CS6220: DATA MINING TECHNIQUES

Matrix Data: Classification: Part 3

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October 1, 2013

Announcement

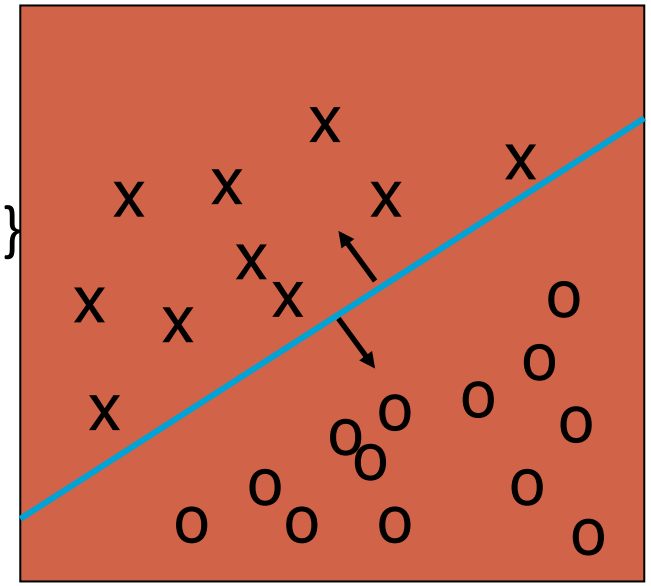
- Assignment 1 is out
  - Deadline (10/14/2013, 11:59pm)

Matrix Data: Classification: Part 3

- SVM (Support Vector Machine)
- kNN (k Nearest Neighbor)
- Other Issues
- Summary

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



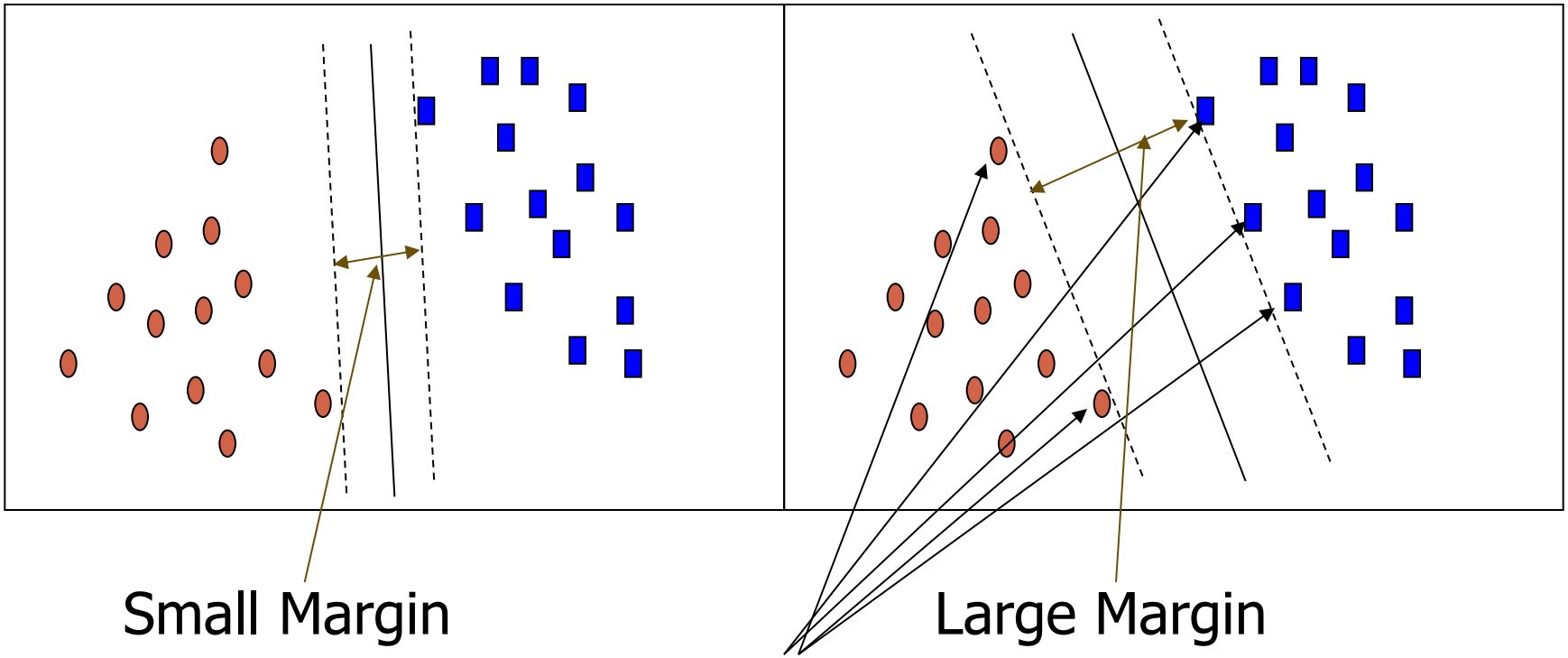
SVM—Support Vector Machines

- 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)

