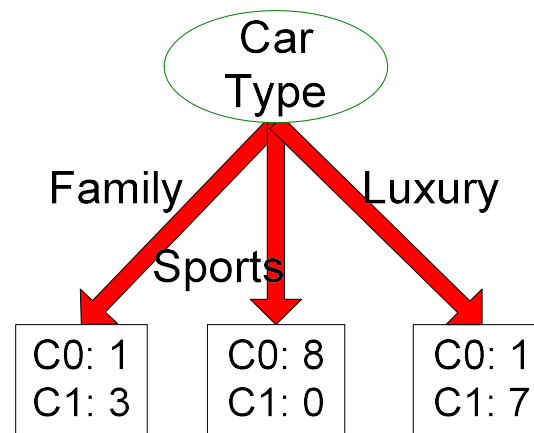
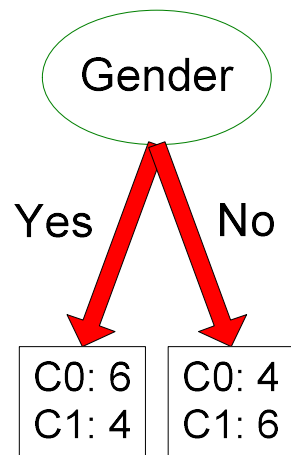
3.2 How to Find the Best Split?

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 | M | Sports | Medium | C0 |
| 4 | M | Sports | Large | C0 |
| 5 | M | Sports | Extra Large | C0 |
| 6 | 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 | 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 | F | Luxury | Small | C1 |
| 17 | F | Luxury | Medium | C1 |
| 18 | F | Luxury | Medium | C1 |
| 19 | F | Luxury | Medium | C1 |
| 20 | 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?

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**

$$\text{Gain} = P - M$$

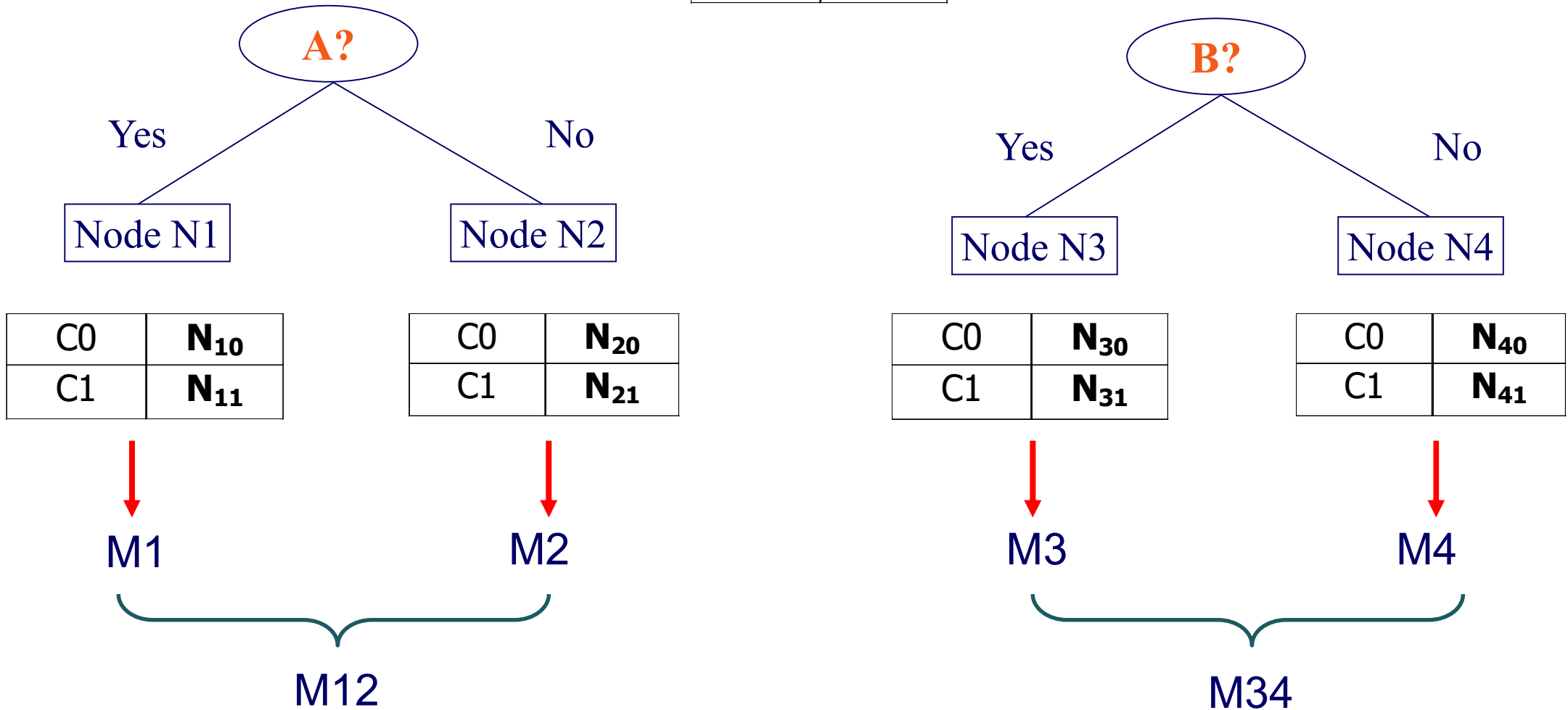
or equivalently, lowest impurity measure after splitting (M)

Comparing Two Splits by Purity Gain

Before Splitting:

| | |
|----|----------|
| C0 | N_{00} |
| C1 | N_{01} |

→ P



Higher purity gain? $P - M12$ or $P - M34$

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

| | |
|-------------------|----------|
| 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

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

| | |
|----|----------|
| C1 | 0 |
| C2 | 6 |

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

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

| | |
|----|----------|
| C1 | 1 |
| C2 | 5 |

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

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

| | |
|----|----------|
| C1 | 2 |
| C2 | 4 |

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

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

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:

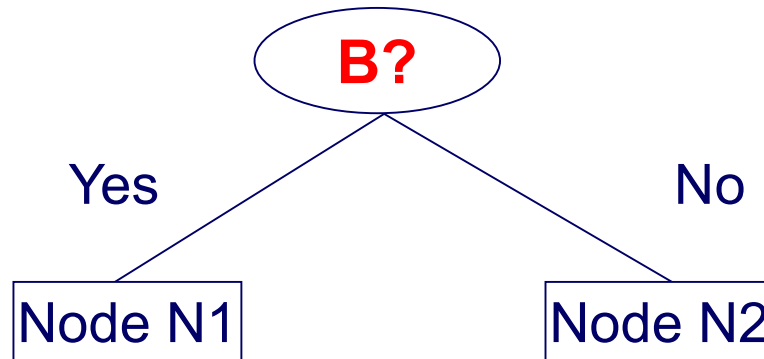
$$GINI_{split} = \sum_{i=1}^k \frac{n_i}{n} GINI(i)$$

