Classification:
Basic Concepts, Model Evaluation and Decision Trees

Classification: Definition

- Given a collection of examples (*dataset*)
  - Each example (record) contains a set of *attributes (features)*, one of the attributes is the *class*.
- Find a *model* (or procedure) to predict the class attribute as a function of the values of other attributes.
- Goal: previously unseen examples should be classified as accurately as possible (generalization).

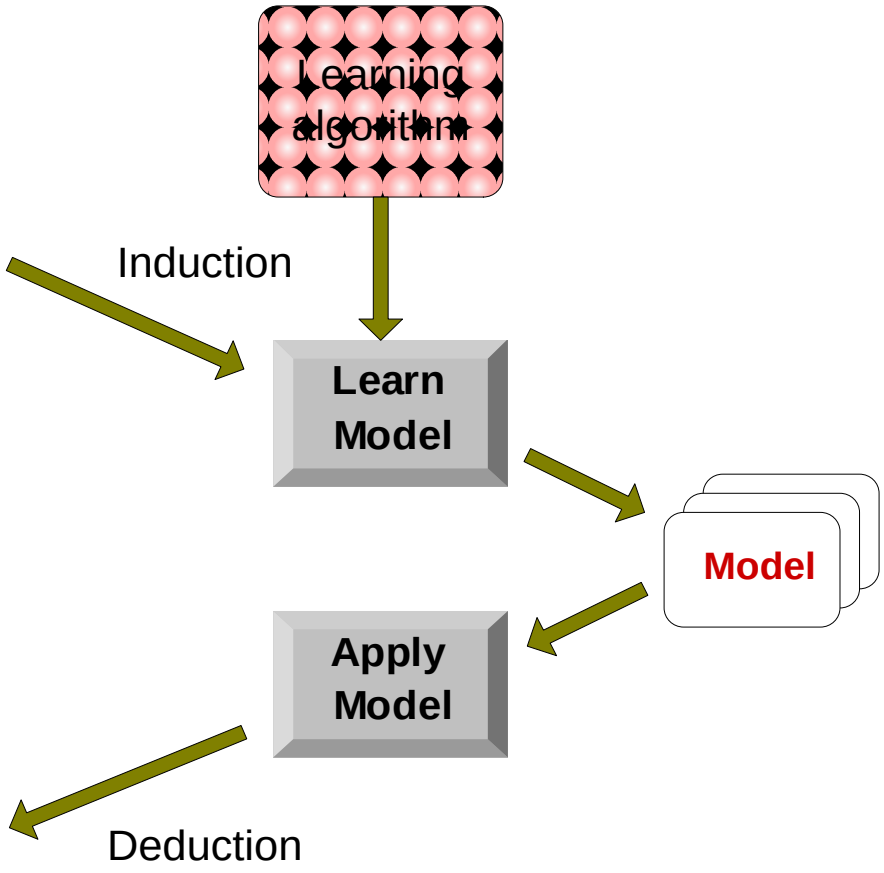
Illustrating Classification Task

Tid	Attrib1	Attrib2	Attrib3	Class
1	Yes	Large	125K	No
2	No	Medium	100K	No
3	No	Small	70K	No
4	Yes	Medium	120K	No
5	No	Large	95K	Yes
6	No	Medium	60K	No
7	Yes	Large	220K	No
8	No	Small	85K	Yes
9	No	Medium	75K	No
10	No	Small	90K	Yes

Training Set

Tid	Attrib1	Attrib2	Attrib3	Class
11	No	Small	55K	?
12	Yes	Medium	80K	?
13	Yes	Large	110K	?
14	No	Small	95K	?
15	No	Large	67K	?

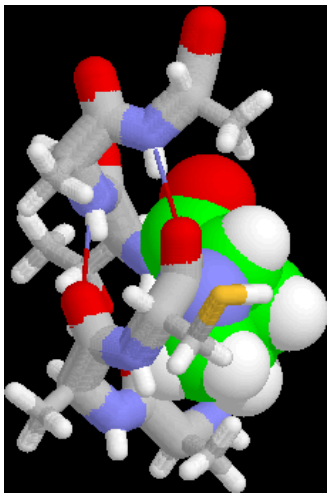
Test Set



Examples of Classification Task

- Predicting tumor cells as benign or malignant
- Classifying credit card transactions as legitimate or fraudulent

- Classifying secondary structures of protein as alpha-helix, beta-sheet, or random coil



- Categorizing news stories as finance, weather, entertainment, sports, etc

Classification Techniques

- Decision Tree based Methods
- Rule-based Methods
- Memory based reasoning
- Linear Classifiers and Neural Networks
- Statistical Methods: eg.Naïve Bayes
- Kernel-Based Methods (e.g. Support Vector Machines)

Measures of Classification Performance

- Confusion Matrix
- Two-class examples

		PREDICTED CLASS	
		Class=Yes	Class=No
ACTUAL CLASS	Class=Yes	a	b
	Class=No	c	d

a: TP (true positive)

b: FN (false negative)

c: FP (false positive)

d: TN (true negative)

Measures of Classification Performance

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

- Most widely-used metric:

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

Limitation of Accuracy

- Consider a 2-class problem
  - Number of Class 0 examples = 9990
  - Number of Class 1 examples = 10

- If model predicts everything to be class 0, accuracy is 9990/10000 = 99.9 %
  - Accuracy is misleading because model does not detect any class 1 example

Other Measures

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

$$\text{Precision (p)} = \frac{a}{a+c}$$

$$\text{Recall (r)} = \frac{a}{a+b}$$

$$\text{F-measure (F1)} = \frac{2rp}{r+p} = \frac{2a}{2a+b+c}$$

- F1 measure is closer to the minimum between p and r

Estimating Generalization

- General idea: use another dataset not used for training
- **Holdout**
  - Split the dataset: a% for training and (100-a)% for testing (depends on randomness)
  - Class analogy should be the same in training and test
- **k-fold Cross validation** (k-fold CV) (usually k=10)
  - Partition the dataset into k disjoint subsets (keep class analogy)
  - k-fold: train on k-1 partitions, test on the remaining one
  - Compute average performance on k-folds (+ std)
  - Expensive: requires training of k models
  - Depends on randomness (although to a smaller degree)
  - Leave-one-out: k=n (deterministic split, heavy computation)
- Stratified cross-validation (random partitioning into folds)

Comparing Performance of two methods

- Or of the same method with different parameters
- If models are generated on the same test sets D1,D2, …, Dk (e.g., via cross-validation)
- Each method produces k models:
  - 1st method produces M11 , M12, …, M1k
  - 2nd method produces M21 , M22, …, M2k
  - For each set: compute $d_j = acc_{1j} – acc_{2j}$
  - d_j has mean d_t and variance σ_t

$$\hat{\sigma}_t^2 = \frac{\sum_{j=1}^{k} (d_j - \overline{d})^2}{k(k-1)}$$

$$d_t = d \pm t_{1-\alpha,k-1} \hat{\sigma}_t$$

  - Interval for *d* contains 0 => difference

may not be statistically significant

The generalization problem

- **Occam's Razor**: Prefer the simplest model that fits well to the data
- Very simple models underfit (bad generalization)
- Complex models overfit (bad generalization)

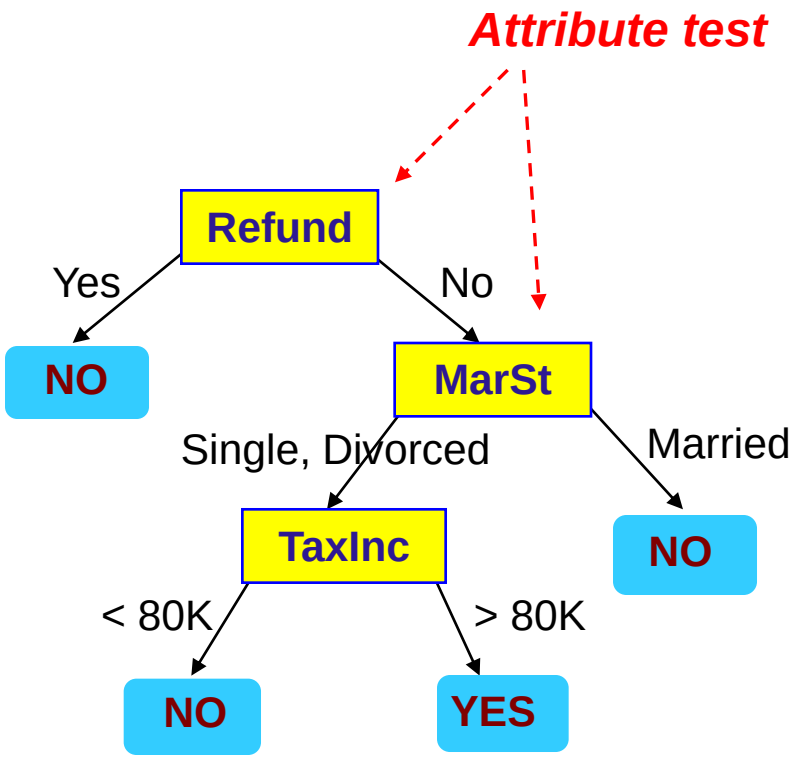
- For a given dataset and type of model, there is an **optimal model complexity** providing **optimal generalization**