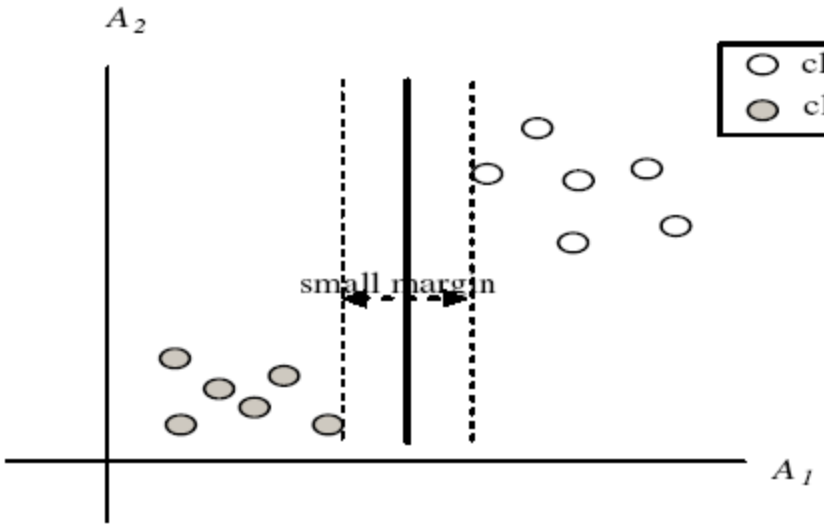
SVM—History and Applications

- 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

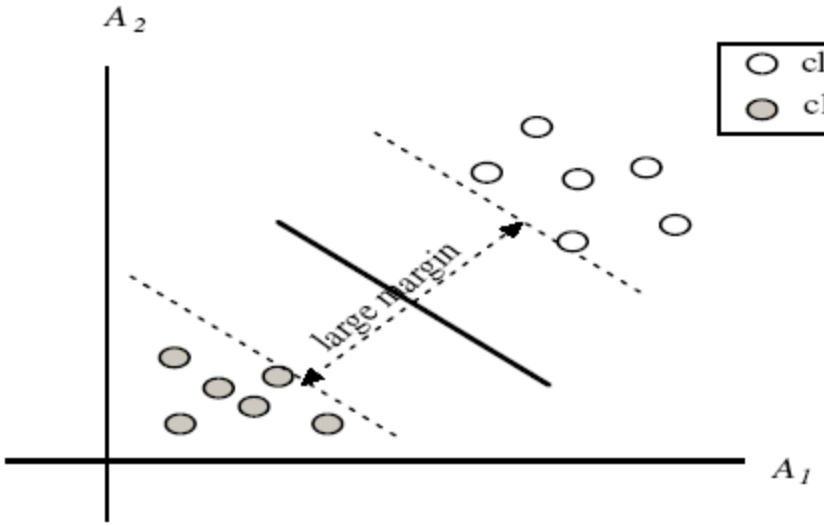
SVM—General Philosophy



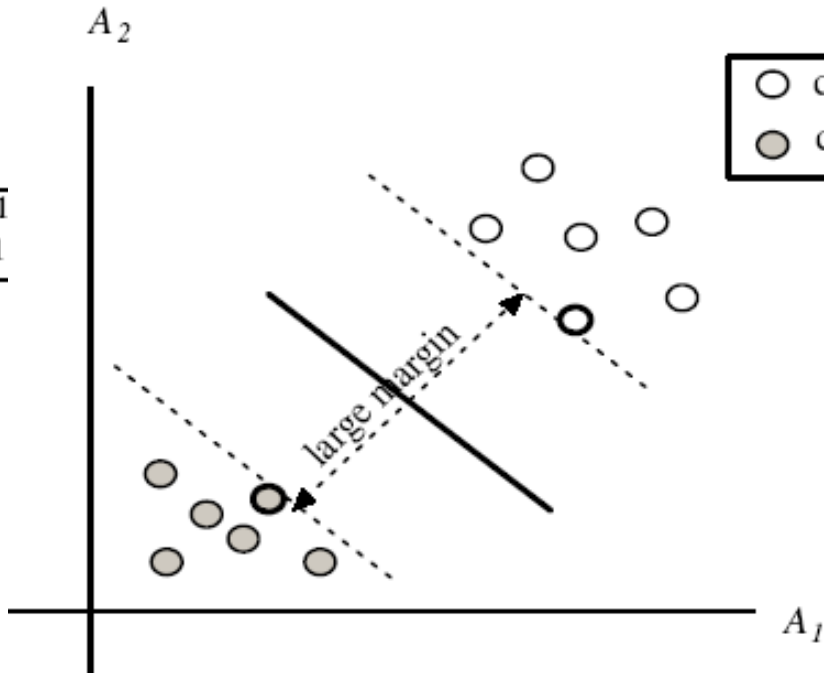
SVM—Margins and Support Vectors



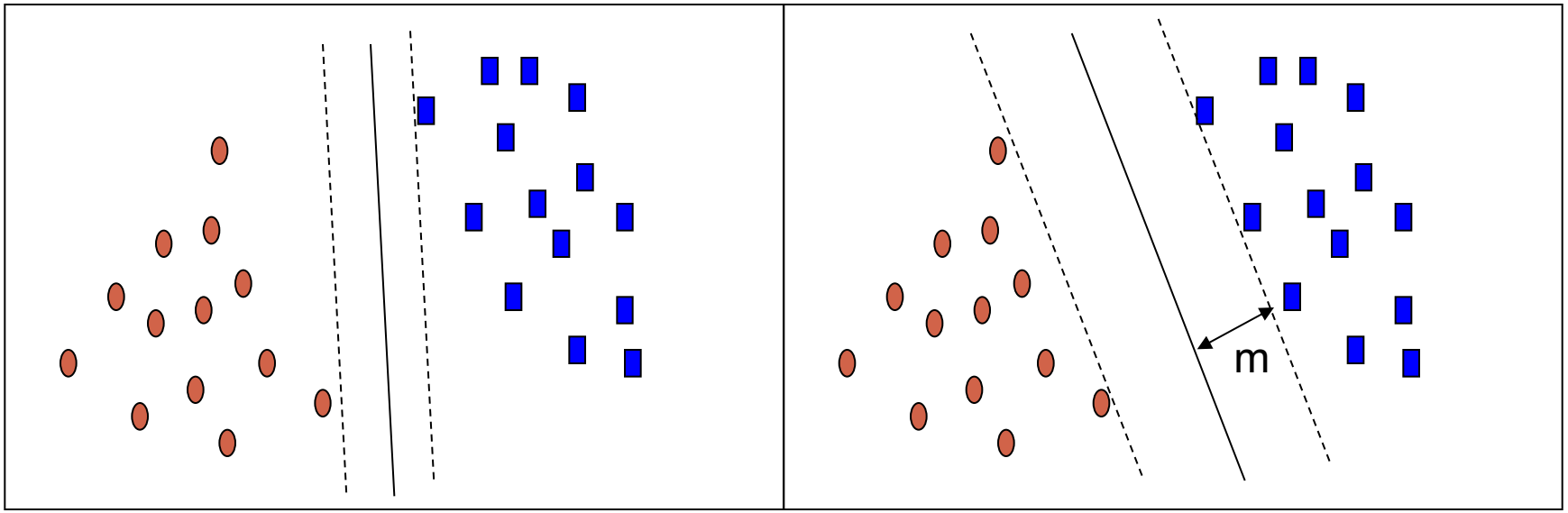
class 1, $y = +1$ (*buys_computer = "yes"*)
class 2, $y = -1$ (*buys_computer = "no"*)



class 1, $y = +1$
class 2, $y = -1$



SVM—When Data Is Linearly Separable



Let data D be ($\mathbf{X}_1$, y_1), …, ($\mathbf{X}_{|D|}$, $y_{|D|}$), 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

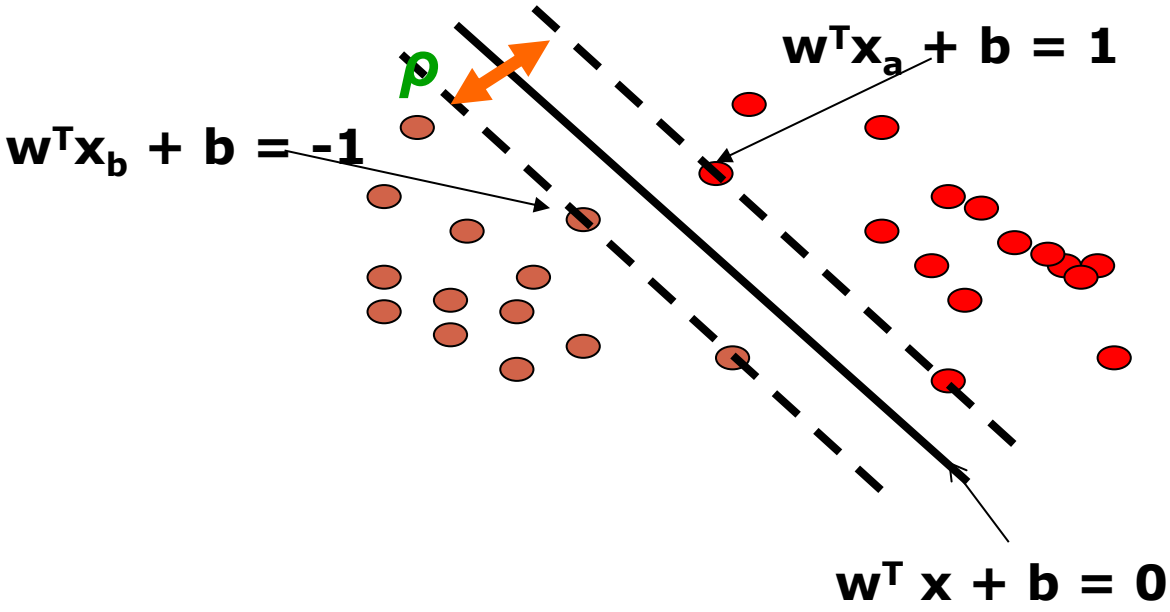
  $w_0 + w_1 x_1 + w_2 x_2 = 0$
- The hyperplane defining the sides of the margin:

