

Chapter 8

Classification (Part 1)

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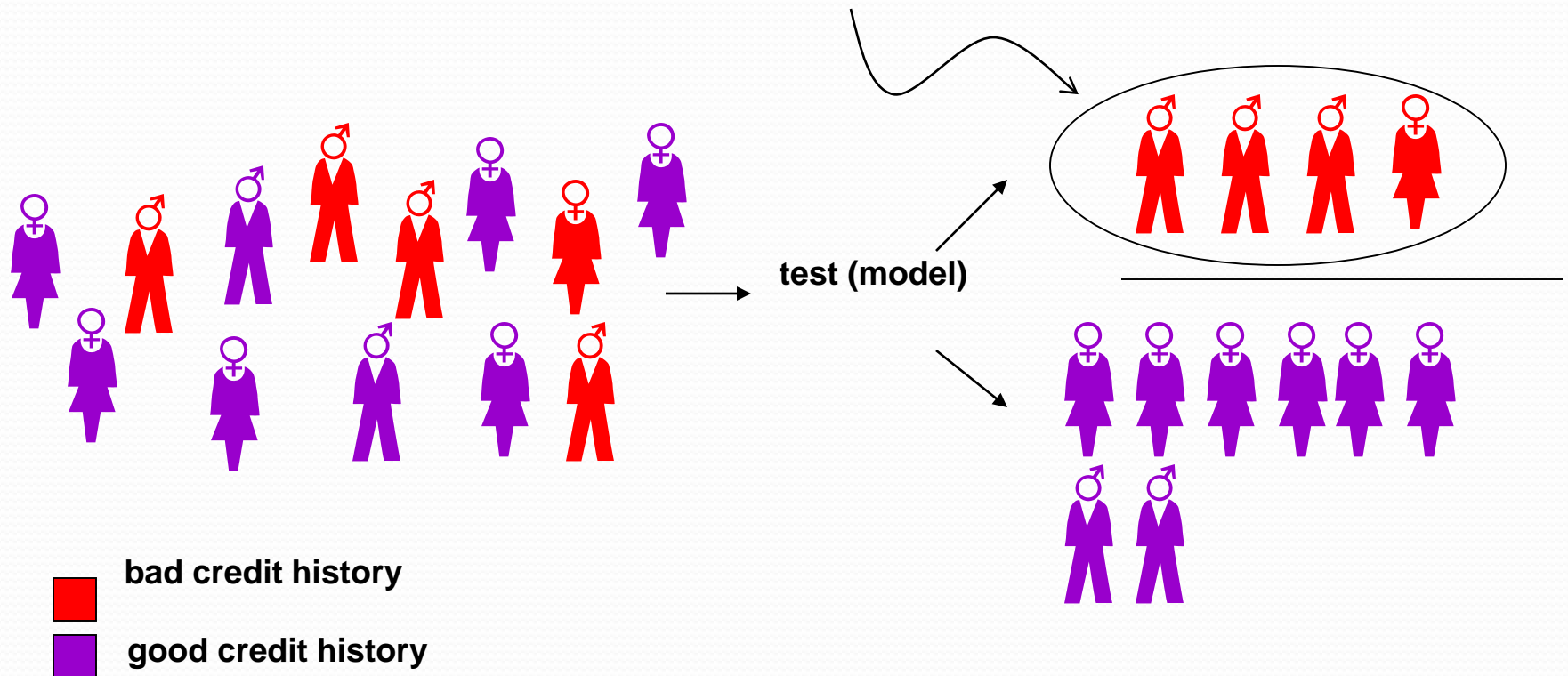
Slides are based on Prof. Ben Kao's work.

Overview

- Basic decision tree classifier (DT) construction
- Some technical issues of DT classification
- Evaluating classifiers

Classification

What common characteristics are shared by the red people, and not by the purple people?



Record id	Age	Income	Student	Credit-rating	Own-computer
1	< 30	High	No	Bad	No
2	< 30	High	No	Good	No
3	30 .. 40	High	No	Bad	Yes
4	> 40	Medium	No	Bad	Yes
5	>40	Low	Yes	Bad	Yes
6	> 40	Low	Yes	Good	No
7	30 .. 40	Low	Yes	Good	Yes
8	< 30	Medium	No	Bad	No
9	< 30	Low	Yes	Bad	Yes
10	> 40	Medium	Yes	Bad	Yes
11	< 30	Medium	Yes	Good	Yes
12	30 .. 40	Medium	No	Good	Yes
13	30 .. 40	High	Yes	Bad	Yes
14	> 40	Medium	No	Good	No

Example rules

- If age < 30 and is not a student \Rightarrow *not a computer owner*
- If age < 30 and is a student \Rightarrow *a computer owner*
- If age is between 30 to 40 \Rightarrow *a computer owner*
- If age > 40 with a good credit rating \Rightarrow *not a computer owner*
- If age > 40 with a bad credit rating \Rightarrow *a computer owner*

Data Model

- a dataset consists of a number of records
- each record consists of a number of attribute values
- one particular attribute is called the *label* (or *class*)
- records that share the same label value form a class
- we want to discover rules that help predict, given a future (unclassified) record, which class the record should belong

Supervised Learning

- our general approach to the classification problem
 - prepare a dataset of labeled records
 - draw a random sample (e.g., 80%), call it the *training set*
 - use the training set to train a classifier
 - apply the classifier to the rest (e.g., 20%) of the records (the *test set*) to evaluate the accuracy of the classifier
 - during the training phase, the classifier is fed with labeled records (*examples of each class*), the learning is supervised. This machine learning approach is called *supervised learning*.

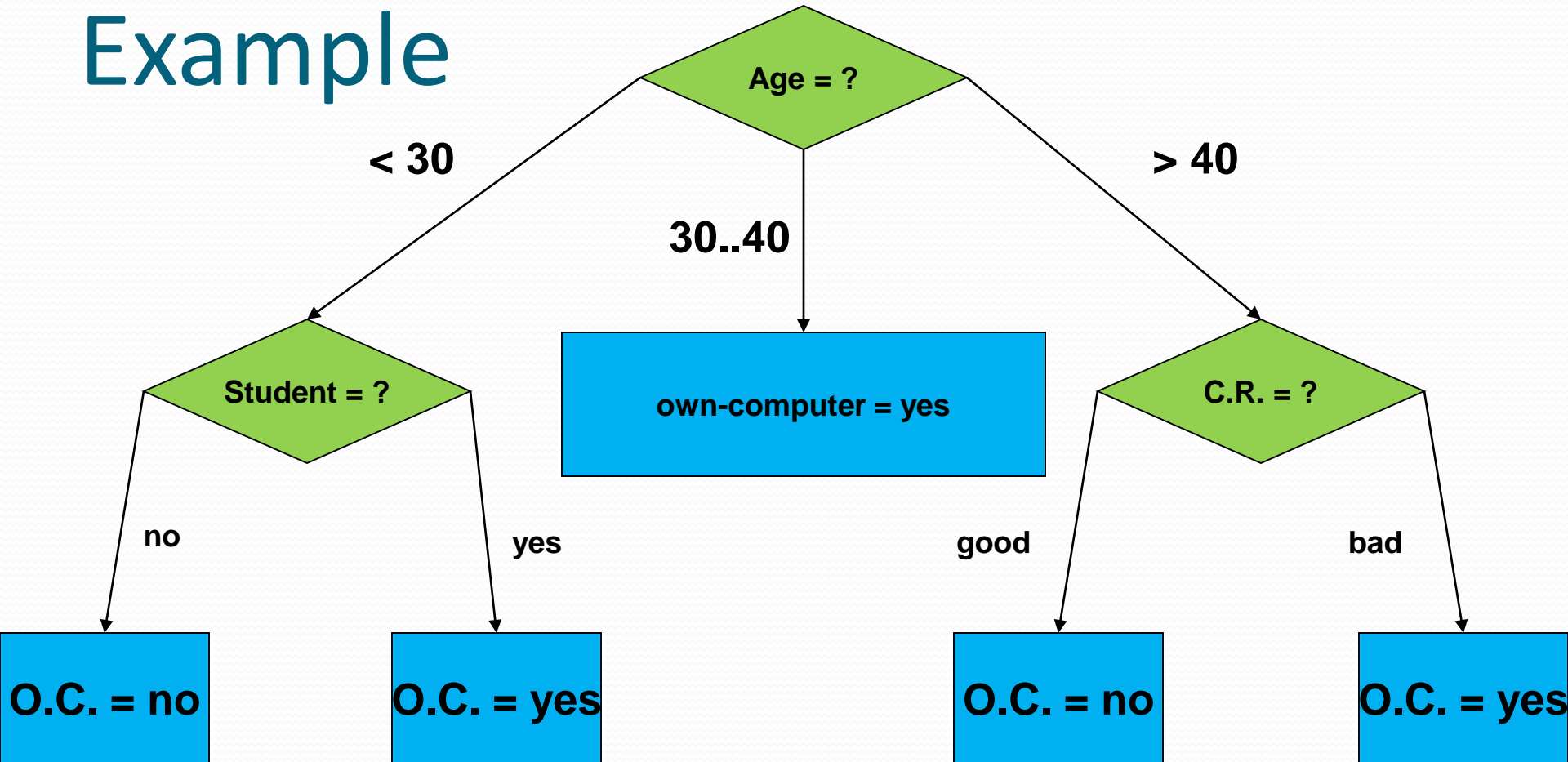
Decision-Tree Classifier (DT)