Example of a Decision Tree

	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

Dataset

Model: Decision Tree



Class Labels at Leaves

Another Example of Decision Tree

	categorical	categorical	continuous	class
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1	Yes	Single	125K	No
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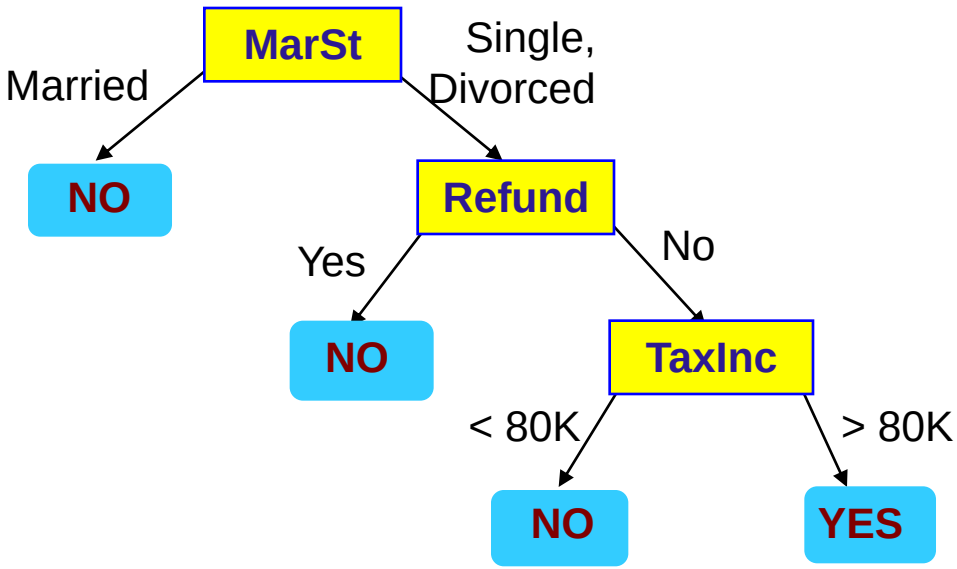

There could be more than one tree that fits the same data!

Decision Tree Classification Task

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Training Set

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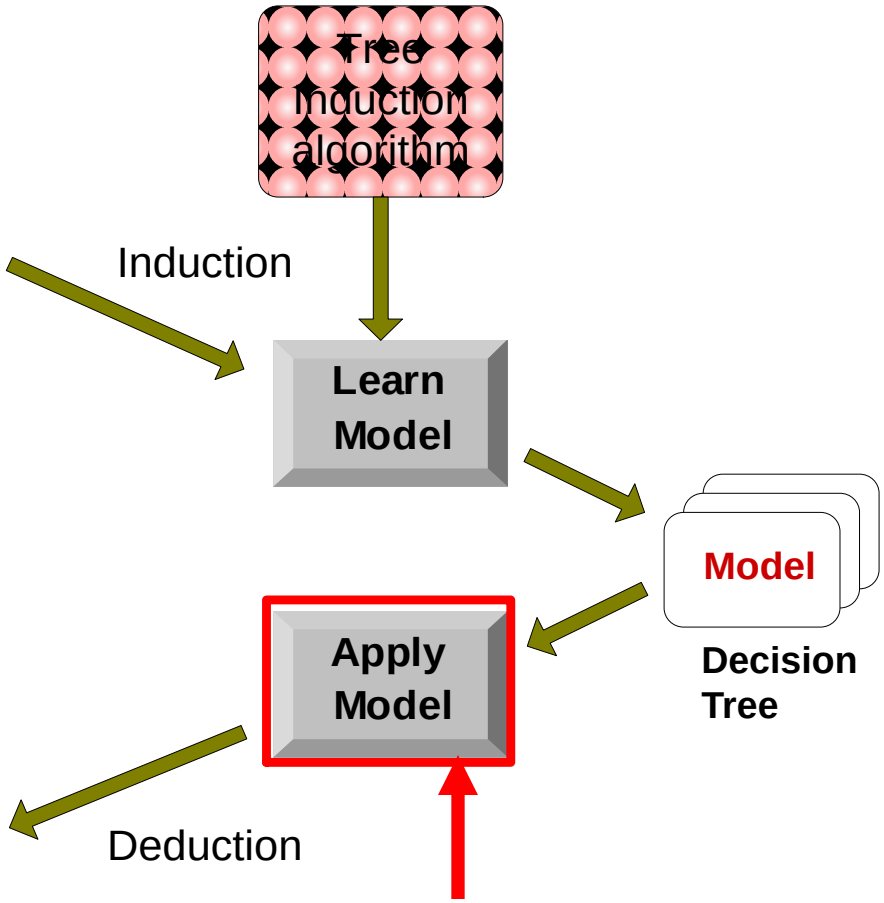
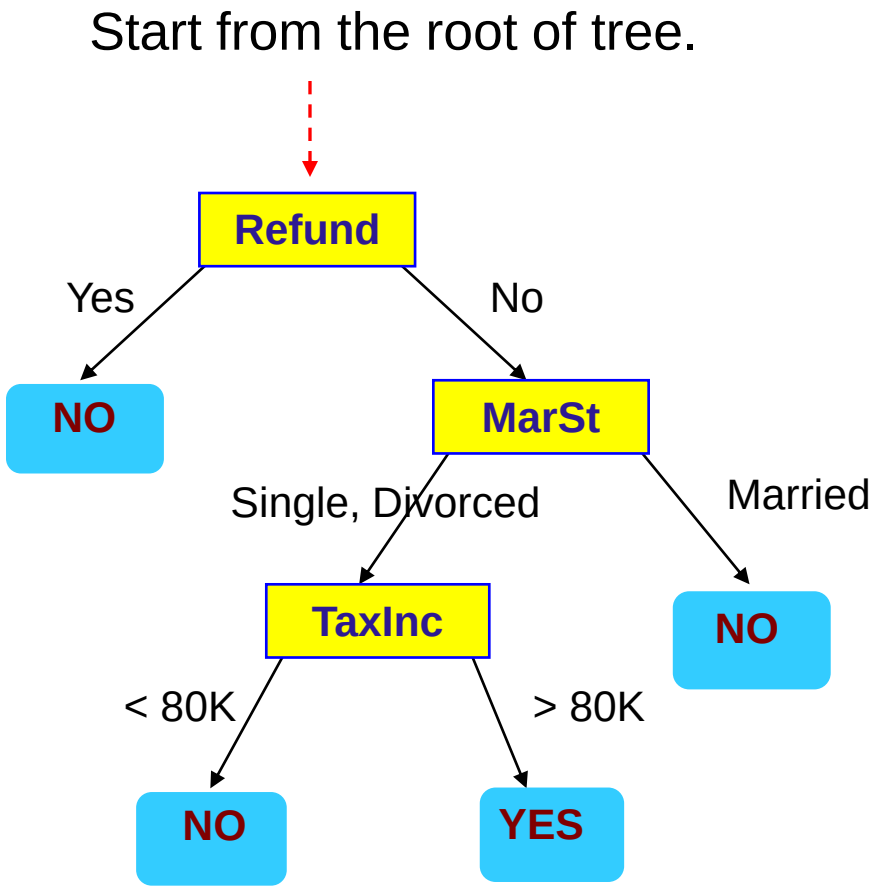


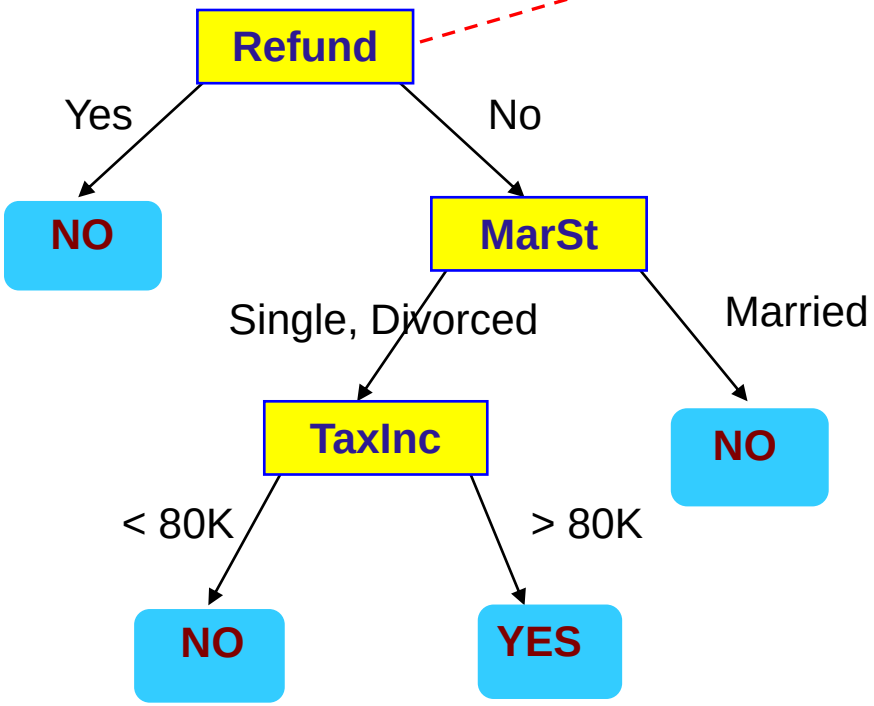
Apply Model to Test Data



Test Data

Refund	Marital Status	Taxable Income	Cheat
No	Married	80K	?