  $H_1: w_0 + w_1 x_1 + w_2 x_2 \geq 1$ 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

Maximum Margin Calculation

- **w**: decision hyperplane normal vector
- $\mathbf{x}_i$: data point *i*
- y_i: class of data point *i* (+1 or -1)



$$\rho = \frac{2}{||w||}$$

SVM as a Quadratic Programming

- QP

Objective: Find $\mathbf{w}$ and b such that $\rho = \frac{2}{||w||}$ is maximized;

Constraints: For all $\{(\mathbf{x_i}, y_i)\}$

$\mathbf{w^T x_i} + b \geq 1$ if $y_i = 1$;

$\mathbf{w^T x_i} + b \leq -1$ if $y_i = -1$

- A better form

Objective: Find $\mathbf{w}$ and b such that $\mathbf{\Phi(w)} = \frac{1}{2}\mathbf{w^T w}$ is minimized;

Constraints: for all $\{(\mathbf{x_i}, y_i)\}$: $y_i(\mathbf{w^T x_i} + b) \geq 1$

Solve QP

- This is now optimizing a *quadratic* function subject to *linear* constraints
- Quadratic optimization problems are a well-known class of mathematical programming problem, and many (intricate) algorithms exist for solving them (with many special ones built for SVMs)
- The solution involves constructing a *dual problem* where a *Lagrange multiplier* α_i is associated with every constraint in the primary problem:

Primal Form and Dual Form

Primal

Objective: Find $\mathbf{w}$ and b such that $\Phi(\mathbf{w}) = \frac{1}{2}\mathbf{w}^T\mathbf{w}$ is minimized;

Constraints: for all $\{(\mathbf{x_i}, y_i)\}$: $y_i(\mathbf{w}^T\mathbf{x_i} + b) \geq 1$

Equivalent under some conditions: KKT conditions

Dual

Objective: Find $\alpha_1 \ldots \alpha_n$ such that
$\mathbf{Q}(\boldsymbol{\alpha}) = \Sigma\alpha_i - \frac{1}{2}\Sigma\Sigma\alpha_i\alpha_j y_i y_j \mathbf{x}_i^T\mathbf{x}_j$ is maximized and

Constraints
(1) $\Sigma\alpha_i y_i = 0$
(2) $\alpha_i \geq 0$ for all α_i

- More derivations: http://cs229.stanford.edu/notes/cs229-notes3.pdf

The Optimization Problem Solution

- The solution has the form:

$$\mathbf{w} = \sum \alpha_i y_i \mathbf{x_i} \qquad b = y_k - \mathbf{w}^T \mathbf{x_k} \text{ for any } \mathbf{x_k} \text{ such that } \alpha_k \neq 0$$

- Each non-zero α_i indicates that corresponding $\mathbf{x_i}$ is a support vector.
- Then the classifying function will have the form:

$$f(\mathbf{x}) = \sum \alpha_i y_i \mathbf{x_i}^T \mathbf{x} + b$$

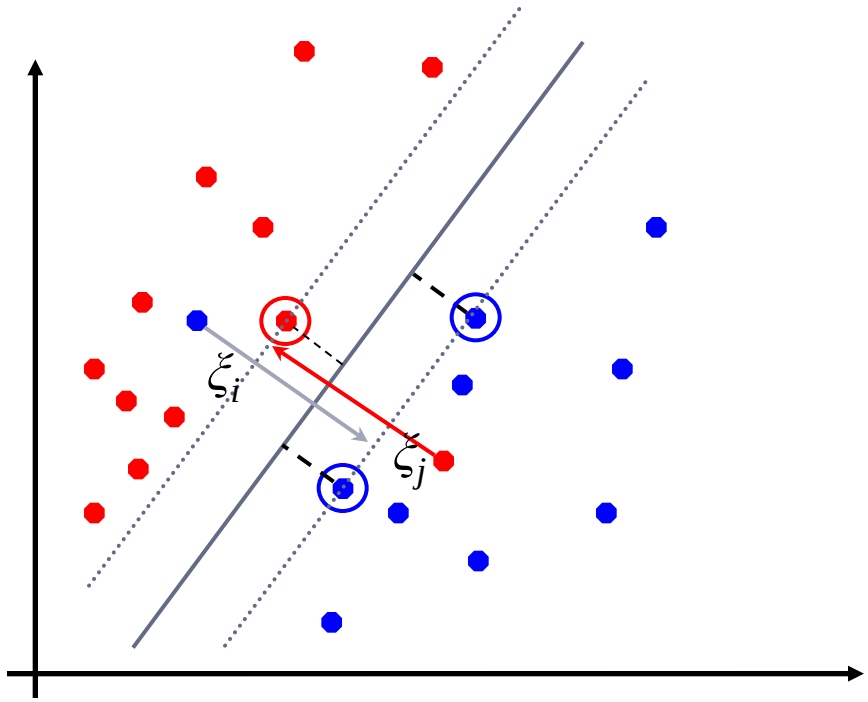
- Notice that it relies on an *inner product* between the test point **x** and the support vectors $\mathbf{x_i}$
  - We will return to this later.
- Also keep in mind that solving the optimization problem involved computing the inner products $\mathbf{x_i}^T \mathbf{x_j}$ between all pairs of training points.

