Classification: Basic Concepts and Decision Trees

Data Mining Techniques

- Classification
- Regression
- Clustering
- Association Rule Discovery
- Anomaly Detection

Classification-Prediction

Classification:

- Estimation of categorical class labels
- Classifies data over the training set (creates a model)

Prediction:

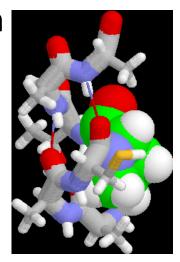
 Models the change of continuous values and predicts missing values or needs to be estimated

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

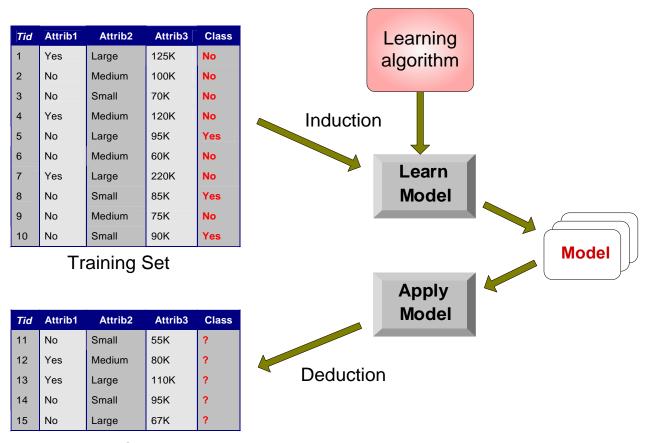


A Classification task

Classification: Definition

- Given a collection of records (training set)
 - Each record contains a set of attributes, one of the attributes is the class.
- Find a *model* for class attribute as a function of the values of other attributes.
- Goal: <u>previously unseen</u> records should be assigned a class as accurately as possible.
 - A test set is used to determine the accuracy of the model.
 Usually, the given data set is divided into training and test
 sets, with training set used to build the model and test set
 used to validate it.

Illustrating Classification Task



Test Set

Classification – Two phases

Model training

- It is known that each row is included in a class, the model is trained by investigating why the row is included in that class.
- The dataset required for model building is called the training set.
- The model is determined by mathematical formulas, decision trees, or rule-based.

Model Testing

- The known real value for the **test set** is compared with the value given by the model.
- The consistency of the model is the sample rate correctly classified by the model.
- The test set must be separate from the training set, otherwise there will be an overfit situation.

Classification Techniques

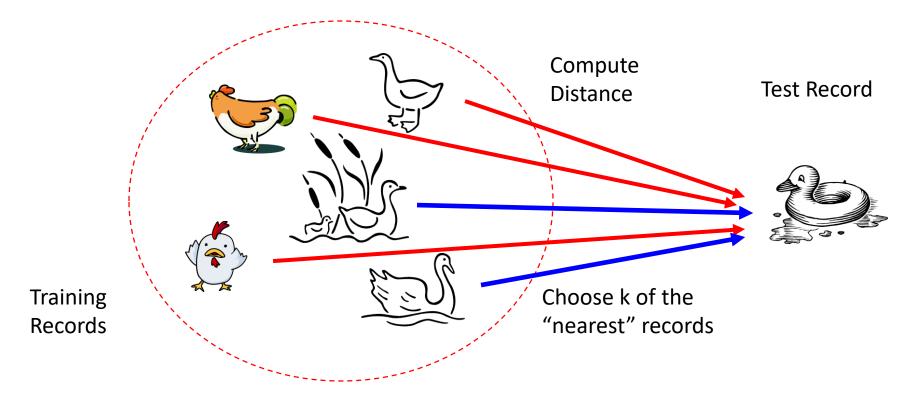
- Rule-based Methods
- Memory based reasoning
- Distance-similarity based methods(Nearest-Neighbor)
- Decision Tree based Methods
- Probabilistic Methods(Naïve Bayes and Bayesian Belief Networks)
- Support Vector Machines
- Artificial Neural Networks
- Ensemle Methods (Bagging Boosting)
 - Random Forest
 - AdaBoost, CatBoost, XGBoost, etc.

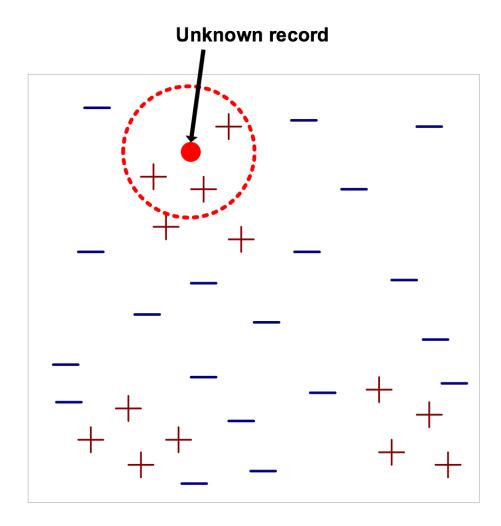
Classification Using Distance

- Place items in class to which they are "closest".
- Must determine distance between an item and a class.
- Classes represented by
 - Centroid: Central value.
 - Medoid: Representative point.
 - Individual points
- Algorithm: KNN

Simple idea:

 If it walks like a duck and sounds like a duck, it's probably a duck.