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 | |

$$\begin{aligned} \text{GINI}_{N1} &= 1 - (5/7)^2 - (2/7)^2 \\ &= 0.408 \end{aligned}$$

$$\begin{aligned} \text{GINI}_{N2} &= 1 - (1/5)^2 - (4/5)^2 \\ &= 0.32 \end{aligned}$$

| | N1 | N2 |
|-------------------|----|----|
| C1 | 5 | 1 |
| C2 | 2 | 4 |
| Gini=0.371 | | |

$$\begin{aligned} \text{GINI}_{\text{Split}} &= 7/12 * 0.408 + \\ &\text{Weights} \rightarrow 5/12 * 0.32 \\ &= 0.371 \end{aligned}$$

$$\text{Purity Gain} = 0.5 - 0.371 = 0.129$$

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 | | |

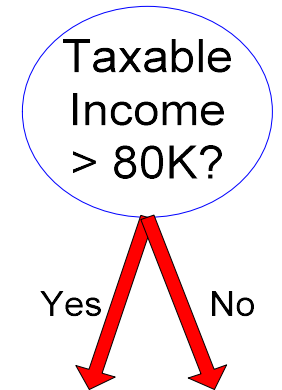
Two-way split
(find best partition of values)

| | 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. choose split positions at the middle between two values
 3. linearly scan these values, each time updating the count matrix and computing the gini index
 4. choose the split position that has the smallest gini index



| Sorted Values Split Positions | | Taxable Income | | | | | | | | | | | | | | | | | | | | | |
|----------------------------------|-------|----------------|-------|----|-------|----|-------|----|-------|----|-------|----|--------------|-----|-------|-----|-------|-----|-------|-----|-------|-----|---|
| | | 60 | | 70 | | 75 | | 85 | | 90 | | 95 | | 100 | | 120 | | 125 | | 220 | | | |
| | | 55 | | 65 | | 72 | | 80 | | 87 | | 92 | | 97 | | 110 | | 122 | | 172 | | 230 | |
| | | <= | > | <= | > | <= | > | <= | > | <= | > | <= | > | <= | > | <= | > | <= | > | <= | > | <= | > |
| Yes | 0 | 3 | 0 | 3 | 0 | 3 | 0 | 3 | 1 | 2 | 2 | 1 | 3 | 0 | 3 | 0 | 3 | 0 | 3 | 0 | 3 | 0 | |
| No | 0 | 7 | 1 | 6 | 2 | 5 | 3 | 4 | 3 | 4 | 3 | 4 | 3 | 4 | 4 | 3 | 5 | 2 | 6 | 1 | 7 | 0 | |
| Gini | 0.420 | | 0.400 | | 0.375 | | 0.343 | | 0.417 | | 0.400 | | <u>0.300</u> | | 0.343 | | 0.375 | | 0.400 | | 0.420 | | |

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 ($\log_2 n_c$) 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 |

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

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

| | |
|----|----------|
| C1 | 1 |
| C2 | 5 |

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

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

| | |
|----|----------|
| C1 | 2 |
| C2 | 4 |

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

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

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!

$$GainRATIO_{split} = \frac{GAIN_{Split}}{SplitINFO}$$

$$SplitINFO = -\sum_{i=1}^k \frac{n_i}{n} \log \frac{n_i}{n}$$

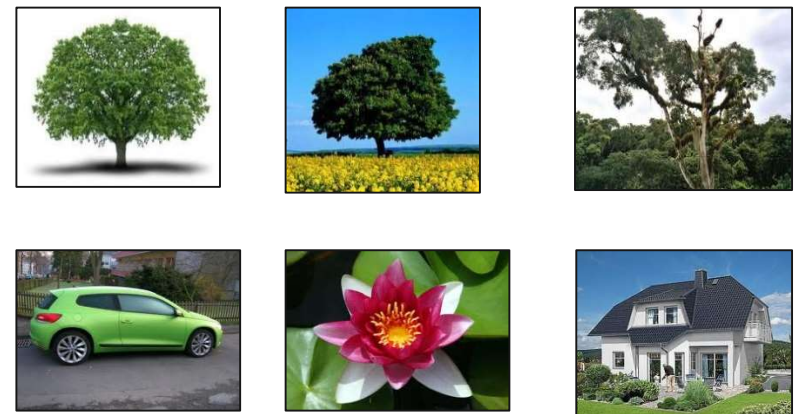
Parent Node p is split into k partitions
 n_i is the number of records in partition i

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 therefore 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:



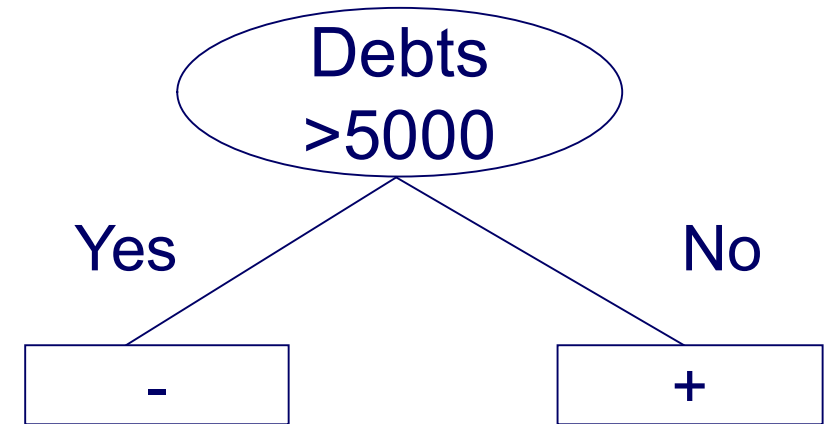
Training data



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

Overfitting: Second Example

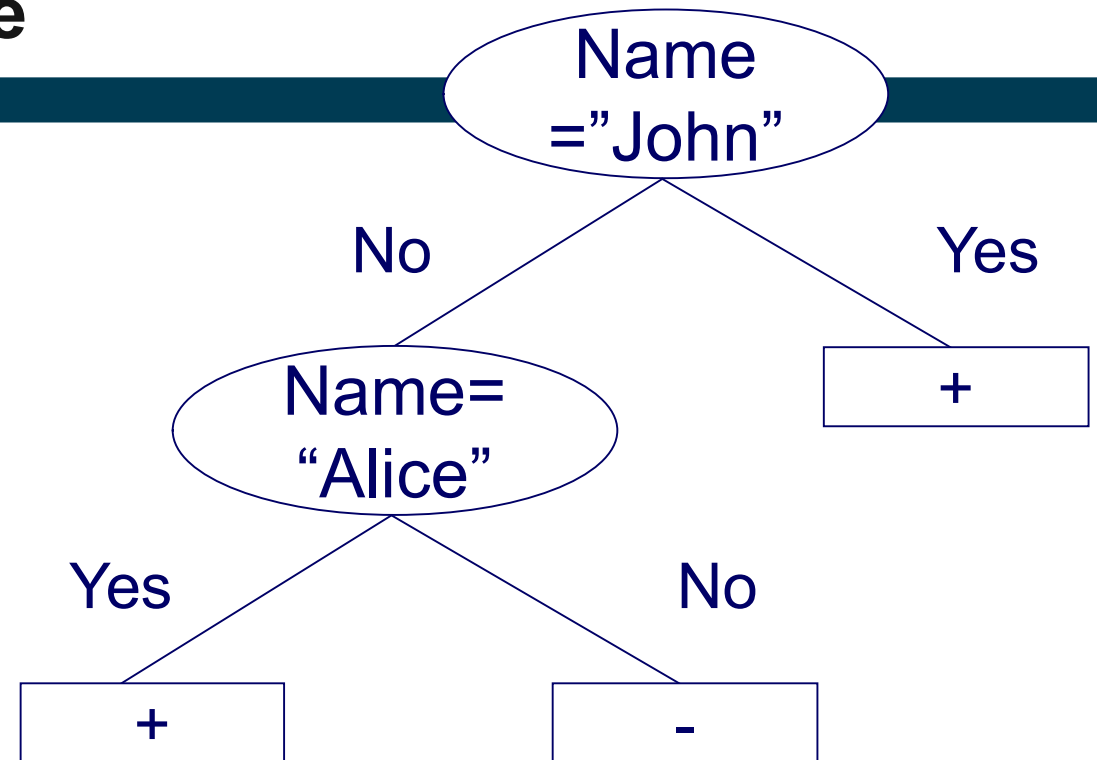
- Example: Predict credit rating
 - possible decision tree:



| 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

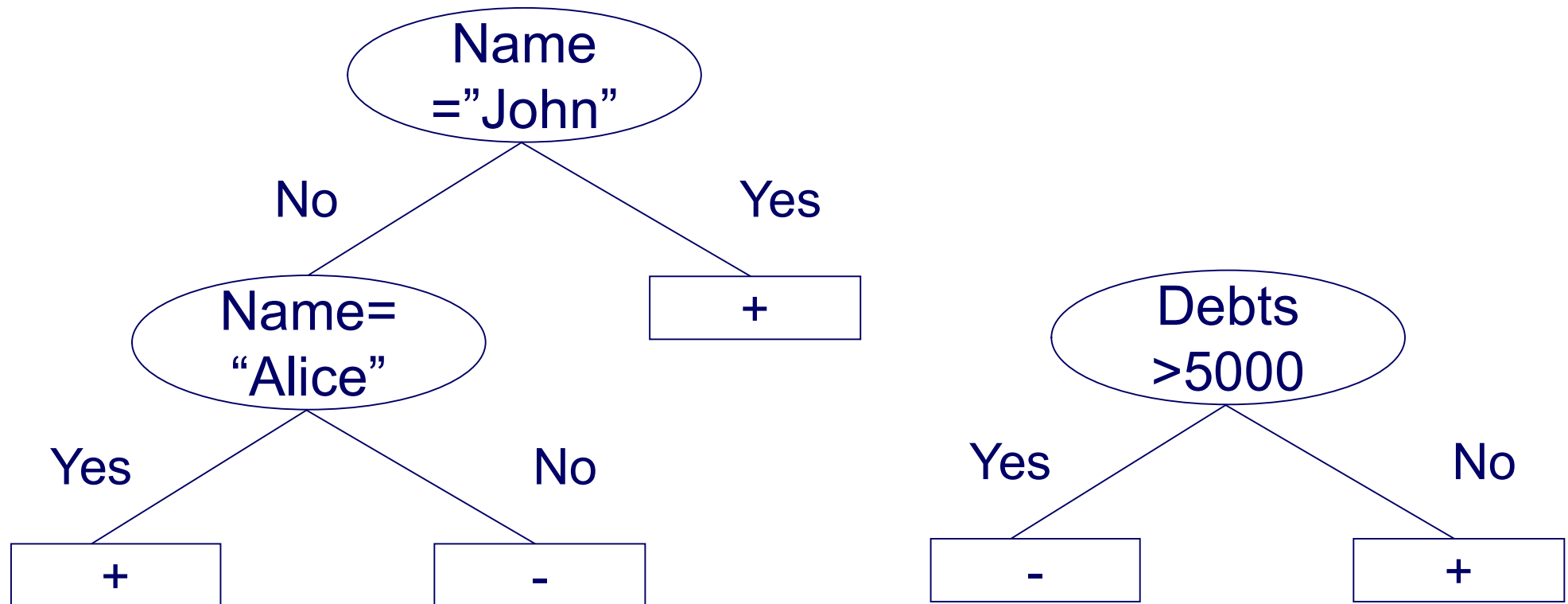
- Example: Predict credit rating
 - alternative decision tree:



| 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 | + |

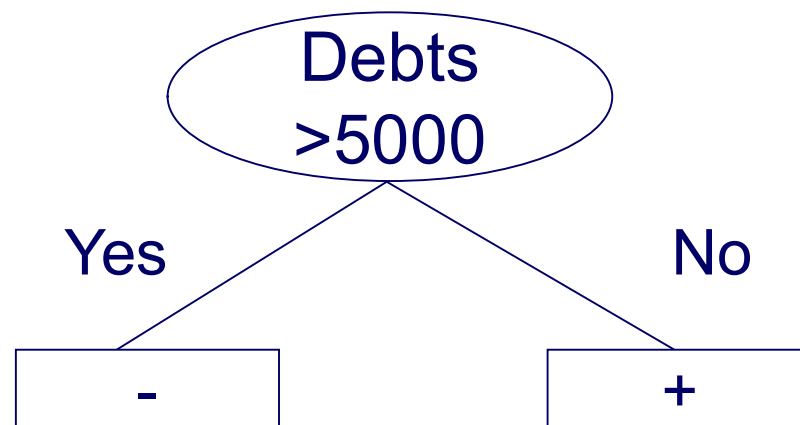
Overfitting: Second Example

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



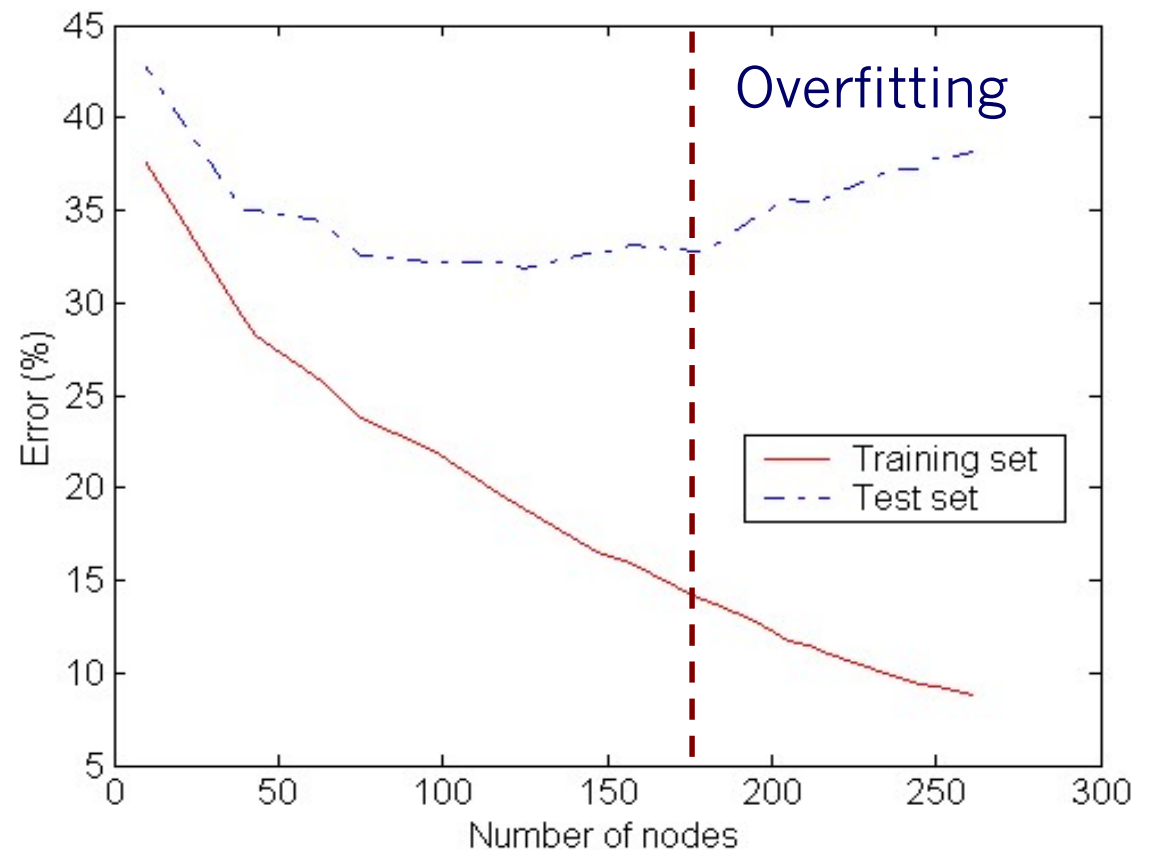
Occam's Razor

- 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



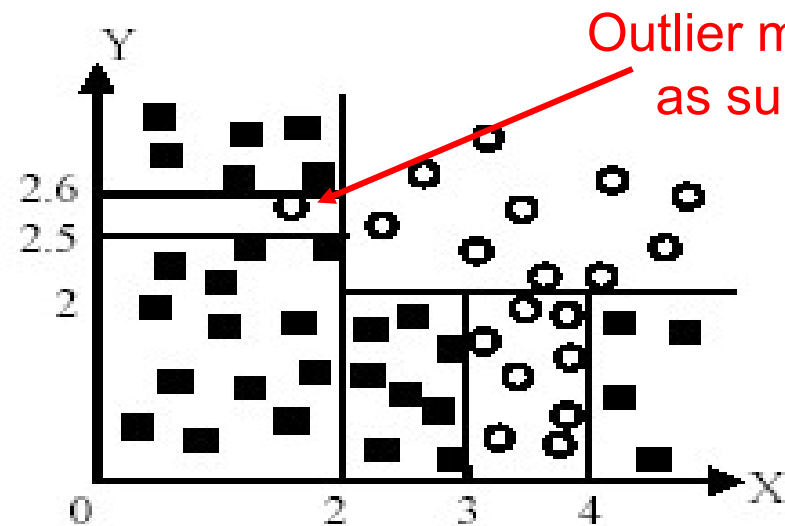
Overfitting: Symptoms and Causes

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

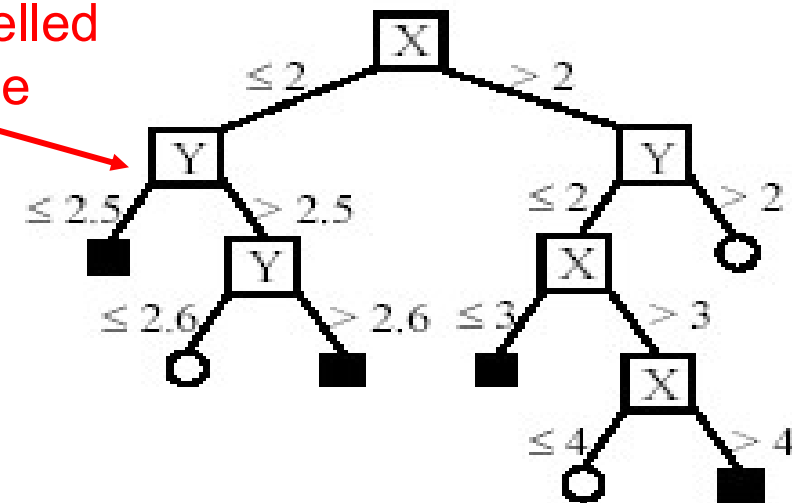


An overfitted model does not **generalize** well to **unseen data**.

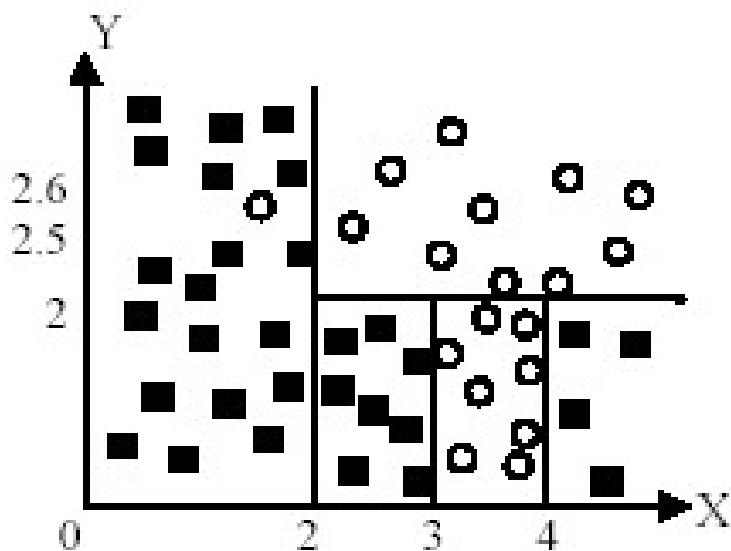
Example of an Outlier causing Overfitting