- we consider how to build a *decision-tree classifier*
- we assume that attributes are all *nominal* – they only take on a finite set of *named-values*
- numeric attributes can be mapped to nominal attributes by *discretization* or *binning*
- example:
 - income can be grouped into
 - low ($< 80K$), medium ($\geq 80K, < 250K$), high ($\geq 250K$)
 - a person's height can be
 - very short, short, average, tall, very tall (with a suitable mapping)

Decision-Tree Classifier

- a decision tree is a tree structure
- properties:
 - each *internal node* denotes a *test* on an attribute
 - each *branch* from a node represents an *outcome* of a test
 - each *leaf node* is associated with a *class label*

Example



Entropy

- entropy is a measure of *uncertainty* or *randomness*
- consider an information source which sends a stream of symbols ('a' or 'b') to a recipient



Entropy

- Q: how certain is the recipient in *predicting* the next symbol the information source would send?
- A: depends on the *probabilities* with which the source sends the symbols

Entropy

- Examples:
 - if the source sends 'a' and 'b' with equal probability, then the recipient is *very uncertain*
 - if the source always sends 'a' and not 'b', then the recipient is *very certain*
 - if the source sends 'a' with a probability of 0.9, and sends 'b' with a probability of 0.1, then the recipient is *pretty certain*
 - what if the source could send 3 symbols 'a', 'b', and 'c' with probabilities 0.3, 0.6, and 0.1, respectively? How certain is the recipient?

Entropy

- entropy is a *numeric measure* to quantify the concept of *uncertainty*
- According to Shannon, the entropy of an information source, S , is defined as:

$$H(S) = \sum_i p_i \log_2 \frac{1}{p_i}$$

where p_i is the probability that the i -th symbol occurs.

- Larger entropy \Leftrightarrow higher uncertainty

Example

- if the information source sends:
 - 'a' (0.5), 'b' (0.5)
 - entropy = $0.5 * \log_2 (1/0.5) + 0.5 * \log_2 (1/0.5) = 1$
 - 'a' (1.0), 'b' (0.0)
 - entropy = $1.0 * \log_2 (1/1.0) = 0$
 - 'a' (0.9), 'b' (0.1)
 - entropy = $0.9 * \log_2 (1/0.9) + 0.1 * \log_2 (1/0.1) = 0.469$
 - 'a' (0.3), 'b' (0.6), 'c' (0.1)
 - entropy = $0.3 * \log_2 (1/0.3) + 0.6 * \log_2 (1/0.6) + 0.1 * \log_2 (1/0.1) = 1.295$

Example

- if the information source sends:

- 'a' (0.5), 'b' (0.5)

- entropy = $0.5 * \log_2 (1/0.5) + 0.5 * \log_2 (1/0.5) = 1$

Very uncertain

- 'a' (1.0), 'b' (0.0)

- entropy = $1.0 * \log_2 (1/1.0) = 0$

Very certain

- 'a' (0.9), 'b' (0.1)

- entropy = $0.9 * \log_2 (1/0.9) + 0.1 * \log_2 (1/0.1) = 0.469$

A bit uncertain

- 'a' (0.3), 'b' (0.6), 'c' (0.1)

- entropy = $0.3 * \log_2 (1/0.3) + 0.6 * \log_2 (1/0.6) + 0.1 * \log_2 (1/0.1) = 1.295$

Very very uncertain

Entropy

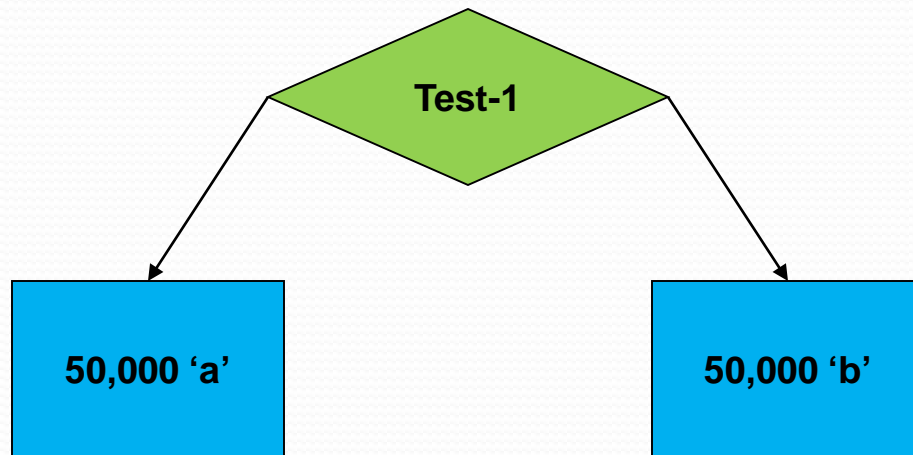
- the concept of entropy is used to select the tests used in a decision tree
- consider a dataset of 100,000 records with
 - 50,000 labeled 'a'
 - 50,000 labeled 'b'
 - if you are given a new record (the 100,001st) and you are asked to give it a label, how uncertain are you?
 - using entropy, your amount of uncertainty (without any additional information) is 1.0

Entropy

- consider a dataset of 100,000 records with
 - 90,000 labeled 'a'
 - 10,000 labeled 'b'
 - if you are given a new record (the 100,001st) and you are asked to give it a label, how uncertain are you?
 - using entropy, your amount of uncertainty (without any additional information) is only 0.469. In fact, you are somewhat sure that the record should be labeled 'a'.

Finding a Good Test

- consider the case with 50,000 'a' records and 50,000 'b' records again
- suppose you come up with a test (Test-1) that partitions the 100,000 records into two groups:



Finding a Good Test

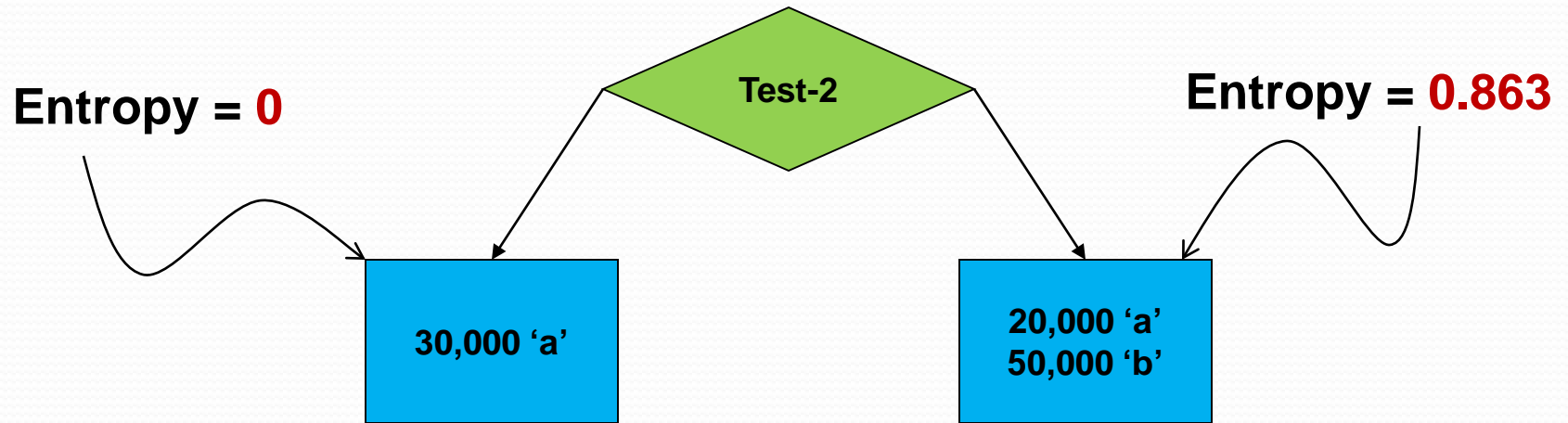
- How good is Test-1?