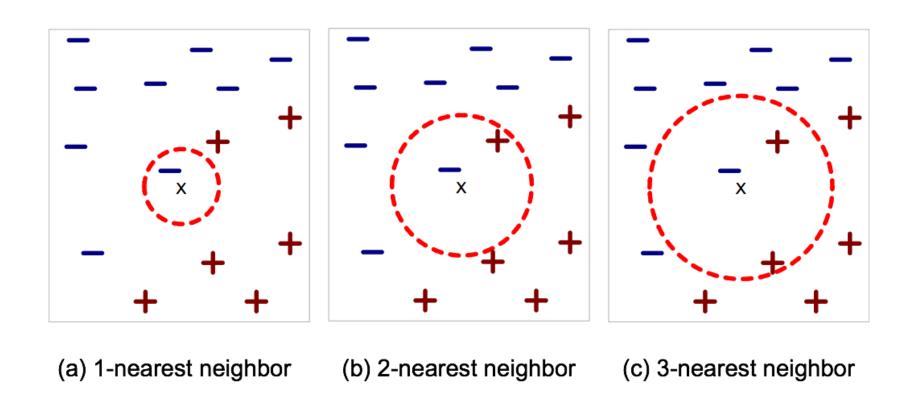
> Three things are required

- Set of records
- Distance metric to find the distance between records
- The number k, which represents the number of nearest records to be evaluated.

To classify an unknown record

- Calculate the distance to other training records
- k nearest neighbors must be determined
- Classification should be made according to the distribution of the nearest classes (for example, the class with the most votes)

Nearest Neighbors



The k-nearest neighbor is the k data points with the nearest distance to that record.

K Nearest Neighbor (KNN):

- Training set includes classes.
- Examine K items near item to be classified.
- New item placed in class with the most number of close items.
- O(q) for each tuple to be classified. (Here q is the size of the training set.)

- To find the distance between two points, one must measure the distance:
 - Euclidean Dist.

$$d(p,q) = \sqrt{\sum_{i} (p_{i} - q_{i})^{2}}$$

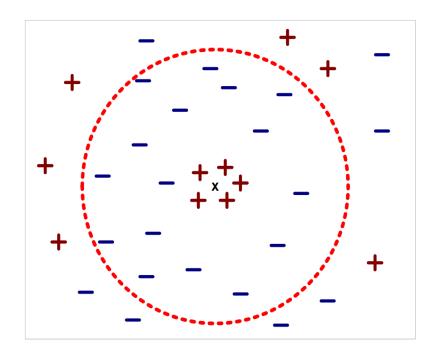
- Find list of nearest classes
 - Choose the class to which it belongs most among k-nearest neighbors
 - Determine the weight effect of neighbors based on distance distance
 - Weight factor, $w = 1/d^2$

Choosing K value:

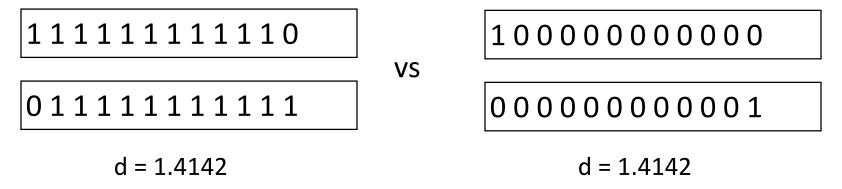
If k is too small, it will be sensitive to outlier values

If k is too large, neighbors contain elements from other

classes



- Issues with Euclidean Distance:
 - High dimentional space
 - curse of dimensionality
 - Can produce logically counterproductive results



Solution: Normalizing vectors to unit length

Scalibility issues

 It may be necessary to normalize and limit attributes so that offsets are not dominated by an attribute.

– Example:

- Average person can have height around 1.5m 1.8m
- Average person can have weight 40kg -150kg
- Average personal income can be \$1K to \$1M

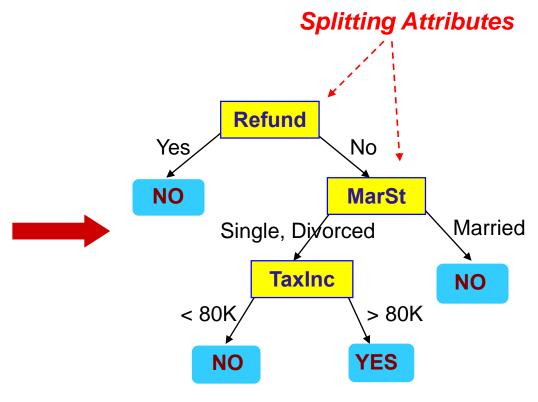
- k-NN Classifiers are called lazy learners
 - They don't need to create a specific model at first,
 such as decision trees or Rule-based systems
 - Classification of unknown values is relatively less costly