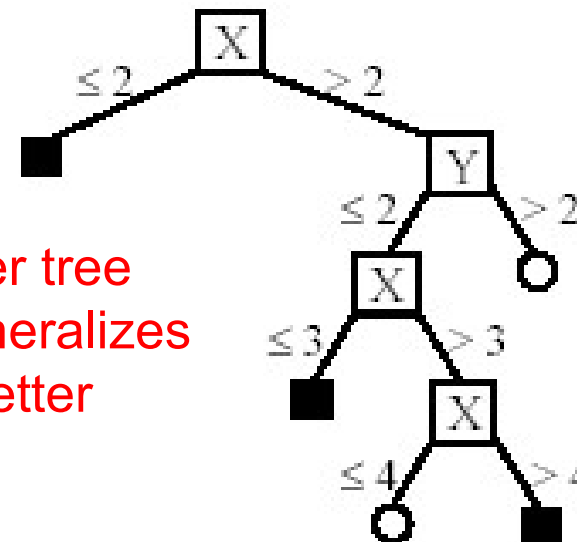
(A) A partition of the data space



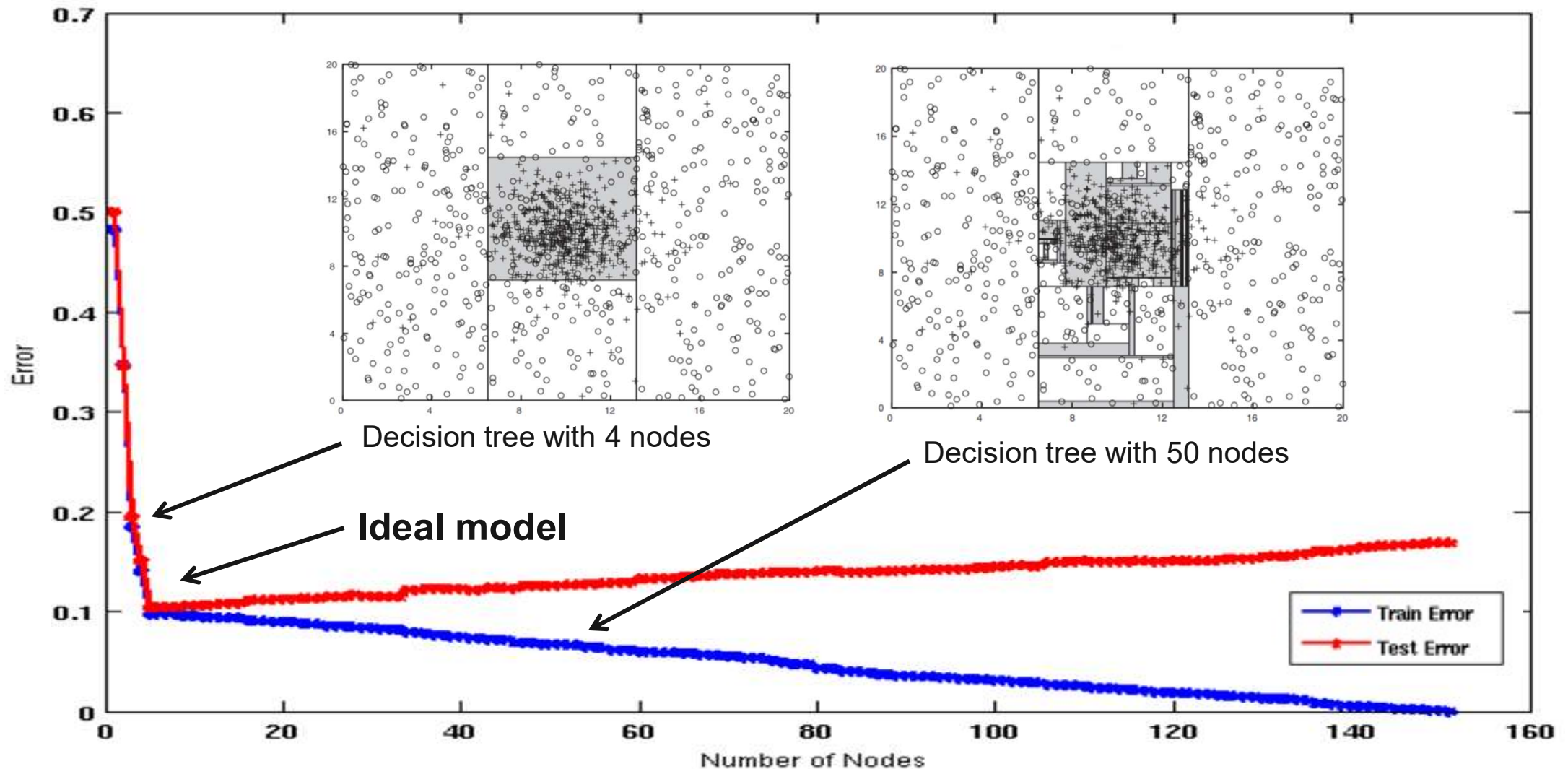
(B). The decision tree



Simpler tree
likely generalizes
better



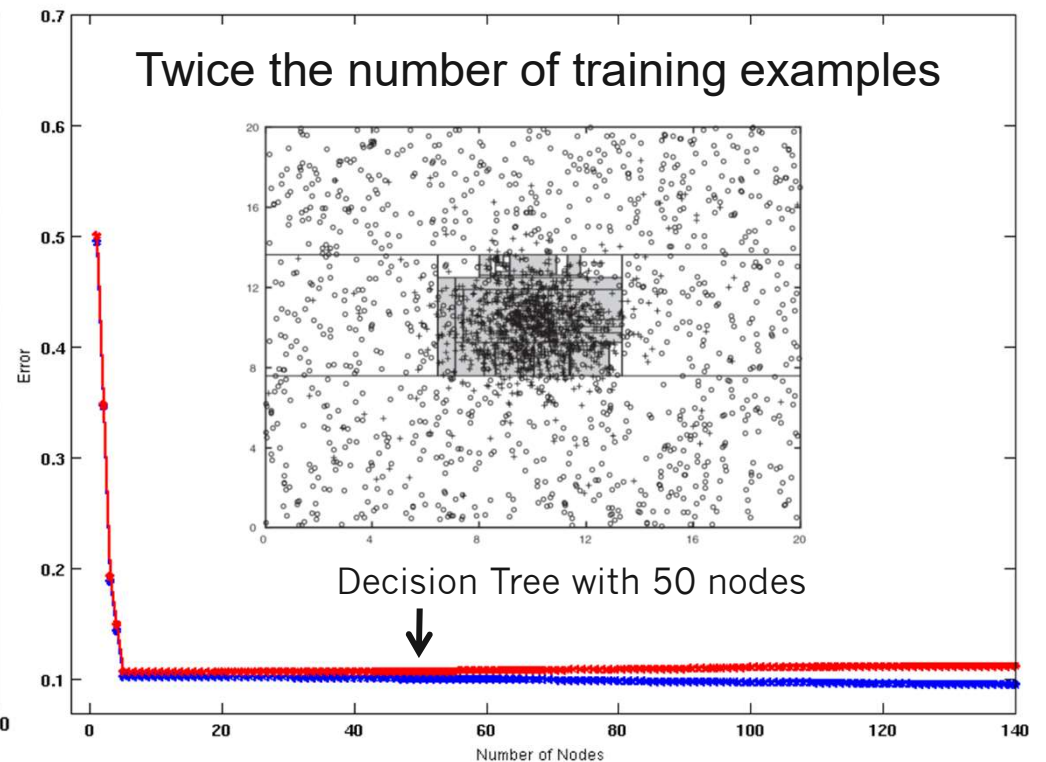
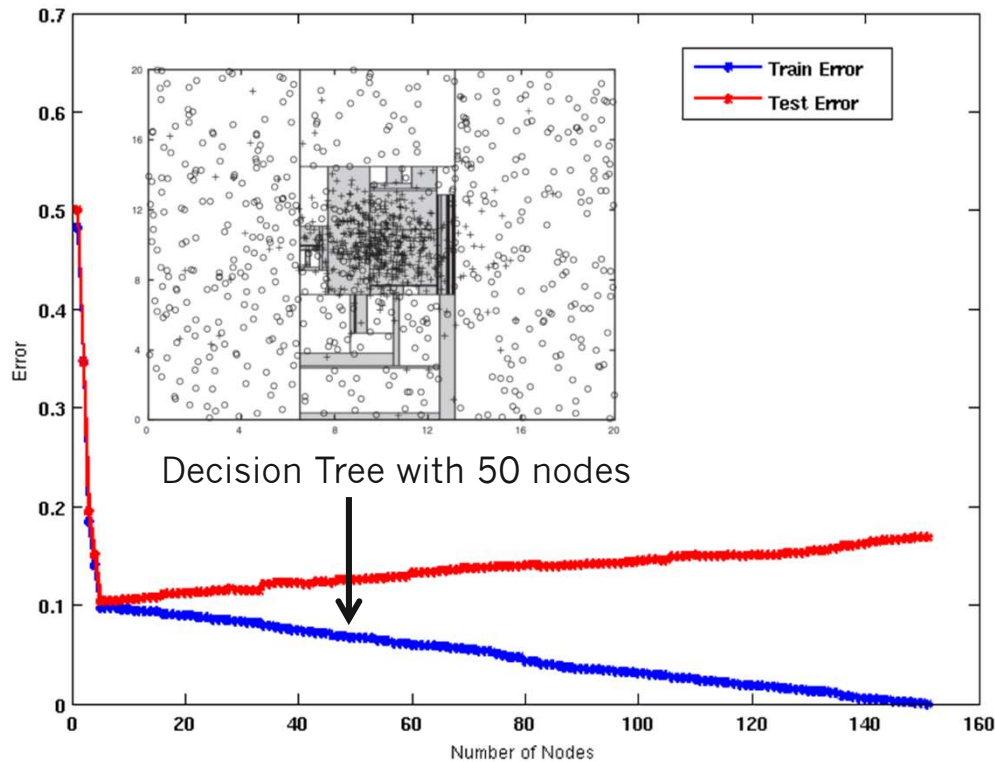
Underfitting versus Overfitting



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



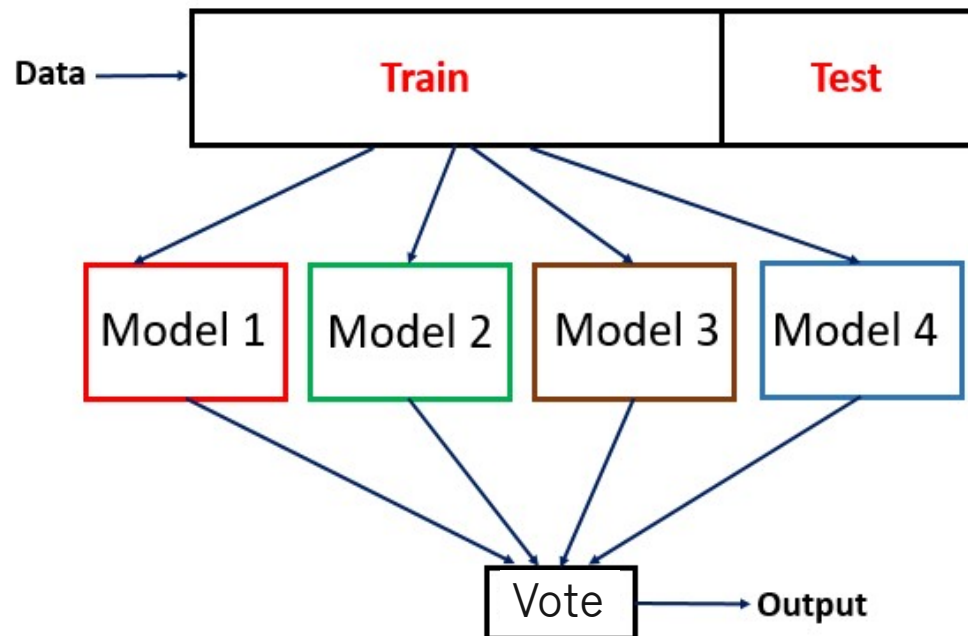
- If training data is **under-representative**, training errors decrease but testing errors increase on increasing number of nodes