Apply Model to Test Data



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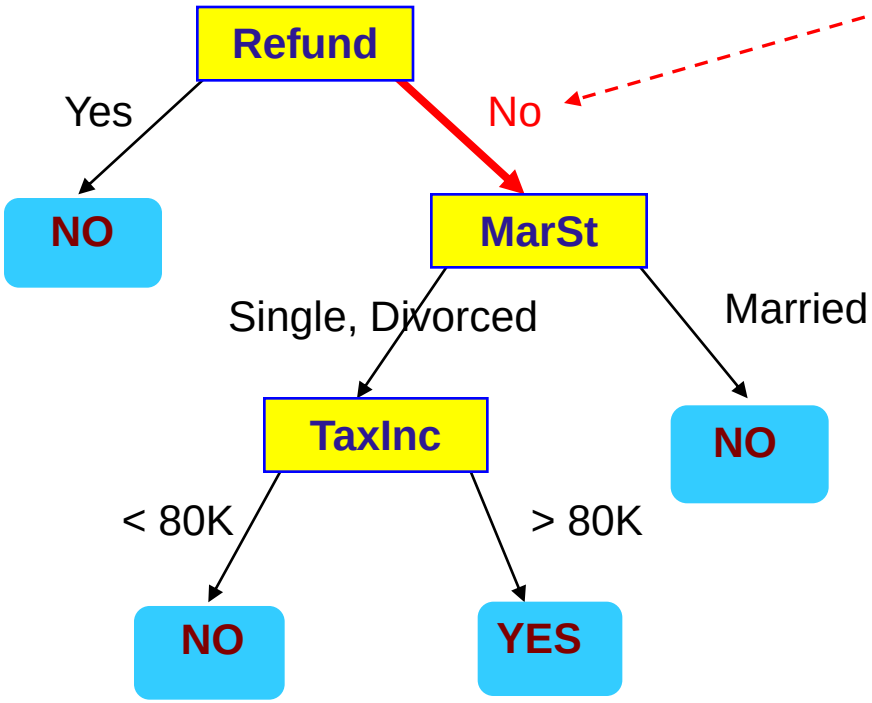

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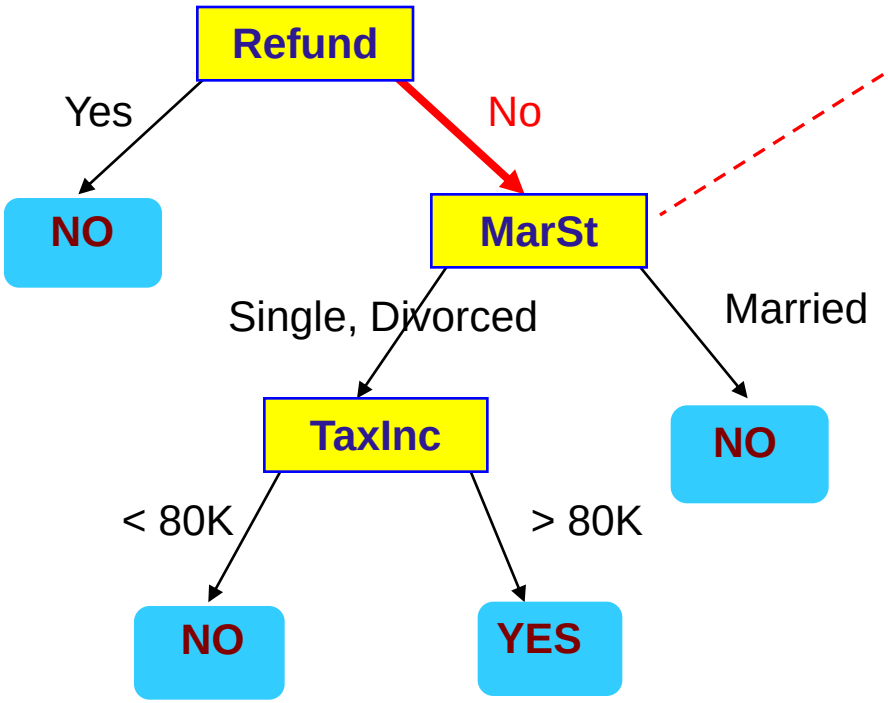

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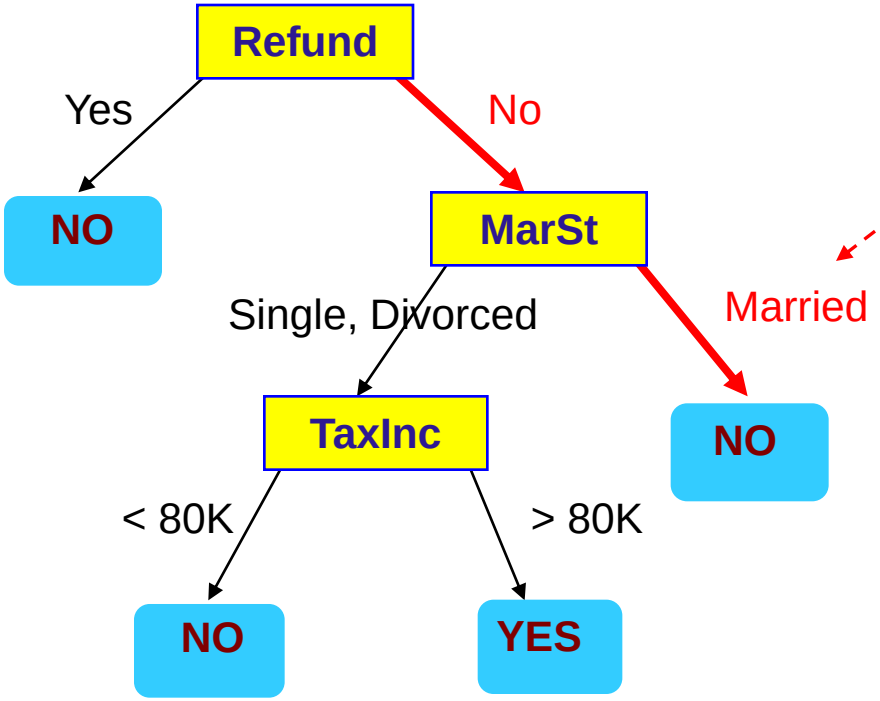

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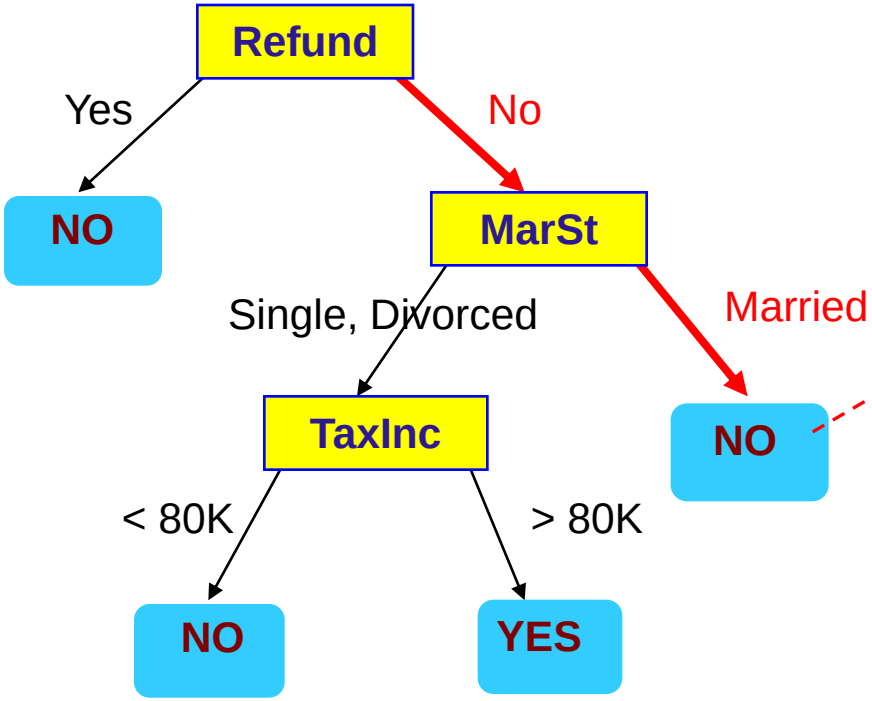

Test Data

Refund	Marital Status	Taxable Income	Cheat
No	Married	80K	?

Assign Cheat to “No”

Decision Tree Classification Task

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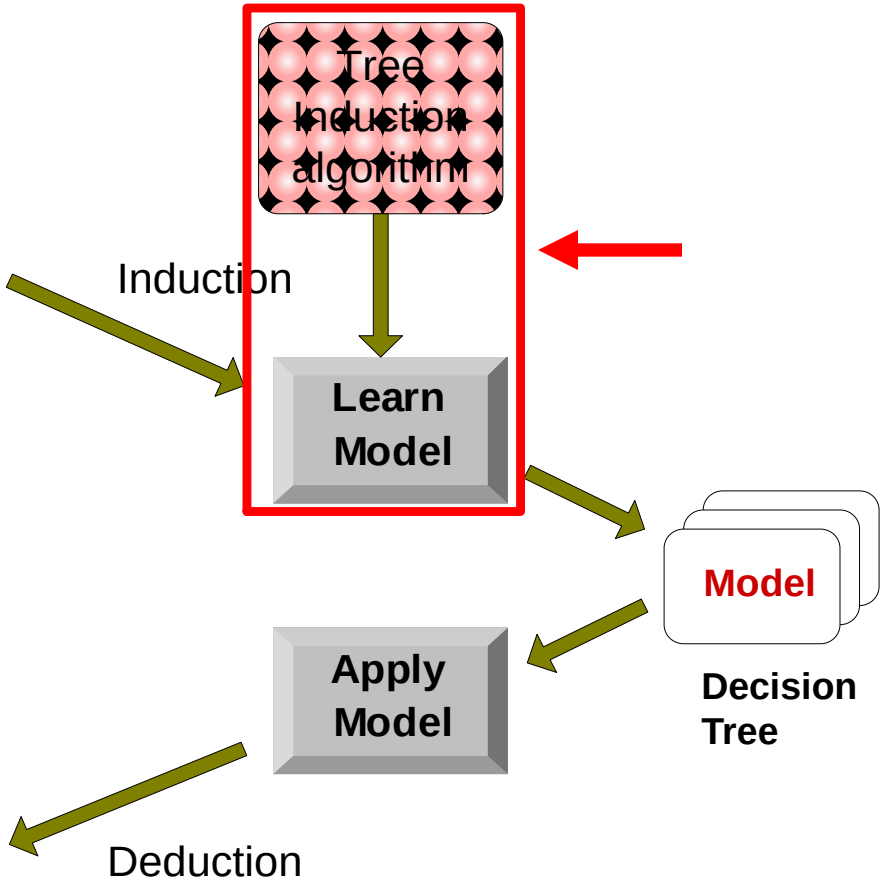