Decision Trees

Example of a Decision Tree

categorical continuous

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



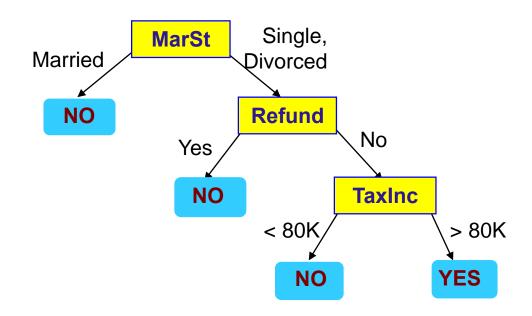
Training Data

Model: Decision Tree

Another Example of Decision Tree

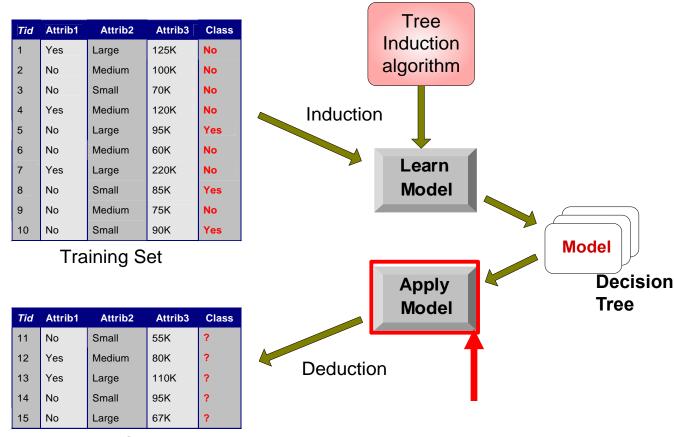
categorical continuous

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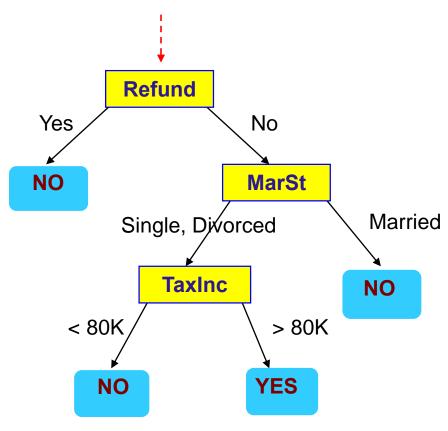
There could be more than one tree that fits the same data!

Decision Tree Classification Task



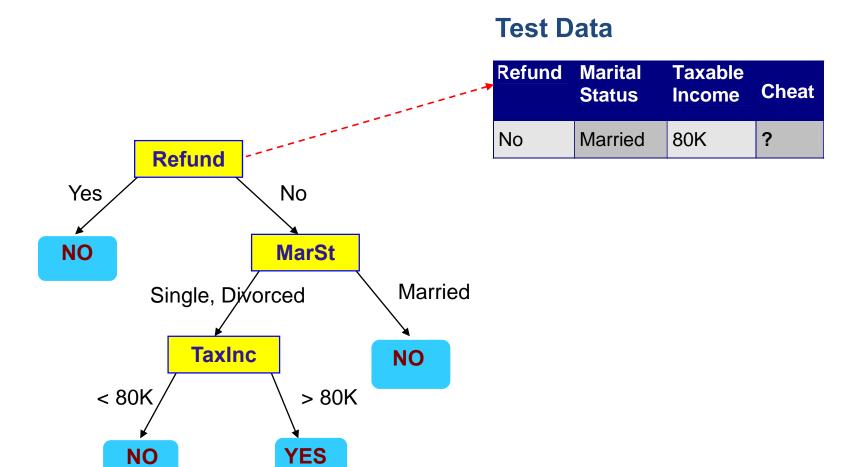
Test Set

Start from the root of tree.