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

Soft Margin Classification

- If the training data is not linearly separable, *slack variables* ξ_i can be added to allow misclassification of difficult or noisy examples.
- Allow some errors
  - Let some points be moved to where they belong, at a cost
- Still, try to minimize training set errors, and to place hyperplane "far" from each class (large margin)



Soft Margin Classification Mathematically

- The old formulation:

Find $\mathbf{w}$ and b such that
$\mathbf{\Phi(w)} = \frac{1}{2}\ \mathbf{w}^T\mathbf{w}$ is minimized and for all $\{(\mathbf{x_i}, y_i)\}$
$y_i\ (\mathbf{w}^T\mathbf{x_i} + b) \geq 1$

- The new formulation incorporating slack variables:

Find $\mathbf{w}$ and b such that
$\mathbf{\Phi(w)} = \frac{1}{2}\ \mathbf{w}^T\mathbf{w} + C\sum\xi_i$ is minimized and for all $\{(\mathbf{x_i}, y_i)\}$
$y_i\ (\mathbf{w}^T\mathbf{x_i} + b) \geq 1 - \xi_i$ and $\xi_i \geq 0$ for all i

- Parameter C can be viewed as a way to control overfitting
  - A regularization term (L1 regularization)

Soft Margin Classification – Solution

- The dual problem for soft margin classification:

Find $\alpha_1 \ldots \alpha_N$ such that
$\mathbf{Q}(\boldsymbol{\alpha}) = \Sigma\alpha_i - \frac{1}{2}\Sigma\Sigma\alpha_i\alpha_j y_i y_j \mathbf{x_i}^T\mathbf{x_j}$ is maximized and
(1) $\Sigma\alpha_i y_i = 0$
(2) $0 \le \alpha_i \le C$ for all α_i

- Neither slack variables ξ_i nor their Lagrange multipliers appear in the dual problem!
- Again, $\mathbf{x_i}$ with non-zero α_i will be support vectors.
- Solution to the dual problem is:

$\mathbf{w} = \Sigma\alpha_i y_i \mathbf{x_i}$
$b = y_k(1-\xi_k) - \mathbf{w}^T\mathbf{x}_k$ where $k = \underset{k'}{\text{argmax}}\ \alpha_{k'}$

w is not needed explicitly for classification!

$f(\mathbf{x}) = \Sigma\alpha_i y_i \mathbf{x_i}^T\mathbf{x} + b$

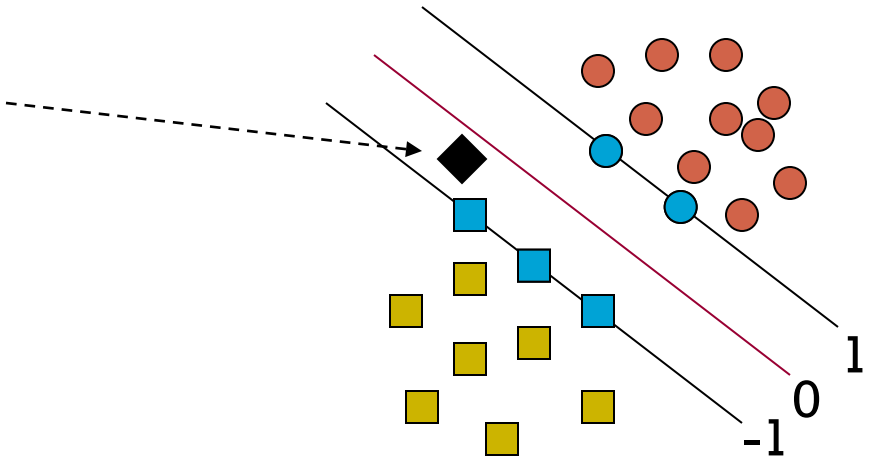
Classification with SVMs

- Given a new point **x**, we can score its projection onto the hyperplane normal:
  - I.e., compute score: $\mathbf{w}^T\mathbf{x} + b = \Sigma\alpha_i y_i \mathbf{x}_i^T\mathbf{x} + b$
    - Decide class based on whether < or > 0
  - Can set confidence threshold t.

Score > t: yes

Score < -t: no

Else: don't know



Linear SVMs: Summary

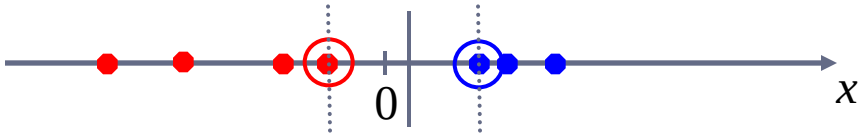
- The classifier is a *separating hyperplane.*
- The most "important" training points are the support vectors; they define the hyperplane.
- Quadratic optimization algorithms can identify which training points $\mathbf{x}_i$ are support vectors with non-zero Lagrangian multipliers α_i.
- Both in the dual formulation of the problem and in the solution, training points appear only inside inner products:

Find $\alpha_1 \ldots \alpha_N$ such that
$\mathbf{Q}(\boldsymbol{\alpha}) = \Sigma\alpha_i - \frac{1}{2}\Sigma\Sigma\alpha_i\alpha_j y_i y_j \mathbf{x}_i^T\mathbf{x}_j$ is maximized and
(1) $\Sigma\alpha_i y_i = 0$
(2) $0 \le \alpha_i \le C$ for all α_i

$$f(\mathbf{x}) = \Sigma\alpha_i y_i \mathbf{x}_i^T\mathbf{x} + b$$

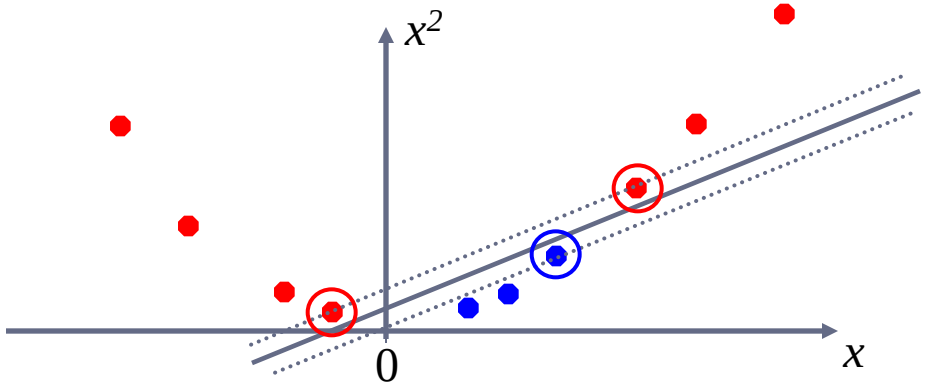
Non-linear SVMs

- Datasets that are linearly separable (with some noise) work out great:



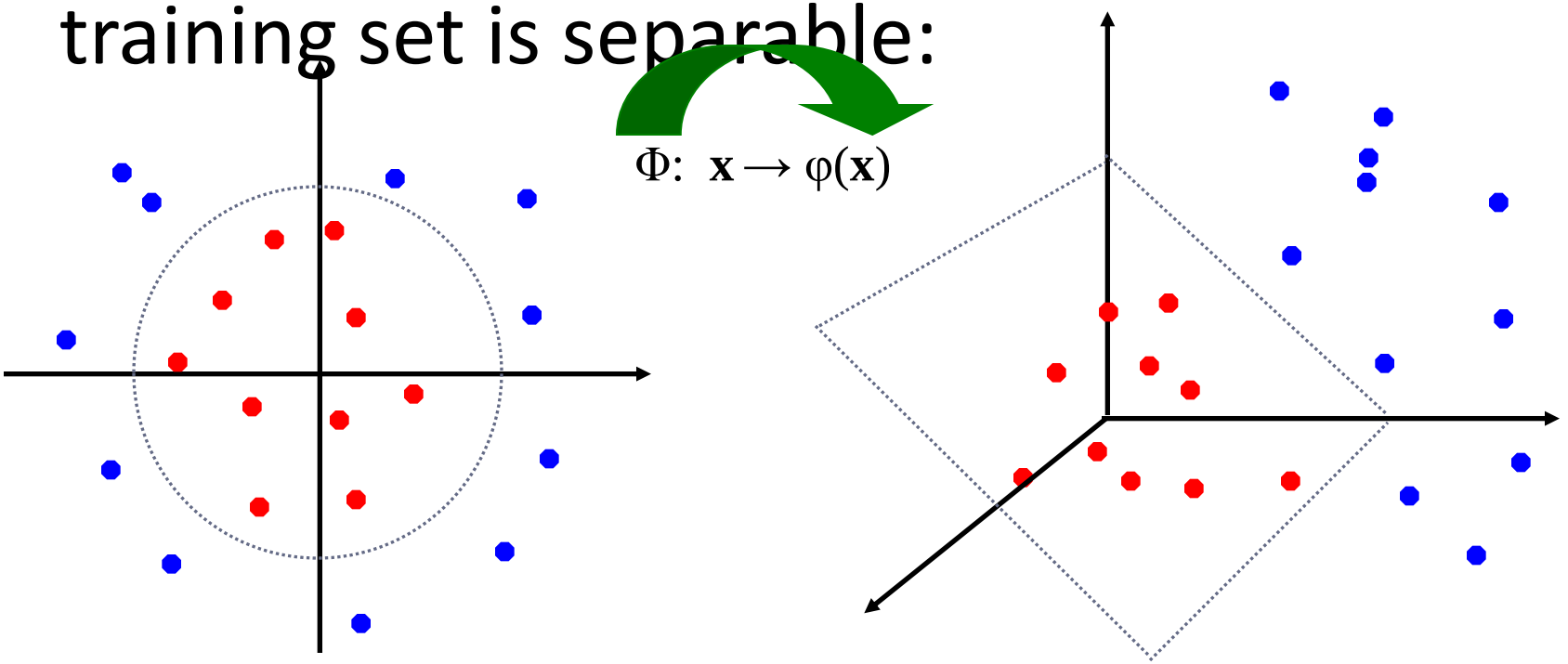
- But what are we going to do if the dataset is just too hard?

- How about … mapping data to a higher-dimensional space:



Non-linear SVMs: Feature spaces

- General idea: the original feature space can always be mapped to some higher-dimensional feature space where the training set is separable:



The "Kernel Trick"

- The linear classifier relies on an inner product between vectors $K(\mathbf{x}_i,\mathbf{x}_j)=\mathbf{x}_i^T\mathbf{x}_j$
- If every data point is mapped into high-dimensional space via some transformation Φ: $\mathbf{x} \rightarrow \phi(\mathbf{x})$, the inner product becomes:

$$K(\mathbf{x}_i,\mathbf{x}_j)= \phi(\mathbf{x}_i)^T\phi(\mathbf{x}_j)$$

- A *kernel function* is some function that corresponds to an inner product in some expanded feature space.
- Example:

  2-dimensional vectors $\mathbf{x}=[x_1 \;\; x_2]$; let $K(\mathbf{x}_i,\mathbf{x}_j)=(1 + \mathbf{x}_i^T\mathbf{x}_j)^2$,

  Need to show that $K(\mathbf{x}_i,\mathbf{x}_j)= \phi(\mathbf{x}_i)^T\phi(\mathbf{x}_j)$:

$$K(\mathbf{x}_i,\mathbf{x}_j)=(1 + \mathbf{x}_i^T\mathbf{x}_j)^2 = 1+ x_{i1}^2x_{j1}^2 + 2\, x_{i1}x_{j1}\, x_{i2}x_{j2}+ x_{i2}^2x_{j2}^2 + 2x_{i1}x_{j1} + 2x_{i2}x_{j2}=$$

$$= [1 \;\; x_{i1}^2 \;\; \sqrt{2}\, x_{i1}x_{i2} \;\; x_{i2}^2 \;\; \sqrt{2}x_{i1} \;\; \sqrt{2}x_{i2}]^T [1 \;\; x_{j1}^2 \;\; \sqrt{2}\, x_{j1}x_{j2} \;\; x_{j2}^2 \;\; \sqrt{2}x_{j1} \;\; \sqrt{2}x_{j2}]$$

$$= \phi(\mathbf{x}_i)^T\phi(\mathbf{x}_j) \quad \text{where } \phi(\mathbf{x}) = [1 \;\; x_1^2 \;\; \sqrt{2}\, x_1x_2 \;\; x_2^2 \;\; \sqrt{2}x_1 \;\; \sqrt{2}x_2]$$

SVM: Different Kernel functions

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

$$\text{Polynomial kernel of degree } h: \quad K(X_i, X_j) = (X_i \cdot X_j + 1)^h$$

$$\text{Gaussian radial basis function kernel}: \quad K(X_i, X_j) = e^{-\|X_i - X_j\|^2 / 2\sigma^2}$$

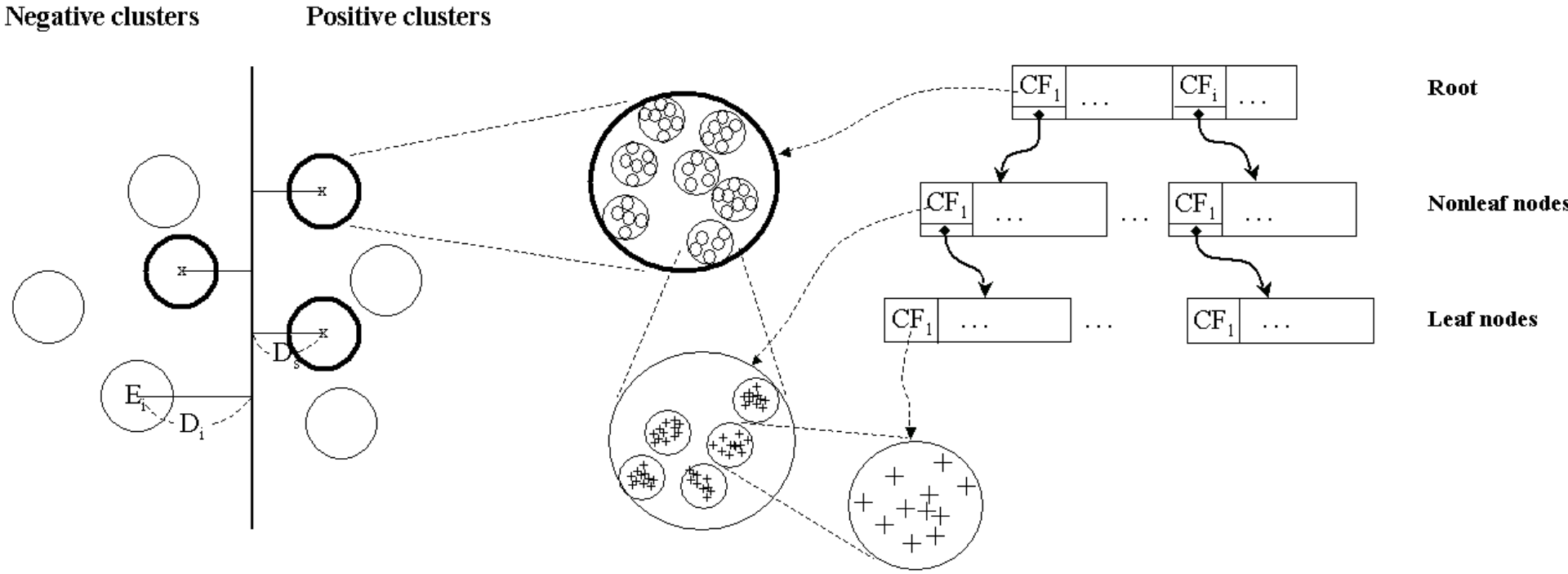
$$\text{Sigmoid kernel}: \quad K(X_i, X_j) = \tanh(\kappa X_i \cdot X_j - \delta)$$

