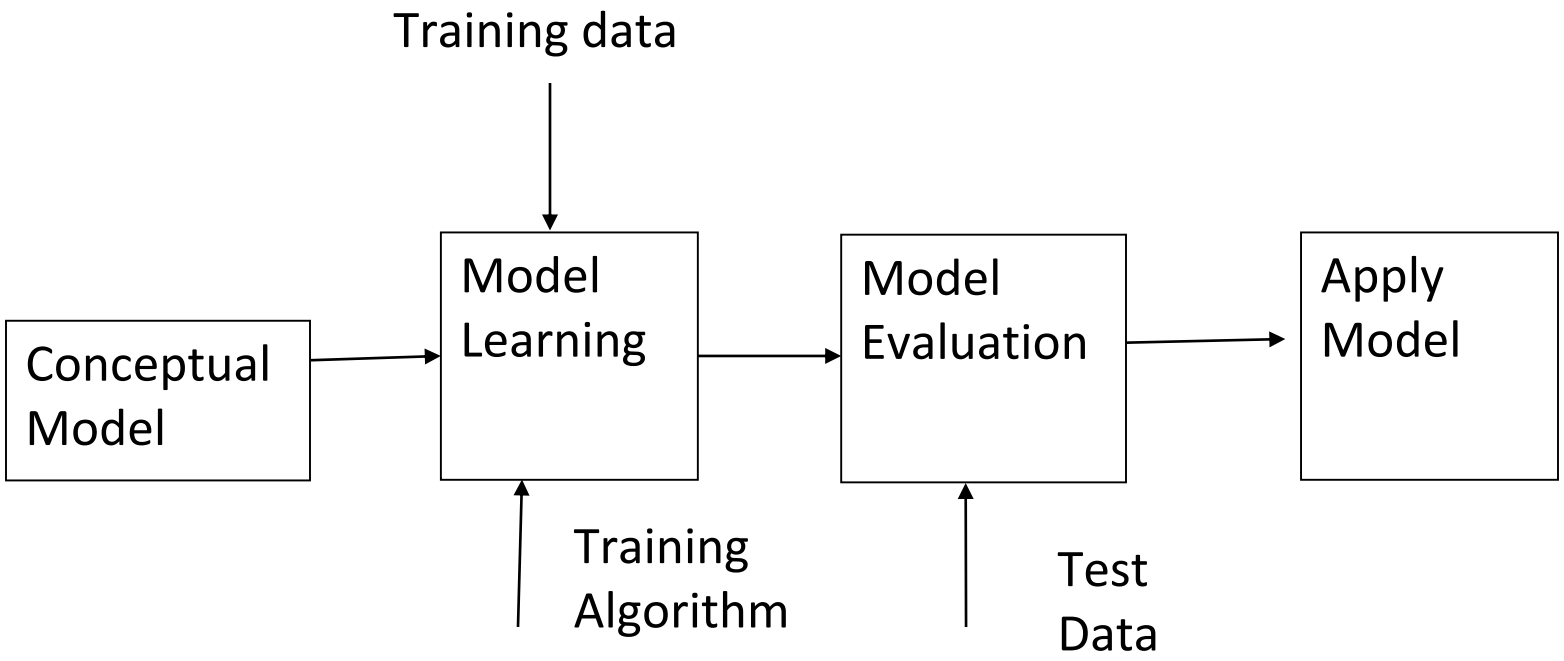
Chapter 3. Classification: Basic Concepts

- Classification: Basic Concepts
- Decision Tree classifier
- Rule Based Classifier
- Nearest Neighbor Classifier
- Bayesian Classifier
- Artificial Neural Network (ANN) Classifier
- Model Evaluation and Selection

Classification: Basic Concepts

- Data analysis can be used for extracting models describing important classes or to predict future data trends.
- These two forms are as follows −
  - Classification
    - Classification models predict categorical class labels
    - For example, we can build a classification model to categorize bank loan applications as either safe or risky,
  - Prediction
    - Prediction models predict continuous valued functions.
    - prediction model to predict the expenditures in dollars of potential customers on computer equipment given their income and occupation.

Concept of Classification



Supervised vs. Unsupervised Learning

- Supervised learning (classification)
  - Supervision: The training data (observations, measurements, etc.) are accompanied by **labels** indicating the class of the observations
  - New data is classified based on the training set
- Unsupervised learning (clustering)
  - The class labels of training data is unknown
  - Given a set of measurements, observations, etc. with the aim of establishing the existence of classes or clusters in the data

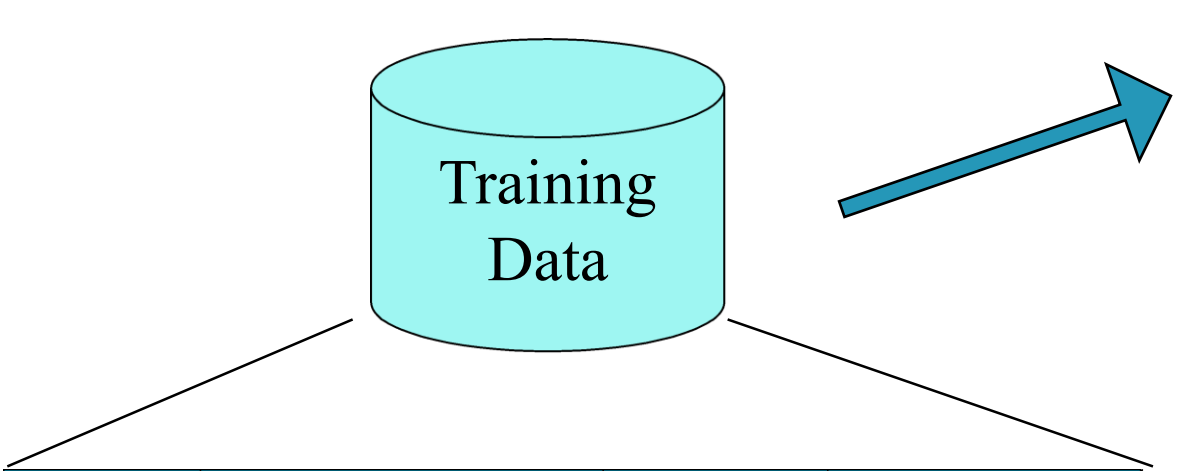
Prediction Problems: Classification vs. Numeric Prediction

- Classification
  - predicts categorical class labels (discrete or nominal)
  - classifies data (constructs a model) based on the training set and the values (class labels) in a classifying attribute and uses it in classifying new data
- Numeric Prediction
  - models continuous-valued functions, i.e., predicts unknown or missing values
- Typical applications
  - Credit/loan approval:
  - Medical diagnosis: if a tumor is cancerous or benign
  - Fraud detection: if a transaction is fraudulent
  - Web page categorization: which category it is