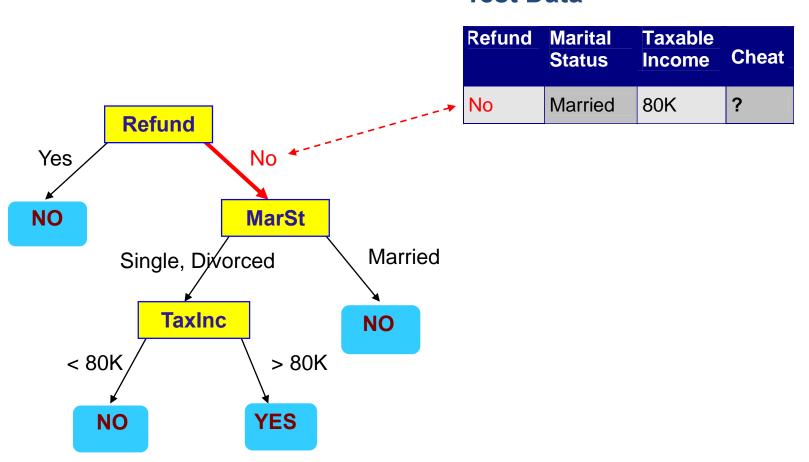


Test Data

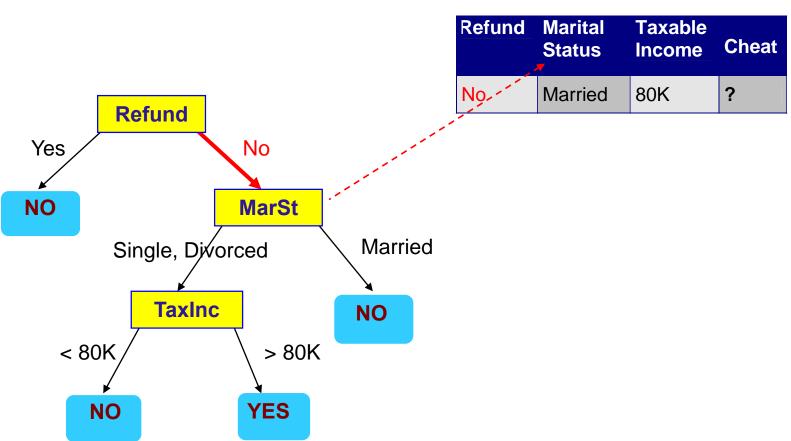
Refund	Marital Status		Cheat
No	Married	80K	?

