Chapter 9. Classification: Advanced Methods

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CS412 Summer 2017:

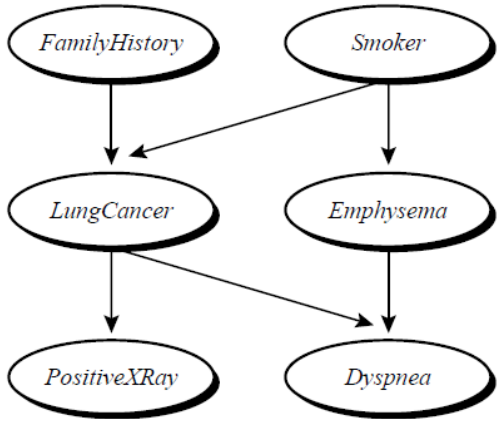
Introduction to Data Mining

Classification: Advanced Methods

- **Bayesian Belief Networks**
- Neural Networks
- Support Vector Machines
- Rule/Pattern-based Classification
- Lazy Learners and K-Nearest Neighbors
- Other Classification Methods: Genetic Algorithms, Fuzzy Sets and Rough Sets
- Additional Topics: Semi-Supervised Methods, Active Learning, etc.

Bayesian Belief Networks

- **Bayesian belief network** (or **Bayesian network, probabilistic network**):
  - allows *class conditional independencies* between *subsets* of variables
- Two components:
  - A *directed acyclic graph* (called a structure)
  - A set of *conditional probability tables* (CPTs)
- A (*directed acyclic*) graphical model of *causal influence* relationships
  - Represents dependency among the variables
  - Gives a specification of joint probability distribution



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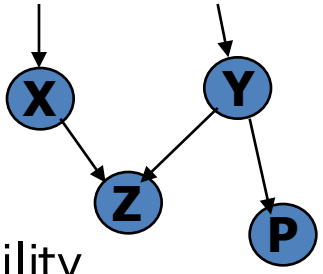


Nodes: random variables

Links: dependency

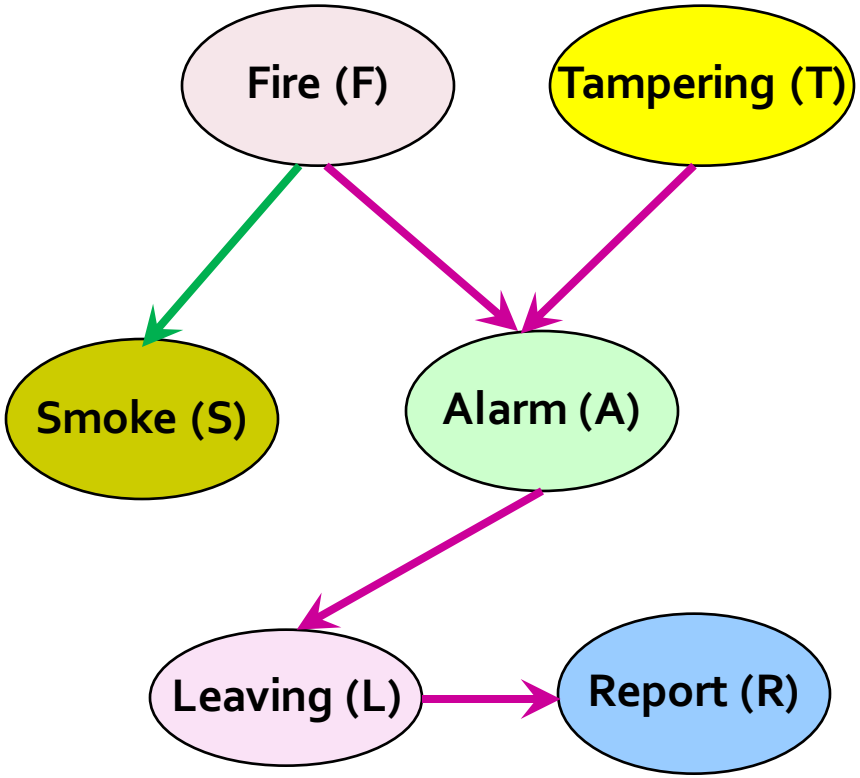
X and Y are the parents of Z, and Y is the parent of P

No dependency between Z and P

Has no loops/cycles

A Bayesian Network and Some of Its CPTs

- Derivation of the probability of a particular combination of values of **X**, from CPT:



- CPT shows the conditional probability for each possible combination of its parents

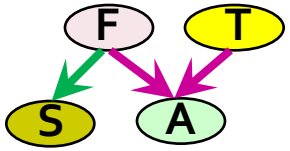
$$P(x_1,\ldots,x_n) = \prod_{i=1}^{n} P(x_i \mid Parents(x_i))$$

CPT: Conditional Probability Tables

Fire	Smoke	$\Theta_{s\|f}$
True	True	.90
False	True	.01

Fire	Tampering	Alarm	$\Theta_{a\|f,t}$
True	True	True	.5
True	False	True	.99
False	True	True	.85
False	False	True	.0001

How Are Bayesian Networks Constructed?



- **Subjective construction**: Identification of (direct) causal structure
  - People are quite good at identifying direct causes from a given set of variables & whether the set contains all relevant direct causes
  - Markovian assumption: Each variable becomes independent of its non-effects once its direct causes are known
    - E.g., S ← F → A ← T, path S → A is blocked once we know F → A
  - HMM (Hidden Markov Model): often used to model dynamic systems whose states are not observable, yet their outputs are
- **Synthesis from other specifications**
  - E.g., from a formal system design: block diagrams & info flow
- **Learning from data** (e.g., from medical records or student admission record)
  - Learn parameters give its structure or learn both structure and parms
  - Maximum likelihood principle: favors Bayesian networks that maximize the probability of observing the given data set

Training Bayesian Networks: Several Scenarios

- Scenario 1: Given both the network structure and all variables observable: *compute only the CPT entries*
- Scenario 2: Network structure known, some variables hidden: *gradient descent* (greedy hill-climbing) method, i.e., search for a solution along the steepest descent of a criterion function
  - Weights are initialized to random probability values
  - At each iteration, it moves towards what appears to be the best solution at the moment, w.o. backtracking
  - Weights are updated at each iteration & converge to local optimum
- Scenario 3: Network structure unknown, all variables observable: search through the model space to *reconstruct network topology*
- Scenario 4: Unknown structure, all hidden variables: No good algorithms known for this purpose
- D. Heckerman. A Tutorial on Learning with Bayesian Networks. In *Learning in Graphical Models*, M. Jordan, ed. MIT Press, 1999.

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- Support Vector Machines
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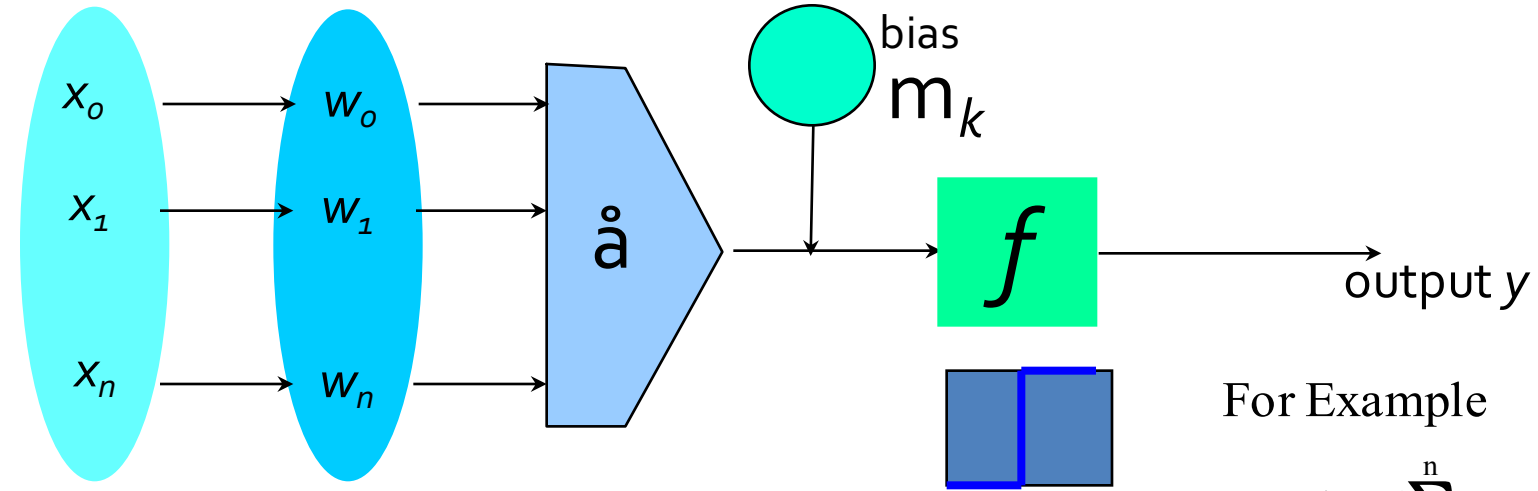
- Additional Topics: Semi-Supervised Methods, Active Learning, etc.

Neural Network for Classification

- Started by psychologists and neurobiologists to develop and test computational analogues of neurons
- A neural network: A set of connected input/output units where 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 the input tuples
- Also referred to as **connectionist learning** due to the connections between units
- Backpropagation: A **neural network** learning algorithm

Neuron: A Hidden/Output Layer Unit

- An *n*-dimensional input vector **x** is mapped into variable y by means of the scalar product and a nonlinear function mapping
- The inputs to unit are outputs from the previous layer. They are multiplied by their corresponding weights to form a weighted sum, which is added to the bias associated with unit. Then a nonlinear activation function is applied to it.