- Increasing the size of training set reduces the difference between training and testing errors at a given number of nodes

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)
 - Stop splitting at a specific depth (e.g. maxDepth = 5)

How to Prevent Overfitting 3: Ensembles

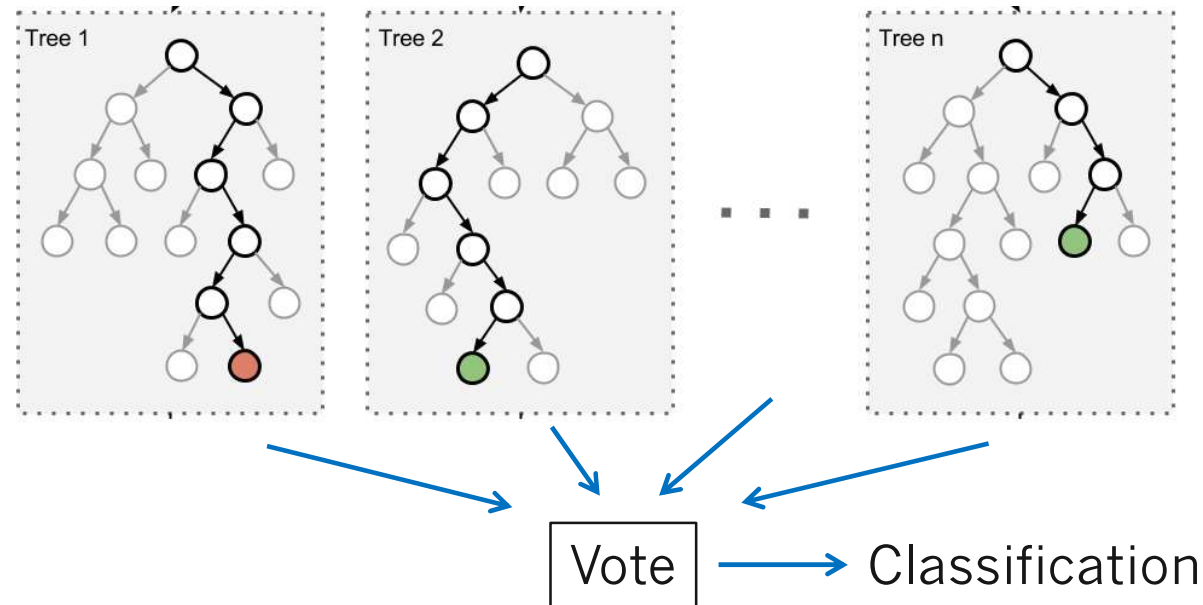
- Learn multiple different models (base learners)
- Have them vote on the final classification decision