Classification—A Two-Step Process

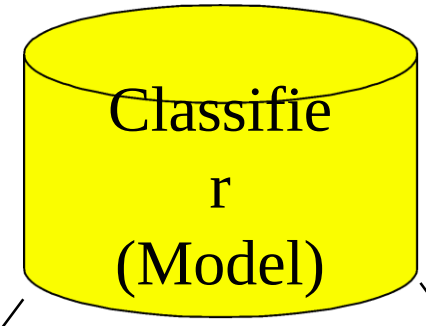
- Model construction: describing a set of predetermined classes
  - Each tuple/sample is assumed to belong to a predefined class, as determined by the class label attribute
  - The set of tuples used for model construction is training set
  - The model is represented as classification rules, decision trees, or mathematical formulae
- Model usage: for classifying future or unknown objects
  - Estimate accuracy of the model
    - The known label of test sample is compared with the classified result from the model
    - Accuracy rate is the percentage of test set samples that are correctly classified by the model
    - Test set is independent of training set (otherwise overfitting)
  - If the accuracy is acceptable, use the model to classify new data
- Note: If *the test set* is used to select models, it is called validation (test) set

Process (1): Model Construction



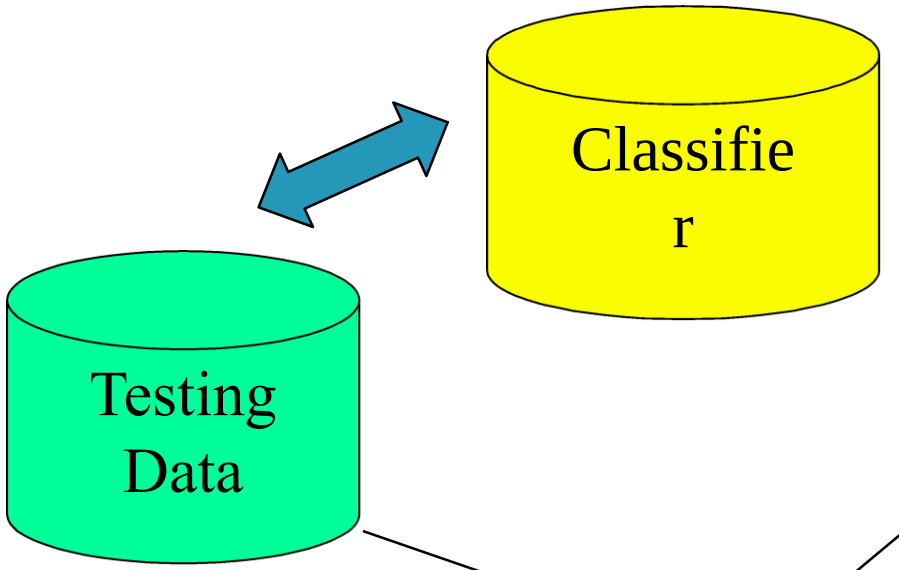
NAME	RANK	YEARS	TENURED
Mike	Assistant Prof	3	no
Mary	Assistant Prof	7	yes
Bill	Professor	2	yes
Jim	Associate Prof	7	yes
Dave	Assistant Prof	6	no
Anne	Associate Prof	3	no

Classification
Algorithms



IF rank = ‘professor’
OR years > 6
THEN tenured = ‘yes’

Process (2): Using the Model in Prediction



NAME	RANK	YEARS	TENURED
Tom	Assistant Prof	2	no
Merlisa	Associate Prof	7	no
George	Professor	5	yes
Joseph	Assistant Prof	7	yes

(Jeff, Professor, 4)

Tenured
?

Classification type

- Decision Tree classifier
- Rule Based Classifier
- Nearest Neighbor Classifier
- Bayesian Classifier
- Artificial Neural Network (ANN) Classifier
- Others

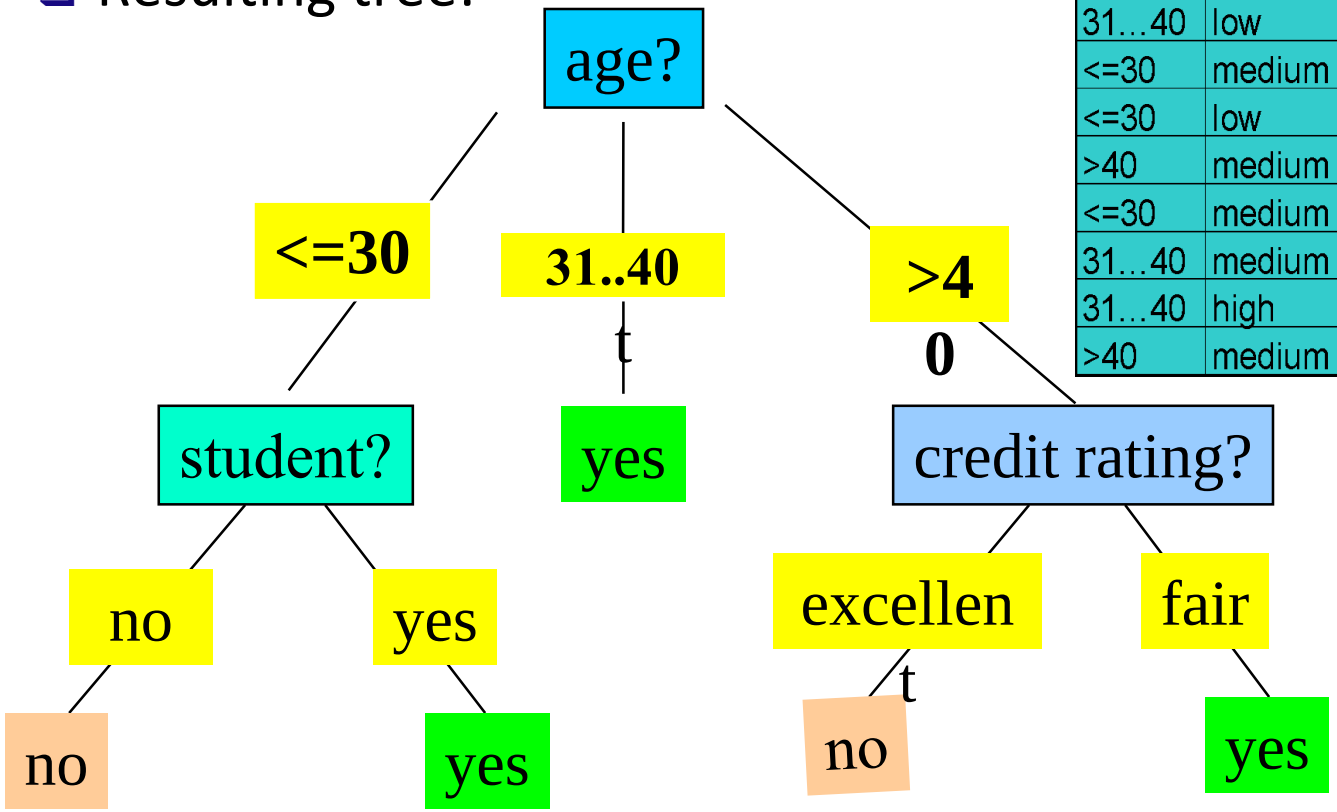
Decision Tree classifier

- A decision tree is tree in which each branch node represents a choice between a number of alternatives and each leaf node represents a classification or decision.
- Decision tree is a classifier in the form of a tree structure where a **leaf node** indicates the class of instances, a **decision node** specifies some test to be carried out on a single attribute value with one branch and sub-tree for each possible outcome of the test.
- A decision tree can be used to classify an instance by starting at root of the tree and moving through it until leaf node. The leaf node provides the corresponding class of instance.