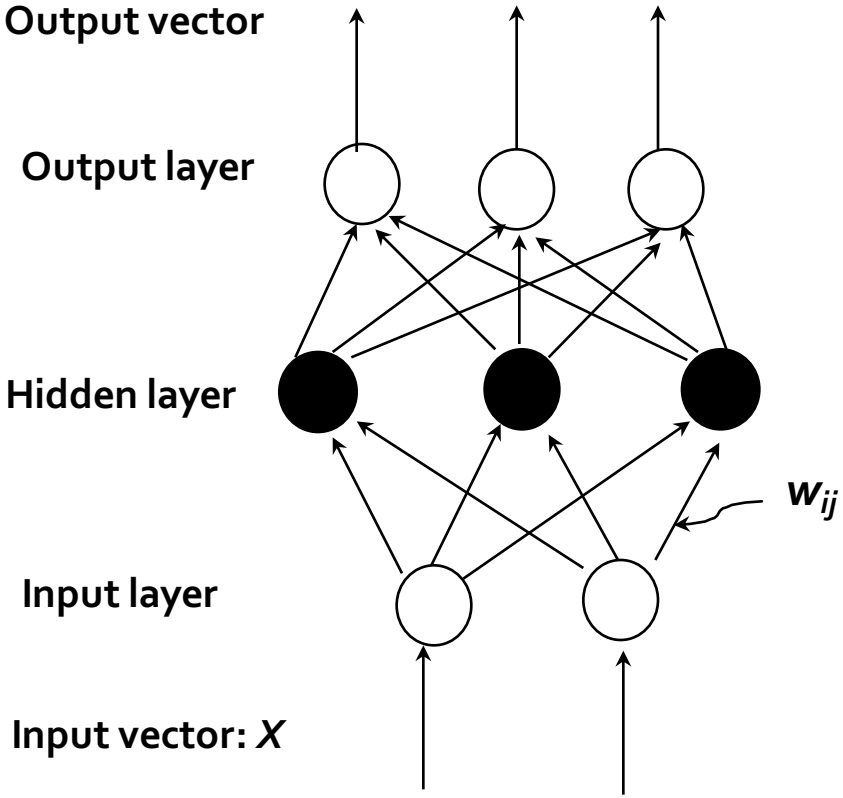


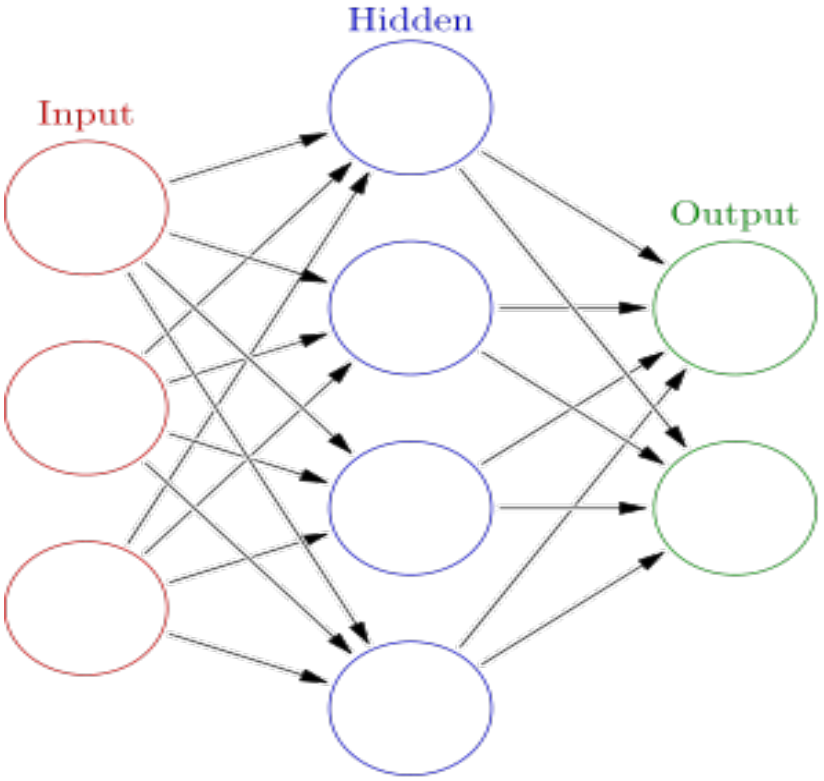
For Example

$$y = \text{sign}\left(\sum_{i=0}^{n} w_i x_i - \mu_k\right)$$

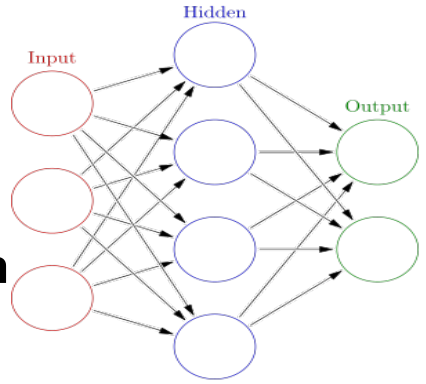
A Multi-Layer Feed-Forward Neural Network

$$w_j^{(k+1)} = w_j^{(k)} + \lambda(y_i - \hat{y}_i^{(k)})x_{ij}$$





How a Multi-Layer Neural Network Works



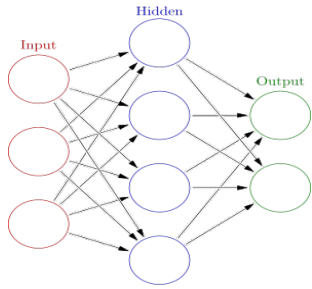
- The **inputs** to the network correspond to the attributes measured for each training tuple
- Inputs are fed simultaneously into the units making up the **input layer**
- They are then weighted and fed simultaneously to a **hidden layer**
- The number of hidden layers is arbitrary, although usually only one
- The weighted outputs of the last hidden layer are input to units making up the **output layer**, which emits the network's prediction
- The network is **feed-forward**: None of the weights cycles back to an input unit or to an output unit of a previous layer
- From a statistical point of view, networks perform **nonlinear regression**
  - Given enough hidden units and enough training samples, they can closely approximate any function

Defining a Network Topology

- Decide the **network topology**
  - Specify # of units in the *input layer*, # of *hidden layers* (if > 1), # of units in *each hidden layer*, and # of units in the *output layer*
- Normalize the input values for each attribute measured in the training tuples to [0.0—1.0]
- One **input** unit per domain value, each initialized to 0
- **Output**, if for classification and more than two classes, one output unit per class is used
- Once a network has been trained and its accuracy is **unacceptable**, repeat the training process with a *different network topology* or a *different set of initial weights*

Back Propagation

- **Back propagation**: Reset weights on the "front" neural units and this is sometimes done in combination with training where the correct result is known
- Iteratively process a set of training tuples & compare the network's prediction with the actual known target value
- For each training tuple, the weights are modified to **minimize the mean squared error** between the network's prediction and the actual target value
- Modifications are made in the "**backwards**" direction: from the output layer, through each hidden layer down to the first hidden layer, hence "**backpropagation**"
- Steps
  - Initialize weights to small random numbers, associated with biases
  - Propagate the inputs forward (by applying activation function)
  - Backpropagate the error (by updating weights and biases)
  - Terminating condition (when error is very small, etc.)



From Neural Networks to Deep Learning

- Train networks with many layers (vs. shallow nets with just a couple of layers)
- Multiple layers work to build an improved feature space
  - First layer learns 1st order features (e.g., edges, …)
  - 2nd layer learns higher order features (combinations of first layer features, combinations of edges, etc.)
  - In current models, layers often learn in an unsupervised mode and discover general features of the input space—serving multiple tasks related to the unsupervised instances (image recognition, etc.)
  - Then final layer features are fed into supervised layer(s)
    - And entire network is often subsequently tuned using supervised training of the entire net, using the initial weightings learned in the unsupervised phase
  - Could also do fully supervised versions (back-propagation)

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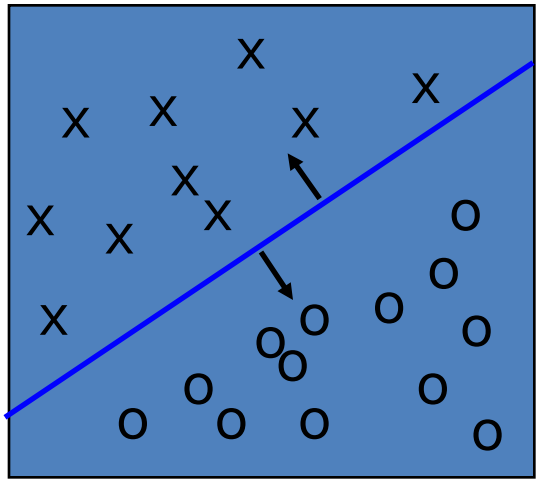
Classification: A Mathematical Mapping

- **Classification:** predicts categorical class labels
  - E.g., Personal homepage classification
    - $x_i = (x_1, x_2, x_3, \ldots)$, $y_i = +1$ or -1
    - x_1 : # of word "homepage"
    - x_2 : # of word "welcome"
- Mathematically, $x \in X = \Re^n$, $y \in Y = \{+1, -1\}$,
  - We want to derive a function f: X → Y
- Linear Classification
  - Binary Classification problem
  - Data above the red line belongs to class 'x'
  - Data below red line belongs to class 'o'
  - Examples: SVM, Perceptron, Probabilistic Classifiers



Discriminative Classifiers

- Advantages
  - Prediction accuracy is generally high
    - As compared to Bayesian methods
  - Robust, works when training examples contain errors
  - Fast evaluation of the learned target function
    - Bayesian networks are normally slow
- Criticism
  - Long training time
  - Difficult to understand the learned function (weights)
    - Bayesian networks can be used easily for pattern discovery
  - Not easy to incorporate domain knowledge
    - Easy in the form of priors on the data or distributions

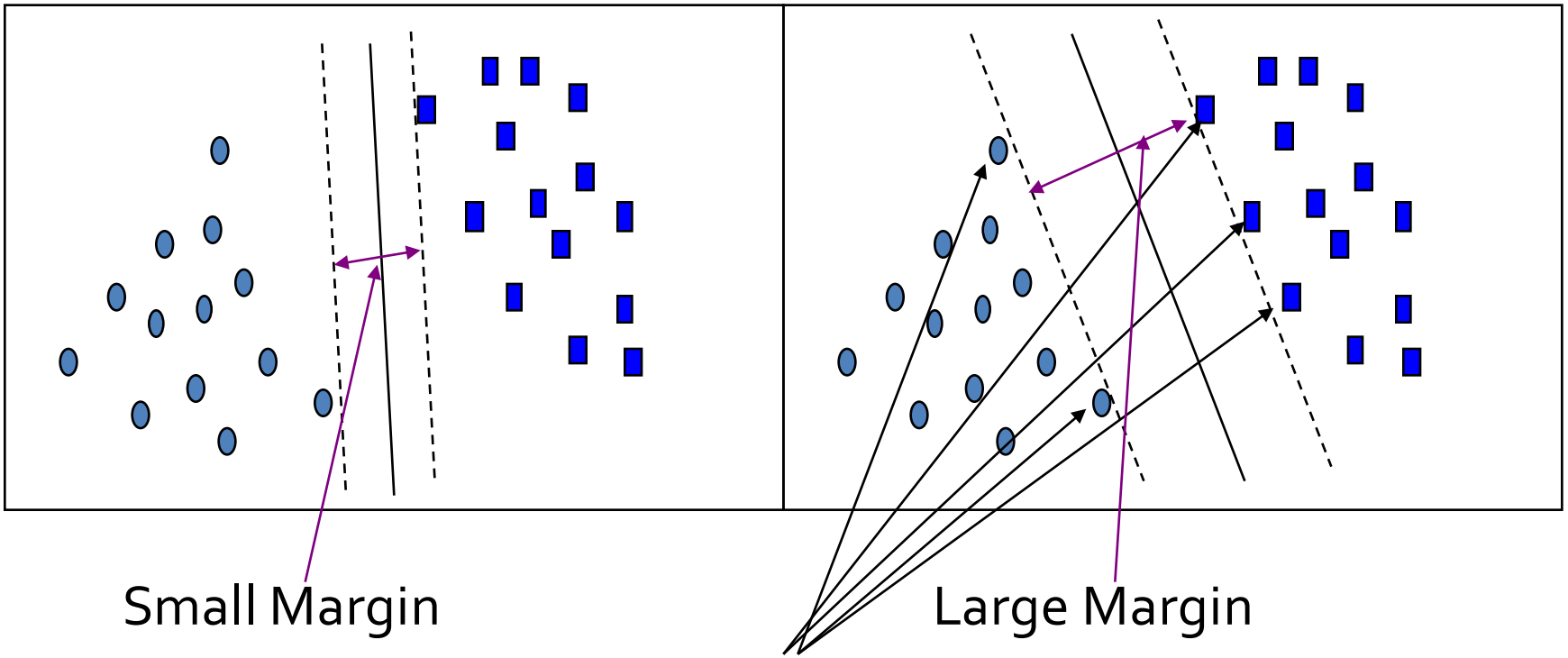
SVM: Support Vector Machines

- A relatively new classification method for both linear and nonlinear data
- It uses a nonlinear mapping to transform the original training data into a higher dimension
- With the new dimension, it searches for the linear optimal separating **hyperplane** (i.e., "decision boundary")
- With an appropriate nonlinear mapping to a sufficiently high dimension, data from two classes can always be separated by a hyperplane
- SVM finds this hyperplane using **support vectors** ("essential" training tuples) and **margins** (defined by the support vectors)