Decision Tree Induction

- Many Algorithms:
  - Hunt's Algorithm (one of the earliest)
  - CART
  - ID3, C4.5
  - SLIQ,SPRINT

General Structure of Hunt's Algorithm

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

Tid	Refund	Marital Status	Taxable Income	Cheat
1	Yes	Single	125K	No
2	No	Married	100K	No
3	No	Single	70K	No
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6	No	Married	60K	No
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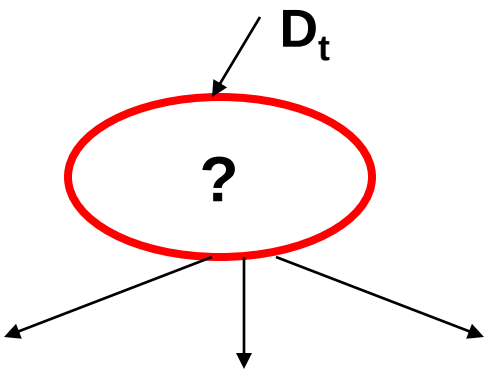
9	No	Married	75K	No
10	No	Single	90K	Yes



Hunt's Algorithm

Tid	Refund	Marital Status	Taxable Income	Cheat
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3	No	Single	70K	No
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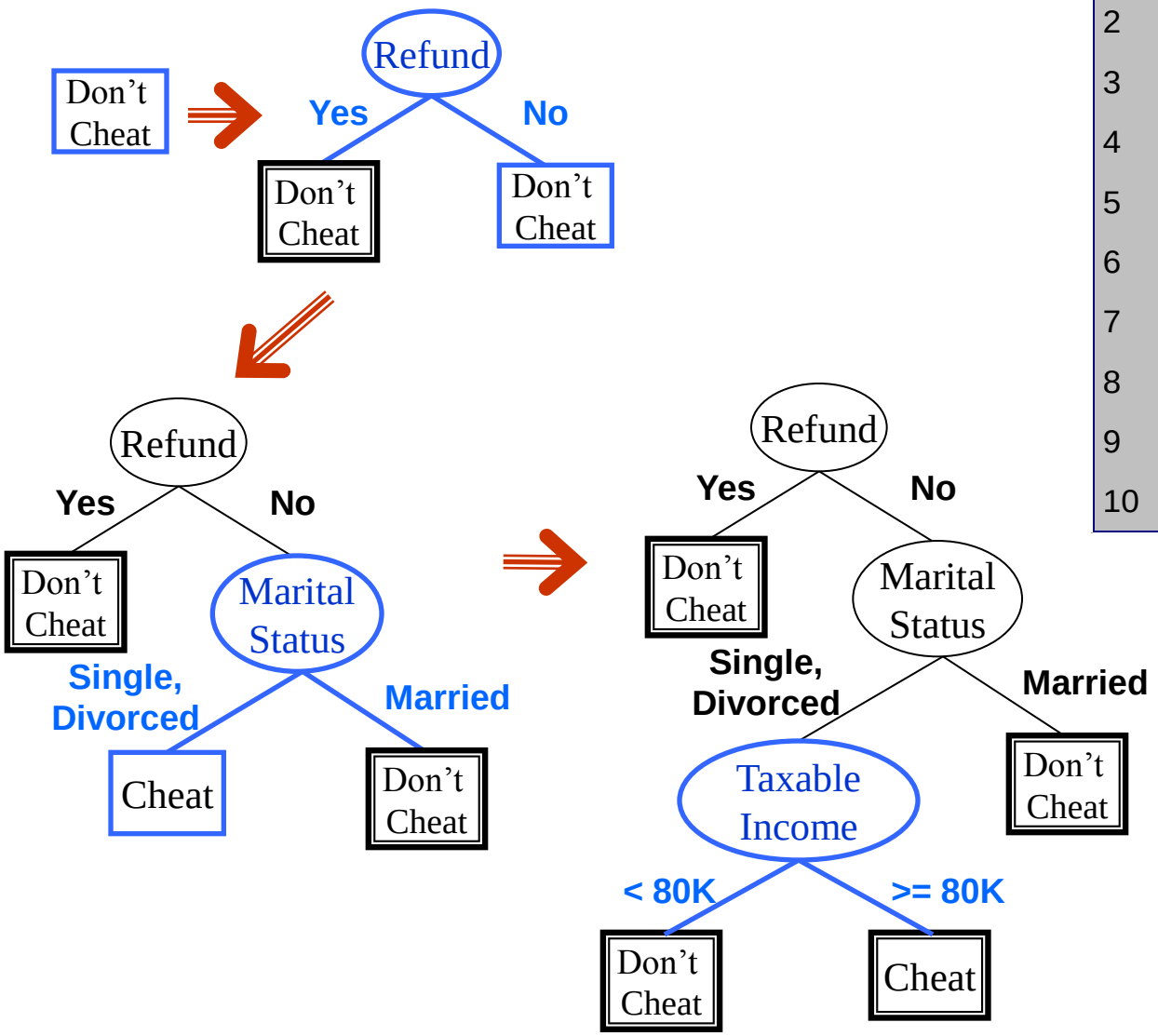

Tree Induction

- Successive Partitioning of the dataset based on attribute tests
- Greedy strategy.
  - Split the records based on the attribute test that optimizes certain criterion.
- Issues
  - Determine how to split the records
    - How to specify the attribute test condition?
    - How to determine the best split?
  - Determine when to stop splitting

Tree Induction

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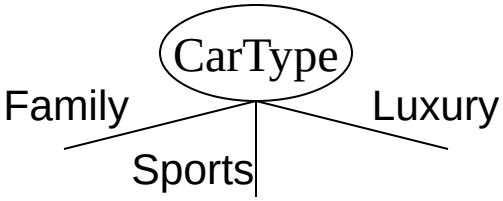
How to Specify Test Condition?

- Depends on attribute types
  - Nominal
  - Ordinal
  - Continuous

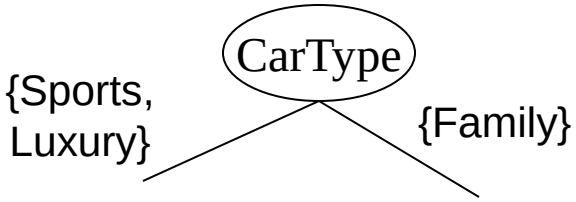
- Depends on number of ways to split
  - 2-way split
  - Multi-way split

Splitting Based on Nominal Attributes

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



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



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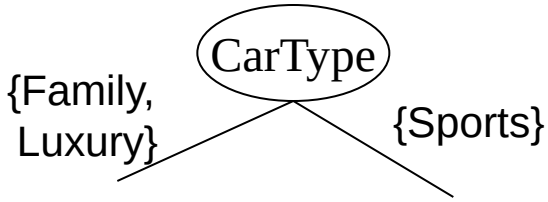
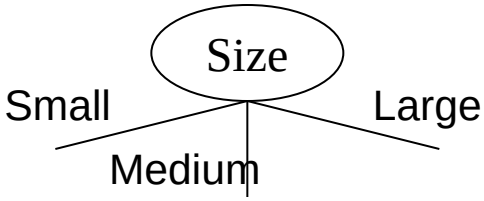
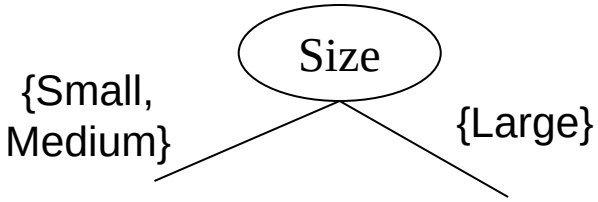


Splitting Based on Ordinal Attributes

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



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



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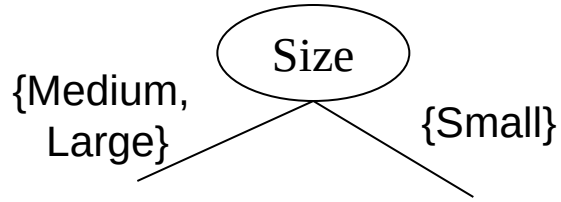
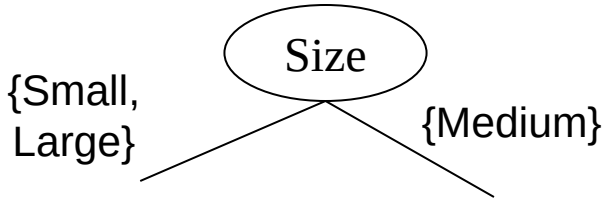


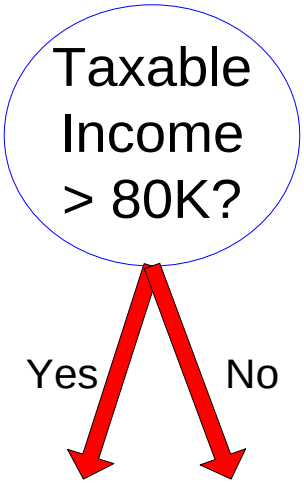
- What about this split?