Finding a Good Test

- How good is Test-1?
 - *it is perfect!*
- Test-1 successfully classified all 100,000 records.
- Given an unlabeled record x , we can apply Test-1 on x .
If Test-1 indicates that x should go to the
 - left group: we are very certain that x should be labeled 'a' because x is sharing the group with 50,000 'a' records and not with any 'b' record
 - right group: x should be labeled 'b'
- Note that the entropy of either group is 0

Finding a Good Test

- consider another test Test-2

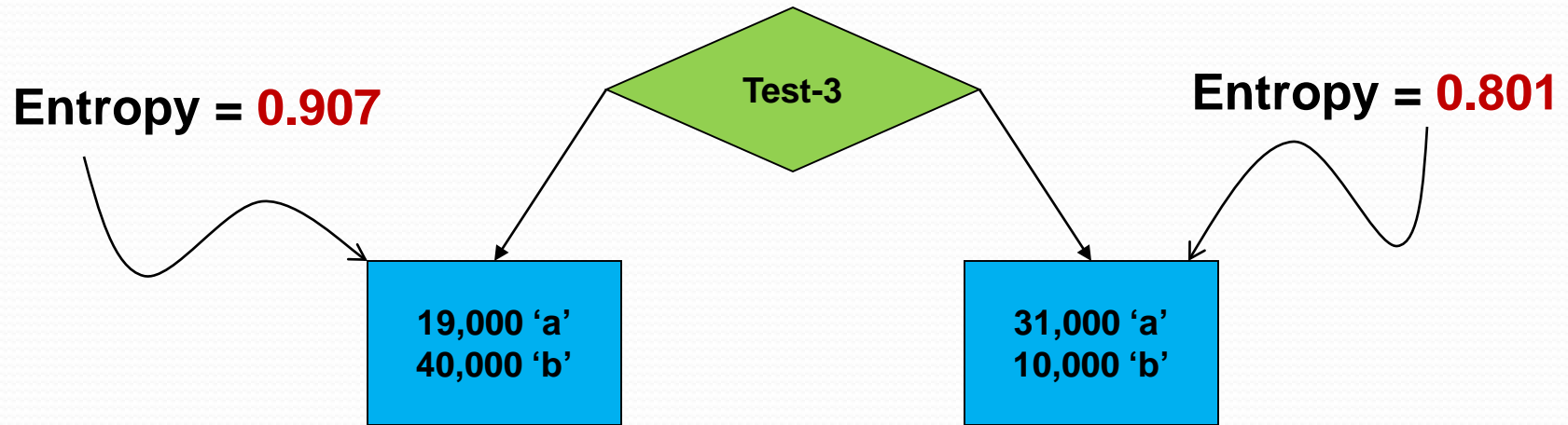


Finding a Good Test

- since 30% of the records are put to the left group by Test2 (and 70% to the right), given a new record, x , we would expect that x will go to the left group (after Test2) with a 30% probability
- the expected entropy (after Test2) is thus:
 - $0.3 * 0 + 0.7 * 0.863 = 0.604$
- Test2 is a *good* test in the sense that it reduces the entropy from 1.0 to 0.604.
- $1 - 0.604 = 0.396$ is called the *information gain* of the test.

Finding a Good Test

- consider yet another test Test-3



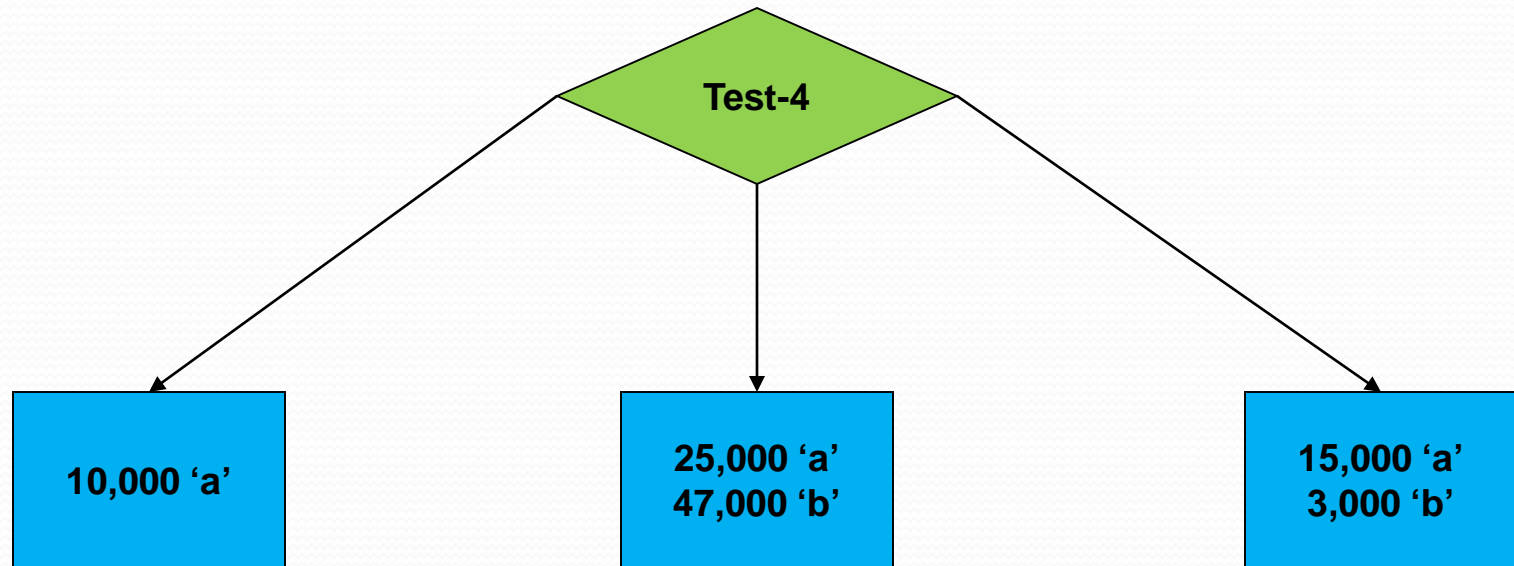
- expected entropy after Test-3:
 - $(59/100) * 0.907 + (41/100) * 0.801 = 0.864$

Finding a Good Test

- ranking the 3 tests:
 - Test-1 is the best (highest information gain)
 - Test-2 is the second best
 - Test-3 is the worst

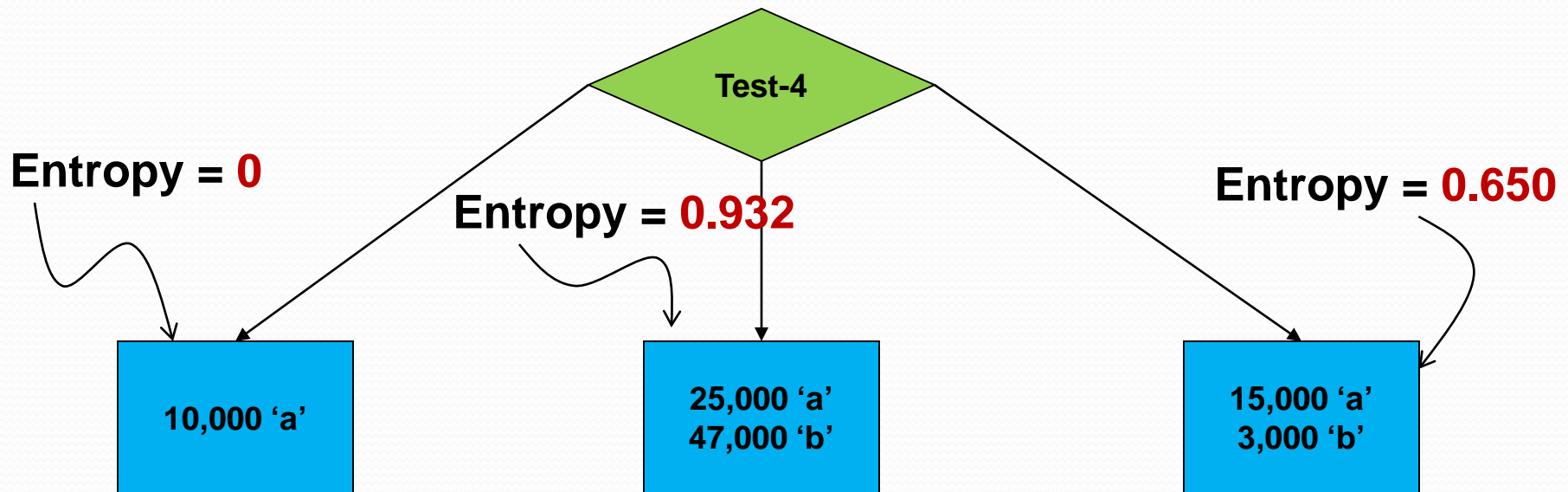
Finding a Good Test

- What about this test?