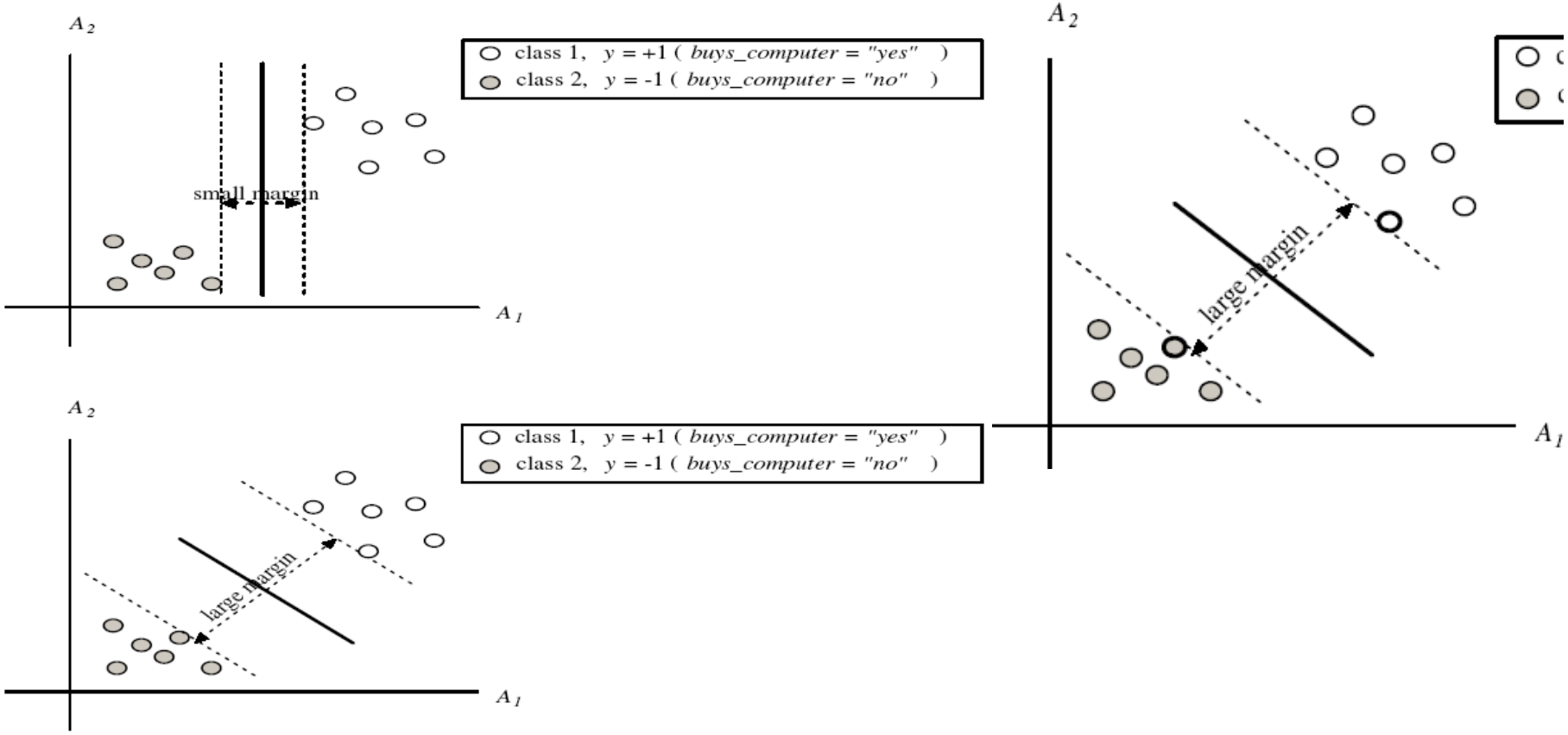
SVM: History and Applications

- Vapnik and colleagues (1992)—groundwork from Vapnik & Chervonenkis' statistical learning theory in 1960s
- Features: training can be slow but accuracy is high owing to their ability to model complex nonlinear decision boundaries (margin maximization)
- Used for: classification and numeric prediction
- Applications:
  - handwritten digit recognition, object recognition, speaker identification, benchmarking time-series prediction tests

SVM: General Philosophy



SVM: Margins and Support Vectors

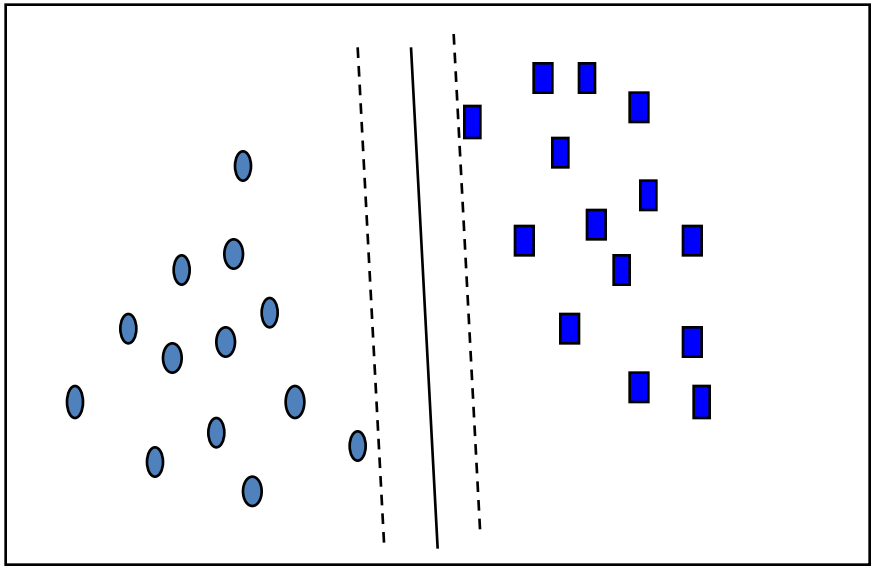


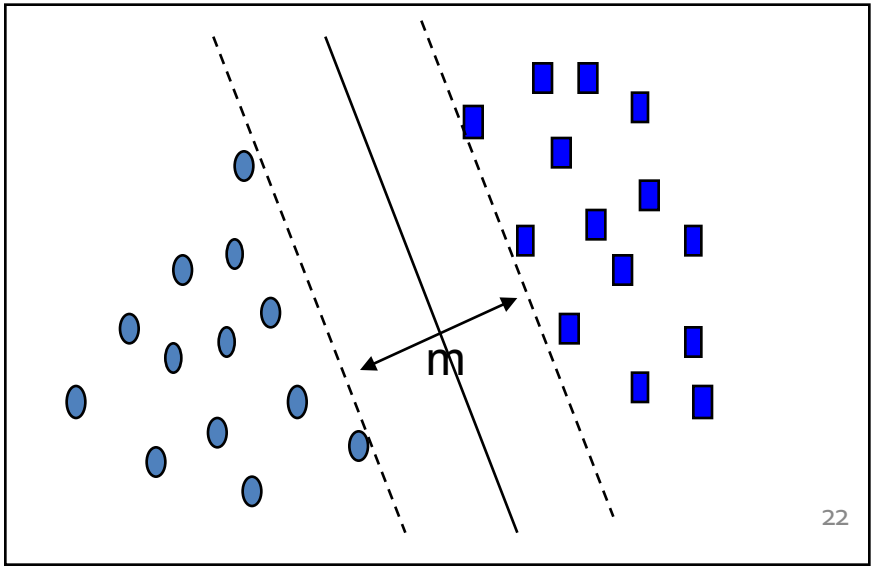
SVM: When Data Is Linearly Separable

Let data D be $(\mathbf{X}_1, y_1), \ldots, (\mathbf{X}_{|D|}, y_{|D|})$, where $\mathbf{X}_i$ is the set of training tuples associated with the class labels y_i

There are infinite lines (hyperplanes) separating the two classes but we want to find the best one (the one that minimizes classification error on unseen data)

SVM searches for the hyperplane with the largest margin, i.e., **maximum marginal hyperplane** (MMH)





SVM: Linearly Separable

- A separating hyperplane can be written as

  $\mathbf{W} \bullet \mathbf{X} + b = 0$

  where $\mathbf{W}=\{w_1, w_2, \ldots, w_n\}$ is a weight vector and b a scalar (bias)
- For 2-D it can be written as: $w_0 + w_1 x_1 + w_2 x_2 = 0$
- The hyperplane defining the sides of the margin:

  $H_1: w_0 + w_1 x_1 + w_2 x_2 \geq 1$ for $y_i = +1$, and

  $H_2: w_0 + w_1 x_1 + w_2 x_2 \leq -1$ for $y_i = -1$
- Any training tuples that fall on hyperplanes H_1 or H_2 (i.e., the sides defining the margin) are **support vectors**
- This becomes a **constrained (convex) quadratic optimization** problem:
  - Quadratic objective function and linear constraints → *Quadratic Programming (QP)* → Lagrangian multipliers

SVM: Linearly Inseparable

- Transform the original input data into a higher dimensional space

Example 6.8 Nonlinear transformation of original input data into a higher dimensional space. Consider the following example. A 3D input vector $\mathbf{X} = (x_1, x_2, x_3)$ is mapped into a 6D space Z using the mappings $\phi_1(\boldsymbol{X}) = x_1, \phi_2(\boldsymbol{X}) = x_2, \phi_3(\boldsymbol{X}) = x_3$, $\phi_4(\boldsymbol{X}) = (x_1)^2, \phi_5(\boldsymbol{X}) = x_1x_2$, and $\phi_6(\boldsymbol{X}) = x_1x_3$. A decision hyperplane in the new space is $d(\mathbf{Z}) = \mathbf{WZ} + b$, where $\mathbf{W}$ and $\mathbf{Z}$ are vectors. This is linear. We solve for $\mathbf{W}$ and b and then substitute back so that we see that the linear decision hyperplane in the new ($\mathbf{Z}$) space corresponds to a nonlinear second order polynomial in the original 3-D input space,

$$\begin{aligned} d(Z) &= w_1x_1 + w_2x_2 + w_3x_3 + w_4(x_1)^2 + w_5x_1x_2 + w_6x_1x_3 + b \\ &= w_1z_1 + w_2z_2 + w_3z_3 + w_4z_4 + w_5z_5 + w_6z_6 + b \end{aligned}$$

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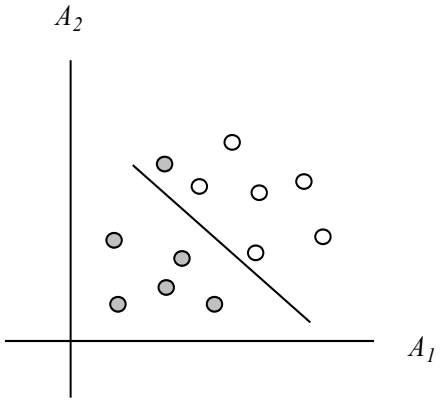


- Search for a linear separating hyperplane in the new space

Why is SVM Effective on High Dimensional Data?