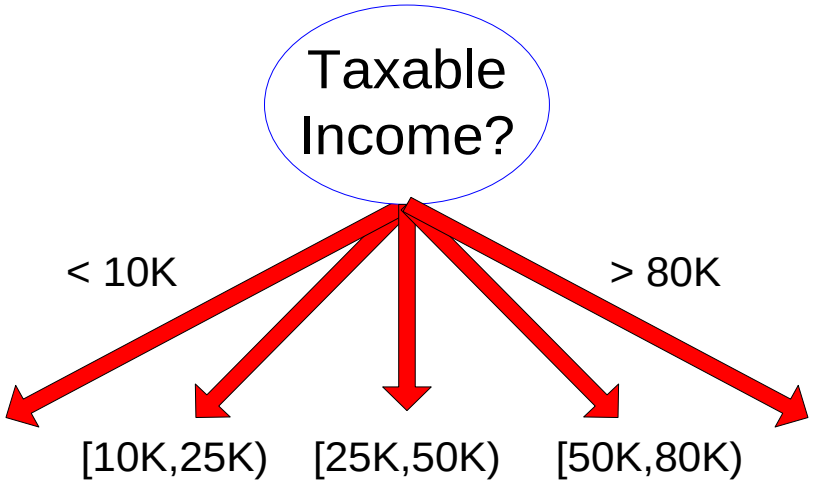
Splitting Based on Continuous Attributes

- Different ways of handling
  - Discretization to form a categorical attribute
    - Static – discretize once at the beginning
    - Dynamic – ranges can be found by equal interval bucketing, equal frequency bucketing (percentiles), or clustering.
  - Binary Decision: $(A < v)$ or $(A \geq v)$
    - consider all possible splits and finds the best cut
    - can be more compute intensive

Splitting Based on Continuous Attributes



(i) Binary split



(ii) Multi-way split

Tree Induction

- Greedy strategy.
  - Split the records based on an attribute test that optimizes certain criterion.

- Issues
  - Determine how to split the records
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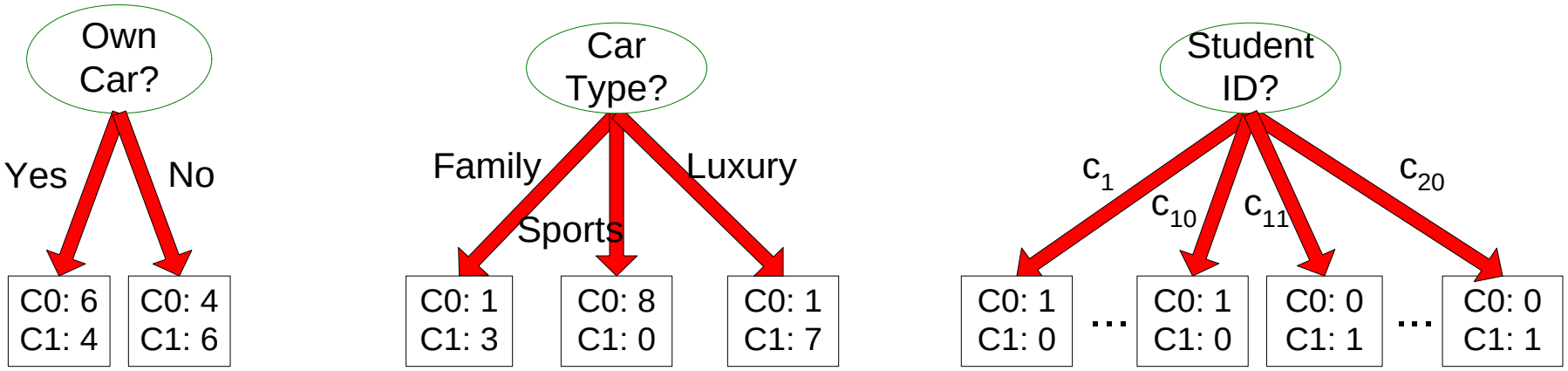
How to determine the Best Split

Before Splitting: 10 records of class 0,
10 records of class 1



Which test condition is the best?

How to determine the Best Split

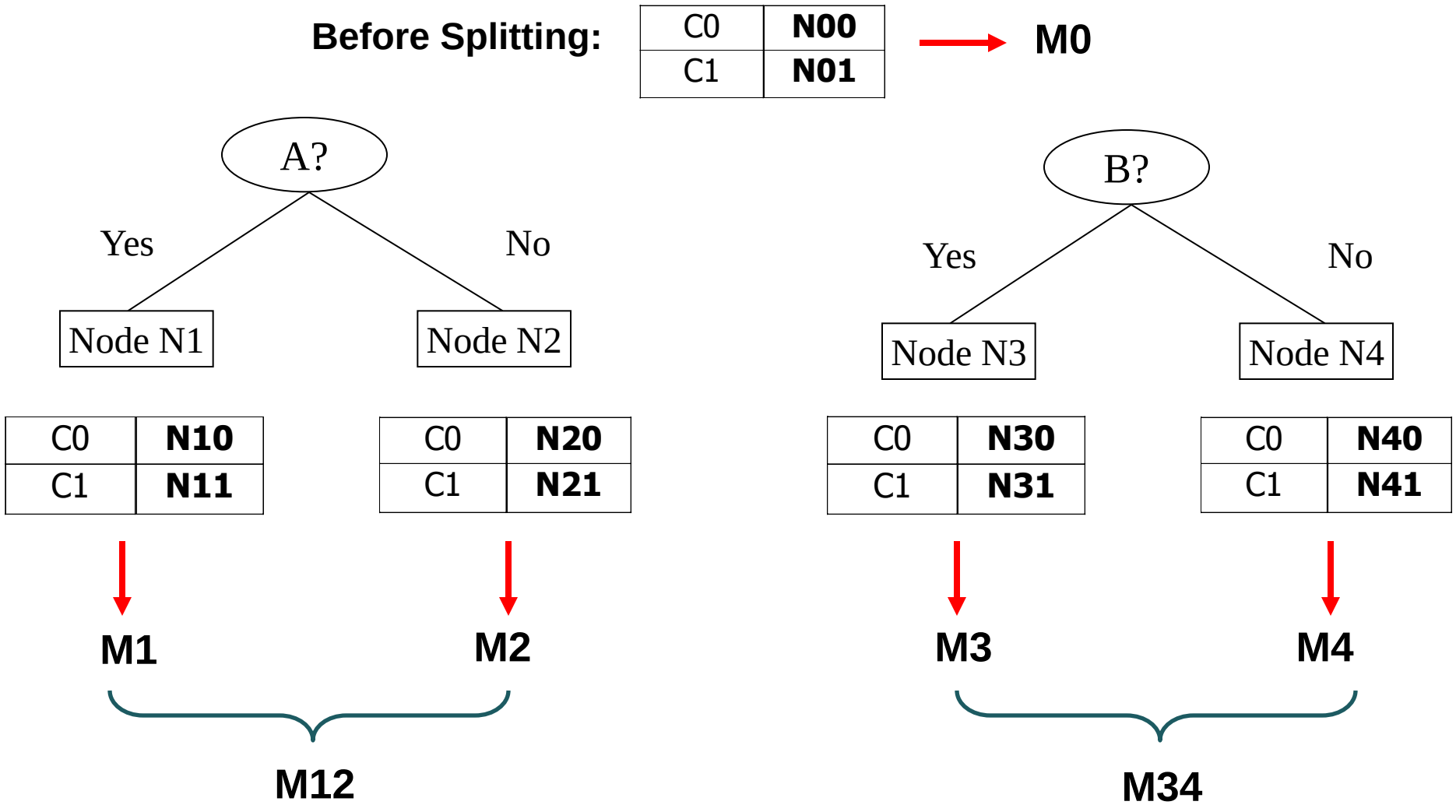
- Nodes with homogeneous class distribution are preferred
- Need a measure of node impurity:

C0: 5 C1: 5	C0: 9 C1: 1
Non-homogeneous, **High degree of impurity**	**Homogeneous,** **Low degree of impurity**

Measures of Node Impurity

- Gini Index
- Entropy
- Misclassification error

How to Find the Best Split



Measure of Impurity: GINI

- Gini Index for a given node n :

$$GINI(n) = 1 - \sum_j [p(j \mid n)]^2$$

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

  - Maximum (1 - 1/n_c) when records are equally distributed among all classes, implying least interesting information
  - Minimum (0.0) when all records belong to one class, implying most interesting information

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

$$GINI(n) = 1 - \sum_j [p(j \mid n)]^2$$

C1	**0**
C2	**6**

P(C1) = 0/6 = 0 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 P(C2) = 5/6

Gini = 1 – (1/6)² – (5/6)² = 0.278

C1	**2**
C2	**4**

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

Gini = 1 – (2/6)² – (4/6)² = 0.444

Splitting Based on GINI

- Used in CART, SLIQ, SPRINT.
- When a node n is split into k partitions (children), the quality of split is computed as,

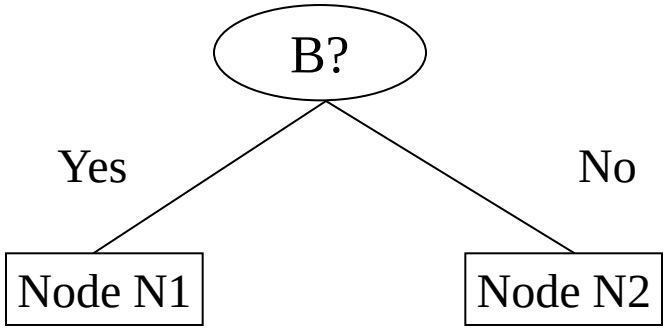
$$GINI_{split} = \sum_{i=1}^{k} \frac{n_i}{n} GINI(i)$$

where, n_i = number of records at child i,

n = number of records at node n.

Binary Attributes:Computing GINI Index

- Splits into two partitions
- Effect of Weighing partitions:
  - Larger and Purer Partitions are sought for.