- *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 the number of data objects in terms of training time and memory usage
- H. Yu, J. Yang, and J. Han, "Classifying Large Data Sets Using SVM with Hierarchical Clusters", KDD'03)
- CB-SVM (Clustering-Based SVM)
  - Given limited amount of system resources (e.g., memory), maximize the SVM performance in terms of accuracy and the training speed
  - Use micro-clustering to effectively reduce the number of points to be considered
  - At deriving support vectors, de-cluster micro-clusters near "candidate vector" to ensure high classification accuracy

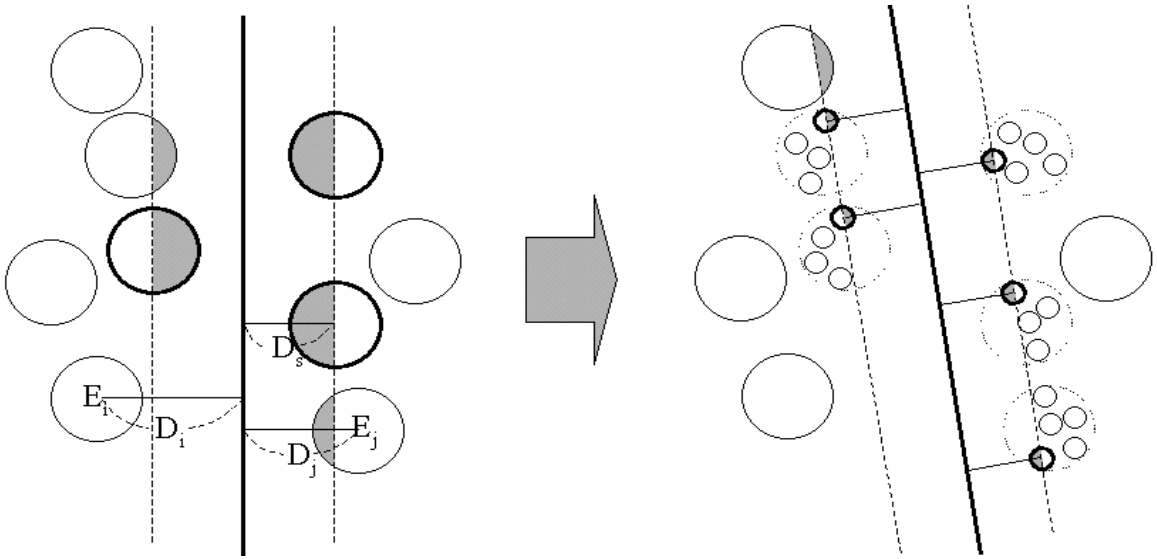
*CF-Tree: Hierarchical Micro-cluster



- Read the data set once, construct a statistical summary of the data (i.e., hierarchical clusters) given a limited amount of memory
- Micro-clustering: Hierarchical indexing structure
  - provide finer samples closer to the boundary and coarser samples farther from the boundary

*Selective Declustering: Ensure High Accuracy

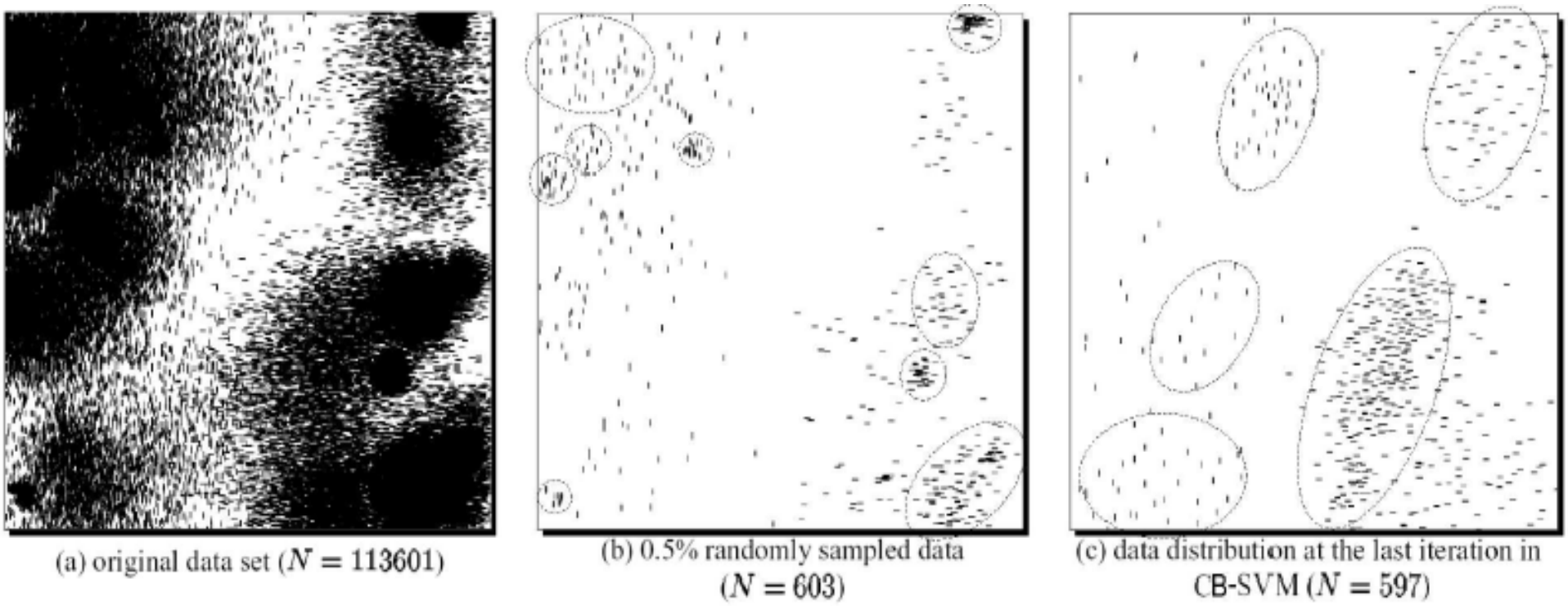
- CF tree is a suitable base structure for selective declustering
- De-cluster only the cluster E_i such that
  - $D_i - R_i < D_s$, where D_i is the distance from the boundary to the center point of E_i and R_i is the radius of E_i
  - Decluster only the cluster whose subclusters have possibilities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