- The **complexity** of trained classifier is characterized by the # of support vectors rather than the dimensionality of the data
- The **support vectors** are the essential or critical training examples —they lie closest to the decision boundary (MMH)
- If all other training examples are removed and the training is repeated, the same separating hyperplane would be found
- The number of support vectors found can be used to compute an (upper) bound on the expected error rate of the SVM classifier, which is independent of the data dimensionality
- Thus, an SVM with a small number of support vectors can have good generalization, even when the dimensionality of the data is high

Kernel Functions for Nonlinear Classification

- Instead of computing the dot product on the transformed data, it is mathatically equivalent to applying a kernel function $K(\mathbf{X}_i, \mathbf{X}_j)$ to the original data, i.e.,
  - $K(\mathbf{X}_i, \mathbf{X}_j) = \Phi(\mathbf{X}_i)\ \Phi(\mathbf{X}_j)$
- Typical Kernel Functions

$$\textbf{Polynomial kernel of degree } h: \quad K(\boldsymbol{X}_i, \boldsymbol{X}_j) = (\boldsymbol{X}_i \cdot \boldsymbol{X}_j + 1)^h$$

$$\textbf{Gaussian radial basis function kernel}: \quad K(\boldsymbol{X}_i, \boldsymbol{X}_j) = e^{-\|\boldsymbol{X}_i - \boldsymbol{X}_j\|^2/2\sigma^2}$$

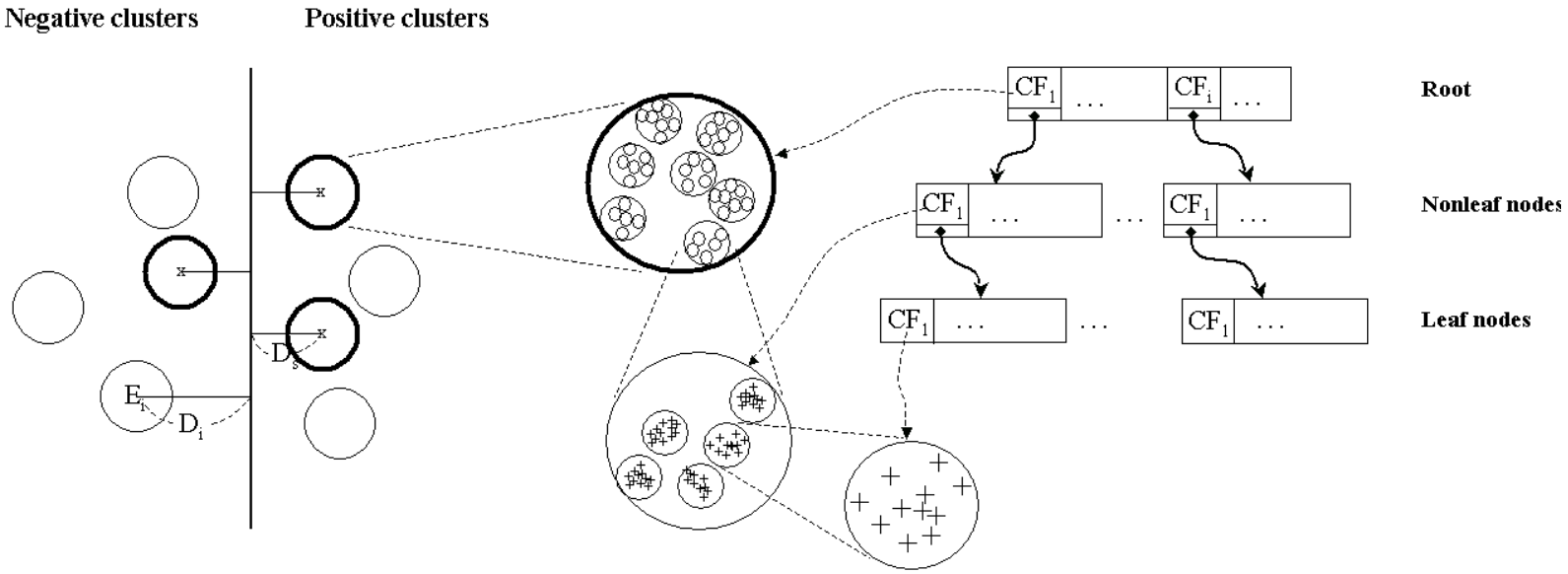
$$\textbf{Sigmoid kernel}: \quad K(\boldsymbol{X}_i, \boldsymbol{X}_j) = \tanh(\kappa \boldsymbol{X}_i \cdot \boldsymbol{X}_j - \delta)$$

- SVM can also be used for classifying multiple (> 2) classes and for regression analysis (with additional parameters)

Scaling SVM by Hierarchical Micro-Clustering

- SVM is not scalable to # of data objects in terms of training time and memory usage
- CB-SVM (Clustering-Based SVM): H. Yu, J. Yang, and J. Han, "Classifying Large Data Sets Using SVM with Hierarchical Clusters", KDD'03
- Clustering-Based SVM: Algorithm outline
  - Construct two CF-trees (hierarchical clusters)
  - Train an SVM from the centroids of the root entries
  - De-cluster the entries near the boundary into the next level
    - The children entries de-clustered from the parent entries are accumulated into the training set with the non-declustered parent entries
  - Repeat until nothing is accumulated
- At deriving support vectors, de-cluster micro-clusters near "candidate vector" to ensure high classification accuracy

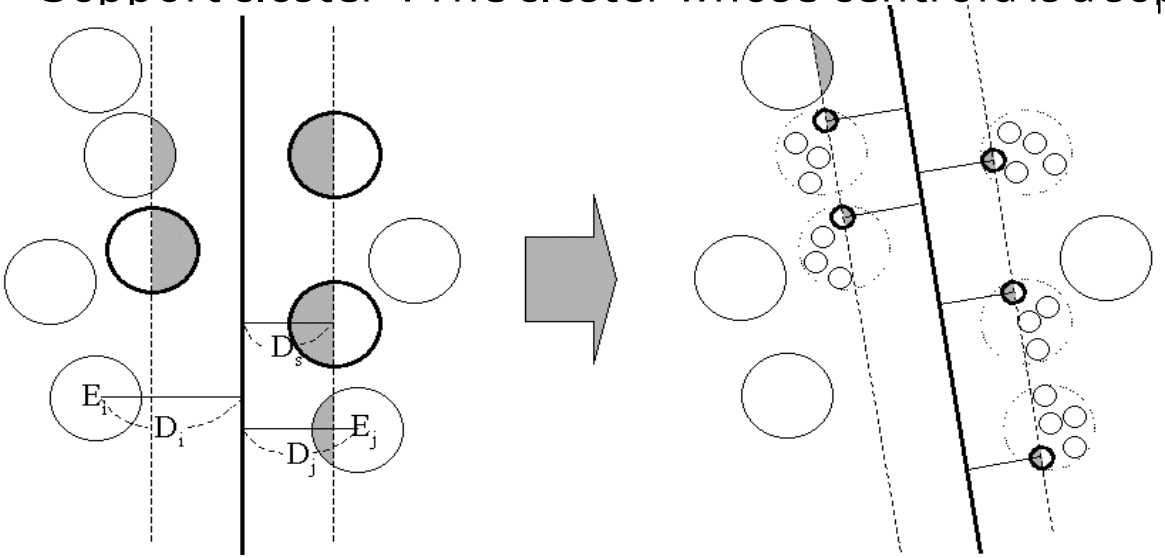
CF-Tree: Hierarchical Micro-cluster



- One scan of the data set: Construct two CF-trees (i.e., statistical summary of the data) from positive and negative data sets independently
- Micro-clustering: Hierarchical indexing structure
  - Provide finer samples closer to the boundary and coarser samples farther from the boundary

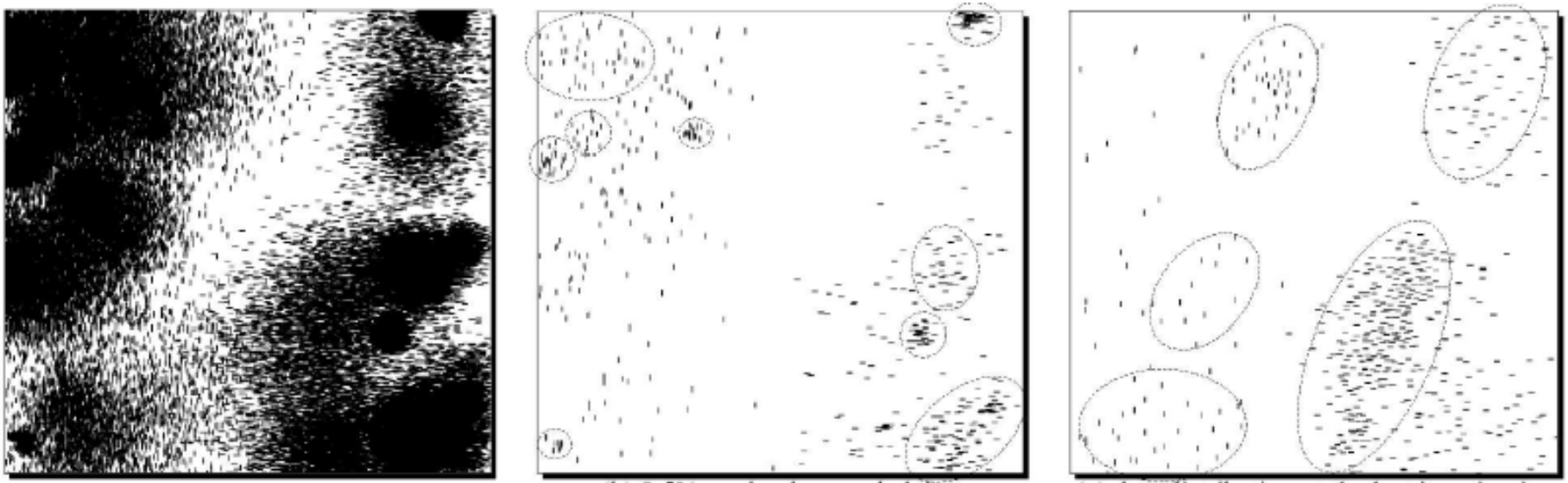
Selective Declustering: Ensure High Accuracy

- CF tree is a suitable base structure for selective declustering
- De-cluster only the cluster E_i such that
  - $D_i - R_i < D_s$, where D_i is the distance from the boundary to the center point of E_i and R_i is the radius of E_i
  - Decluster only the cluster whose subclusters have possibilities to be the support cluster of the boundary
    - "Support cluster": The cluster whose centroid is a support vector



Accuracy and Scalability on Synthetic Dataset

- Experiments on large synthetic data sets shows better accuracy than random sampling approaches and far more scalable than the original SVM algorithm



(a) original data set ($N = 113601$)

(b) 0.5% randomly sampled data ($N = 603$)

(c) data distribution at the last iteration in CB-SVM ($N = 597$)

Figure 6: Synthetic data set in a two-dimensional space. '|': positive data; '−': negative data

SVM Related Links

- SVM Website: http://www.kernel-machines.org/
- Representative implementations
  - **LIBSVM**: an efficient implementation of SVM, multi-class classifications, nu-SVM, one-class SVM, including also various interfaces with java, python, etc.
  - **SVM-light**: simpler but performance is not better than LIBSVM, support only binary classification and only in C
  - **SVM-torch**: another recent implementation also written in C

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Using IF-THEN Rules for Classification