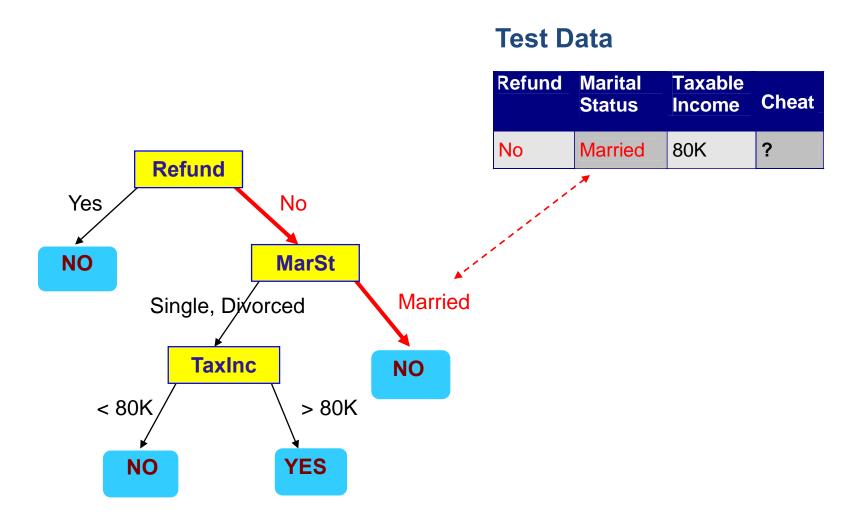


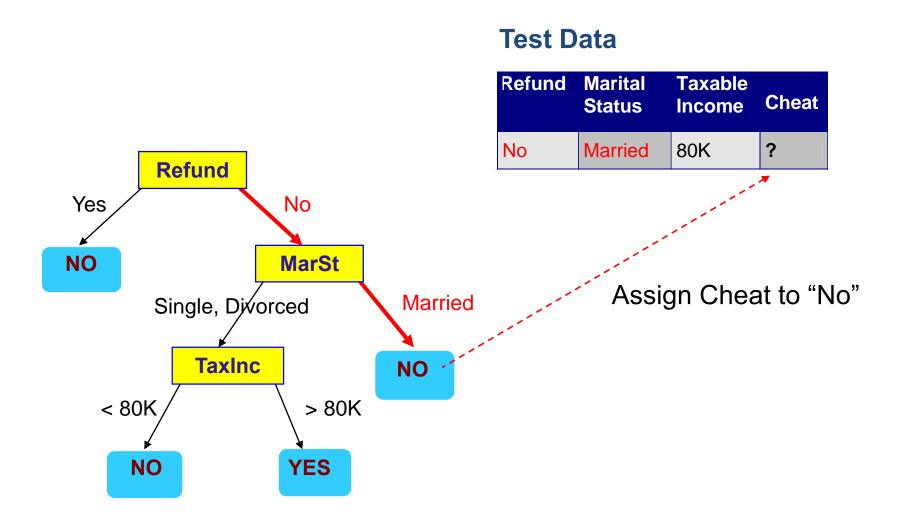
Test Data



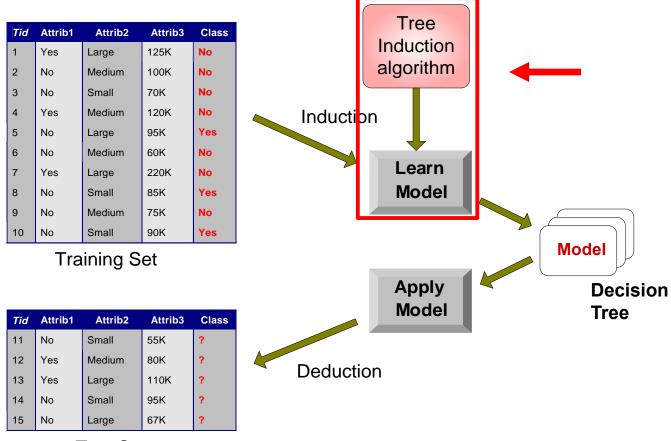
Test Data







Decision Tree Classification Task



Test Set

Decision Tree Induction

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

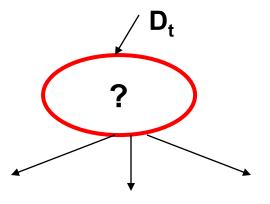
General Structure of Hunt's Algorithm

 Let D_t be the set of training records that reach a node t

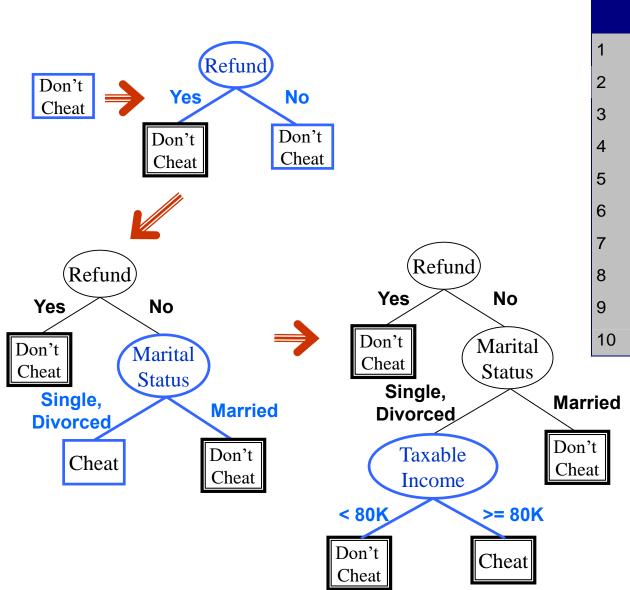
General Procedure:

- 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.

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10	No	Single	90K	Yes



Hunt's Algorithm



Tid	Refund	Marital Status	Taxable Income	Cheat
1	Yes	Single	125K	No
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10	No	Single	90K	Yes

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

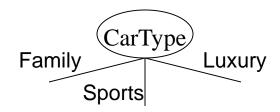
How to Specify Test Condition?

- 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.

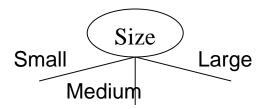


Binary split: Divides values into two subsets.
 Need to find optimal partitioning.

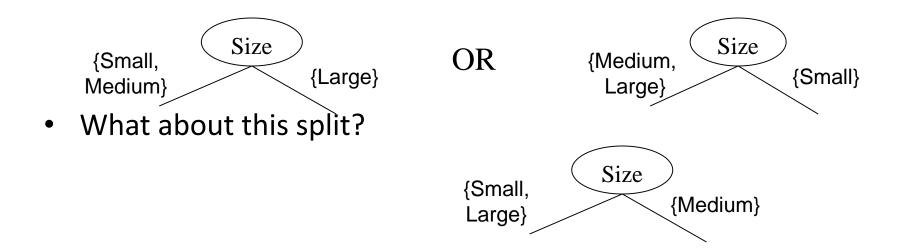


Splitting Based on Ordinal Attributes

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



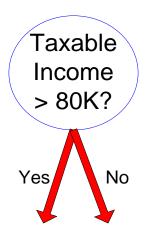
Binary split: Divides values into two subsets.
 Need to find optimal partitioning.



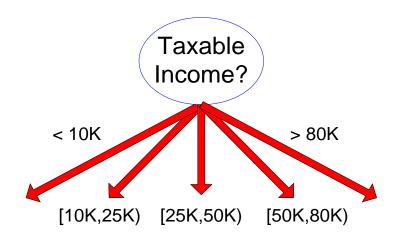
Splitting Based on Continuous Attributes

- Different ways of handling
 - Discretization to form an ordinal 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 ≥ 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

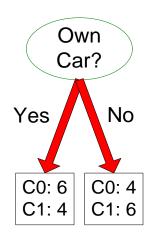
Tree Induction

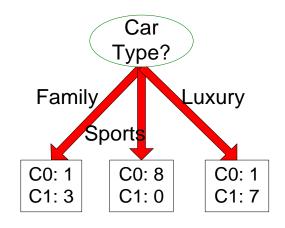
- Greedy strategy.
 - Split the records based on an attribute test that optimizes certain criterion.

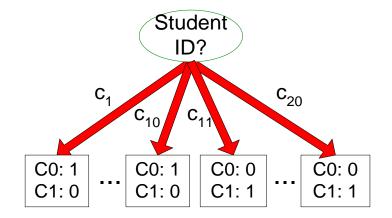
- Issues
 - Determine how to split the records
 - How to specify the attribute test condition?
 - How to determine the best split?
 - Determine when to stop splitting