Finding a Good Test

- What about this test?




$$\text{expected entropy} = 0.1 * 0 + 0.72 * 0.932 + 0.18 * 0.65 = 0.788$$

Build a Decision Tree

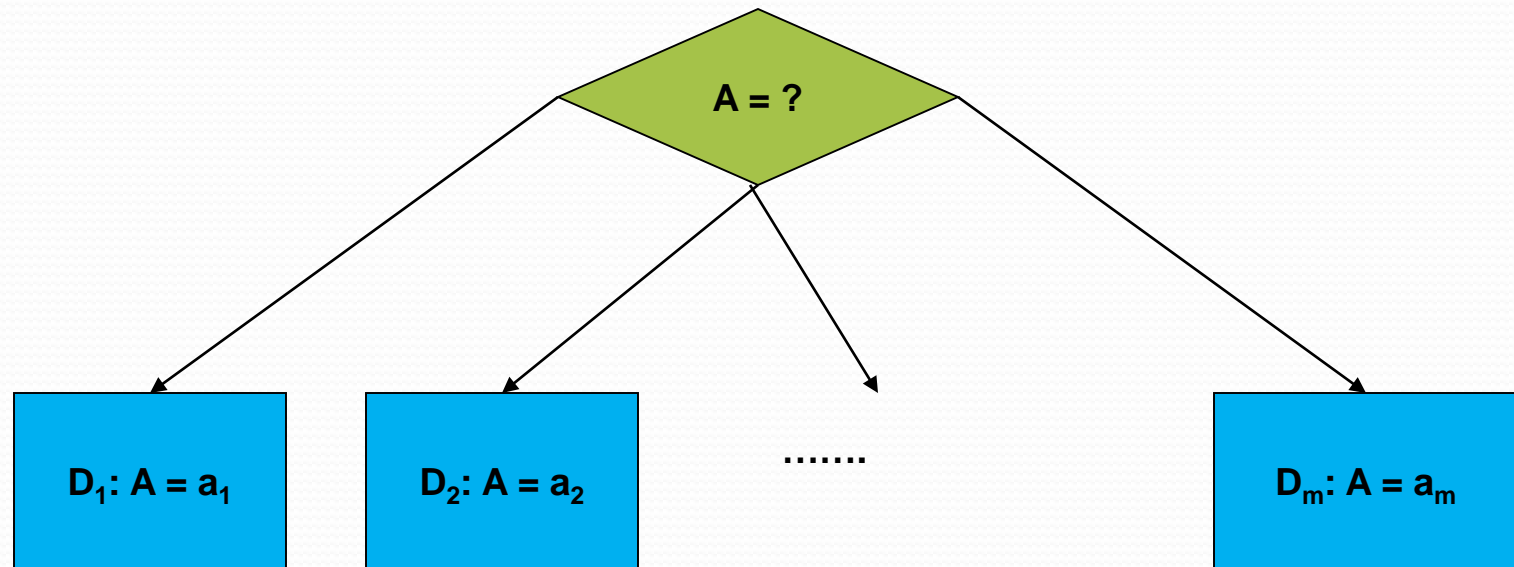
- base on the concept of test and entropy
- call our algorithm $\text{build-tree}(D, L)$ where
 - D is a training set of data records
 - L is a list of nominal attributes
- want to build a decision tree using tests on attributes' values
- A recursive construction algorithm

Procedure (base cases)

- if ...
 - all records in D are of the same label K
 - $\text{build-tree}(D, L)$ returns a tree with only a leaf node labeled K .
No test is needed
 - L is empty \Rightarrow no tests can be derived
 - $\text{build-tree}(D, L)$ returns a tree with only a leaf node labeled M ,
where M = most common label among the records in D .
 - all records in D share the same attribute values for all attributes in $L \Rightarrow$ no meaningful tests can be derived
 - repeat the action of the 2nd case.
- 

Procedure (recursive case)

- otherwise, compute the most effective (i.e., most entropy reducing) test that can be derived from the attributes in L . Let the test be



Procedure

- suppose the test divides D into m groups: $D_1 \dots D_m$
- create a node labeled “ $A=?$ ”
- for each group, D_i ,
 - if D_i is empty, create a subtree T_i with a lone leaf node labeled M , where M is the most common label among the records in D
 - else
 - recursively call $\text{build-tree}(D_i, L-\{A\})$ to build a subtree T_i ,
 - connect the test node “ $A=?$ ” to T_i by a branch labeled “ a_i ”

Record id	Age	Income	Student	Credit-rating	Own-computer
1	< 30	High	No	Bad	No
2	< 30	High	No	Good	No
3	30 .. 40	High	No	Bad	Yes
4	> 40	Medium	No	Bad	Yes
5	>40	Low	Yes	Bad	Yes
6	> 40	Low	Yes	Good	No
7	30 .. 40	Low	Yes	Good	Yes
8	< 30	Medium	No	Bad	No
9	< 30	Low	Yes	Bad	Yes
10	> 40	Medium	Yes	Bad	Yes
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12	30 .. 40	Medium	No	Good	Yes
13	30 .. 40	High	Yes	Bad	Yes
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Example

- Dataset D :
 - 14 records
 - label attribute: “Own-computer”
 - 9 computer owners, 5 non-owners
 - entropy of D
 - $5/14 * \log_2 (14/5) + 9/14 * \log_2 (14/9) = 0.940$
 - 4 nominal attributes for deriving tests
 - $L = \{\text{‘Age’, ‘Income’, ‘Student’, ‘Credit-rating’}\}$
 - goal: to derive rules that would classify a person as a computer owner or not

Example

- determine the effectiveness of 4 tests
- the test: “Age = ?”, e.g., divides D into 3 groups:

Group 1: Age < 30

Record id	Age	Income	Student	Credit-rating	Own-computer
1	< 30	High	No	Bad	No
2	< 30	High	No	Good	No
8	< 30	Medium	No	Bad	No
9	< 30	Low	Yes	Bad	Yes
11	< 30	Medium	Yes	Good	Yes

Group 2: Age: 30..40

Record id	Age	Income	Student	Credit-rating	Own-computer
3	30 .. 40	High	No	Bad	Yes
7	30 .. 40	Low	Yes	Good	Yes
12	30 .. 40	Medium	No	Good	Yes
13	30 .. 40	High	Yes	Bad	Yes

Group 3: Age > 40

Record id	Age	Income	Student	Credit-rating	Own-computer
4	> 40	Medium	No	Bad	Yes
5	>40	Low	Yes	Bad	Yes
6	> 40	Low	Yes	Good	No
10	> 40	Medium	Yes	Bad	Yes
14	> 40	Medium	No	Good	No

Example

- entropy of:
 - group 1 = $2/5 * \log_2 (5/2) + 3/5 * \log_2 (5/3) = 0.971$
 - group 2 = 0
 - group 3 = $2/5 * \log_2 (5/2) + 3/5 * \log_2 (5/3) = 0.971$
- expected entropy (after test using the “Age” attribute)
=
 $(5/14 * 0.971) + (4/14 * 0) + (5/14 * 0.971) = \boxed{0.694}$

Example

attribute test	expected entropy
Age	0.694
Income	0.911
Student	0.788
Credit-rating	0.892

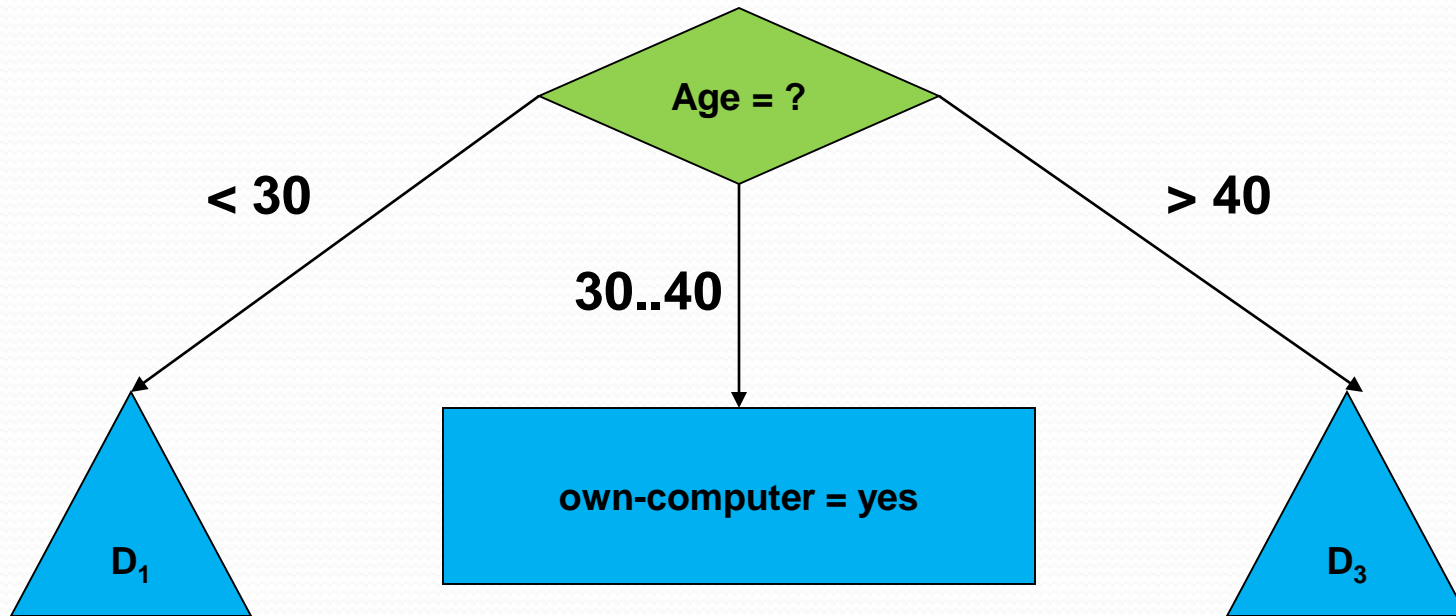
Best



Example

- “Age” wins out.
- D is divided into 3 groups:
 - D_1 (Age < 30) = {1, 2, 8, 9, 11}
 - D_2 (Age: 30..40) = {3, 7, 12, 13}
 - D_3 (Age > 40) = {4, 5, 6, 10, 14}
- we recursively apply build-tree to the three datasets, with $L = \{\text{“Income”, “Student”, “Credit-rating”}\}$
- Since all records in D_2 are of the same label (own-computer = yes), a node is created labeled “own-computer = yes”