*CB-SVM Algorithm: Outline

- Construct two CF-trees from positive and negative data sets independently
  - Need one scan of the data set
- 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
- Train an SVM again from the centroids of the entries in the training set
- Repeat until nothing is accumulated

*Accuracy and Scalability on Synthetic Dataset



(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

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

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

Matrix Data: Classification: Part 3

- SVM (Support Vector Machine)
- kNN (k Nearest Neighbor) 
- Other Issues
- Summary

Lazy vs. Eager Learning

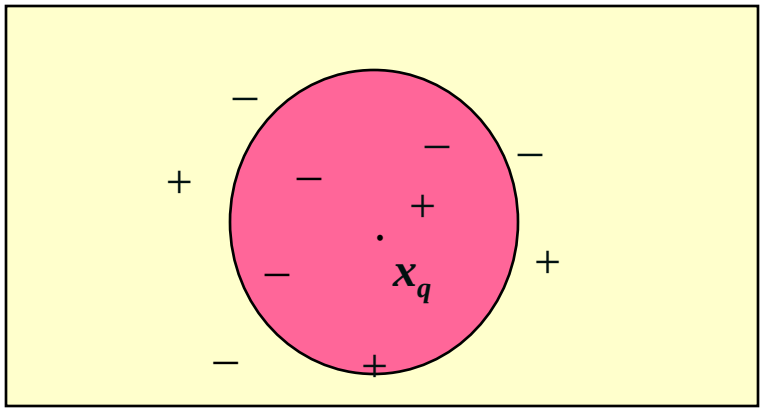
- Lazy vs. eager learning
  - **Lazy learning** (e.g., instance-based learning): Simply stores training data (or only minor processing) and waits until it is given a test tuple
  - **Eager learning** (the above discussed methods): Given a set of training tuples, constructs a classification model before 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

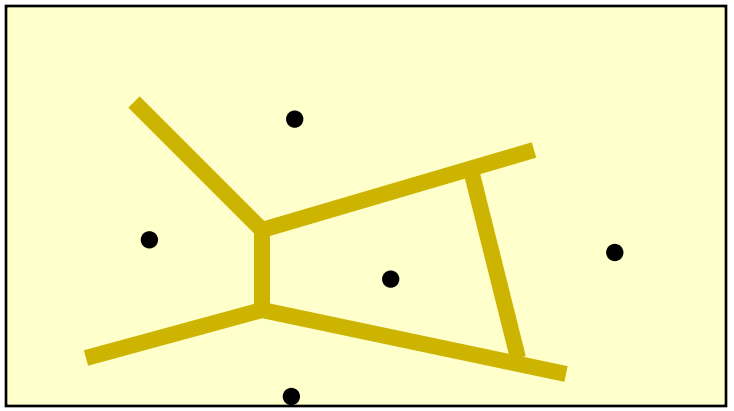
Lazy Learner: Instance-Based Methods

- 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

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
    - $y_q = \frac{\sum w_i y_i}{\sum w_i}$, where x_i's are x_q's nearest 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

Similarity and Dissimilarity

- **Similarity**
  - Numerical measure of how alike two data objects are
  - Value is higher when objects are more alike
  - Often falls in the range [0,1]
- **Dissimilarity** (e.g., distance)
  - Numerical measure of how different two data objects are
  - Lower when objects are more alike
  - Minimum dissimilarity is often 0
  - Upper limit varies
- **Proximity** refers to a similarity or dissimilarity

Data Matrix and Dissimilarity Matrix

- Data matrix
  - n data points with p dimensions
  - Two modes

$$\begin{bmatrix} x_{11} & \cdots & x_{1f} & \cdots & x_{1p} \\ \cdots & \cdots & \cdots & \cdots & \cdots \\ x_{i1} & \cdots & x_{if} & \cdots & x_{ip} \\ \cdots & \cdots & \cdots & \cdots & \cdots \\ x_{n1} & \cdots & x_{nf} & \cdots & x_{np} \end{bmatrix}$$

- Dissimilarity matrix
  - n data points, but registers only the distance
  - A triangular matrix
  - Single mode

$$\begin{bmatrix} 0 & & & & \\ d(2,1) & 0 & & & \\ d(3,1) & d(3,2) & 0 & & \\ \vdots & \vdots & \vdots & & \\ d(n,1) & d(n,2) & \cdots & \cdots & 0 \end{bmatrix}$$

Proximity Measure for Nominal Attributes

- Can take 2 or more states, e.g., red, yellow, blue, green (generalization of a binary attribute)
- Method 1: Simple matching
  - m: # of matches, p: total # of variables

$$d(i, j) = \frac{p - m}{p}$$

- Method 2: Use a large number of binary attributes
  - creating a new binary attribute for each of the M nominal states

Proximity Measure for Binary Attributes

- A contingency table for binary data

Object *i* \ Object *j*	1	0	sum
1	q	r	$q+r$
0	s	t	$s+t$
sum	$q+s$	$r+t$	p

- Distance measure for symmetric binary variables:

$$d(i,j) = \frac{r+s}{q+r+s+t}$$

- Distance measure for asymmetric binary variables:

$$d(i,j) = \frac{r+s}{q+r+s}$$

- Jaccard coefficient (*similarity* measure for *asymmetric* binary variables):

$$sim_{Jaccard}(i,j) = \frac{q}{q+r+s}$$

- Note: Jaccard coefficient is the same as "coherence":

$$coherence(i,j) = \frac{sup(i,j)}{sup(i)+sup(j)-sup(i,j)} = \frac{q}{(q+r)+(q+s)-q}$$

Dissimilarity between Binary Variables

- Example

Name	Gender	Fever	Cough	Test-1	Test-2	Test-3	Test-4
Jack	M	Y	N	P	N	N	N
Mary	F	Y	N	P	N	P	N
Jim	M	Y	P	N	N	N	N