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

- Greedy approach:
 - 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

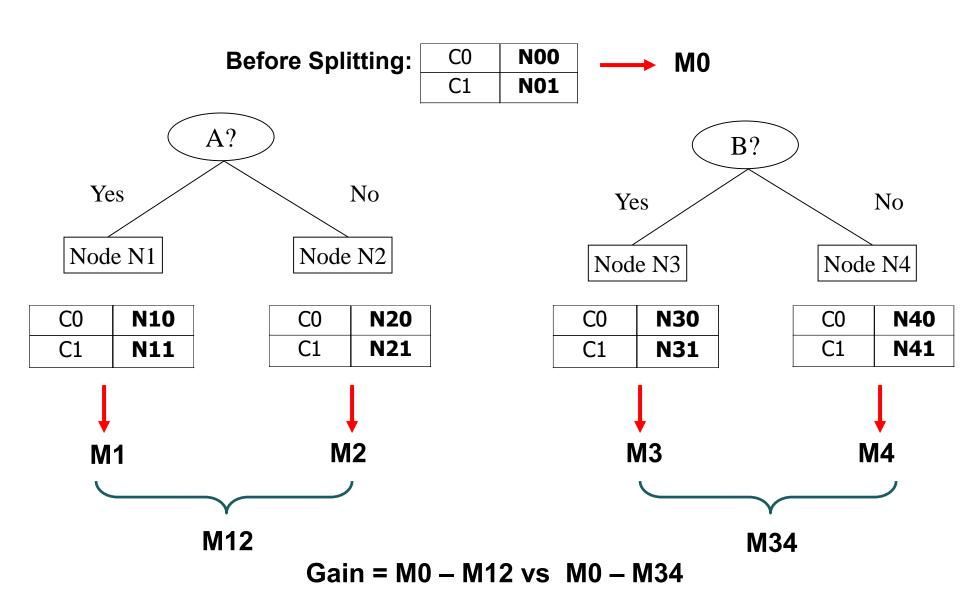
Measures of Node Impurity

Gini Index

Entropy

Misclassification error

How to Find the Best Split



Measure of Impurity: GINI

Gini Index for a given node t :

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

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

- 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

Gini=	0.000
C2	6
C1	0

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

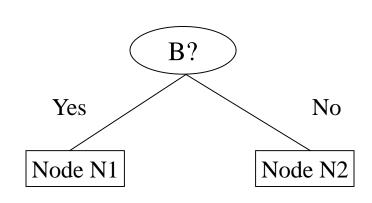
- Used in CART, SLIQ, SPRINT.
- When a node p is split into k partitions (children), the quality of split is computed as,

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

where, n_i = number of records at child i, n_i = number of records at node p.

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)

$$= 1 - (5/7)^2 - (2/7)^2$$

= 0.408

Gini(N2)

$$= 1 - (1/5)^2 - (4/5)^2$$

= 0.320

	N1	N2				
C1	5	1				
C2	2	4				
Gini=0.371						

Gini(Children)

= 7/12 * 0.408 + 5/12 * 0.320

= 0.371

Categorical Attributes: Computing Gini Index

- For each distinct value, gather counts for each class in the dataset
- Use the count matrix to make decisions

Multi-way split

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

Two-way split (find best partition of values)

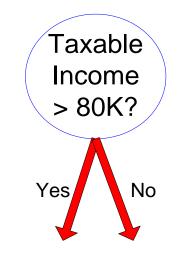
	CarType							
	{Sports, Luxury}	{Family}						
C1	3	1						
C2	2 4							
Gini	0.400							

	CarType							
	{Sports}	{Family, Luxury}						
C 1	2 2							
C2	1 5							
Gini	0.419							

Continuous Attributes: Computing Gini Index

- Use Binary Decisions based on one value
- Several Choices for the splitting value
 - Number of possible splitting valuesNumber of distinct values
- Each splitting value has a count matrix associated with it
 - Class counts in each of the partitions, A < v
 and A ≥ v
- Simple method to choose best v
 - For each v, scan the database to gather count matrix and compute its Gini index
 - Computationally Inefficient! Repetition of work.

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1	Yes	Single	125K	No			
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3	No	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			



Continuous Attributes: Computing Gini Index...

- For efficient computation: for each attribute,
 - Sort the attribute on values
 - Linearly scan these values, each time updating the count matrix and computing gini index
 - Choose the split position that has the least gini index

		No No)	No		Ye	es Ye		s	Yes		N	0	No		No		No				
•	Taxable Income																						
Sorted Values 60 70 75 85 90 95 100 120 125														220									
Split Positions _		55		6	65 72		2	80		8	87		92		97 1		10 1:		22 17		72 230		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	43	0.4	117	0.4	100	<u>0.</u>	<u>300</u>	0.3	43	0.3	75	0.4	00	0.4	20

Alternative Splitting Criteria based on INFO

Entropy at a given node t:

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

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

- 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

$$Entropy(t) = -\sum_{j} p(j | t) \log_{2} p(j | t)$$

C1	0
C2	6

$$P(C1) = 0/6 = 0$$
 $P(C2) = 6/6 = 1$
Entropy = $-0 \log 0 - 1 \log 1 = -0 - 0 = 0$

Entropy =
$$-0 \log 0 - 1 \log 1 = -0 - 0 = 0$$

C1	1
C2	5

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

$$P(C1) = 1/6$$
 $P(C2) = 5/6$
Entropy = - (1/6) log_2 (1/6) - (5/6) log_2 (1/6) = 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 INFO...