A partially-built tree



Example

- For D_1 , we have

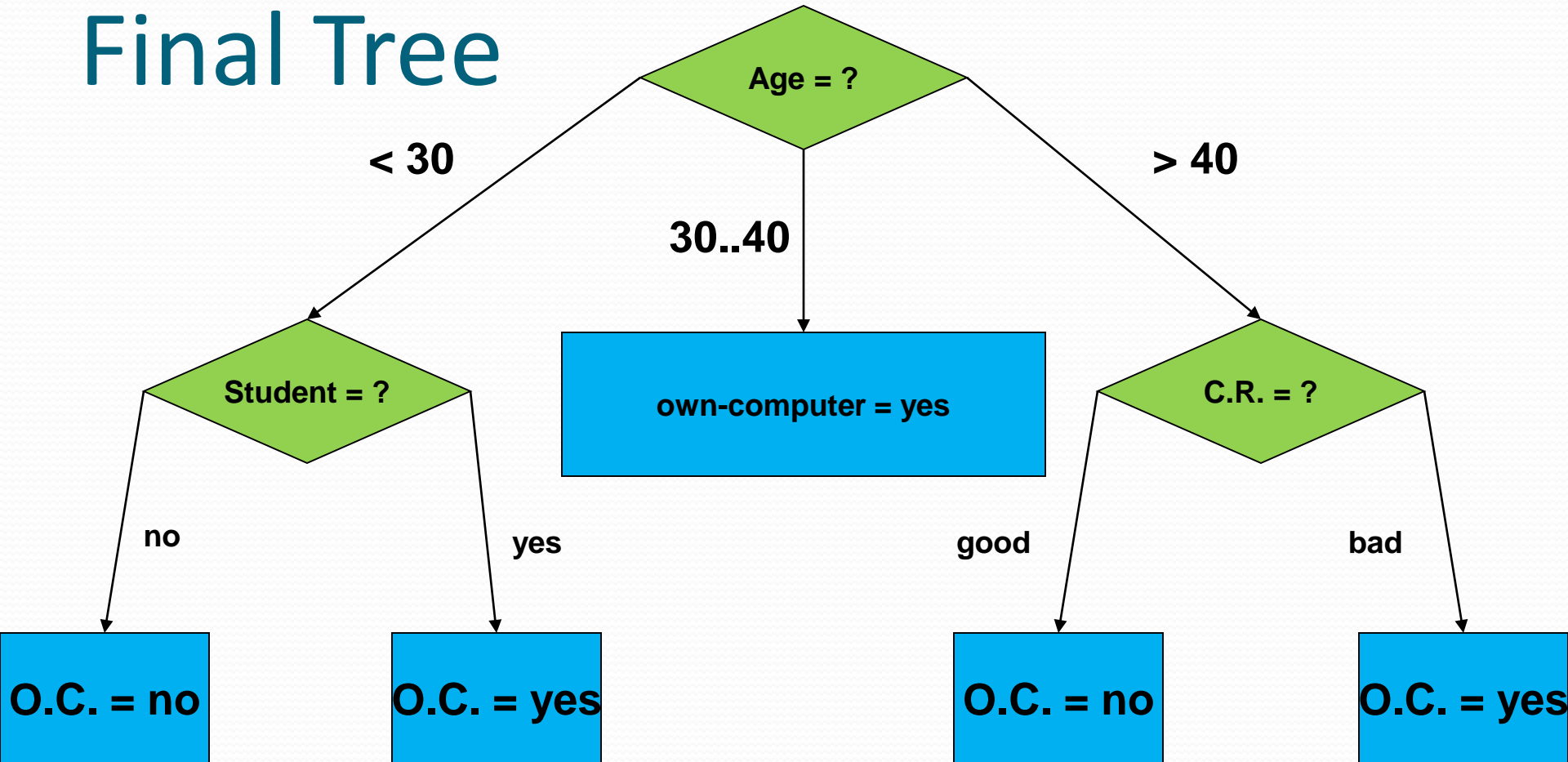
attribute test	expected entropy
Income	0.4
Student	0
Credit-rating	0.951

Example

- For D_3 , we have

attribute test	expected entropy
Income	0.951
Student	0.951
Credit-rating	0

Final Tree



Rules

- We derive classification rules from the decision tree by *walking* the tree from the root to every leaf.
 - If age < 30 and is not a student \Rightarrow not a computer owner
 - If age < 30 and is a student \Rightarrow a computer owner
 - If age is between 30 to 40 \Rightarrow a computer owner
 - If age > 40 with a good credit rating \Rightarrow not a computer owner
 - If age > 40 with a bad credit rating \Rightarrow a computer owner

Applying Rules

- Given a record X :

<i>Age</i>	<i>Income</i>	<i>Student</i>	<i>Credit-rating</i>
< 30	medium	yes	fair

is X a computer-owner or not?

Algorithm build-tree(D, L) {

Begin

If all records in D share the same label 'K'

Return a leaf node with the label 'K';

If ((L is empty) || (all records in D share the same attribute values)) {

Let 'K' be the most common label in D;

Return a leaf node with the label 'K';

}

For each attribute A in L do

Compute the expected entropy achieved by using A as the test on D;

Let A be the attribute which achieves the smallest expected entropy;

Create a node N with label "A = ?";

Assume A has n possible values a_1, \dots, a_n

Partition D into D_1, \dots, D_n , where D_i contains all the records with $A = a_i$;

For each a_i do {

If D_i is empty {

Let 'K' be the most common label in D;

Attach a leaf node to N labeled 'K';

}

Else

Attach the sub-tree obtained by calling build-tree(D_i , L-{A}) to N;

}

Return the tree rooted at N;

End

Issues

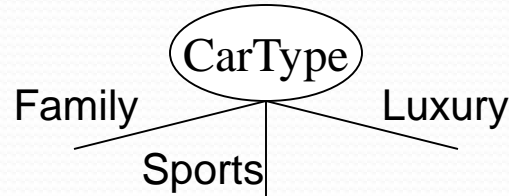
- How to derive a test based on an attribute?
- How to measure the purity (certainty, uncertainty) of a dataset?
- How to measure the performance of a classifier?
- Numerical attribute
- Overfitting

How to derive a test?

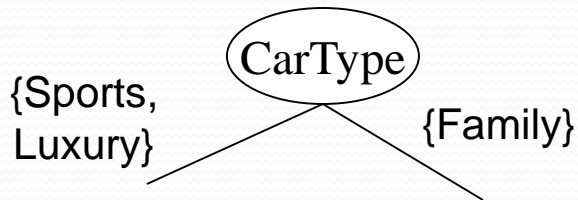
- Depends on attribute types
 - Nominal
 - Ordinal
 - Continuous (numerical)
- Depends on number of ways to split
 - 2-way split
 - Multi-way split

Splitting (Nominal Attributes)

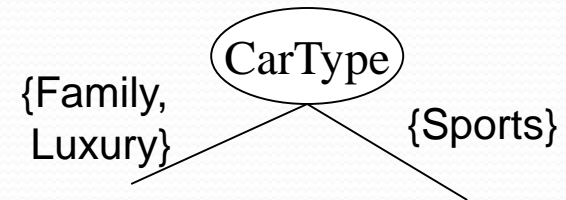
- *Multi-way split*: Use as many partitions as distinct values.