Decision Tree Induction: An Example

- Training data set: Buys_computer
- The data set follows an example of Quinlan's ID3 (Playing Tennis)
- Resulting tree:

age	income	student	credit_rating	buys_computer
<=30	high	no	fair	no
<=30	high	no	excellent	no
31…40	high	no	fair	yes
>40	medium	no	fair	yes
>40	low	yes	fair	yes
>40	low	yes	excellent	no
31…40	low	yes	excellent	yes
<=30	medium	no	fair	no
<=30	low	yes	fair	yes
>40	medium	yes	fair	yes
<=30	medium	yes	excellent	yes
31…40	medium	no	excellent	yes
31…40	high	yes	fair	yes
>40	medium	no	excellent	no



Decision Tree Algorithm

- Hunt's Algorithm
- ID3, J48, C4.5 (Based on Entropy Calculation)
- SLIQ,SPRINT,CART (Based on Gini-Index)

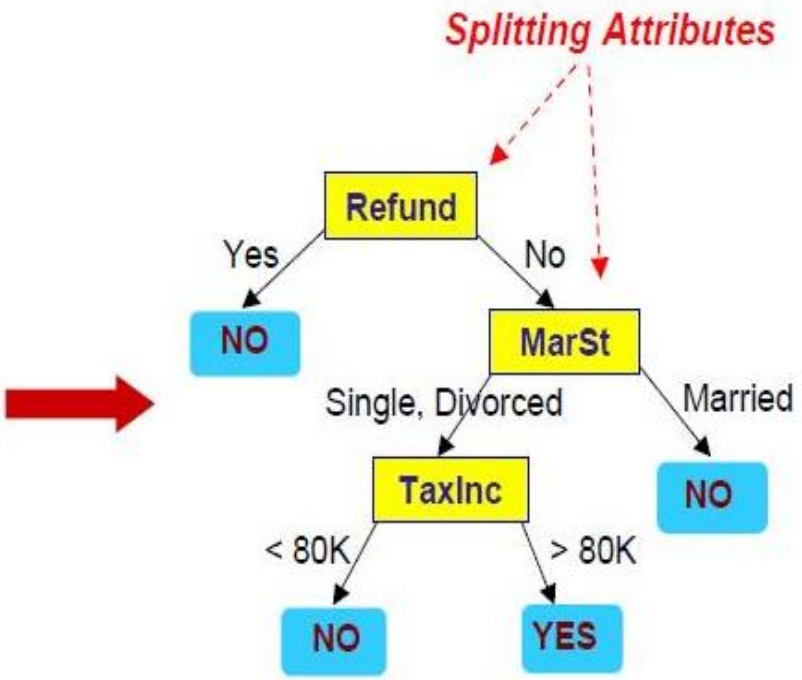
Hunt's Algorithm

- Hunt's algorithm grows a decision tree in a recursive fashion by partitioning the training data into successively into subsets.
- Let Dt be the set of training data that reach a node '**t**'. The general recursive procedure is defined as:
  - If Dt contains records that belong the same class y_t, then t is a leaf node labeled as y_t.
  - If Dt is an empty set, then t is a leaf node labeled by the default class, y_d
  - If Dt contains records that belong to more than one class, use an attribute test to split the data into smaller subsets.
- It recursively applies the procedure to each subset until all the records in the subset belong to the same class.
- The Hunt's algorithm assumes that each combination of attribute sets has a unique class label during the procedure.
- If all the records associated with Dt have identical attribute values except for the class label, then it is not possible to split these records any future. In this case, the node is declared a leaf node with the same class label as the majority class of training records associated with this node.

Example

Tid	Refund	Marital Status	Taxable Income	Cheat
	categorical	categorical	continuous	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	No	Single	90K	Yes

Training Data



Model: Decision Tree

Tree Induction:

- Tree induction is based on Greedy Strategy i.e. split the records based on an attribute test that optimize certain criterion.
- **Issues:**
  - **How to split the record?**
  - **How to specify the attribute test condition?**
    - Depends on attribute types and number of ways to split the record i.e. 2-ways split /multi-way split.
    - Depends upon attribute types. (Nominal, Ordinal, Continuous)
  - **When to stop splitting?**
    - When all records are belongs to the same class or all records have similar attributes.
  - **How to determine the best split?**
    - Nodes with homogenous class distribution are preferred.
    - Measure the node impurity.
      - Gini-Index
      - Entropy
      - Misclassification Error

Gini Index (CART, IBM IntelligentMiner)

- If a data set D contains examples from n classes, gini index, $gini(D)$ is defined as

$$gini(D) = 1 - \sum_{j=1}^{n} p_j^2$$

  where p_j is the relative frequency of class j in D

- If a data set D is split on A into two subsets D_1 and D_2, the *gini* index $gini(D)$ is defined as

$$gini_A(D) = \frac{|D_1|}{|D|} gini(D_1) + \frac{|D_2|}{|D|} gini(D_2)$$

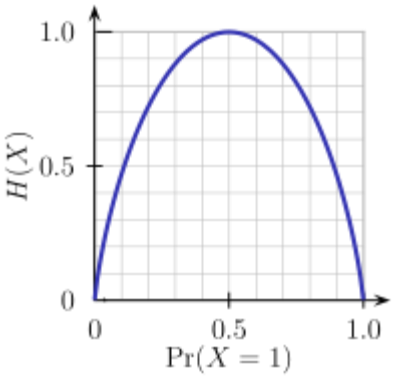
- Reduction in Impurity:

$$\Delta gini(A) = gini(D) - gini_A(D)$$

- The attribute provides the smallest $gini_{split}(D)$ (or the largest reduction in impurity) is chosen to split the node (*need to enumerate all the possible splitting points for each attribute*)

Brief Review of Entropy

- Entropy (Information Theory)
  - A measure of uncertainty associated with a random variable
  - Calculation: For a discrete random variable *Y* taking *m* distinct values $\{y_1, \ldots, y_m\}$,
    - $H(Y) = -\sum_{i=1}^{m} p_i \log(p_i)$, where $p_i = P(Y = y_i)$
  - Interpretation:
    - Higher entropy => higher uncertainty
    - Lower entropy => lower uncertainty
- Conditional Entropy
  - $H(Y|X) = \sum_x p(x) H(Y|X = x)$



m = 2

Algorithm for Decision Tree Induction

- Basic algorithm (a greedy algorithm)
  - Tree is constructed in a top-down recursive divide-and-conquer manner
  - At start, all the training examples are at the root
  - Attributes are categorical (if continuous-valued, they are discretized in advance)
  - Examples are partitioned recursively based on selected attributes
  - Test attributes are selected on the basis of a heuristic or statistical measure (e.g., information gain)
- Conditions for stopping partitioning
  - All samples for a given node belong to the same class
  - There are no remaining attributes for further partitioning – majority voting is employed for classifying the leaf
  - There are no samples left

ID3 Algorithm

- The ID3 algorithm begins with the original dataset as the root node.
- On each iteration of the algorithm, it iterates through every unused attribute of the dataset and calculates the entropy (or information gain) of that attribute.
- It then selects the attribute which has the smallest entropy (or largest information gain) value.
- The dataset is then split by the selected attribute to produce subsets of the data.
- The algorithm continues to recur on each subset, considering only attributes never selected before. Recursion on a subset may stop in one of these cases:

ID3 Algorithm

- Every element in the subset belongs to the same class , then the node is turned into a leaf and labeled with the class of the examples
- If the examples do not belong to the same class ,
- Calculate entropy and hence information gain to select the best node to split data.
- Partition the data into subset.
- Recursively repeat until all data are correctly classified

Throughout the algorithm, the decision tree is constructed with each non-terminal node representing the selected attribute on which the data was split, and terminal nodes representing the class label of the final subset of this branch.