- 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 a 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

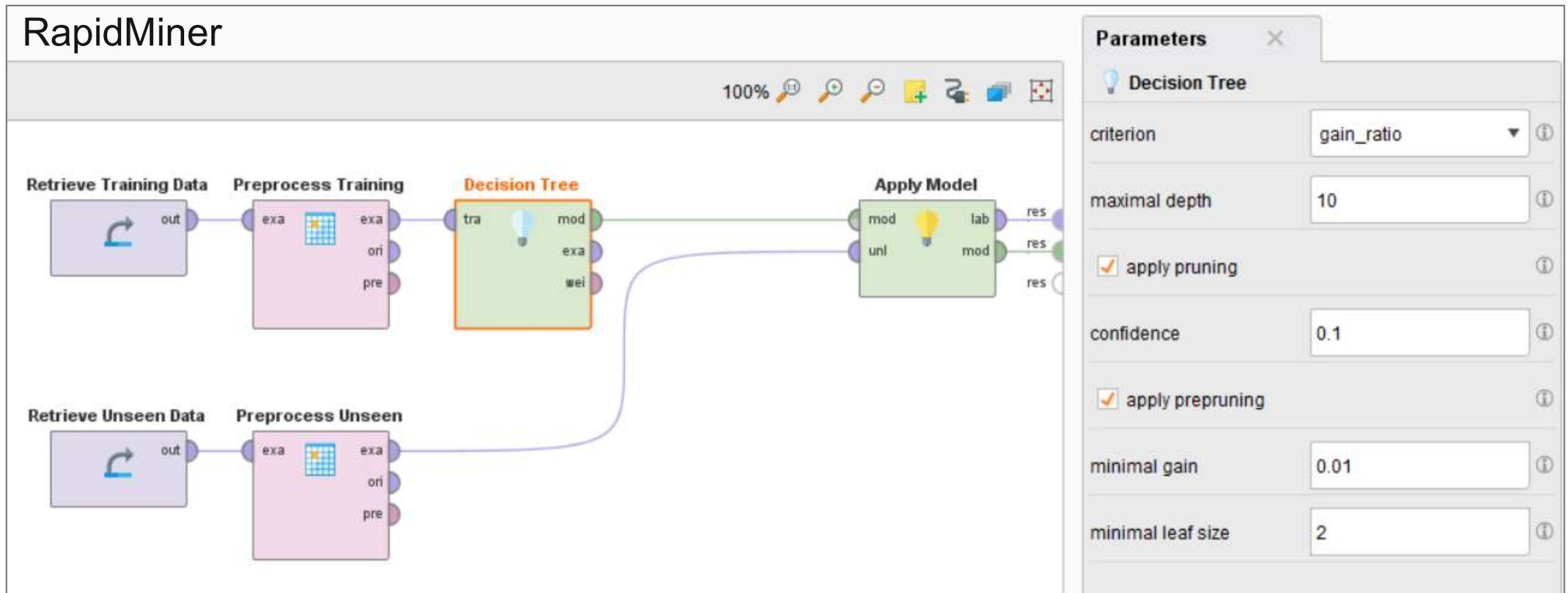
Python

```
from sklearn.tree import DecisionTreeClassifier

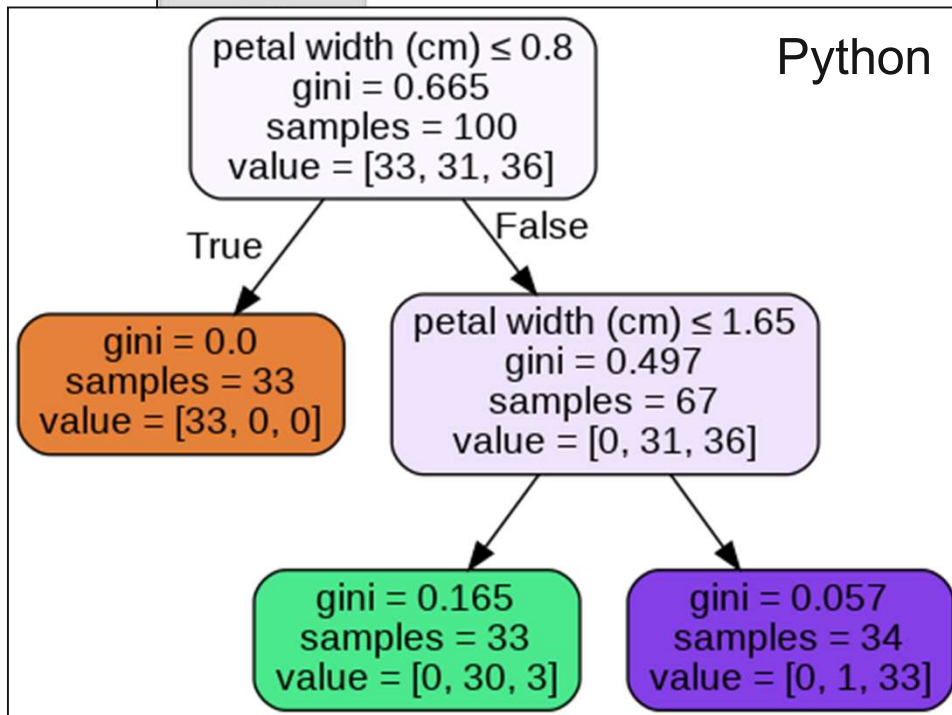
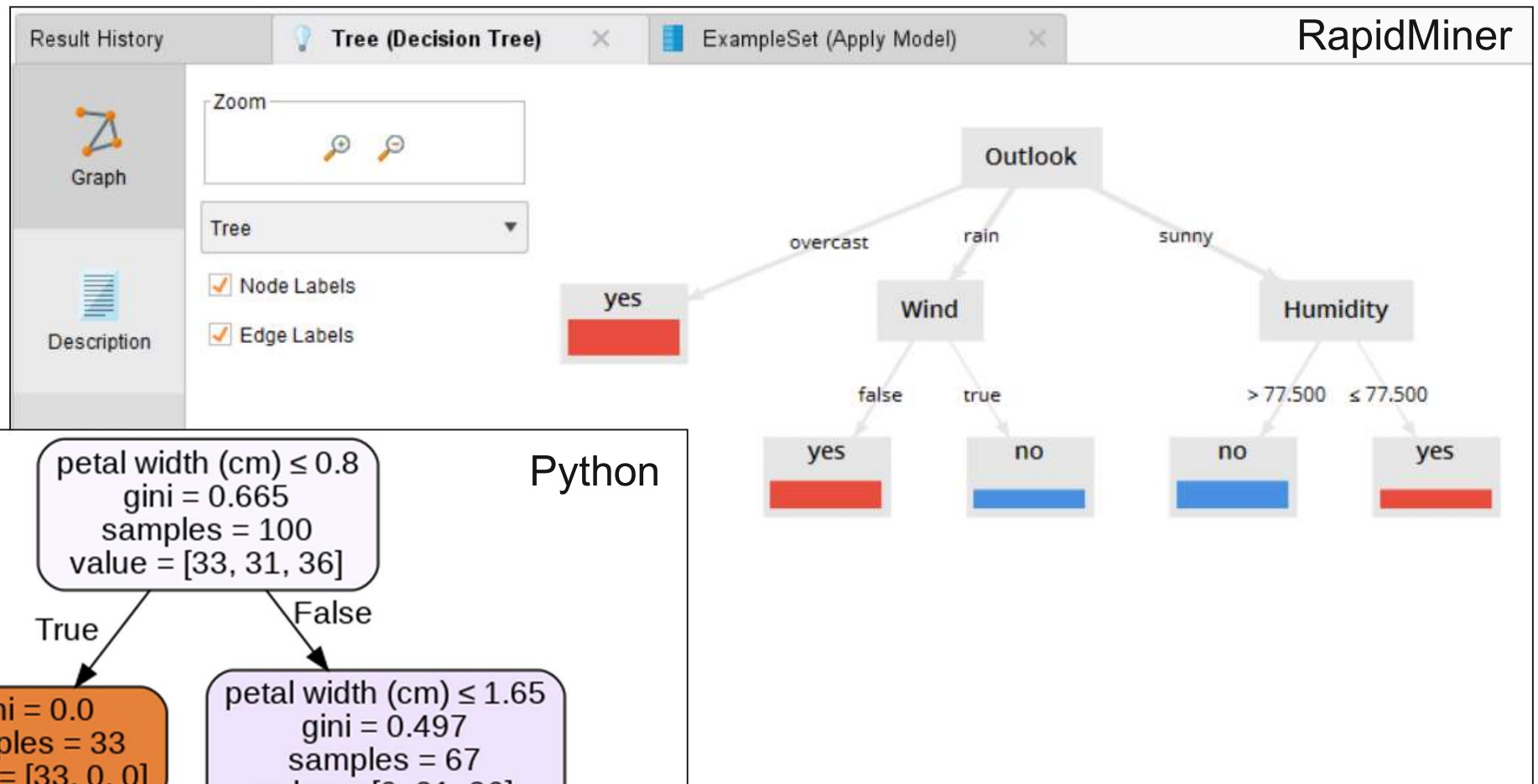
# Train classifier
dt_learner = DecisionTreeClassifier(criterion='gini', max_depth=10)
dt_learner.fit(preprocessed_training_data, training_labels)

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