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

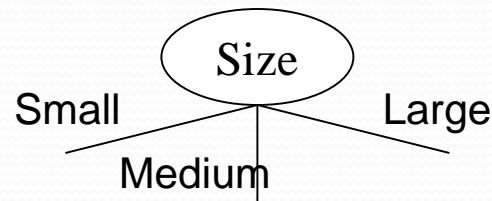


OR



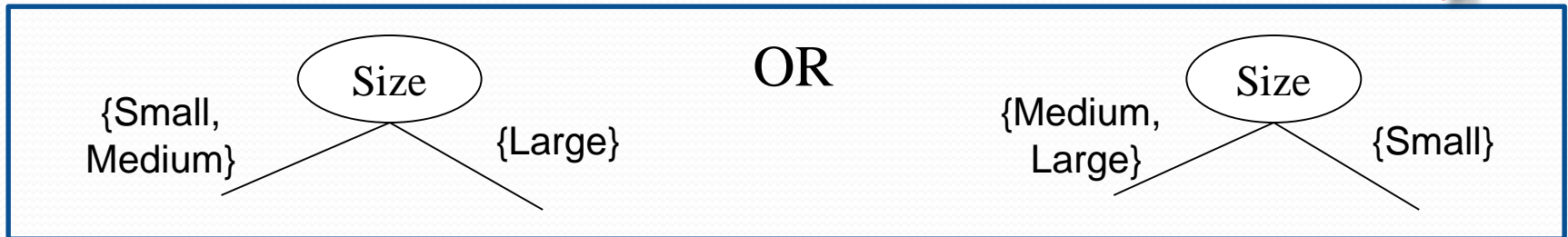
Splitting (Ordinal Attributes)

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

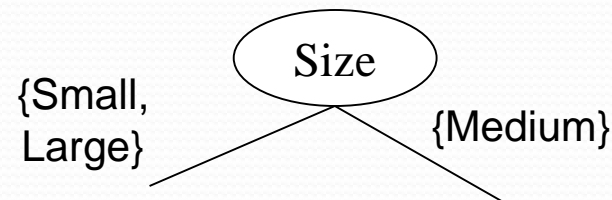


Order preserving

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



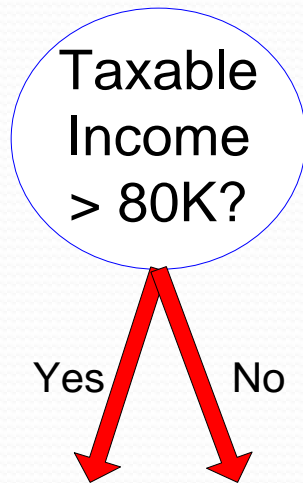
- What about this split?



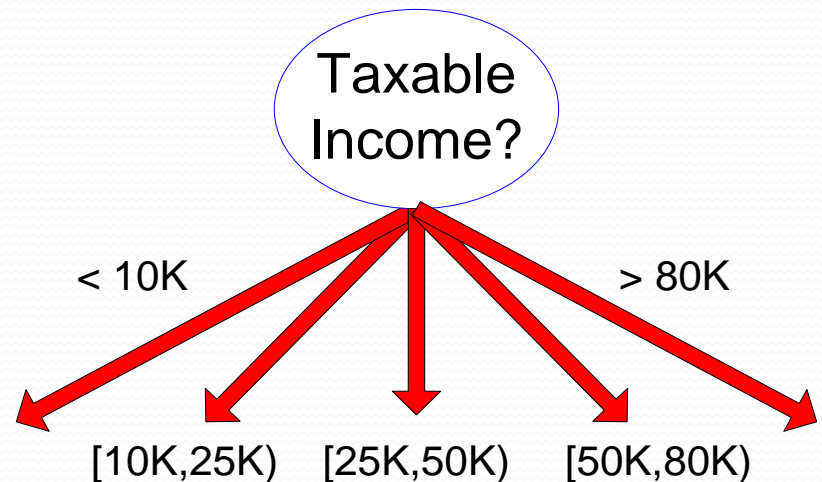
Splitting (Continuous Attributes)

- *Discretization*: transform it to an ordinal attribute
- *Binary Decision*: $(A < v)$ or $(A \geq v)$
 - consider all possible splits and finds the best cut
 - can be more computationally expensive

Splitting (Continuous Attributes)



(i) Binary split



(ii) Multi-way split

Impurity measures

- Entropy (Information Gain) – ID₃
- Gain Ratio – C4.5
- Gini Index - CART
- Classification error

Entropy/Information gain

- Disadvantage: Tends to prefer splits that result in large number of partitions, each being small but pure.

Gain Ratio

- Gain Ratio:

$$GainRATIO = \frac{GAIN}{SplitINFO}$$

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

- Parent Node, p is split into k partitions
- n_i is the number of records in partition i
- Gain = reduction in entropy due to the test.
- Adjusts Information Gain by the entropy of the partitioning (SplitINFO). Higher entropy partitioning (large number of small partitions) is penalized!
- Used in C4.5
- Designed to overcome the disadvantage of Information Gain

Before Splitting:

C0	N00
C1	N01

→ M0

A?

Yes

No

Node N1

Node N2

C0	N10
C1	N11

C0	N20
C1	N21

M1

M2

M12

B?

Yes

No

Node N3

Node N4

C0	N30
C1	N31

C0	N40
C1	N41

M3

M4

M34

Gain = M0 – M12 vs M0 – M34

GINI

- Used in CART
- Given a set S :

$$GINI(S) = 1 - \sum_i (p_i)^2$$

- Maximum $(1 - 1/n_c)$, where n_c is the number of classes
- Minimum (0.0) when all records belong to one class

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	

$$GINI(S) = 1 - \sum_i (p_i)^2$$

Example (GINI)

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

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

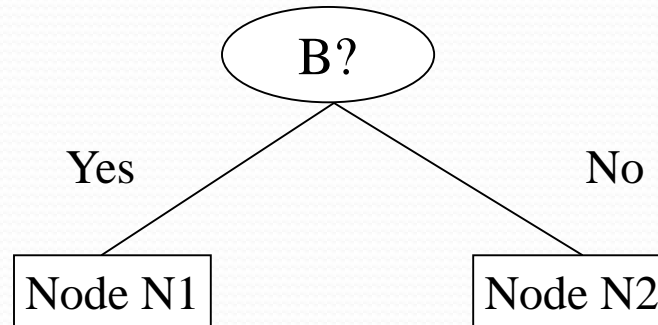
$$Gini = 1 - (1/6)^2 - (5/6)^2 = 0.278$$

C1	2
C2	4

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

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

Example (GINI)



$$\begin{aligned} \text{Gini(N1)} &= 1 - (5/7)^2 - (2/7)^2 \\ &= 0.194 \end{aligned}$$

$$\begin{aligned} \text{Gini(N2)} &= 1 - (1/5)^2 - (4/5)^2 \\ &= 0.528 \end{aligned}$$

	N1	N2
C1	5	1
C2	2	4
Gini=0.333		

	Parent
C1	6
C2	6
Gini = 0.500	

$$\begin{aligned} \text{Gini(Children)} &= 7/12 * 0.194 + \\ &\quad 5/12 * 0.528 \\ &= 0.333 \end{aligned}$$

Classification Error

- Given a set S :

$$Error(S) = 1 - \max_i P_i$$

- Measures misclassification error made by a node, where n_c is the number of classes
 - Maximum ($1 - 1/n_c$)
 - Minimum (0.0)

Example (Classification Error)