Attribute Selection Measure: Information Gain (ID3/C4.5)

- Select the attribute with the highest information gain
- Let p_i be the probability that an arbitrary tuple in D belongs to class C_i, estimated by $|C_{i,D}|/|D|$
- Expected information (entropy) needed to classify a tuple in D:

$$Info(D) = -\sum_{i=1}^{m} p_i \log_2(p_i)$$

- Information needed (after using A to split D into v partitions) to classify D:

$$Info_A(D) = \sum_{j=1}^{v} \frac{|D_j|}{|D|} \times Info(D_j)$$

- Information gained by branching on attribute A

$$Gain(A) = Info(D) - Info_A(D)$$

Attribute Selection: Information Gain

- Class P: buys_computer = "yes"
- Class N: buys_computer = "no"

$$Info(D) = I(9,5) = -\frac{9}{14}\log_2(\frac{9}{14}) - \frac{5}{14}\log_2(\frac{5}{14}) = 0.940$$

age	p_i	n_i	$I(p_i, n_i)$
<=30	2	3	0.971
31…40	4	0	0
>40	3	2	0.971

age	income	student	credit_rating	buys_computer
<=30	high	no	fair	no
<=30	high	no	excellent	no
31…40	high	no	fair	yes
>40	medium	no	fair	yes
>40	low	yes	fair	yes
>40	low	yes	excellent	no
31…40	low	yes	excellent	yes
<=30	medium	no	fair	no
<=30	low	yes	fair	yes
>40	medium	yes	fair	yes
<=30	medium	yes	excellent	yes
31…40	medium	no	excellent	yes
31…40	high	yes	fair	yes
>40	medium	no	excellent	no

$$Info_{age}(D) = \frac{5}{14}I(2,3) + \frac{4}{14}I(4,0) + \frac{5}{14}I(3,2) = 0.694$$

$\frac{5}{14}I(2,3)$ means "age <=30" has 5 out of 14 samples, with 2 yes'es and 3 no's. Hence

$$Gain(age) = Info(D) - Info_{age}(D) = 0.246$$

Similarly,

$$Gain(income) = 0.029$$
$$Gain(student) = 0.151$$
$$Gain(credit\_rating) = 0.048$$

Computing Information-Gain for Continuous-Valued Attributes

- Let attribute A be a continuous-valued attribute
- Must determine the *best split point* for A
  - Sort the value A in increasing order
  - Typically, the midpoint between each pair of adjacent values is considered as a possible *split point*
    - $(a_i+a_{i+1})/2$ is the midpoint between the values of a_i and a_{i+1}
  - The point with the *minimum expected information requirement* for A is selected as the split-point for A
- Split:
  - D1 is the set of tuples in D satisfying A $\leq$ split-point, and D2 is the set of tuples in D satisfying A > split-point

Gain Ratio for Attribute Selection (C4.5)

- Information gain measure is biased towards attributes with a large number of values
- C4.5 (a successor of ID3) uses gain ratio to overcome the problem (normalization to information gain)

$$SplitInfo_A(D) = -\sum_{j=1}^{v} \frac{|D_j|}{|D|} \times \log_2\left(\frac{|D_j|}{|D|}\right)$$

  - GainRatio(A) = Gain(A)/SplitInfo(A)
- Ex.

$$SplitInfo_{income}(D) = -\frac{4}{14} \times \log_2\left(\frac{4}{14}\right) - \frac{6}{14} \times \log_2\left(\frac{6}{14}\right) - \frac{4}{14} \times \log_2\left(\frac{4}{14}\right) = 1.557$$

  - gain_ratio(income) = 0.029/1.557 = 0.019
- The attribute with the maximum gain ratio is selected as the splitting attribute

Gini Index (CART, IBM IntelligentMiner)

- If a data set D contains examples from n classes, gini index, $gini(D)$ is defined as

$$gini(D) = 1 - \sum_{j=1}^{n} p_j^2$$

  where p_j is the relative frequency of class j in D

- If a data set D is split on A into two subsets D_1 and D_2, the *gini* index $gini(D)$ is defined as

$$gini_A(D) = \frac{|D_1|}{|D|} gini(D_1) + \frac{|D_2|}{|D|} gini(D_2)$$

- Reduction in Impurity:

$$\Delta gini(A) = gini(D) - gini_A(D)$$

- The attribute provides the smallest $gini_{split}(D)$ (or the largest reduction in impurity) is chosen to split the node (*need to enumerate all the possible splitting points for each attribute*)

Computation of Gini Index

- Ex. D has 9 tuples in buys_computer = "yes" and 5 in "no"

$$gini(D) = 1 - \left(\frac{9}{14}\right)^2 - \left(\frac{5}{14}\right)^2 = 0.459$$

- Suppose the attribute income partitions D into 10 in D_1: {low, medium} and 4 in D_2

$$gini_{income \in \{low,medium\}}(D) = \left(\frac{10}{14}\right) Gini(D_1) + \left(\frac{4}{14}\right) Gini(D_2)$$

$$= \frac{10}{14}\left(1 - \left(\frac{7}{10}\right)^2 - \left(\frac{3}{10}\right)^2\right) + \frac{4}{14}\left(1 - \left(\frac{2}{4}\right)^2 - \left(\frac{2}{4}\right)^2\right)$$

$$= 0.443$$

$$= Gini_{income \in \{high\}}(D).$$

  $Gini_{\{low,high\}}$ is 0.458; $Gini_{\{medium,high\}}$ is 0.450. Thus, split on the {low,medium} (and {high}) since it has the lowest Gini index

- All attributes are assumed continuous-valued
- May need other tools, e.g., clustering, to get the possible split values
- Can be modified for categorical attributes

Comparing Attribute Selection Measures

- The three measures, in general, return good results but
  - **Information gain**:
    - biased towards multivalued attributes
  - **Gain ratio**:
    - tends to prefer unbalanced splits in which one partition is much smaller than the others
  - **Gini index**:
    - biased to multivalued attributes
    - has difficulty when # of classes is large
    - tends to favor tests that result in equal-sized partitions and purity in both partitions

Overfitting and Tree Pruning

- Overfitting: An induced tree may overfit the training data
  - Too many branches, some may reflect anomalies due to noise or outliers
  - Poor accuracy for unseen samples
- Two approaches to avoid overfitting
  - Prepruning: *Halt tree construction early*—do not split a node if this would result in the goodness measure falling below a threshold
    - Difficult to choose an appropriate threshold
  - Postpruning: *Remove branches* from a "fully grown" tree—get a sequence of progressively pruned trees
    - Use a set of data different from the training data to decide which is the "best pruned tree"

Enhancements to Basic Decision Tree Induction

- Allow for **continuous-valued attributes**
  - Dynamically define new discrete-valued attributes that partition the continuous attribute value into a discrete set of intervals
- Handle **missing attribute values**
  - Assign the most common value of the attribute
  - Assign probability to each of the possible values
- **Attribute construction**
  - Create new attributes based on existing ones that are sparsely represented
  - This reduces fragmentation, repetition, and replication