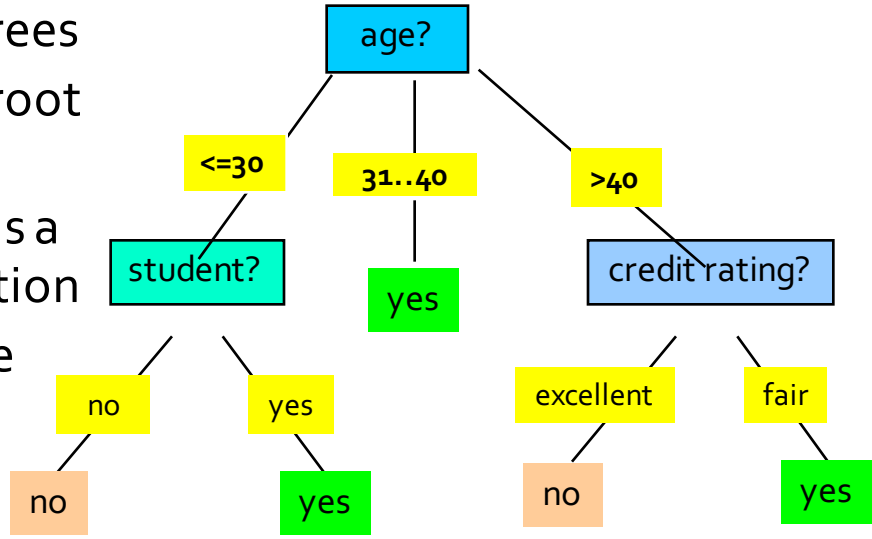
- Represent the knowledge in the form of **IF-THEN** rules
  R_1: IF *age* = youth AND *student* = yes THEN *buys_computer* = yes
  - Rule antecedent/precondition vs. rule consequent
- Assessment of a rule: *coverage* and *accuracy*
  - n_{covers} = # of tuples covered by R_1
  - $n_{correct}$ = # of tuples correctly classified by R_1

  coverage(R_1) = n_{covers}/|D| /* D: training data set */

  accuracy(R_1) = $n_{correct}$ / 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



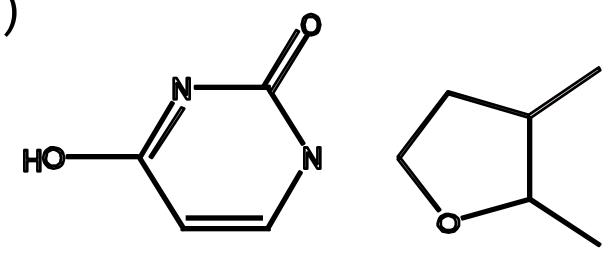
IF *age* = young AND *student* = *no* THEN *buys_computer* = *no*
IF *age* = young AND *student* = *yes* THEN *buys_computer* = *yes*
IF *age* = mid-age THEN *buys_computer* = *yes*
IF *age* = old AND *credit_rating* = *excellent* THEN *buys_computer* = *no*
IF *age* = old AND *credit_rating* = *fair*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

Rule Induction: Sequential Covering Method

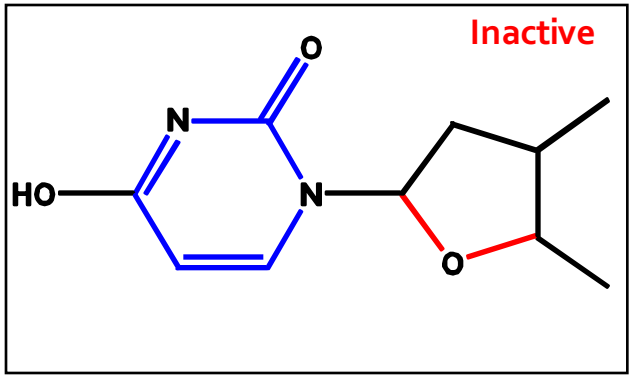
- Sequential covering algorithm: Extracts rules directly from training data
- Typical sequential covering algorithms: FOIL, AQ, CN2, RIPPER
- Rules are learned *sequentially*, each for a given class C_i will cover many tuples of C_i but none (or few) of the tuples of other classes
- Steps:
  - Rules 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*

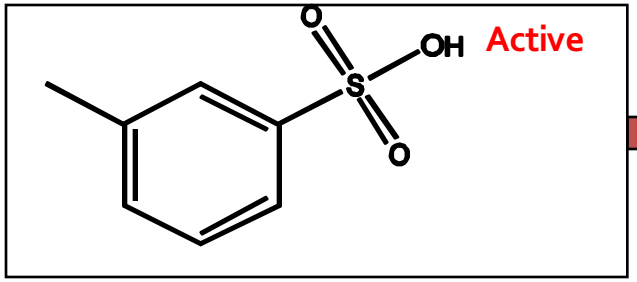
Pattern-Based Classification, Why?

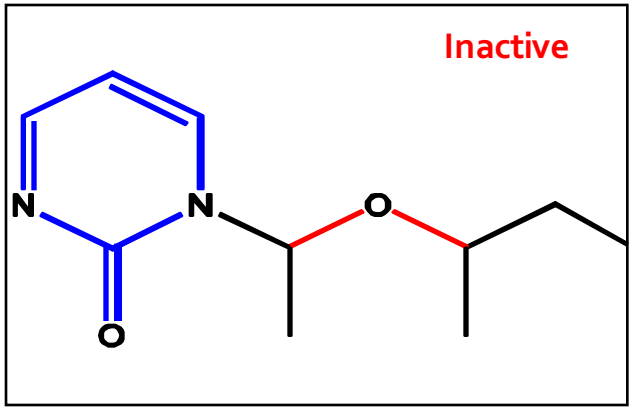
- **Pattern-based classification:** An integration of both themes
- **Why pattern-based classification?**
  - **Feature construction**
    - Higher order; compact; discriminative
    - E.g., single word → phrase (Apple pie, Apple i-pad)
  - **Complex data modeling**
    - Graphs (no predefined feature vectors)
    - Sequences
    - Semi-structured/unstructured Data



Pattern-Based Classification on Graphs



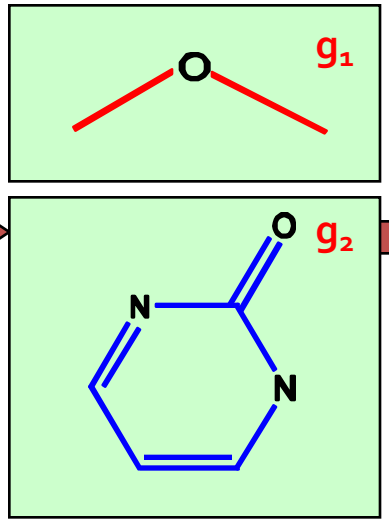




Mining

min_sup=2

Frequent subgraphs



Transform

Use frequent patterns as features for classification

g_1	g_2	Class
1	1	0
0	0	1
1	1	0

Associative or Pattern-Based Classification

- **Data:** Transactions, microarray data, … → **Patterns or association rules**
- **Classification Methods** (Some interesting work):
  - CBA [Liu, Hsu & Ma, KDD'98]: Use high-conf., high-support *class association rules* to build classifiers
  - Emerging patterns [Dong & Li, KDD'99]: Patterns whose support changes significantly between the two classes
  - CMAR [Li, Han & Pei, ICDM'01]: Multiple rules in prediction
  - CPAR [Yin & Han, SDM'03]: Beam search on multiple prediction rules
  - RCBT [Cong et al., SIGMOD'05]: Build classifier based on mining top-k covering rule groups with row enumeration (for high-dimensional data)
  - Lazy classifier [Veloso, Meira & Zaki, ICDM'06]: For a test t, project training data D on t, mine rules from D_t , predict on the best rule
  - Discriminative pattern-based classification [Cheng et al., ICDE'07]

CBA: Classification Based on Associations

- CBA [Liu, Hsu and Ma, KDD'98]
- Method
  - Mine high-confidence, high-support class association rules
  - LHS: conjunctions of attribute-value pairs); RHS: class labels

    $p_1 \wedge p_2 \ldots \wedge p_l \rightarrow$ "$A_{\text{class-label}} = C$" (confidence, support)
  - Rank rules in descending order of confidence and support
  - Classification: Apply the first rule that matches a test case; o.w. apply the default rule
  - Effectiveness: Often found more accurate than some traditional classification methods, such as C4.5
  - Why? — Exploring high confident associations among multiple attributes may overcome some constraints introduced by some classifiers that consider only one attribute at a time

CMAR: Classification Based on Multiple Association Rules

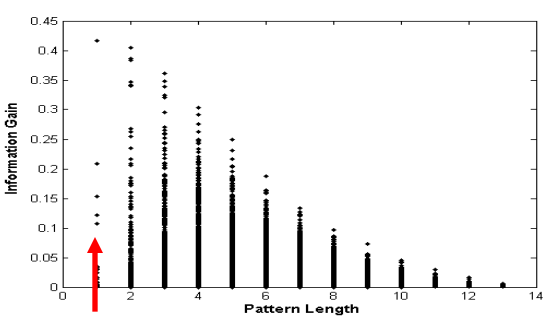
- Rule pruning whenever a rule is inserted into the tree
  - Given two rules, R_1 and R_2, if the antecedent of R_1 is more general than that of R_2 and $conf(R_1) \geq conf(R_2)$, then prune R_2
  - Prunes rules for which the rule antecedent and class label are not positively correlated, based on the χ^2 test of statistical significance
- Classification based on generated/pruned rules
  - If only *one rule* satisfies tuple X, assign the class label of the rule
  - If a *rule set* S satisfies X
    - Divide S into groups according to class labels
    - Use a weighted χ^2 measure to find the strongest group of rules, based on the statistical correlation of rules within a group
    - Assign X the class label of the strongest group
- CMAR improves model construction efficiency and classification accuracy

Discriminative Pattern-Based Classification

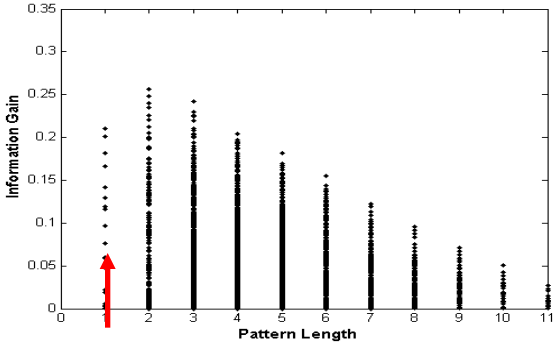
- Discriminative patterns as features for classification [Cheng et al., ICDE'07]
- **Principle:** Mining discriminative frequent patterns as high-quality features and then apply any classifier
- **Framework (PatClass)**
  - Feature construction by *frequent itemset mining*
  - Feature selection (e.g., using Maximal Marginal Relevance (MMR))
    - Select discriminative features (i.e., that are relevant but minimally similar to the previously selected ones)
    - Remove redundant or closely correlated features
  - Model learning
    - Apply a general classifier, such as SVM or C4.5, to build a classification model