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; 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)
- Used in ID3 and C4.5
- Disadvantage: Tends to prefer splits that result in large number of partitions, each being small but pure.

Splitting Based on INFO...

Gain Ratio:

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

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

- 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

Splitting Criteria based on Classification Error

Classification error at a node t :

$$Error(t) = 1 - \max_{i} P(i \mid t)$$

- 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 =
$$1 - \max(0, 1) = 1 - 1 = 0$$

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

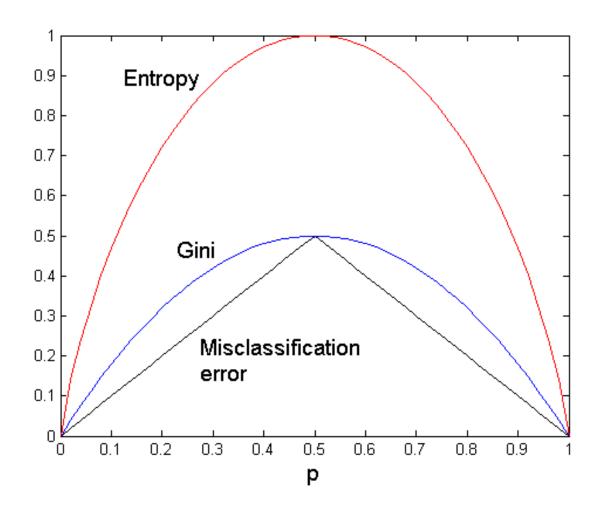
Error =
$$1 - \max(1/6, 5/6) = 1 - 5/6 = 1/6$$

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

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
 - using hyperparametes such as max_depth,min_samples_leaf, min_samples_split, etc.

Decision Tree Based Classification

Advantages:

- Inexpensive to construct
- Extremely fast at classifying unknown records
- Easy to interpret for small-sized trees
- Accuracy is comparable to other classification techniques for many simple data sets

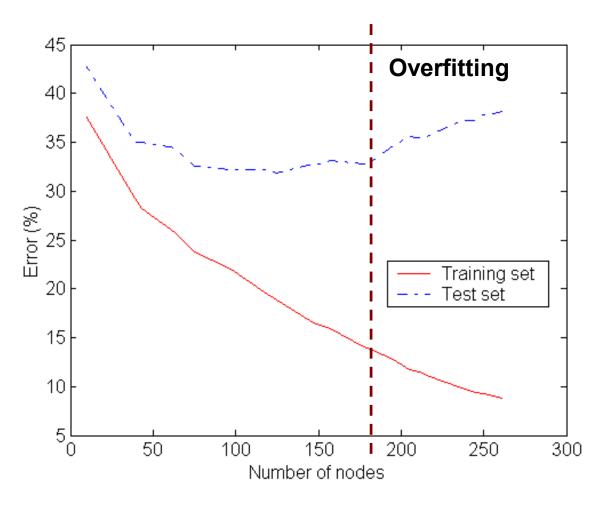
Practical Issues of Classification

Underfitting and Overfitting

Missing Values

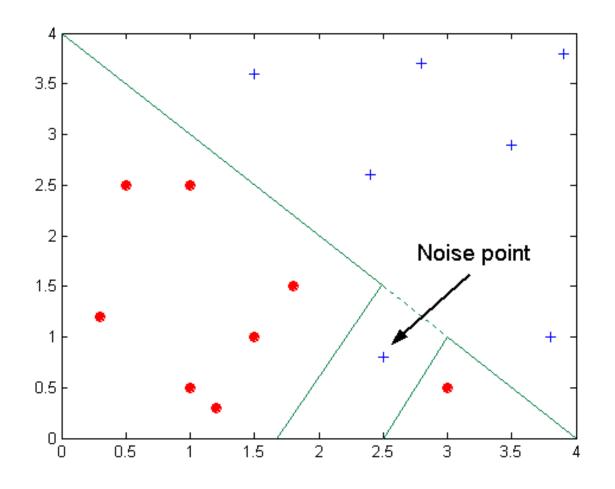
Costs of Classification

Underfitting and Overfitting



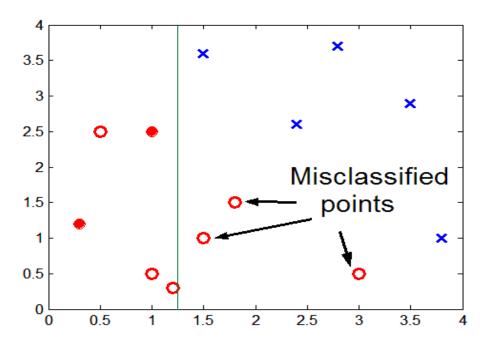
Underfitting: when model is too simple, both training and test errors are large

Overfitting due to Noise



Decision boundary is distorted by noise point

Overfitting due to Insufficient Examples



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

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

Notes on Overfitting

 Overfitting results in decision trees that are more complex than necessary

 Training error no longer provides a good estimate of how well the tree will perform on previously unseen records