Advantages of Decision Tree Classifier

- Inexpensive to construct
- Extremely fast at classifying unknown records
- Easy to interpret for small-sized trees
- Accuracy is

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Using IF-THEN Rules for Classification

- Represent the knowledge in the form of IF-THEN rules

  R: IF *age* = youth AND *student* = yes THEN *buys_computer* = yes

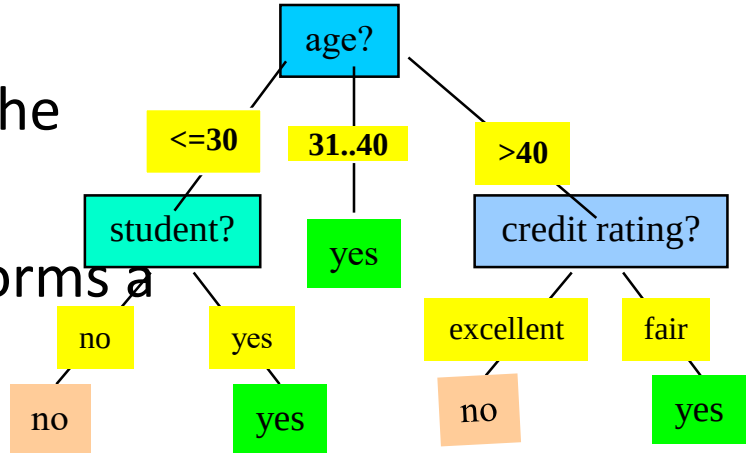
  - Rule antecedent/precondition vs. rule consequent
- Assessment of a rule: *coverage* and *accuracy*
  - n_{covers} = # of tuples covered by R
  - $n_{correct}$ = # of tuples correctly classified by R

  coverage(R) = n_{covers} /|D| /* D: training data set */

  accuracy(R) = $n_{correct}$ / n_{covers}
- If more than one rule are triggered, need **conflict resolution**
  - Size ordering: assign the highest priority to the triggering rules that has the "toughest" requirement (i.e., with the *most attribute tests*)
  - Class-based ordering: decreasing order of *prevalence or misclassification cost per class*
  - Rule-based ordering (**decision list**): rules are organized into one long priority list, according to some measure of rule quality or by experts

Rule Extraction from a Decision Tree

- Rules are *easier to understand* than large trees
- One rule is created *for each path* from the root to a leaf
- Each attribute-value pair along a path forms a conjunction: the leaf holds the class prediction
- Rules are mutually exclusive and exhaustive



- Example: Rule extraction from our *buys_computer* decision-tree

IF *age* = young AND *student* = *no* THEN *buys_computer* = *no*
IF *age* = young AND *student* = *yes* THEN *buys_computer* = *yes*
IF *age* = mid-age THEN *buys_computer* = *yes*
IF *age* = old AND *credit_rating* = *excellent* THEN *buys_computer* = *no*
IF *age* = old AND *credit_rating* = *fair* THEN *buys_computer* = *yes*

Rule Induction: Sequential Covering Method

- Sequential covering algorithm: Extracts rules directly from training data
- Typical sequential covering algorithms: FOIL, AQ, CN2, RIPPER
- Rules are learned *sequentially*, each for a given class C_i will cover many tuples of C_i but none (or few) of the tuples of other classes
- Steps:
  - Rules are learned one at a time
  - Each time a rule is learned, the tuples covered by the rules are removed
  - Repeat the process on the remaining tuples until *termination condition*, e.g., when no more training examples or when the quality of a rule returned is below a user-specified threshold
- Comp. w. decision-tree induction: learning a set of rules *simultaneously*

Characteristics of Rule-Based Classifier

- **Mutually exclusive Rules**
  - Classifier contains mutually exclusive rules if all the rules are independent of each other.
  - Every record is covered by at most one rule.
  - Rules are no longer mutually exclusive if a record may triggered by more than one rule. To make mutually exclusive we apply rule ordering.
- **Exhaustive Rules**
  - Classifier has exhaustive coverage if it accounts for every possible combination of attribute values (every possible rule).
  - Each record is covered by at least one rule.
  - Rules are no longer exhaustive if a record may bit trigger any rules. To make rules exhaustive use default class.

Building Classification Rules

Two approaches are used to build classification rules.

- **Direct Method**
  - Extract rules directly from data. It is an inductive and sequential approach.
- ***Sequential Covering***
- Start from an empty rule
- Grow a rule using the Learn-One-Rule function
- Remove training records covered by the rule
- Repeat Step (2) and (3) until stopping criterion is met

Aspects of Sequential Covering

- Rule Growing
- Instance Elimination
- Rule Evaluation
- Stopping Criterion
- Rule Pruning

Rule Growing

- ***CN2 Algorithm:***
- Start from an empty conjunct: {}
- Add conjuncts that minimizes the entropy measure: {A}, {A,B}, …
- Determine the rule consequent by taking majority class of instances covered by the rule

Rule Growing

- ***RIPPER Algorithm:***
  - Start from an empty rule: {} => class
  - Add conjuncts that maximize FOIL's information gain measure:
  - R0: {} => class (initial rule)
  - R1: {A} => class (rule after adding conjunct)
  - Gain (R0, R1) = t [log (p1/(p1+n1)) – log (p0/(p0 + n0))]

Where,

t: number of positive instances covered by both R0 and R1

p0: number of positive instances covered by R0

n0: number of negative instances covered by R0

p1: number of positive instances covered by R1

n1: number of negative instances covered by R1

Instance Elimination

- We need to eliminate instances otherwise; the next rule is identical to previous rule.
- We remove positive instances to ensure that the next rule is different.
- We remove negative instances to prevent underestimating accuracy of rule

Rule Evaluation

- Metrics:
  - Accuracy $= \frac{n_c}{n}$
  - Laplace $= \frac{n_c + 1}{n + k}$
  - M-estimate $= \frac{n_c + kp}{n + k}$