On the Power of Discriminative Patterns

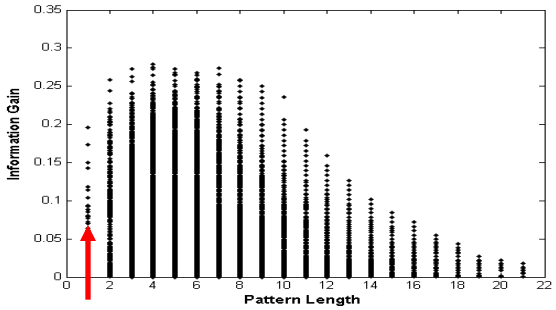
- K-itemsets are often more informative than single features (1-itemsets) in classification
- Computation on real datasets shows: The discriminative power of k-itemsets (for $k > 1$ but often ≤ 10) is higher than that of single features



(a) Austral



(b) Cleve

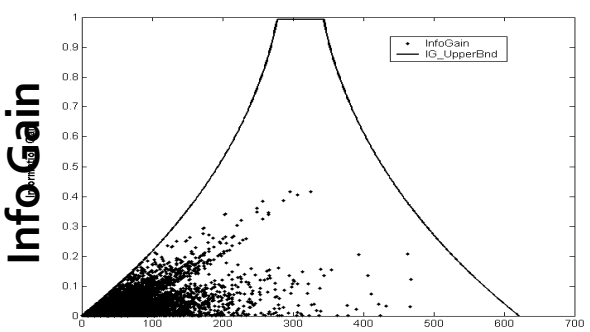


(c) Sonar

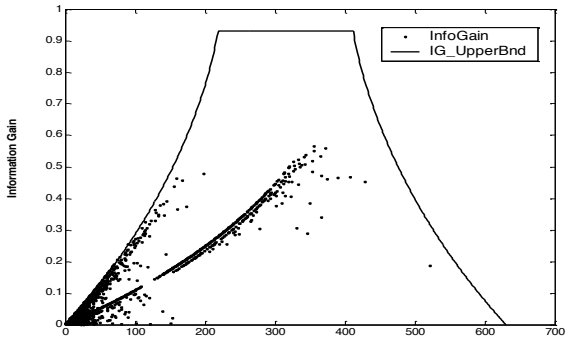
Information Gain vs. Pattern Length

Information Gain vs. Pattern Frequency

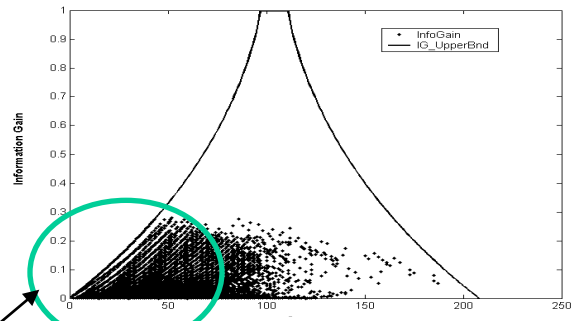
- Computation on real datasets shows: Pattern frequency (but not too frequent) is strongly tied with the discriminative power (information gain)
- Information gain upper bound monotonically increases with pattern frequency



(a) Austral



(b) Breast



(c) Sonar

Low support, low info gain

Information Gain Formula: $IG(C \mid X) = H(C) - H(C \mid X)$

Conditional entropy of study focus

Entropy of given data

$$H(C) = -\sum_{i=1}^{m} p_i \log_2(p_i)$$

$$H(C \mid X) = \sum_j P(X = x_j) H(Y \mid X = x_j)$$

Discriminative Pattern-Based Classification: Experimental Results

Table 1. Accuracy by SVM on Frequent Combined Features vs. Single Features

Data	Single Feature			Freq. Pattern	
	Item_All	*Item_FS*	*Item_RBF*	*Pat_All*	*Pat_FS*
anneal	**99.78**	**99.78**	99.11	99.33	99.67
austral	85.01	85.50	85.01	81.79	**91.14**
auto	83.25	84.21	78.80	74.97	**90.79**
breast	97.46	97.46	96.98	96.83	**97.78**
cleve	84.81	84.81	85.80	78.55	**95.04**
diabetes	74.41	74.41	74.55	77.73	**78.31**
glass	75.19	75.19	74.78	79.91	**81.32**
heart	84.81	84.81	84.07	82.22	**88.15**
hepatic	84.50	89.04	85.83	81.29	**96.83**
horse	83.70	84.79	82.36	82.35	**92.39**
iono	93.15	94.30	92.61	89.17	**95.44**
iris	94.00	**96.00**	94.00	95.33	**96.00**
labor	89.99	91.67	91.67	94.99	**95.00**
lymph	81.00	81.62	84.29	83.67	**96.67**
pima	74.56	74.56	76.15	76.43	**77.16**
sonar	82.71	86.55	82.71	84.60	**90.86**
vehicle	70.43	72.93	72.14	73.33	**76.34**
wine	98.33	99.44	98.33	98.30	**100**
zoo	97.09	97.09	95.09	94.18	**99.00**

Table 2. Accuracy by C4.5 on Frequent Combined Features vs. Single Features

Dataset	Single Features		Frequent Patterns	
	Item_All	*Item_FS*	*Pat_All*	*Pat_FS*
anneal	98.33	98.33	97.22	**98.44**
austral	84.53	84.53	84.21	**88.24**
auto	71.70	77.63	71.14	**78.77**
breast	95.56	95.56	95.40	**96.35**
cleve	80.87	80.87	80.84	**91.42**
diabetes	**77.02**	**77.02**	76.00	76.58
glass	75.24	75.24	76.62	**79.89**
heart	81.85	81.85	80.00	**86.30**
hepatic	78.79	85.21	80.71	**93.04**
horse	83.71	83.71	84.50	**87.77**
iono	92.30	92.30	92.89	**94.87**
iris	**94.00**	**94.00**	93.33	93.33
labor	86.67	86.67	**95.00**	91.67
lymph	76.95	77.62	74.90	**83.67**
pima	75.86	75.86	76.28	**76.72**
sonar	80.83	81.19	**83.67**	**83.67**
vehicle	70.70	71.49	**74.24**	73.06
wine	95.52	93.82	96.63	**99.44**
zoo	91.18	91.18	95.09	**97.09**

Discriminative Pattern-Based Classification: Scalability Tests

Table 3. Accuracy & Time on Chess Data

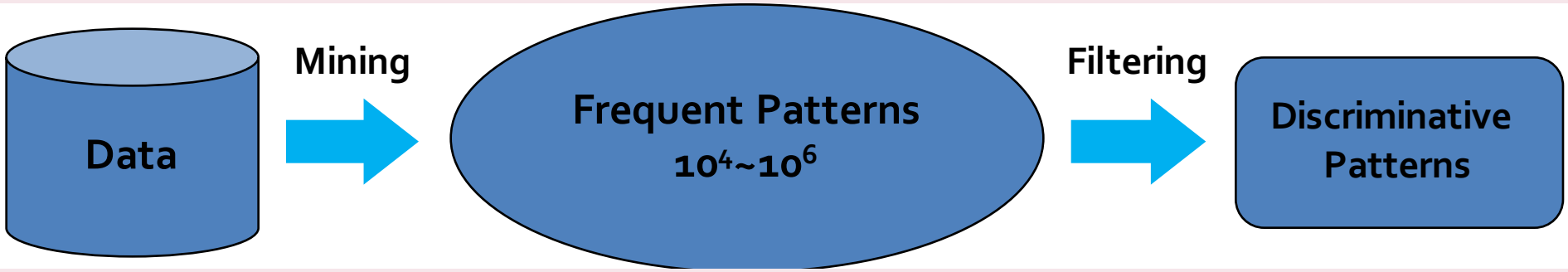
min_sup	#Patterns	Time (s)	SVM (%)	C4.5 (%)
1	N/A	N/A	N/A	N/A
2000	68,967	44.703	92.52	97.59
2200	28,358	19.938	91.68	97.84
2500	6,837	2.906	91.68	97.62
2800	1,031	0.469	91.84	97.37
3000	136	0.063	91.90	97.06

Table 4. Accuracy & Time on Waveform Data

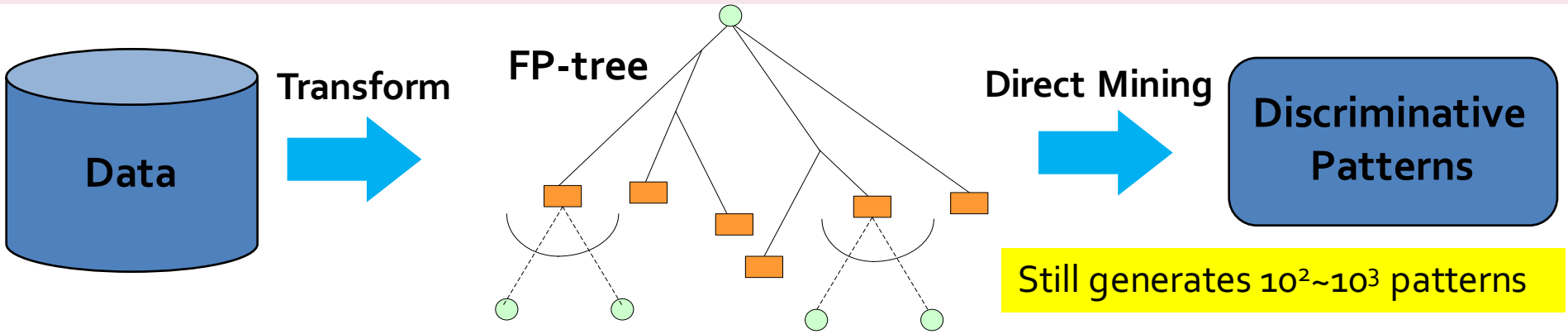
min_sup	#Patterns	Time (s)	SVM (%)	C4.5 (%)
1	9,468,109	N/A	N/A	N/A
80	26,576	176.485	92.40	88.35
100	15,316	90.406	92.19	87.29
150	5,408	23.610	91.53	88.80
200	2,481	8.234	91.22	87.32

Mining Concise Set of Discriminative Patterns

Frequent pattern mining, then getting discriminative patterns: Expensive, large model



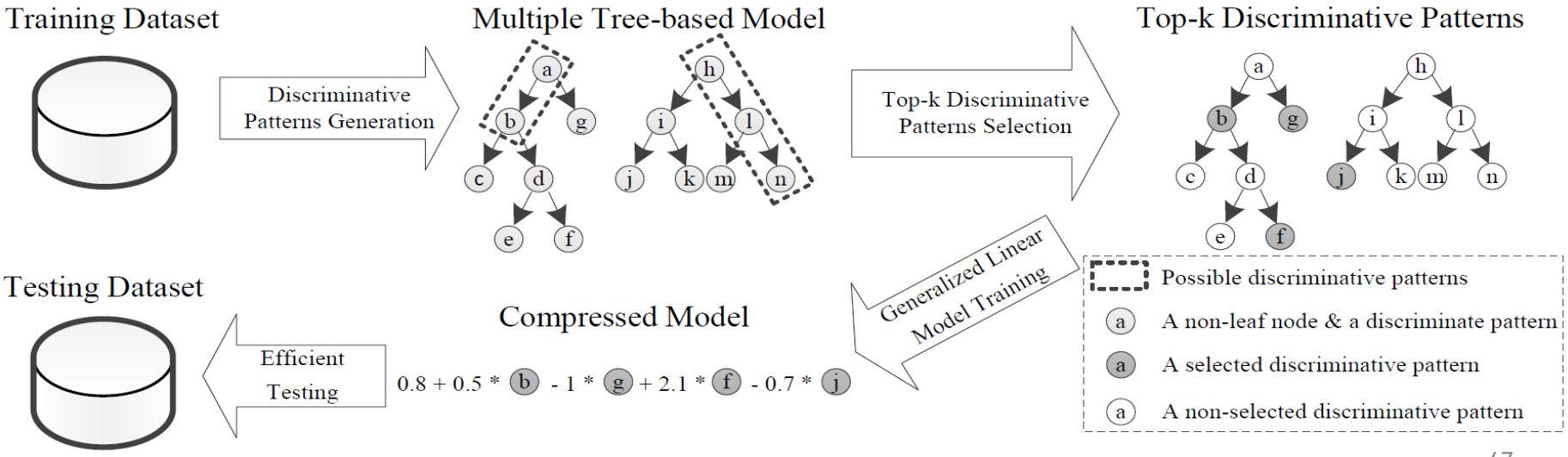
DDPMine [Cheng et al., ICDE'08]: Direct mining of discriminative patterns: Efficient