C1	0
C2	6

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

$$\text{Error} = 1 - \max(0, 1) = 1 - 1 = 0$$

C1	1
C2	5

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

$$\text{Error} = 1 - \max(1/6, 5/6) = 1 - 5/6 = 1/6$$

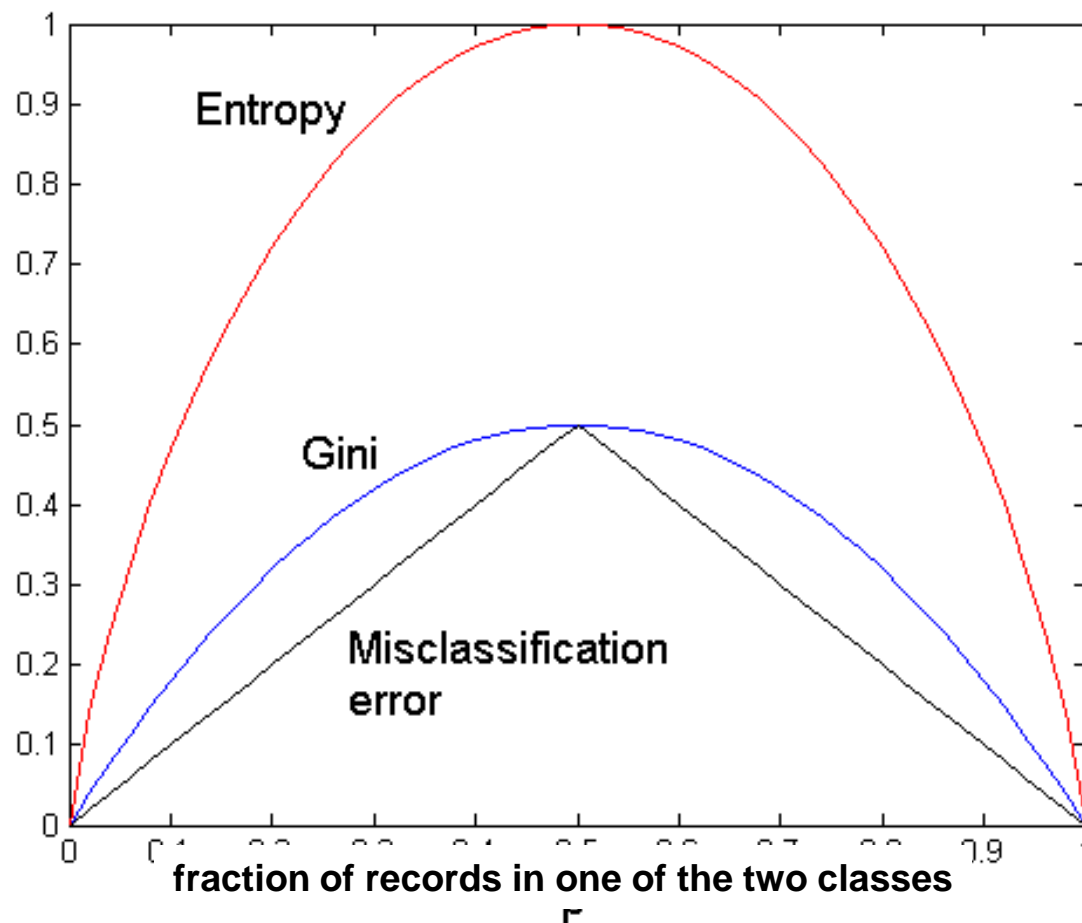
C1	2
C2	4

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

$$\text{Error} = 1 - \max(2/6, 4/6) = 1 - 4/6 = 1/3$$

Comparison

For a 2-class problem:



Exercise

Q1. It is important to calculate the worst-case computational complexity of the decision tree algorithm. Given data set D , the number of attributes n , and the number of training tuples $|D|$, show that the computational cost of growing a tree is at most $n \times |D| \times \log(|D|)$.

Evaluating Classifiers

- Accuracy metrics
- Training set vs. test set

Accuracy metrics

- Use test data of known class labels
- Confusion Matrix:

ACTUAL CLASS	PREDICTED CLASS	
	Class=Yes	Class=No
Class=Yes	<i>a</i>	<i>b</i>
Class=No	<i>c</i>	<i>d</i>

a: TP (true positive)
b: FN (false negative)
c: FP (false positive)
d: TN (true negative)

correct

incorrect

Accuracy

ACTUAL CLASS	PREDICTED CLASS		
		Class=Yes	Class=No
	Class=Yes	a (TP)	b (FN)
	Class=No	c (FP)	d (TN)

$$\text{Accuracy} = \frac{a + d}{a + b + c + d} = \frac{TP + TN}{TP + TN + FP + FN}$$

$$\text{Error rate (e)} = 1 - \text{accuracy}$$

The simple “accuracy” measure may be misleading especially when the classes are “imbalanced”.

Other metrics

- Assume two class labels (positive, negative)
- $\text{precision} = \text{TP} / (\text{TP} + \text{FP})$
 - The fraction of “positive class predictions” that are truly positives.
- $\text{recall} = \text{TP} / (\text{TP} + \text{FN})$
 - The fraction of “positives” that are predicted positives.
- $\text{F measure} = (2 * \text{precision} * \text{recall}) / (\text{precision} + \text{recall})$

ACTUAL CLASS	PREDICTED CLASS	
	Class=Yes	Class=No
	Class=Yes	Class=No
	a (TP)	b (FN)
	c (FP)	d (TN)

Getting a (training set, test set) pair

- Holdout
- Random subsampling
- Cross validation
- Bootstrap

Holdout Method

- Given a set of N labeled records (examples)
- Reserve $2/3$ for training and $1/3$ for testing
- Limitations
 - fewer labeled examples available for training
 - Larger training set \Rightarrow more accurate model built, but fewer test examples to give a good accuracy evaluation ... (and vice versa)

Random subsampling

- Repeated holdout
- Repeat experiment k times, each with a different sample of the data as holdout
- Classifier's accuracy = average accuracy of classifier on samples
- Limitations
 - some records may be used more often than others in training/testing

Cross-validation

- k -fold cross-validation:
 - Divide the examples into k partitions
 - Run classifier by using $k-1$ partitions as training data and one partition as test data
 - Repeat for all combinations of $k-1$ partitions and measure average accuracy

Bootstrap approach

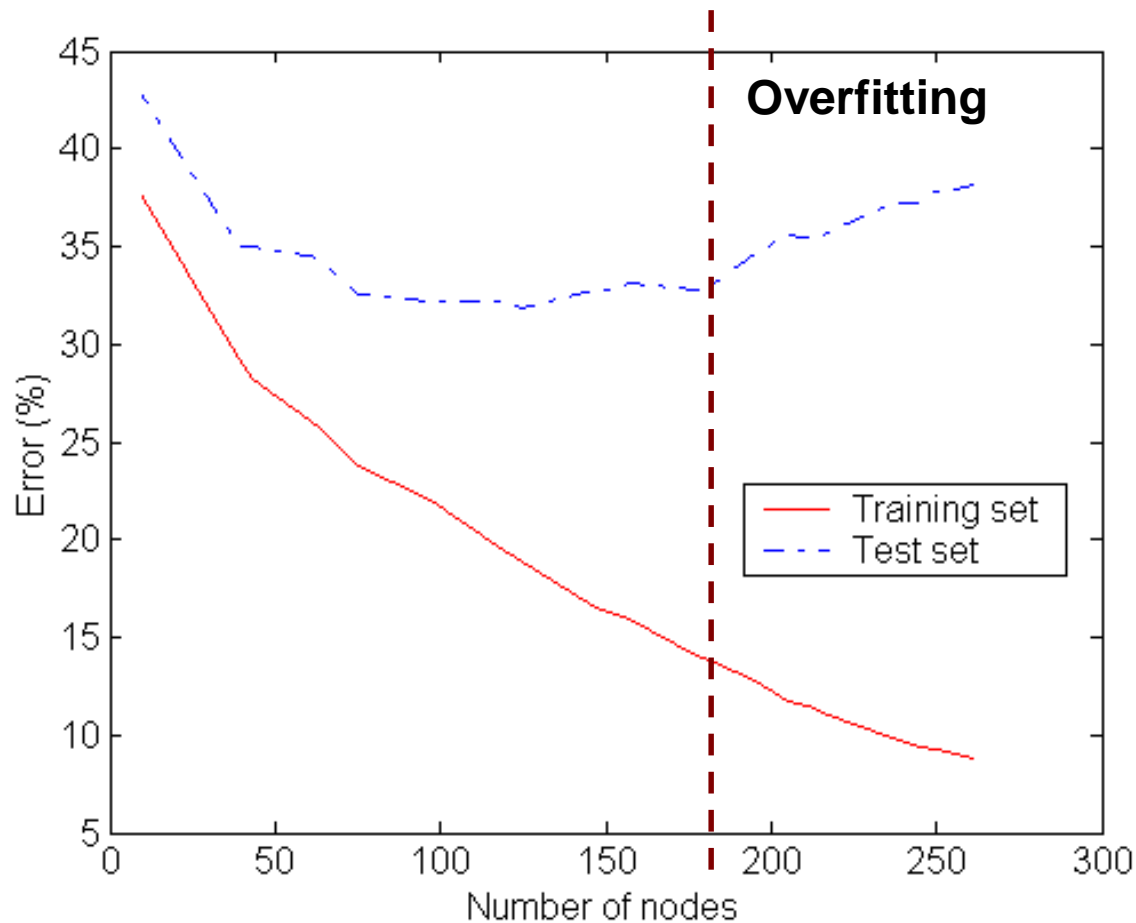
- Sample with replacement
- An N -sized sample contains 63.2% of the data
- Repeat b times and compute average accuracy

Training error vs. Generalization error

- Given a training set X , we derive a model M
- We can apply the model M on X and measure the error of the model in classifying X 's records.
 - The error is called *training error* e_X
- We can apply the model M on a test set Y
 - The error is called *test error* e_Y
- *Generalization error* (e_G) = expected error when M is applied to a future unseen record.
- Since M is derived from X , it naturally fits X .
- In general, $e_G > e_X$
- We hope that $e_G \approx e_Y$