n : Number of instances

n_c: Number of instances covered by rule

k: Number of classes

p: Prior probability

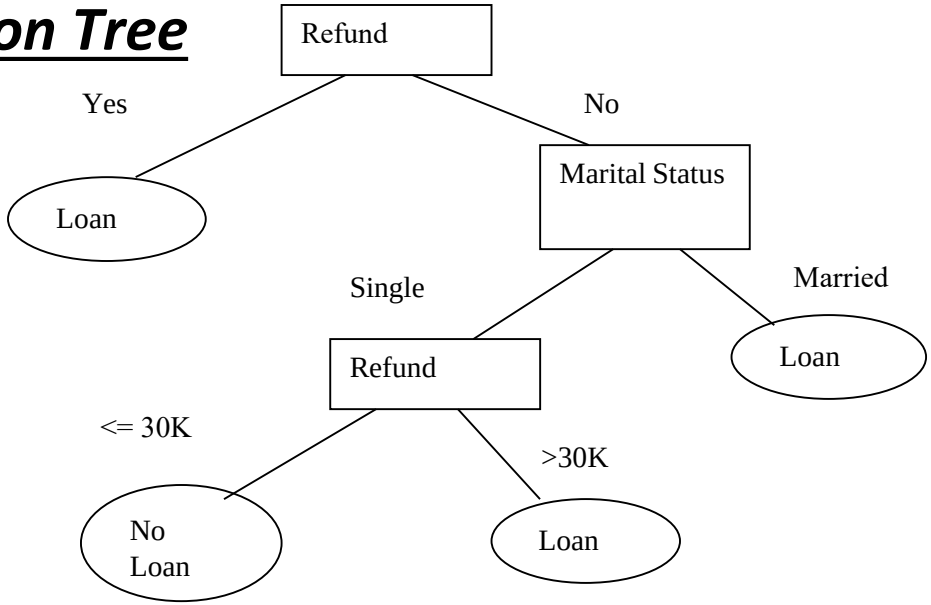
Stopping Criterion and Rule Pruning

- ***Stopping criterion***
  - Compute the gain
  - If gain is not significant, discard the new rule.
- ***Rule Pruning***
  - Similar to post-pruning of decision trees.
  - Reduced Error Pruning:
  - Remove one of the conjuncts in the rule
  - Compare error rate on validation set before and after pruning
  - If error improves, prune the conjunct

Indirect Method:

- Extract rules from other classification models (e.g. decision trees, neural networks, etc).

Eg; Rule Extraction from Decision Tree



Rules:
R1: (Refund = Yes) => Loan
R2: (Refund = No) ^ (Marital Status = Married) => Loan

Rule simplification

Complex rules can be simplified. In above example R2 can be simplified as:
r2: (Marital Status = Married) => Loan

Advantages of Rule-Based Classifiers

- As highly expressive as decision trees
- Easy to interpret
- Easy to generate
- Can classify new instances rapidly
- Performance comparable to decision trees

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Instance Based Classifier

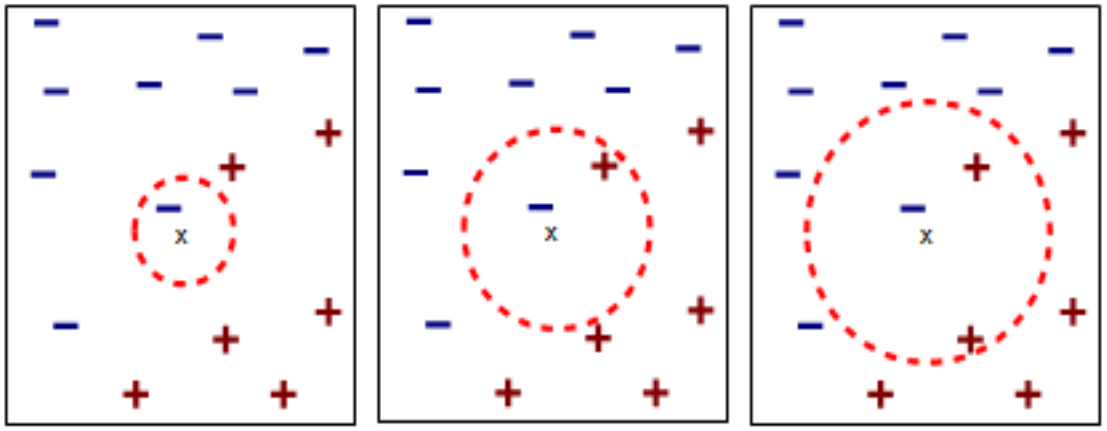
- **Rote-learner**
  - Memorizes entire training data and performs classification only if attributes of record match one of the training examples exactly
- **Nearest neighbor**
  - Uses k "closest" points (nearest neighbors) for performing classification. K-closet neighbor of a record 'X' are data points that have the K-smallest distance of 'X'.
  - Classification based on learning by analogy i.e. by comparing a given test tuple with training tuple that are similar to it.
  - Training tuples are described by n-attributes.
  - When given an unknown tuple, a k-nearest- neighbor classifier searches the pattern space for the k-training tuples that are closest to the unknown tuple.

Nearest neighbor

- Nearest neighbor classifier requires:
  - Set of stored records
  - Distance metric to compute distance between records. For distance calculation any standard approach can be used such as Euclidean distance.
  - The value of ‘K’, the number of nearest neighbor to retrieve.
  - To classify the unknown records
  - Compute distance to other training records.
  - Identify the k-nearest neighbor.
  - Use class label nearest neighbors to determine the class label of unknown record. In case of conflict, use majority vote for classification.

Issues of classification using k-nearest neighbor classification

- **Choosing the value of K**
  - One of challenge in classification is to choose the appropriate value of K. If K is too small, it is sensitive to noise points. If K is too large, neighbor may include points from other classes.
  - With the change of value of K, the classification result may vary.



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

Issues of classification using k-nearest neighbor classification

- **Scaling Issue**
  - Attribute may have to be scaled to prevent distance measure from being dominated by one of attributes. Eg. Height, Temperature etc.
- **Distance computing for non-numeric data.**
  - Use Distance as 0 for the same data and maximum possible distance for different data.
- **Missing values**
  - Use maximum possible distance

Disadvantages

- Poor accuracy when data have noise and irrelevant attributes.
- Slow when classifying test tuples.
- Classifying unknown records are relatively expensive.

Chapter 3. Classification: Basic Concepts

- Classification: Basic Concepts
- Decision Tree classifier
- Rule Based Classifier
- Nearest Neighbor Classifier
- Bayesian Classifier 
- Artificial Neural Network (ANN) Classifier
- Model Evaluation and Selection

Bayesian Classification: Why?

- A statistical classifier: performs *probabilistic prediction*, *i.e.*, predicts class membership probabilities
- Foundation: Based on Bayes' Theorem.
- Performance: A simple Bayesian classifier, *naïve Bayesian classifier*, has comparable performance with decision tree and selected neural network classifiers
- Incremental: Each training example can incrementally increase/decrease the probability that a hypothesis is correct — prior knowledge can be combined with observed data
- Standard: Even when Bayesian methods are computationally intractable, they can provide a standard of optimal decision making against which other methods can be measured

Bayes' Theorem: Basics

- Total probability Theorem: $P(B) = \sum_{i=1}^{M} P(B|A_i)P(A_i)$
- Bayes' Theorem: $P(H|\mathbf{X}) = \frac{P(\mathbf{X}|H)P(H)}{P(\mathbf{X})} = P(\mathbf{X}|H) \times P(H) / P(\mathbf{X})$
  - Let **X** be a data sample ("*evidence*"): class label is unknown
  - Let H be a *hypothesis* that X belongs to class C
  - Classification is to determine P(H|**X**), (i.e., *posteriori probability):* the probability that the hypothesis holds given the observed data sample **X**
  - P(H) (*prior probability*): the initial probability
    - E.g., **X** will buy computer, regardless of age, income, …
  - P(**X**): probability that sample data is observed
  - P(**X**|H) (likelihood): the probability of observing the sample **X**, given that the hypothesis holds
    - E.g., Given that **X** will buy computer, the prob. that X is 31..40, medium income

Prediction Based on Bayes' Theorem

- Given training data **X**, *posteriori probability of a hypothesis* H, P(H|**X**), follows the Bayes' theorem

$$P(H|\mathbf{X}) = \frac{P(\mathbf{X}|H)P(H)}{P(\mathbf{X})} = P(\mathbf{X}|H) \times P(H) / P(\mathbf{X})$$