Need new ways for estimating errors

Estimating Generalization Errors

- Re-substitution errors: error on training (Σ e(t))
- Generalization errors: error on testing (Σ e'(t))
- Methods for estimating generalization errors:
 - Optimistic approach: e'(t) = e(t)
 - Pessimistic approach:
 - For each leaf node: e'(t) = (e(t)+0.5)
 - Total errors: $e'(T) = e(T) + N \times 0.5$ (N: number of leaf nodes)
 - For a tree with 30 leaf nodes and 10 errors on training (out of 1000 instances):
 Training error = 10/1000 = 1%

 Generalization error = (10 + 30×0.5)/1000 = 2.5%
 - Reduced error pruning (REP):
 - uses validation data set to estimate generalization error

Occam's Razor

 Given two models of similar generalization errors, one should prefer the simpler model over the more complex model

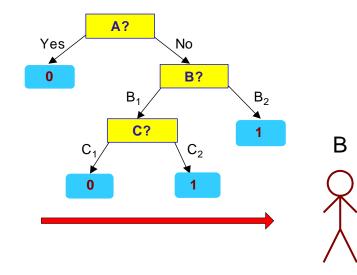
 For complex models, there is a greater chance that it was fitted accidentally by errors in data

 Therefore, one should include model complexity when evaluating a model

Minimum Description Length (MDL)

X	y
X_1	1
X ₂	0
X_3	0
X_4	1
X _n	1





X	у
X_1	
X_2	?
X_3	?
X_4	?
X _n	?

- Cost(Model, Data) = Cost(Data | Model) + Cost(Model)
 - Cost is the number of bits needed for encoding.
 - Search for the least costly model.
- Cost(Data | Model) encodes the misclassification errors.
- Cost(Model) uses node encoding (number of children) plus splitting condition encoding.

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 class distribution of instances are independent of the available features (e.g., using χ^2 test)
 - Stop if expanding the current node does not improve impurity measures (e.g., Gini or information gain).

How to Address Overfitting...

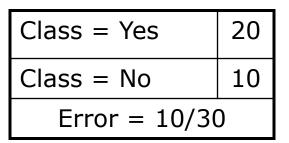
Post-pruning

- 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
- Can use MDL or Cost complexity pruning (ccp-alpha) for post-pruning



Example of Post-Pruning

A?



Training Error (Before splitting) = 10/30

Pessimistic error = (10 + 0.5)/30 = 10.5/30

Training Error (After splitting) = 9/30

Pessimistic error (After splitting)

$$= (9 + 4 \times 0.5)/30 = 11/30$$

PRUNE!

Class = Yes	8
Class = No	4

Class = Yes	3
Class = No	4

A1

Class = Yes	4
Class = No	1

Class = Yes	5
Class = No	1

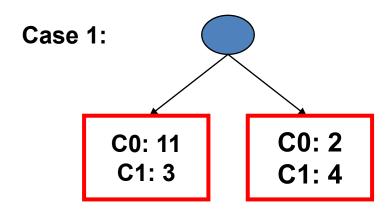
Examples of Post-pruning

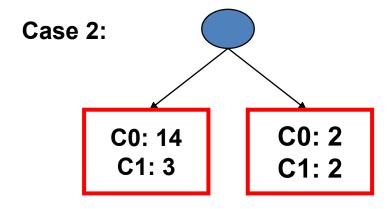
Optimistic error?Don't prune for both cases

Pessimistic error?Don't prune case 1, prune case 2

– Reduced error pruning?

Depends on validation set





Handling Missing Attribute Values

- Missing values affect decision tree construction in three different ways:
 - Affects how impurity measures are computed
 - Affects how to distribute instance with missing value to child nodes
 - Affects how a test instance with missing value is classified

Computing Impurity Measure

Tid	Refund	Marital Status	Taxable Income	Class
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	?	Single	90K	Yes

Missing value

Before Splitting:

Entropy(Parent)

$$= -0.3 \log(0.3) - (0.7) \log(0.7) = 0.8813$$

	Class = Yes	Class = No
Refund=Yes	0	3
Refund=No	2	4
Refund=?	1	0

Split on Refund:

$$= -(2/6)\log(2/6) - (4/6)\log(4/6) = 0.9183$$

Entropy(Children)

$$= 0.3 (0) + 0.6 (0.9183) = 0.551$$

Gain =
$$0.9 \times (0.8813 - 0.551) = 0.3303$$

Distribute Instances

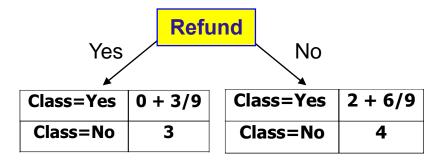
Tid	Refund	Marital Status	Taxable Income	Class
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6	No	Married	60K	No
7	Yes	Divorced	220K	No
8	No	Single	85K	Yes
9	No	Married	75K	No



Class=Yes	0
Class=No	3

Cheat=Yes	2
Cheat=No	4

Tid	Refund		Taxable Income	Class
10	?	Single	90K	Yes



Probability that Refund=Yes is 3/9 Probability that Refund=No is 6/9

Assign record to the left child with weight = 3/9 and to the right child with weight = 6/9

Classify Instances