RapidMiner



Examples of Learned Decision Trees



Random Forests in RapidMiner and Python

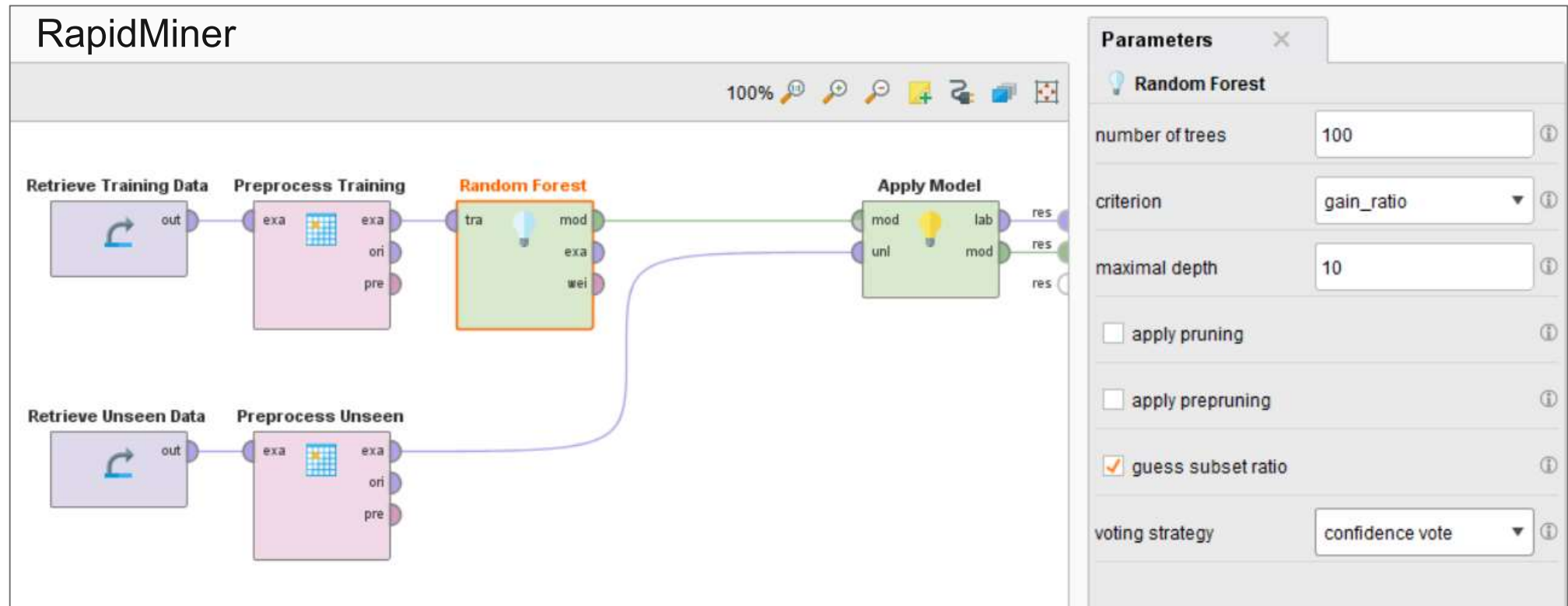
Python

```
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)
```

RapidMiner



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)
- Ignore irrelevant attributes (automatic feature selection)
- 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 consider 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