- Informally, this can be viewed as

  posteriori = likelihood x prior/evidence

- Predicts **X** belongs to C_i iff the probability $P(C_i|\mathbf{X})$ is the highest among all the $P(C_k|X)$ for all the *k* classes
- Practical difficulty: It requires initial knowledge of many probabilities, involving significant computational cost

Classification Is to Derive the Maximum Posteriori

- Let D be a training set of tuples and their associated class labels, and each tuple is represented by an n-D attribute vector **X** = (x_1, x_2, …, x_n)
- Suppose there are *m* classes C_1, C_2, …, C_m.
- Classification is to derive the maximum posteriori, i.e., the maximal $P(C_i|\mathbf{X})$
- This can be derived from Bayes' theorem

$$P(C_i|\mathbf{X}) = \frac{P(\mathbf{X}|C_i)P(C_i)}{P(\mathbf{X})}$$

- Since P(X) is constant for all classes, only

$$P(C_i|\mathbf{X}) = P(\mathbf{X}|C_i)P(C_i)$$

needs to be maximized

Naïve Bayes Classifier

- A simplified assumption: attributes are conditionally independent (i.e., no dependence relation between attributes):

$$P(\mathbf{X}|C_i) = \prod_{k=1}^{n} P(x_k|C_i) = P(x_1|C_i) \times P(x_2|C_i) \times \ldots \times P(x_n|C_i)$$

- This greatly reduces the computation cost: Only counts the class distribution
- If A_k is categorical, $P(x_k|C_i)$ is the # of tuples in C_i having value x_k for A_k divided by $|C_{i,D}|$ (# of tuples of C_i in D)
- If A_k is continous-valued, $P(x_k|C_i)$ is usually computed based on Gaussian distribution with a mean μ and standard deviation σ

and $P(x_k|C_i)$ is

$$g(x, \mu, \sigma) = \frac{1}{\sqrt{2\pi}\sigma} e^{-\frac{(x-\mu)^2}{2\sigma^2}}$$

$$P(\mathbf{X}|C_i) = g(x_k, \mu_{C_i}, \sigma_{C_i})$$

Naïve Bayes Classifier: Training Dataset

Class:
C1:buys_computer = ‘yes’
C2:buys_computer = ‘no’

Data to be classified:
X = (age <=30,
Income = medium,
Student = yes
Credit_rating = Fair)

age	income	student	credit_rating	comp
<=30	high	no	fair	no
<=30	high	no	excellent	no
31…40	high	no	fair	yes
>40	medium	no	fair	yes
>40	low	yes	fair	yes
>40	low	yes	excellent	no
31…40	low	yes	excellent	yes
<=30	medium	no	fair	no
<=30	low	yes	fair	yes
>40	medium	yes	fair	yes
<=30	medium	yes	excellent	yes
31…40	medium	no	excellent	yes
31…40	high	yes	fair	yes
>40	medium	no	excellent	no

Naïve Bayes Classifier: An Example

age	income	student	credit_rating	com
<=30	high	no	fair	no
<=30	high	no	excellent	no
31…40	high	no	fair	yes
>40	medium	no	fair	yes
>40	low	yes	fair	yes
>40	low	yes	excellent	no
31…40	low	yes	excellent	yes
<=30	medium	no	fair	no
<=30	low	yes	fair	yes
>40	medium	yes	fair	yes
<=30	medium	yes	excellent	yes
31…40	medium	no	excellent	yes
31…40	high	yes	fair	yes
>40	medium	no	excellent	no

- $P(C_i)$: P(buys_computer = "yes") = 9/14 = 0.643
  P(buys_computer = "no") = 5/14= 0.357
- Compute $P(X|C_i)$ for each class
  P(age = "<=30" | buys_computer = "yes") = 2/9 = 0.222
  P(age = "<= 30" | buys_computer = "no") = 3/5 = 0.6
  P(income = "medium" | buys_computer = "yes") = 4/9 = 0.444
  P(income = "medium" | buys_computer = "no") = 2/5 = 0.4
  P(student = "yes" | buys_computer = "yes) = 6/9 = 0.667
  P(student = "yes" | buys_computer = "no") = 1/5 = 0.2
  P(credit_rating = "fair" | buys_computer = "yes") = 6/9 = 0.667
  P(credit_rating = "fair" | buys_computer = "no") = 2/5 = 0.4
- **X = (age <= 30 , income = medium, student = yes, credit_rating = fair)**

$P(X|C_i)$: P(X|buys_computer = "yes") = 0.222 x 0.444 x 0.667 x 0.667 = 0.044
P(X|buys_computer = "no") = 0.6 x 0.4 x 0.2 x 0.4 = 0.019

$P(X|C_i)*P(C_i)$: P(X|buys_computer = "yes") * P(buys_computer = "yes") = 0.028
P(X|buys_computer = "no") * P(buys_computer = "no") = 0.007

Therefore, X belongs to class ("buys_computer = yes")

Avoiding the Zero-Probability Problem

- Naïve Bayesian prediction requires each conditional prob. be **non-zero**. Otherwise, the predicted prob. will be zero

$$P(X \mid C_i) = \prod_{k=1}^{n} P(x_k \mid C_i)$$

- Ex. Suppose a dataset with 1000 tuples, income=low (0), income= medium (990), and income = high (10)
- Use **Laplacian correction** (or Laplacian estimator)
  - *Adding 1 to each case*

    Prob(income = low) = 1/1003

    Prob(income = medium) = 991/1003

    Prob(income = high) = 11/1003
  - The "corrected" prob. estimates are close to their "uncorrected" counterparts

Naïve Bayes Classifier: Comments

- Advantages
  - Easy to implement
  - Good results obtained in most of the cases
- Disadvantages
  - Assumption: class conditional independence, therefore loss of accuracy
  - Practically, dependencies exist among variables
    - E.g., hospitals: patients: Profile: age, family history, etc.

      Symptoms: fever, cough etc., Disease: lung cancer, diabetes, etc.
    - Dependencies among these cannot be modeled by Naïve Bayes Classifier
- How to deal with these dependencies? Bayesian Belief Networks (Chapter 9)

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Artificial Neural Network (ANN) Classifier

- It is set of connected i/o units in which each connection has a weight associated with it.
- During the learning phase the network learns by adjusting the weights so as to be able to predict the correct class label of i/p labels.
- It also referred as connectionist learning due to connection between units.
- It has long training time and poor interpretability but has tolerance to noisy data.
- It can classify pattern on which they have not been trained.
- Well suited for continuous valued i/ps.
- It has parallel topology and processing.

Artificial Neural Network (ANN) Classifier

- Before training the network topology must be designed by:
  - ***Specifying number of i/p nodes/units:*** Depends upon number of independent variable in data set.
  - ***Number of hidden layers:*** Generally only layer is considered in most of the problem. Two layers can be designed for complex problem. Number of nodes in the hidden layer can be adjusted iteratively.
  - ***Number of output nodes/units:*** Depends upon number of class labels of the data set.
  - ***Learning rate:*** Can be adjusted iteratively.
  - ***Learning algorithm*:** Any appropriate learning algorithm can be selected during training phase.
  - ***Bias value***: Can be adjusted iteratively.
- During training the connection weights must be adjusted to fit i/p values with the o/p values.