DPClass [Shang et al, SDM'16]: A better solution — Efficient, effective, and generating a very limited number of (such as only 20 or so) patterns

DPClass: Discriminative Pattern-based Classification

- Input: A feature table for training data
- Adopt every prefix path in an (extremely) random forest as a candidate pattern
  - The split points of continuous variables are automatically chosen by random forest → No discretization!
- Run top-k (e.g., top-20) pattern selection based on training data
- Train a generalized linear model (e.g., logistic regression) based on "bag-of-patterns" representations of training data



Explanatory Discriminative Patterns: Generation

- Example: For each patient, we have several uniformly sampled features as follows
  - Age (A): Positive Integers no more than 60
  - Gender (G): Male or Female.
  - Lab Test 1 (LT1): Categorical values from (A, B, O, AB)
  - Lab Test 2 (LT2): Continuous values in [0..1]
- The positive label of the hypo-disease will be given when at least one of the following rules holds
  - (age > 18) and (gender = Male) and (LT1 = AB) and (LT2 ≥ 0.6)
  - (age > 18) and (gender = Female) and (LT1 = O) and (LT2 ≥ 0.5)
  - (age ≤ 18) and (LT2 ≥ 0.9)
- Training: 10^5 random patients + 0.1% noise
  - Flip the binary labels with 0.1% probability
- Testing: 5×10^4 random patients in test

Explanatory Discriminative Patterns: Evaluation

- Accuracy:
  - **DPClass 99.99% (perfect)**
  - DDPMine 95.64% (reasonable)
- Top-3 Discriminative Patterns:
  - **DPClass (perfect):**
    - (age > 18) and (gender = Female) and (LT1 = O) and (LT2 ≥ 0.496)
    - (age ≤ 18) and (LT2 ≥ 0.900)
    - (age > 18) and (gender = Male) and (LT1 = AB) and (LT2 ≥ 0.601)
  - DDPMine (poor):
    - (LT2 > 0.8)
    - (gender = Male) and (LT1 = AB) and (LT2 ≥ 0.6) and (LT2 < 0.8)
    - (gender = Female) and (LT1 = O) and (LT2 ≥ 0.6) and (LT2 < 0.8)

A Comparison on Classification Accuracy

- DPClass: Discriminative & frequent at the same time, then select top-k
  - Only top-20 patterns are used in DPClass
- Two methods on pattern selection
  - Forward vs. LASSO
  - In comparison with DDPMine and Random Forest, DPClass maintains high accuracy
- An extension of DPClass has been applied to health study
  - Cheng et al, "Mining Discriminative Patterns to Predict Health Status for Cardiopulmonary Patients", *ACM-BCB'16*

	Dataset	DPClass (Forward)	DPClass (LASSO)	DDPMine	Random Forest
low-dimensional data	adult	**85.66%**	84.33%	83.42%	85.45%
	hypo	**99.58%**	99.28%	92.69%	97.22%
	sick	98.35%	**98.87%**	93.82%	94.03%
	crx	**89.35%**	87.96%	87.96%	**89.35%**
	sonar	**85.29%**	83.82%	73.53%	83.82%
	chess	92.25%	92.05%	90.04%	**94.22%**
high-dimensional data	namao	97.17%	96.94%	96.83%	**97.86%**
	musk	95.92%	95.71%	93.29%	**96.60%**
	madelon	74.50%	**76.00%**	59.84%	56.50%

Classification: Advanced Methods

- Bayesian Belief Networks
- Neural Networks
- Support Vector Machines
- Rule/Pattern-based Classification
- **Lazy Learners and K-Nearest Neighbors**
- Other Classification Methods: Genetic Algorithms, Fuzzy Sets and Rough Sets
- Additional Topics: Semi-Supervised Methods, Active Learning, etc.

Lazy vs. Eager Learning

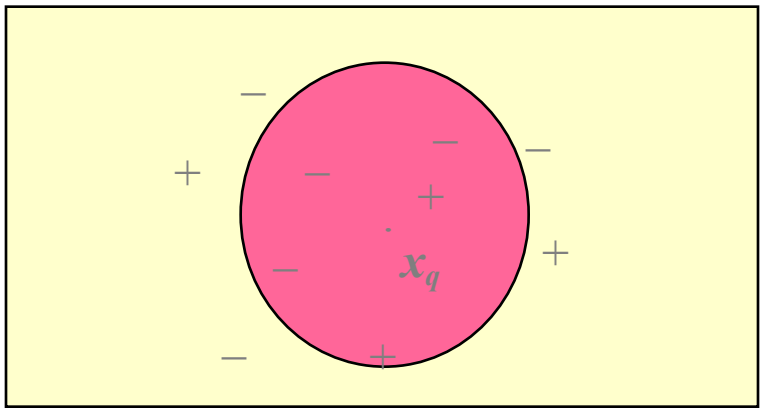
- Lazy vs. eager learning
  - **Lazy learning** (e.g., instance-based learning): Simply stores training data (or only minor processing) and waits until it is given a test tuple
  - **Eager learning** (the above discussed methods): Given a set of training tuples, constructs a classification model before receiving new (e.g., test) data to classify
- Lazy: less time in training but more time in predicting
- Accuracy
  - Lazy method effectively uses a richer hypothesis space since it uses many local linear functions to form an implicit global approximation to the target function
  - Eager: must commit to a single hypothesis that covers the entire instance space

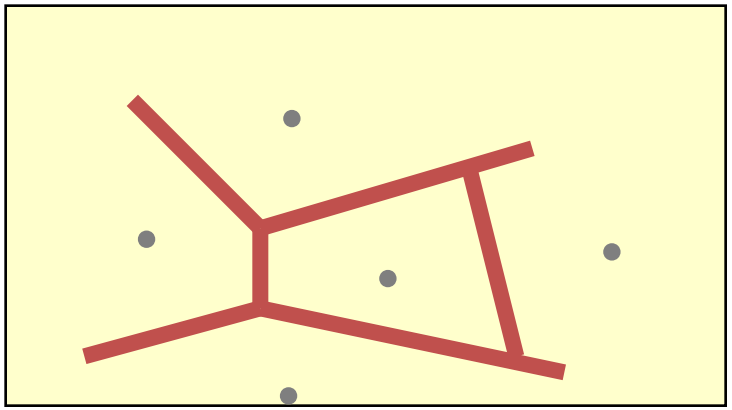
Lazy Learner: Instance-Based Methods

- Instance-based learning:
  - Store training examples and delay the processing ("lazy evaluation") until a new instance must be classified
- Typical approaches
  - *k*-nearest neighbor approach
    - Instances represented as points in a Euclidean space.
  - Locally weighted regression
    - Constructs local approximation
  - Case-based reasoning
    - Uses symbolic representations and knowledge-based inference

The *k*-Nearest Neighbor Algorithm

- All instances correspond to points in the n-D space
- The nearest neighbor are defined in terms of Euclidean distance, dist($\mathbf{X}_1$, $\mathbf{X}_2$)
- Target function could be discrete- or real- valued
- For discrete-valued, *k*-NN returns the most common value among the *k* training examples nearest to x_q
- Vonoroi diagram: the decision surface induced by 1-NN for a typical set of training examples





Discussion on the *k*-NN Algorithm

- *k*-NN for real-valued prediction for a given unknown tuple
  - Returns the mean values of the *k* nearest neighbors
- Distance-weighted nearest neighbor algorithm
  - Weight the contribution of each of the *k* neighbors according to their distance to the query x_q
    - Give greater weight to closer neighbors $w \equiv \frac{1}{d(x_q, x_i)^2}$
- Robust to noisy data by averaging *k*-nearest neighbors
- Curse of dimensionality: distance between neighbors could be dominated by irrelevant attributes
  - To overcome it, axes stretch or elimination of the least relevant attributes

Case-Based Reasoning (CBR)

- **CBR**: Uses a database of problem solutions to solve new problems
- Store symbolic description (tuples or cases)—not points in a Euclidean space
- Applications: Customer-service (product-related diagnosis), legal ruling
- Methodology
  - Instances represented by rich symbolic descriptions (e.g., function graphs)
  - Search for similar cases, multiple retrieved cases may be combined
  - Tight coupling between case retrieval, knowledge-based reasoning, and problem solving
- Challenges
  - Find a good similarity metric
  - Indexing based on syntactic similarity measure, and when failure, backtracking, and adapting to additional cases

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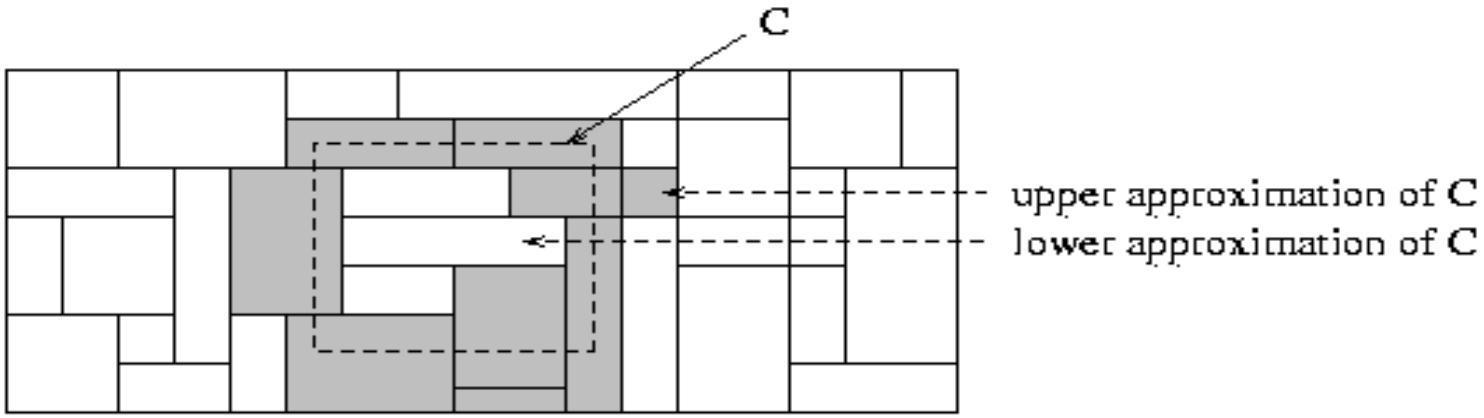
- Additional Topics: Semi-Supervised Methods, Active Learning, etc.