	Parent
C1	**6**
C2	**6**
Gini = 0.500	

Gini(N1)
= 1 – (5/6)² – (2/6)²
= 0.194

Gini(N2)
= 1 – (1/6)² – (4/6)²
= 0.528

	N1	N2
C1	**5**	**1**
C2	**2**	**4**
Gini=0.333		

Gini(Children)
= 7/12 * 0.194 +
5/12 * 0.528
= 0.333

Continuous Attributes: Computing Gini Index

- Use Binary Decisions based on one value
- Simple method to choose best v
  - For each v, scan the database to gather count matrix and compute its Gini index
  - Computationally Inefficient (may be used if the computational load is affordable)

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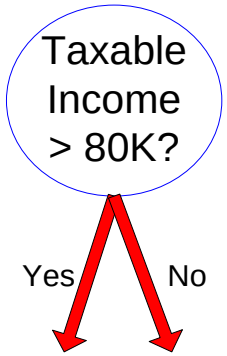


Alternative Splitting Criteria

- Entropy at a given node n:

$$Entropy(n) = -\sum_{j} p(j \mid n) \log p(j \mid n)$$

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

  - Measures homogeneity of a node.
    - Maximum (log n_c) when records are equally distributed among all classes implying least information
    - Minimum (0.0) when all records belong to one class, implying most information
  - Entropy based computations are similar to the GINI index computations

Examples for computing Entropy

$$Entropy(n) = -\sum_j p(j \mid n) \log_2 p(j \mid n)$$

C1	**0**
C2	**6**

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

Entropy = – 0 log 0 – 1 log 1 = – 0 – 0 = 0

C1	**1**
C2	**5**

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

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

C1	**2**
C2	**4**

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:

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

Parent Node, p is split into k partitions;

n_i is number of records in partition i

  - Measures Reduction in Entropy achieved because of the split. Choose the split that achieves most reduction (maximizes GAIN)
  - Disadvantage: Tends to prefer splits that result in large number of partitions, each being small but pure.

Splitting Based on Information Gain

- Gain Ratio:

$$GainRATIO_{split} = \frac{GAIN_{Split}}{SplitINFO} \qquad SplitINFO = -\sum_{i=1}^{k} \frac{n_i}{n} \log \frac{n_i}{n}$$

Parent Node, p is split into k partitions

n_i is the number of records in partition i

- Adjusts Information Gain by the entropy of the partitioning (SplitINFO). Higher entropy partitioning (large number of small partitions) is penalized!
- Designed to overcome the disadvantage of Information Gain

Splitting Criteria based on Classification Error

- Classification error at a node t :

$$Error(n) = 1 - \max_i P(i \mid n)$$

- Measures misclassification error made by a node.
  - Maximum (1 - 1/n_c) when records are equally distributed among all classes, implying least interesting information
  - Minimum (0.0) when all records belong to one class, implying most interesting information

Examples for Computing Error

$$Error(t) = 1 - \max_i P(i \mid t)$$

C1	**0**
C2	**6**

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

Error = 1 – max (0, 1) = 1 – 1 = 0

C1	**1**
C2	**5**

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

Error = 1 – max (1/6, 5/6) = 1 – 5/6 = 1/6

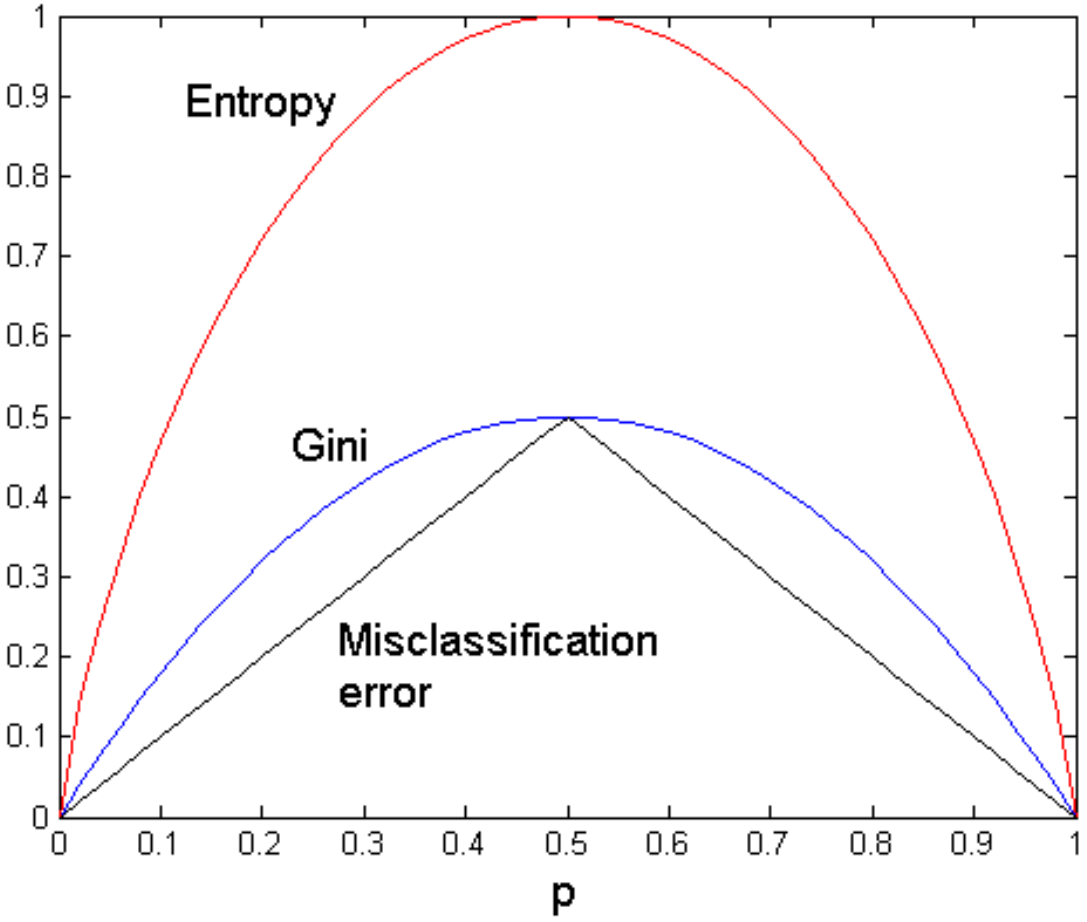
C1	**2**
C2	**4**

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

Error = 1 – max (2/6, 4/6) = 1 – 4/6 = 1/3

Comparison among Splitting Criteria

For a 2-class problem:



Tree Induction

- Greedy strategy.
  - Split the records based on an attribute test that optimizes certain criterion.

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

Stopping Criteria for Tree Induction

- Stop expanding a node when all the records belong to the same class
- Stop expanding a node when all the records have similar attribute values
- Early termination (needs an estimate of generalization)

Decision Tree Based Classification

- Advantages:
  - Relatively inexpensive to construct
  - Extremely fast at classifying unknown records
  - Easy to interpret for small-sized trees
  - Accuracy is comparable to other classification techniques for several data sets

Example: C4.5

- Simple depth-first construction.
- Uses Information Gain
- Sorts Continuous Attributes at each node.

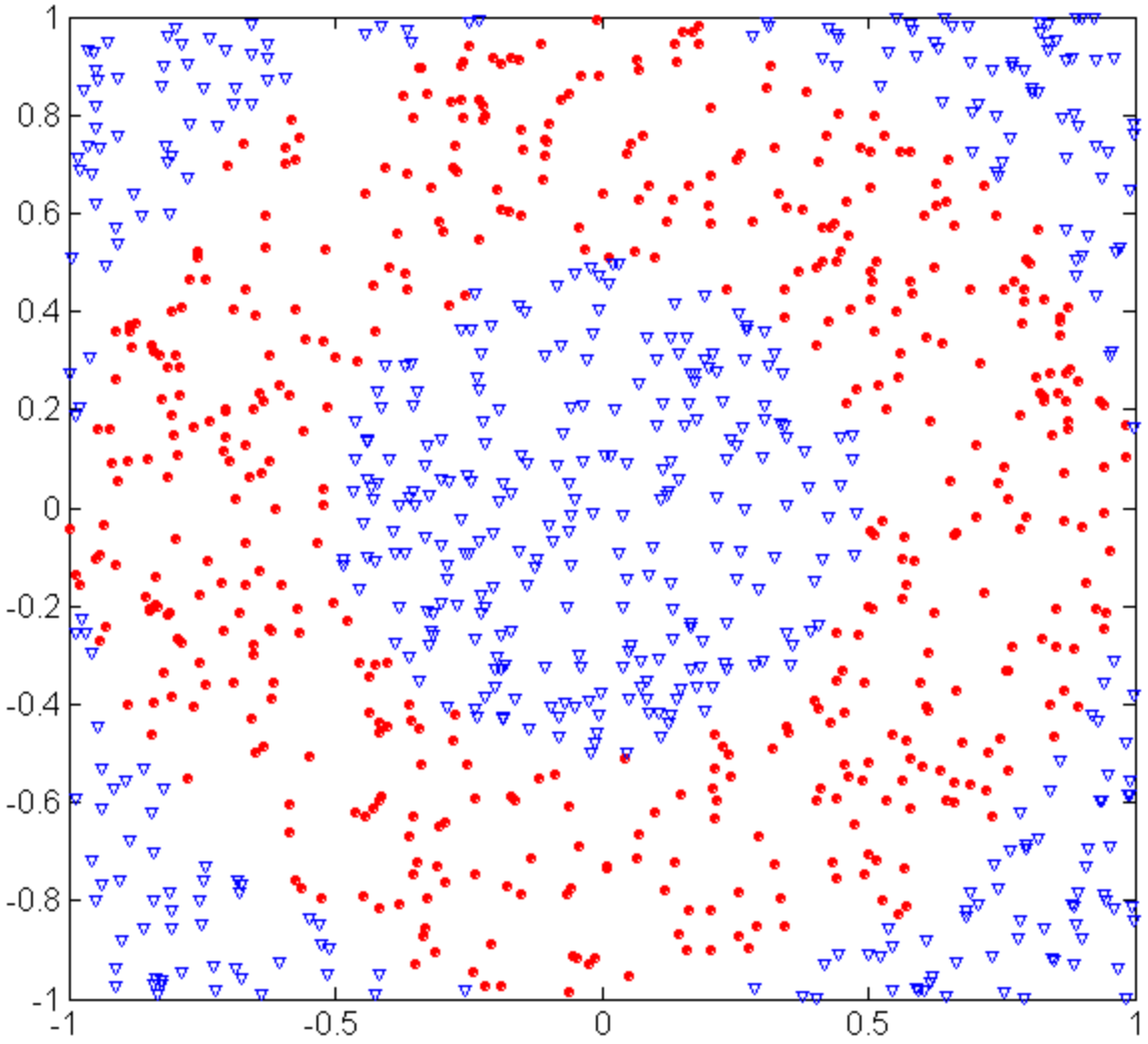
- You can download the software from: http://www.cse.unsw.edu.au/~quinlan/c4.5r8.tar.gz

The generalization problem (again)

- **Occam's Razor**: Prefer the simplest model that fits well to the data
- Very simple models underfit (bad generalization)
- Complex models overfit (bad generalization)

- For a given dataset and type of model, there is an **optimal model complexity** providing **optimal generalization**

Underfitting and Overfitting (Example)



500 circular and 500 triangular data points.