Back propagation algorithm

- ***Step 1: Initialization:***
  - Set all the weights and thresholds levels of the network to random numbers uniformly distributed inside a small range.
- ***Step 2: Activation:***
  - Activate the back propagation neural network by applying i/ps and desired o/ps.
  - Calculate the actual o/ps of the neurons in the hidden layers.
  - Calculate the actual o/ps of the neurons in the o/p layers.
- ***Step 3: Weight training:***
  - Updates weights in the back propagation network by propagating backwards the errors associated with the o/p neurons.
  - Calculate error gradient of o/p layer and hence of neurons in the hidden layer.
- ***Step 4: Iteration:***
  - Increase iteration by repeating steps 2 and 3 until selected error criteria is satisfied.

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Model Evaluation and Selection

- Evaluation metrics: How can we measure accuracy? Other metrics to consider?
- Use **validation test set** of class-labeled tuples instead of training set when assessing accuracy
- Methods for estimating a classifier's accuracy:
  - Holdout method, random subsampling
  - Cross-validation
  - Bootstrap
- Comparing classifiers:
  - Confidence intervals
  - Cost-benefit analysis and ROC Curves

Classifier Evaluation Metrics: Confusion Matrix

Confusion Matrix:

Actual class\Predicted class	C_1	¬ C_1
C_1	**True Positives (TP)**	**False Negatives (FN)**
¬ C_1	**False Positives (FP)**	**True Negatives (TN)**

Example of Confusion Matrix:

Actual class\Predicted class	buy_computer = yes	buy_computer = no	Total
buy_computer = yes	**6954**	**46**	7000
buy_computer = no	**412**	**2588**	3000
Total	7366	2634	10000

- Given *m* classes, an entry, $\boldsymbol{CM_{i,j}}$ in a **confusion matrix** indicates # of tuples in class *i* that were labeled by the classifier as class *j*
- May have extra rows/columns to provide totals

Classifier Evaluation Metrics: Accuracy, Error Rate, Sensitivity and Specificity

A\P	C	¬C	
C	**TP**	**FN**	**P**
¬C	**FP**	**TN**	**N**
	P'	**N'**	**All**

- **Classifier Accuracy,** or recognition rate: percentage of test set tuples that are correctly classified

  Accuracy = (TP + TN)/All

- **Error rate:** *1 – accuracy*, or

  Error rate = (FP + FN)/All

- **Class Imbalance Problem**:
  - One class may be *rare*, e.g. fraud, or HIV-positive
  - Significant *majority of the negative class* and minority of the positive class
  - **Sensitivity**: True Positive recognition rate
    - **Sensitivity = TP/P**
  - **Specificity**: True Negative recognition rate
    - **Specificity = TN/N**

Classifier Evaluation Metrics: Precision and Recall, and F-measures

- **Precision**: exactness – what % of tuples that the classifier labeled as positive are actually positive

$$precision = \frac{TP}{TP + FP}$$

- **Recall:** completeness – what % of positive tuples did the classifier label as positive?
- Perfect score is 1.0

$$recall = \frac{TP}{TP + FN}$$

- Inverse relationship between precision & recall
- ***F* measure (*F_1* or *F*-score)**: harmonic mean of precision and recall,

$$F = \frac{2 \times precision \times recall}{precision + recall}$$

- ***$F_ß$*:** weighted measure of precision and recall
  - assigns ß times as much weight to recall as to precision

$$F_\beta = \frac{(1 + \beta^2) \times precision \times recall}{\beta^2 \times precision + recall}$$

Classifier Evaluation Metrics: Example

Actual Class\Predicted class	cancer = yes	cancer = no	Total	Recognition(%)
cancer = yes	**90**	**210**	300	30.00 (*sensitivity*
cancer = no	**140**	**9560**	9700	98.56 (*specificity)*
Total	230	9770	10000	96.40 (*accuracy*)

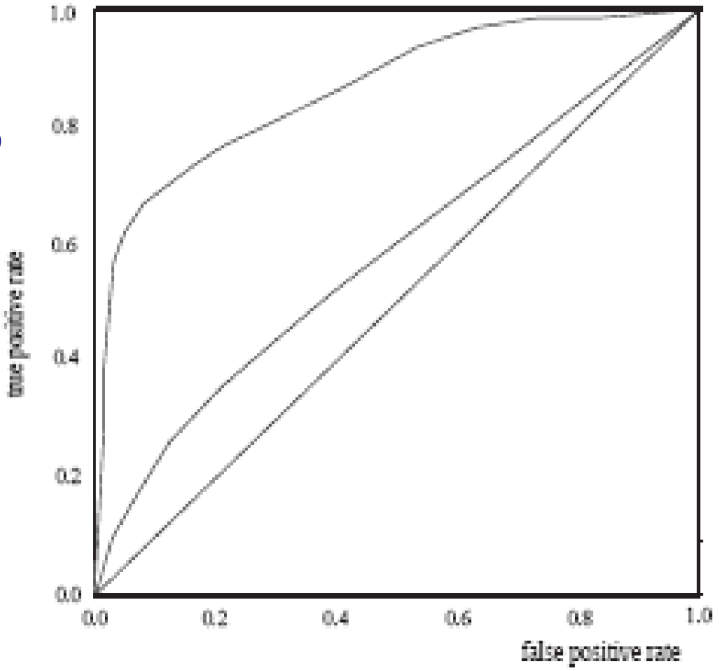
- *Precision* = 90/230 = 39.13% *Recall* = 90/300 = 30.00%

Evaluating Classifier Accuracy: Holdout & Cross-Validation Methods

- **Holdout method**
  - Given data is randomly partitioned into two independent sets
    - Training set (e.g., 2/3) for model construction
    - Test set (e.g., 1/3) for accuracy estimation
  - Random sampling: a variation of holdout
    - Repeat holdout k times, accuracy = avg. of the accuracies obtained
- **Cross-validation** (*k*-fold, where k = 10 is most popular)
  - Randomly partition the data into *k mutually exclusive* subsets, each approximately equal size
  - At *i*-th iteration, use D_i as test set and others as training set
  - Leave-one-out: *k* folds where *k* = # of tuples, for small sized data
  - ***Stratified cross-validation***: folds are stratified so that class dist. in each fold is approx. the same as that in the initial data

Model Selection: ROC Curves

- **ROC** (Receiver Operating Characteristics) curves: for visual comparison of classification models
- Originated from signal detection theory
- Shows the trade-off between the true positive rate and the false positive rate
- The area under the ROC curve is a measure of the accuracy of the model
- Rank the test tuples in decreasing order: the one that is most likely to belong to the positive class appears at the top of the list
- The closer to the diagonal line (i.e., the closer the area is to 0.5), the less accurate is the model



- Vertical axis represents the true positive rate
- Horizontal axis rep. the false positive rate
- The plot also shows a diagonal line
- A model with perfect accuracy will have an area of 1.0

Issues Affecting Model Selection

- **Accuracy**
  - classifier accuracy: predicting class label
- **Speed**
  - time to construct the model (training time)
  - time to use the model (classification/prediction time)
- **Robustness**: handling noise and missing values
- **Scalability**: efficiency in disk-resident databases
- **Interpretability**
  - understanding and insight provided by the model
- Other measures, e.g., goodness of rules, such as decision tree size or compactness of classification rules