Genetic Algorithms (GA)

- Genetic Algorithm: based on an analogy to biological evolution
- An initial **population** is created consisting of randomly generated rules
  - Each rule is represented by a string of bits
  - E.g., if A_1 and $\neg A_2$ then C_2 can be encoded as 100
  - If an attribute has $k > 2$ values, k bits can be used
- Based on the notion of survival of the **fittest**, a new population is formed to consist of the fittest rules and their offspring
- The *fitness of a rule* is represented by its classification accuracy on a set of training examples
- Offspring are generated by *crossover* and *mutation*
- The process continues until a population P evolves *when each rule in P satisfies a pre-specified threshold*
- Slow but easily parallelizable

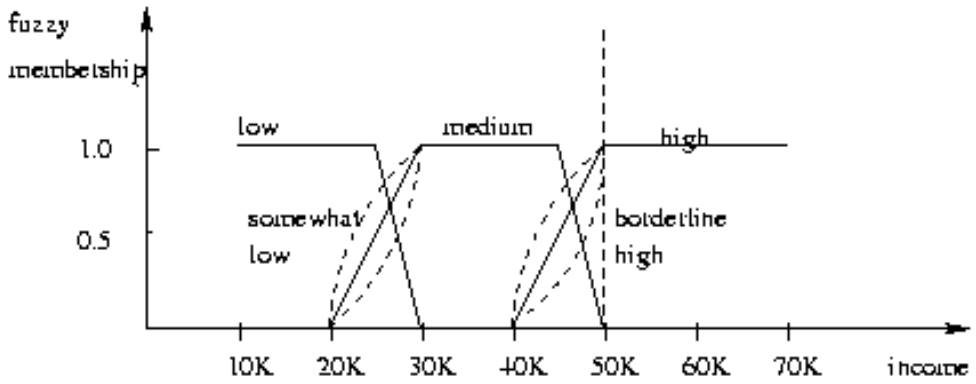
Rough Set Approach

- Rough sets are used to **approximately or "roughly" define equivalent classes**
- A rough set for a given class C is approximated by two sets: a lower approximation (certain to be in C) and an upper approximation (cannot be described as not belonging to C)
- Finding the minimal subsets (**reducts**) of attributes for feature reduction is NP-hard but a **discernibility matrix** (which stores the differences between attribute values for each pair of data tuples) is used to reduce the computation intensity



Fuzzy Set Approaches

- Fuzzy logic uses truth values between 0.0 and 1.0 to represent the degree of membership (such as in a *fuzzy membership graph*)
- Attribute values are converted to fuzzy values. Ex.:
  - Income, *x*, is assigned a fuzzy membership value to each of the discrete categories {low, medium, high}, e.g. $49K belongs to "medium income" with fuzzy value 0.15 but belongs to "high income" with fuzzy value 0.96
  - Fuzzy membership values do not have to sum to 1.
- Each applicable rule contributes a vote for membership in the categories
- Typically, the truth values for each predicted category are summed, and these sums are combined



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Multiclass Classification

- Classification involving more than two classes (i.e., > 2 Classes)
- Method 1. **One-vs.-all** (OVA): Learn a classifier one at a time
  - Given m classes, train m classifiers: one for each class
  - Classifier j: treat tuples in class j as *positive* & all others as *negative*
  - To classify a tuple **X**, the set of classifiers vote as an ensemble
- Method 2. **All-vs.-all** (AVA): Learn a classifier for each pair of classes
  - Given m classes, construct m(m-1)/2 binary classifiers
  - A classifier is trained using tuples of the two classes
  - To classify a tuple **X**, each classifier votes
    - X is assigned to the class with maximal vote
- Comparison
  - All-vs.-all tends to be superior to one-vs.-all
  - Problem: Binary classifier is sensitive to errors, and errors affect vote count

Error-Correcting Codes for Multiclass Classification

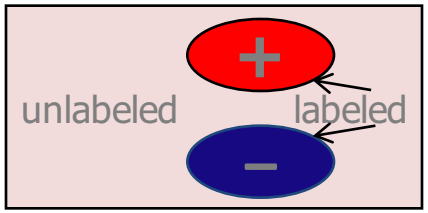
- Originally designed to correct errors during data transmission for communication tasks by exploring data redundancy
- Example
  - A 7-bit codeword associated with classes 1-4

Class	Error-Corr. Codeword						
C_1	1	1	1	1	1	1	1
C_2	0	0	0	0	1	1	1
C_3	0	0	1	1	0	0	1
C_4	0	1	0	1	0	1	0

  - Given a unknown tuple **X**, the 7-trained classifiers output: 0001010
  - Hamming distance: # of different bits between two codewords
  - H(**X**, C_1) = 5, by checking # of bits between [1111111] & [0001010]
  - H(**X**, C_2) = 3, H(**X**, C_3) = 3, H(**X**, C_4) = 1, thus C_4 as the label for **X**
- Error-correcting codes can correct up to (h – 1)/2 1-bit error, where h is the minimum Hamming distance between any two codewords
- If we use 1-bit per class, it is equiv. to one-vs.-all approach, the code are insufficient to self-correct
- When selecting error-correcting codes, there should be good row-wise and col.-wise separation between the codewords

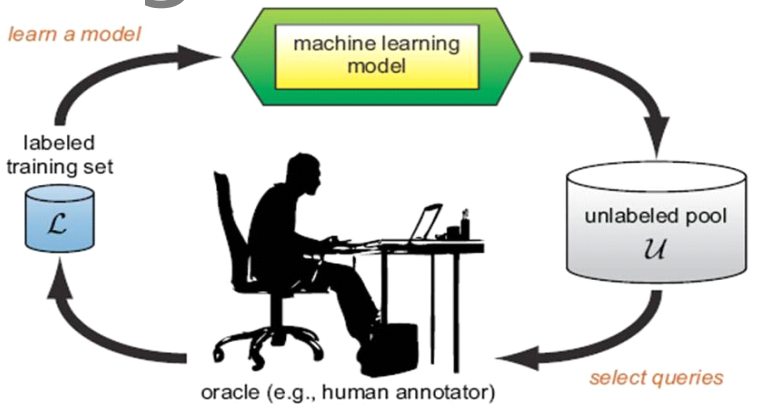
Semi-Supervised Classification

- Semi-supervised: Uses labeled and unlabeled data to build a classifier



- Self-training:
  - Build a classifier using the labeled data
  - Use it to label the unlabeled data, and those with the most confident label prediction are added to the set of labeled data
  - Repeat the above process
  - Adv: easy to understand; disadv: may reinforce errors
- Co-training: Use two or more classifiers to teach each other
  - Each learner uses a mutually independent set of features of each tuple to train a good classifier, say f_1
  - Then f_1 and f_2 are used to predict the class label for unlabeled data X
  - Teach each other: The tuple having the most confident prediction from f_1 is added to the set of labeled data for f_2 & vice versa
- Other methods, e.g., joint probability distribution of features and labels

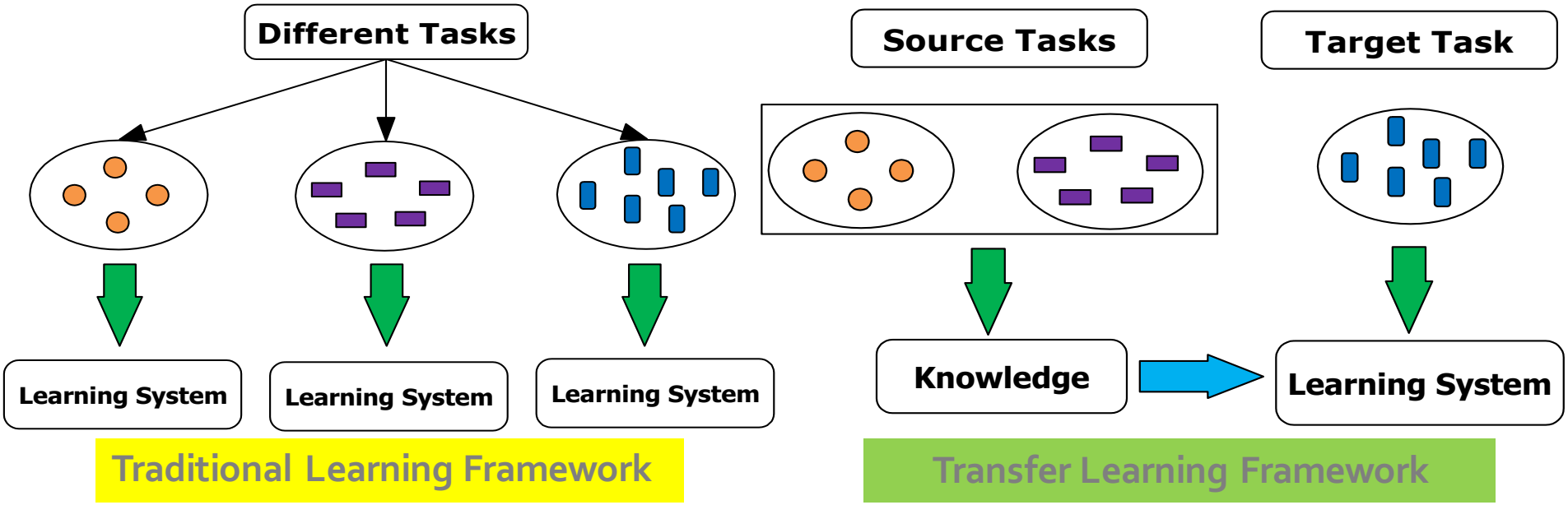
Active Learning



- Class labels are expensive to obtain
- Active learner: query human (oracle) for labels
- Pool-based approach: Uses a pool of unlabeled data
  - L: a small subset of D is labeled, U: a pool of unlabeled data in D
  - Use a query function to carefully select one or more tuples from U and request labels from an oracle (a human annotator)
  - The newly labeled samples are added to L, and learn a model
  - Goal: Achieve high accuracy using as few labeled data as possible
- Evaluated using *learning curves*: Accuracy as a function of the number of instances queried (# of tuples to be queried should be small)
- Research issue: How to choose the data tuples to be queried?
  - Uncertainty sampling: choose the least certain ones
  - Reduce *version space*, the subset of hypotheses consistent w. the training data
  - Reduce expected entropy over U: Find the greatest reduction in the total number of incorrect predictions

Transfer Learning: Conceptual Framework

- Transfer learning: Extract knowledge from one or more source tasks and apply the knowledge to a target task
- Traditional learning: Build a new classifier for each new task
- Transfer learning: Build new classifier by applying existing knowledge learned from source tasks



Transfer Learning: Methods and Applications

- Applications: Especially useful when data is outdated or distribution changes, e.g., Web document classification, e-mail spam filtering
- *Instance-based transfer learning*: Reweight some of the data from source tasks and use it to learn the target task
- TrAdaBoost (Transfer AdaBoost)
  - Assume source and target data each described by the same set of attributes (features) & class labels, but rather diff. distributions
  - Require only labeling a small amount of target data
  - Use source data in training: When a source tuple is misclassified, reduce the weight of such tupels so that they will have less effect on the subsequent classifier
- Research issues
  - Negative transfer: When it performs worse than no transfer at all
  - Heterogeneous transfer learning: Transfer knowledge from different feature space or multiple source domains
  - Large-scale transfer learning

Summary

- Effective and advanced classification methods
  - Bayesian belief network (probabilistic networks)
  - Backpropagation (Neural networks)
  - Support Vector Machine (SVM)
  - Pattern-based classification
  - Other classification methods: lazy learners (KNN, case-based reasoning), genetic algorithms, rough set and fuzzy set approaches
- Additional Topics on Classification
  - Multiclass classification
  - Semi-supervised classification
  - Active learning
  - Transfer learning

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