Circular points:

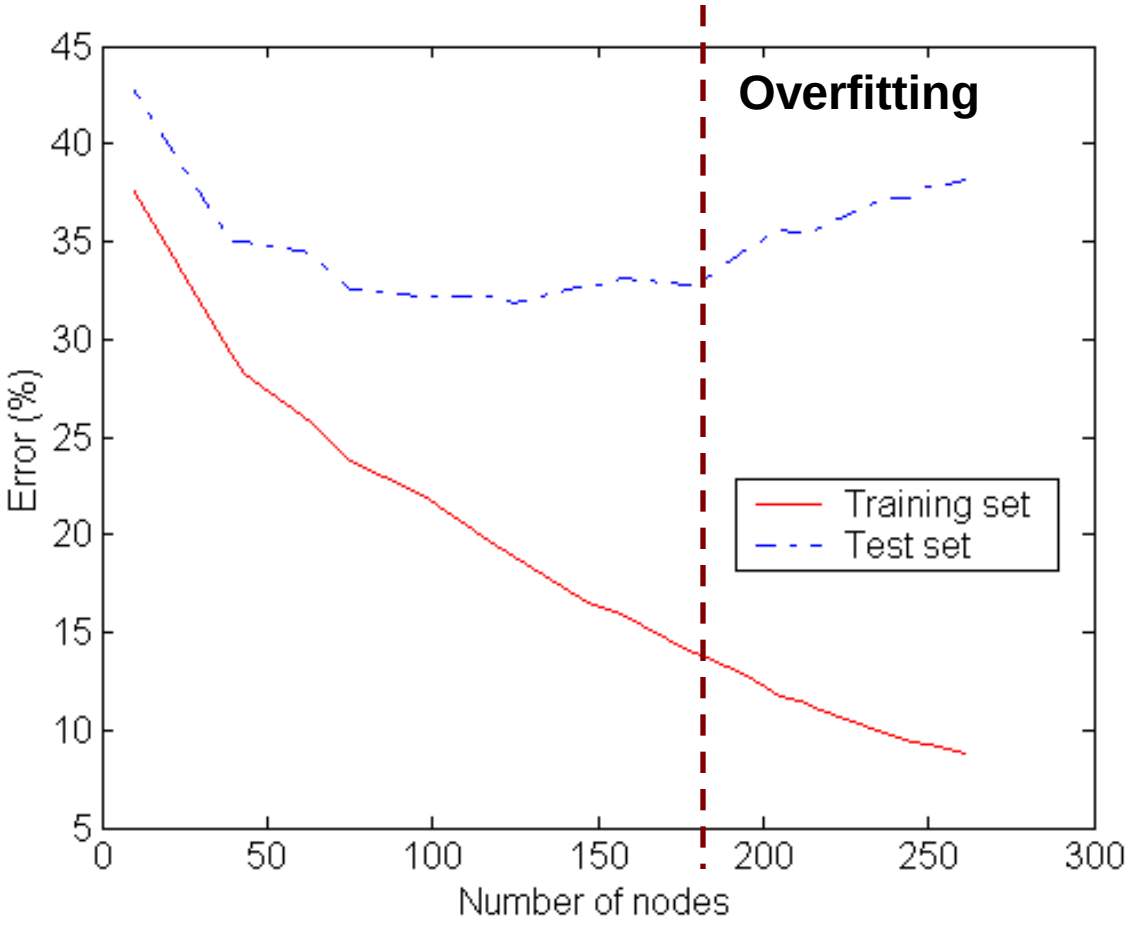
$0.5 \leq \text{sqrt}(x_1^2+x_2^2) \leq 1$

Triangular points:

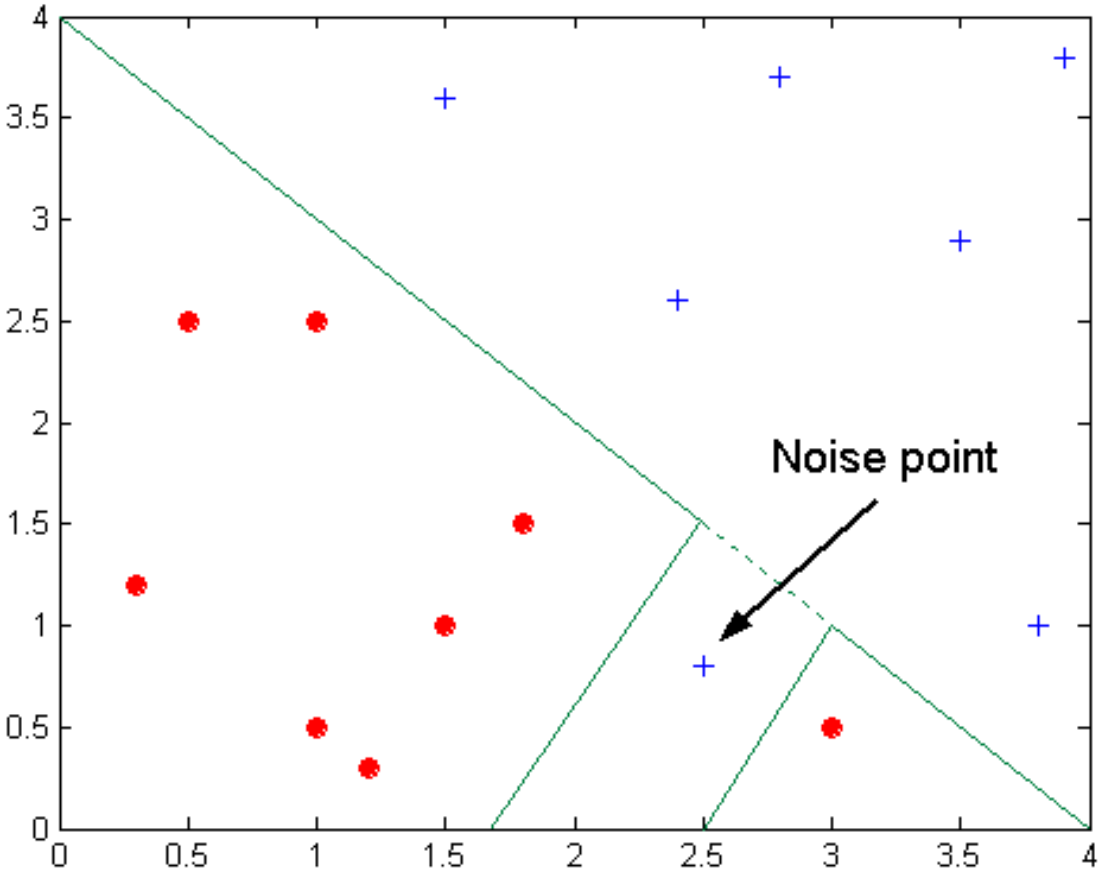
$\text{sqrt}(x_1^2+x_2^2) > 0.5$ or

$\text{sqrt}(x_1^2+x_2^2) < 1$

Underfitting and Overfitting

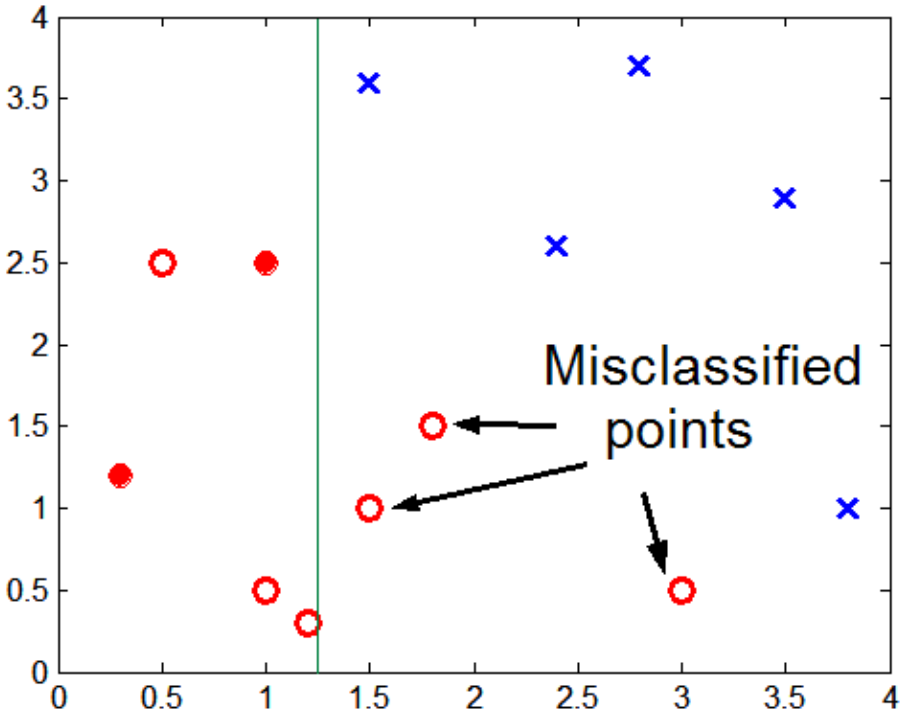


Overfitting due to Noise



Decision boundary is distorted by noise point

Insufficient Examples



Lack of data points in the lower half of the diagram **affects generalization**: makes it difficult to predict correctly the class labels of that region

- Insufficient number of examples in the region causes the decision tree to predict the test examples using other examples that are irrelevant to the classification task

Minimum Description Length (MDL)

- An alternative formulation of Occam's razor
- Cost(Model,Data) = Cost(Data|Model) + Cost(Model)
  - Cost is the number of bits needed for encoding.
- Cost(Data|Model) encodes the misclassification errors in the dataset.
- Cost(Model) uses node encoding (number of children) plus splitting condition encoding (penalty term).
- Search for the least costly model.