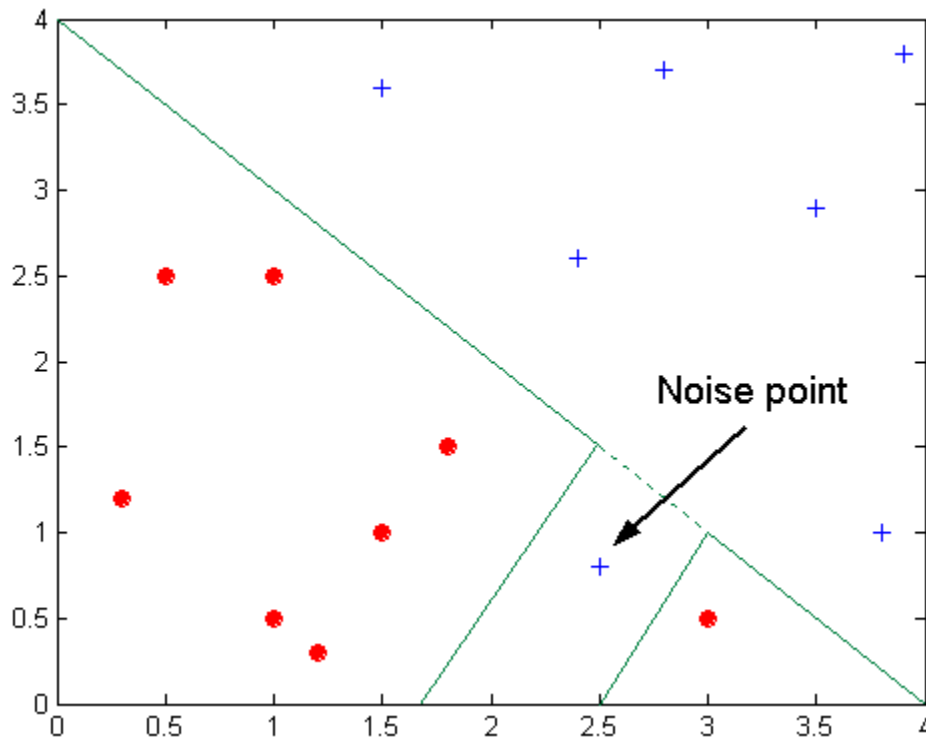
Overfitting and Underfitting

- When we build M , we aim at reducing the impurity of a tree node. Essentially, we are building an M that reduces e_X .
- Issue: M may be fitting the training set too well that it becomes *too specific* to the training set. This issue is called *model overfitting*.
- Model overfitting $\Rightarrow M$ is not generally applicable to records other than the training set \Rightarrow large e_G .



Underfitting: when model is too simple, both training and test errors are large

Overfitting due to noise



- **Overfitting results in decision trees that are more complex than necessary**

Decision boundary is distorted by noise point

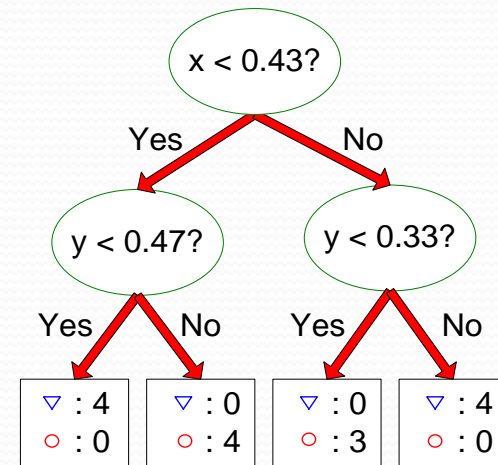
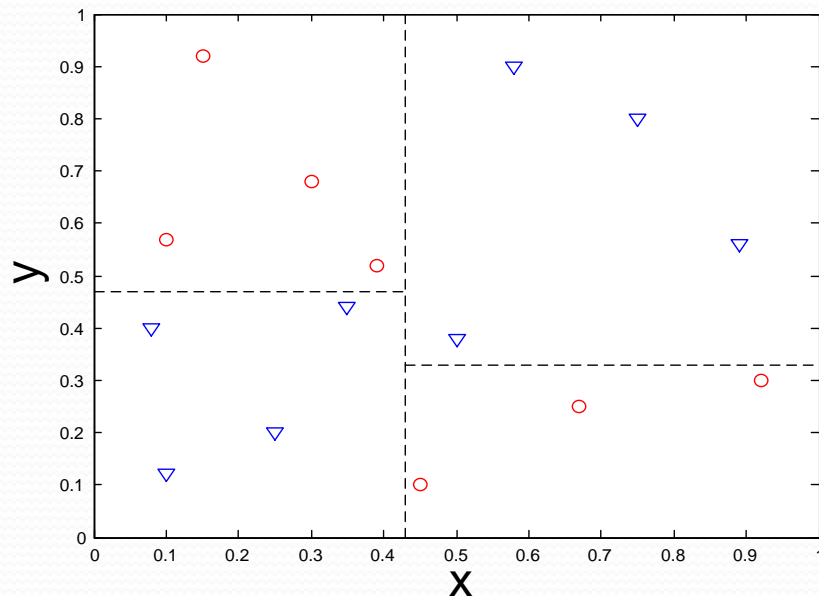
Handling overfitting

- Pre-Pruning (Early Stopping Rule)
 - Stop the algorithm before it becomes a fully-grown tree
 - Typical stopping conditions for a node:
 - Stop if all instances belong to the same class
 - Stop if all the attribute values are the same
 - More restrictive conditions:
 - Stop if **number of instances is less** than some user-specified threshold
 - Stop if **expanding the current node does not improve impurity measures** (e.g., Gini or information gain) by much.

Handling overfitting

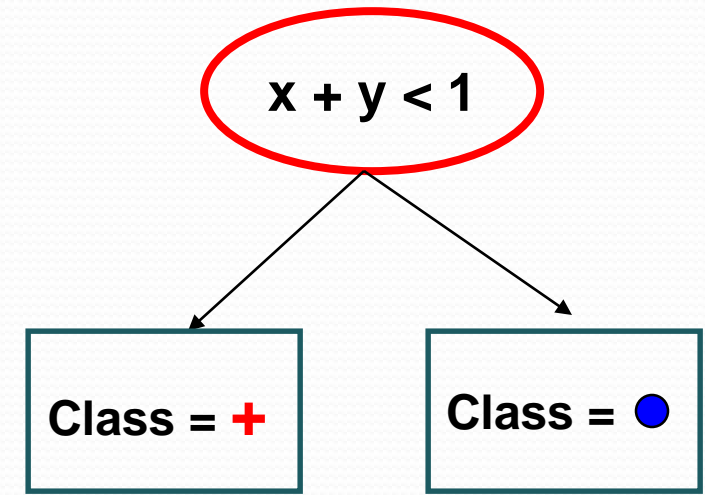
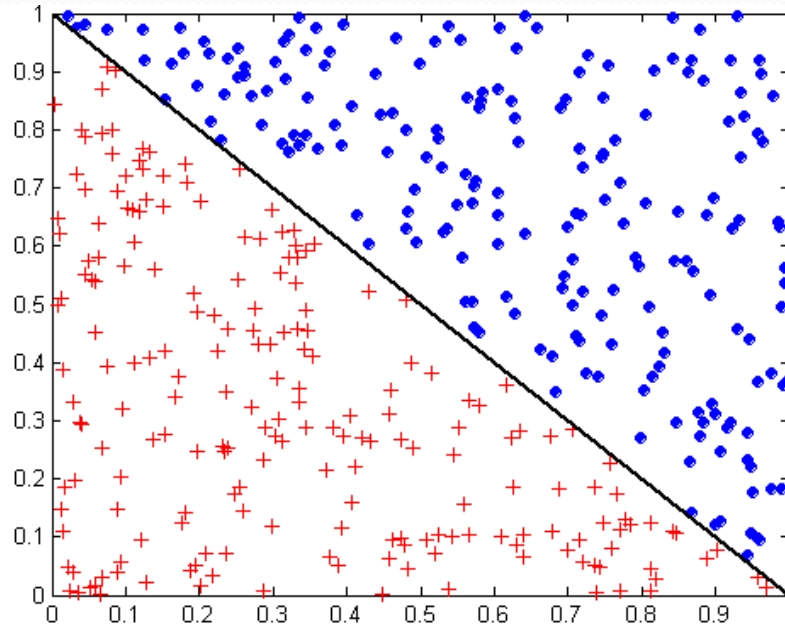
- Post-pruning
 - Grow decision tree to its entirety
 - Trim the nodes of the decision tree in a bottom-up fashion
 - Class label of leaf node is determined from majority class of instances in the sub-tree
 - Basic idea: given a tree T and a node v to be pruned to obtain a pruned tree T' :
 - Estimate a cost complexity (cc):
 - More node: \uparrow cc; Larger error: \uparrow cc
 - If $\text{cc of } T' < \text{cc of } T$, prune v .

Decision Boundary



- Border line between two neighboring regions of different classes is known as decision boundary
- Decision boundary is parallel to axes because test condition involves a single attribute at-a-time

Oblique Decision Trees



- Test condition may involve multiple attributes

Decision Tree Based Classification

- Advantages:
 - Non-parametric
 - Inexpensive to construct
 - Extremely fast at classifying unknown records
 - Easy to interpret small-sized trees
 - Accuracy is comparable to other classification techniques for many simple data sets
- Disadvantages
 - Subject to overfitting
 - Do not generalize well for some discrete-valued functions (e.g. parity functions)
 - Decision boundaries are only rectilinear