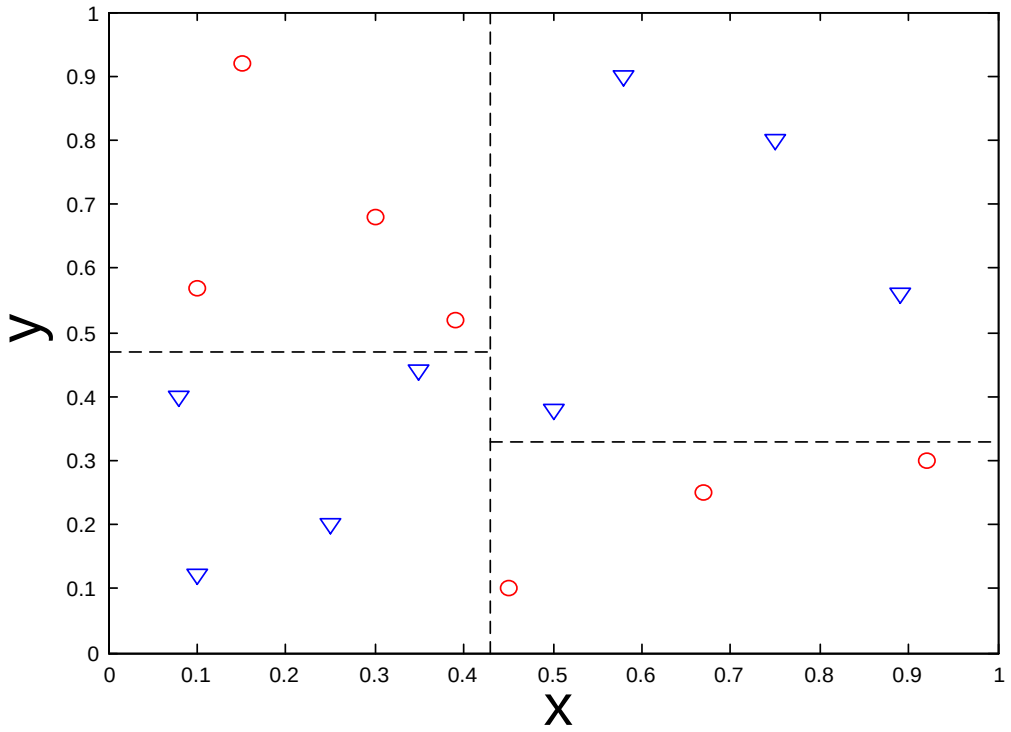
How to Address Overfitting

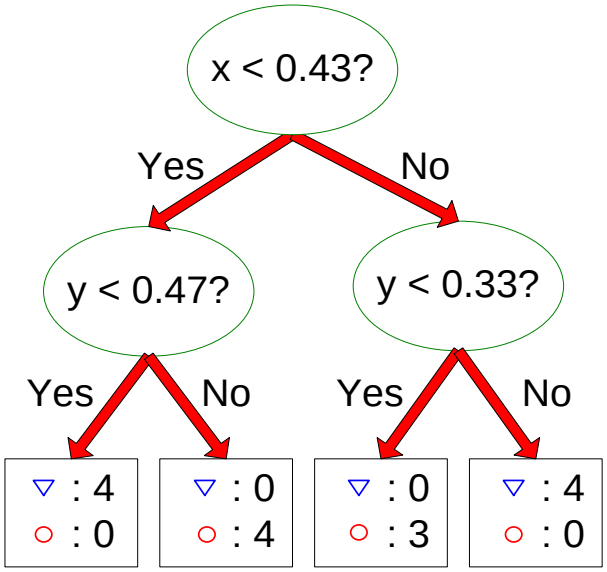
- Pre-Pruning (Early Stopping Rule)
  - Stop the algorithm before it becomes a fully-grown tree
  - Typical stopping conditions for a node:
    - Stop if all instances belong to the same class
    - Stop if all the attribute values are the same
  - More restrictive conditions:
    - Stop if number of 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).

How to Address Overfitting…

- Post-pruning
  - Grow decision tree to its entirety
  - Trim the nodes of the decision tree in a bottom-up fashion
  - If generalization error improves after trimming, replace sub-tree by a leaf node.
  - Class label of leaf node is determined from majority class of instances in the sub-tree
  - Estimate generalization error using a validation set (hold out some training examples for validation)
  - Validation set is different from test set.

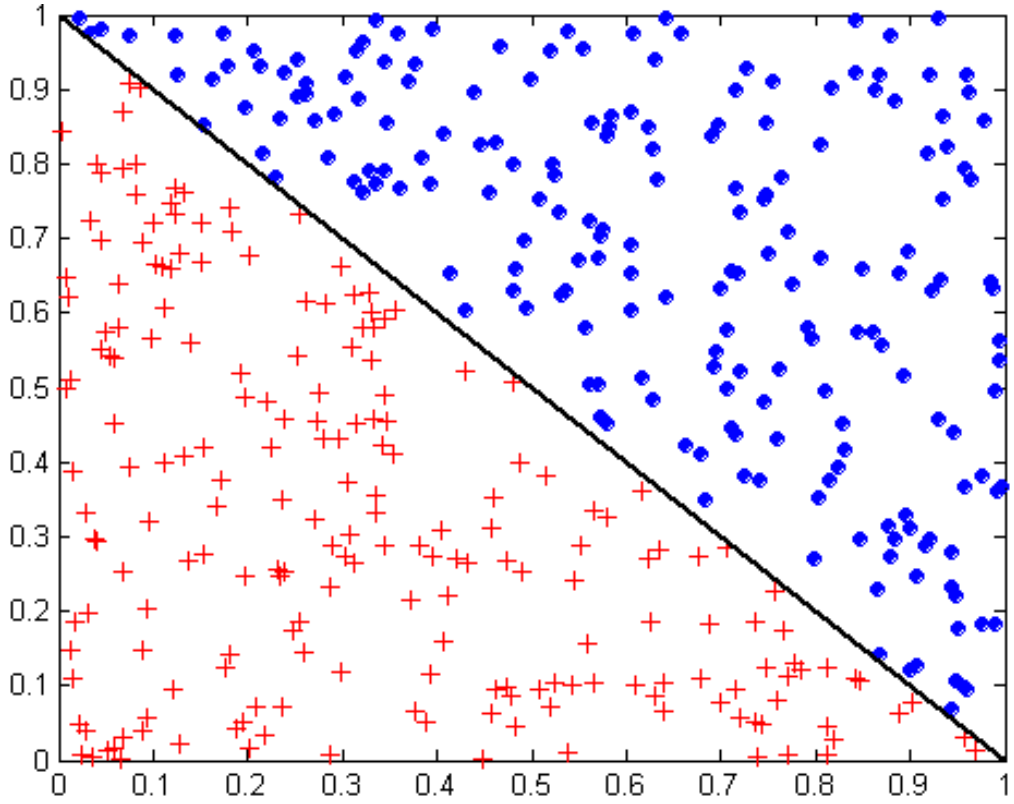
Decision Boundary (continuous attributes)

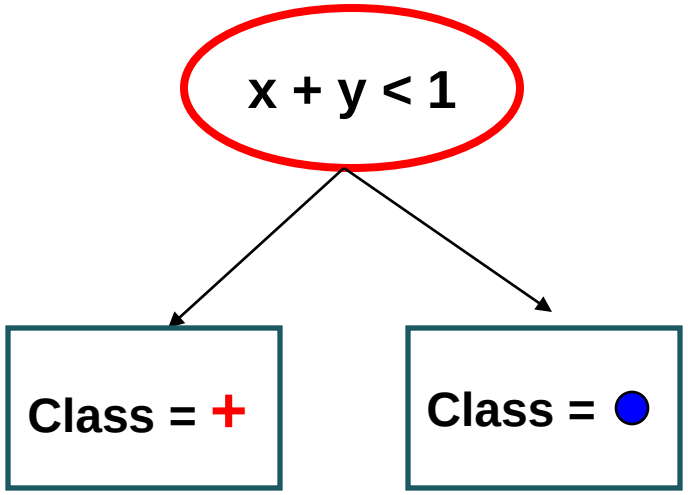




- **Border line between two neighboring regions of different classes is known as decision boundary**
- **Decision boundary is parallel to axes because test condition involves a single attribute at-a-time**

Oblique Decision Trees





- Test condition may involve multiple attributes
- More expressive representation
- Finding optimal test condition is computationally expensive