  - Gender is a symmetric attribute
  - The remaining attributes are asymmetric binary
  - Let the values Y and P be 1, and the value N 0

$$d(jack, mary) = \frac{0+1}{2+0+1} = 0.33$$

$$d(jack, jim) = \frac{1+1}{1+1+1} = 0.67$$

$$d(jim, mary) = \frac{1+2}{1+1+2} = 0.75$$

Standardizing Numeric Data

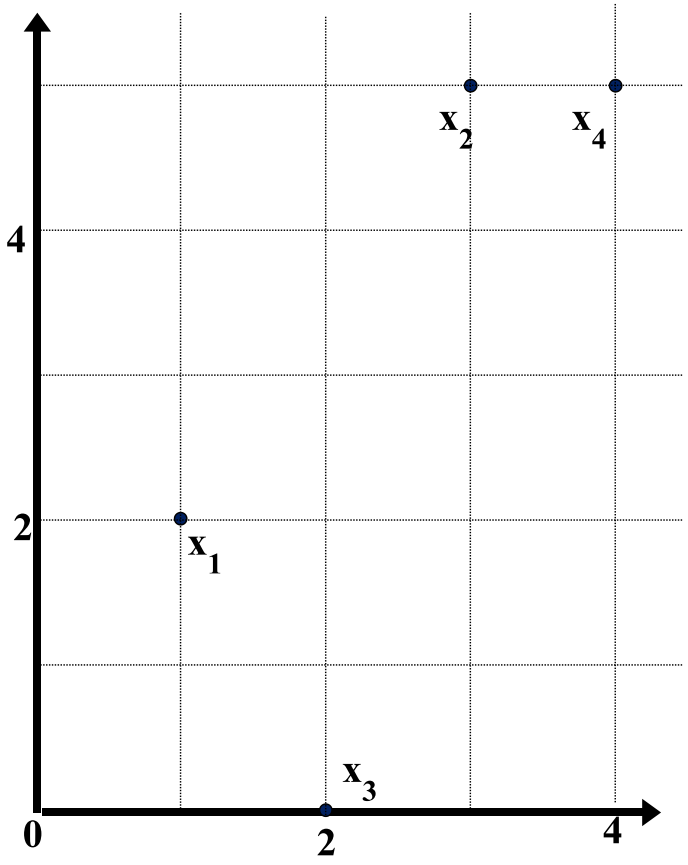
- Z-score: $$z = \frac{x - \mu}{\sigma}$$
  - X: raw score to be standardized, μ: mean of the population, σ: standard deviation
  - the distance between the raw score and the population mean in units of the standard deviation
  - negative when the raw score is below the mean, "+" when above
- An alternative way: Calculate the mean absolute deviation

$$s_f = \frac{1}{n}(|x_{1f} - m_f| + |x_{2f} - m_f| + \ldots + |x_{nf} - m_f|)$$

where $$m_f = \frac{1}{n}(x_{1f} + x_{2f} + \ldots + x_{nf})$$

  - standardized measure (*z-score*): $$z_{if} = \frac{x_{if} - m_f}{s_f}$$
- Using mean absolute deviation is more robust than using standard deviation

Example:
Data Matrix and Dissimilarity Matrix



Data Matrix

point	attribute1	attribute2
x1	1	2
x2	3	5
x3	2	0
x4	4	5

Dissimilarity Matrix

(with Euclidean Distance)

	x1	*x2*	*x3*	*x4*
x1	0			
x2	3.61	0		
x3	2.24	5.1	0	
x4	4.24	1	5.39	0

Distance on Numeric Data: Minkowski Distance

- *Minkowski distance*: A popular distance measure

$$d(i, j) = \sqrt[h]{|x_{i1} - x_{j1}|^h + |x_{i2} - x_{j2}|^h + \cdots + |x_{ip} - x_{jp}|^h}$$

where $i = (x_{i1}, x_{i2}, \ldots, x_{ip})$ and $j = (x_{j1}, x_{j2}, \ldots, x_{jp})$ are two p-dimensional data objects, and h is the order (the distance so defined is also called L-h norm)

- Properties
  - $d(i, j) > 0$ if $i \neq j$, and $d(i, i) = 0$ (Positive definiteness)
  - $d(i, j) = d(j, i)$ (Symmetry)
  - $d(i, j) \leq d(i, k) + d(k, j)$ (Triangle Inequality)
- A distance that satisfies these properties is a metric

Special Cases of Minkowski Distance

- *h* = 1: Manhattan (city block, L_1 norm) distance
  - E.g., the Hamming distance: the number of bits that are different between two binary vectors

$$d(i,j) = |x_{i_1} - x_{j_1}| + |x_{i_2} - x_{j_2}| + \ldots + |x_{i_p} - x_{j_p}|$$

- *h* = 2: (L_2 norm) Euclidean distance

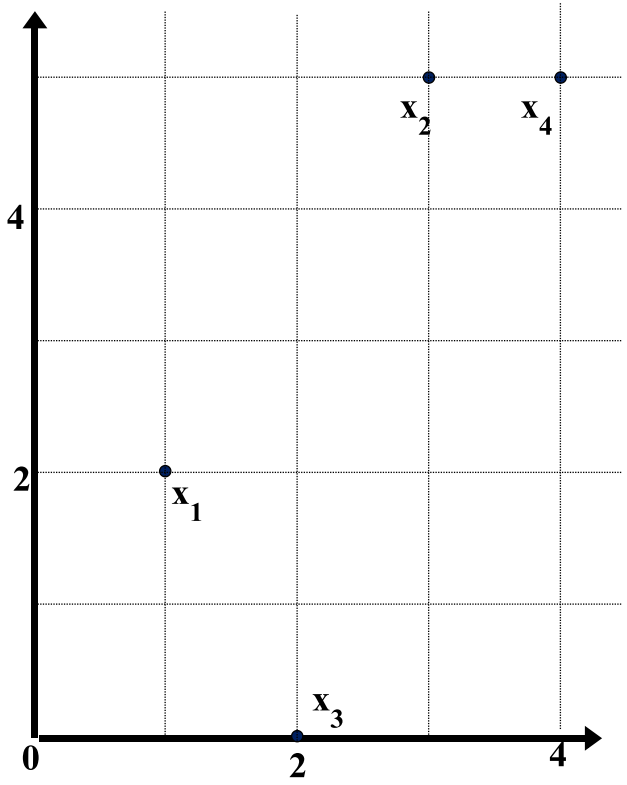
$$d(i,j) = \sqrt{(|x_{i_1} - x_{j_1}|^2 + |x_{i_2} - x_{j_2}|^2 + \ldots + |x_{i_p} - x_{j_p}|^2)}$$

- $h \to \infty$. "supremum" (L_{max} norm, L_∞ norm) distance.
  - This is the maximum difference between any component (attribute) of the vectors

$$d(i,j) = \lim_{h \to \infty} \left(\sum_{f=1}^{p} |x_{if} - x_{jf}|^h \right)^{\frac{1}{h}} = \max_{f}^{p} |x_{if} - x_{jf}|$$

Example: Minkowski Distance

point	attribute 1	attribute 2
x1	1	2
x2	3	5
x3	2	0
x4	4	5



Dissimilarity Matrices

Manhattan (L_1)

L	x1	x2	x3	x4
x1	0			
x2	5	0		
x3	3	6	0	
x4	6	1	7	0

Euclidean (L_2)

L2	x1	x2	x3	x4
x1	0			
x2	3.61	0		
x3	2.24	5.1	0	
x4	4.24	1	5.39	0

Supremum

L_∞	x1	x2	x3	x4
x1	0			
x2	3	0		
x3	2	5	0	
x4	3	1	5	0

Ordinal Variables

- An ordinal variable can be discrete or continuous
- Order is important, e.g., rank
- Can be treated like interval-scaled
  - replace x_{if} by their rank $r_{if} \in \{1, \ldots, M_f\}$
  - map the range of each variable onto [0, 1] by replacing *i*-th object in the *f*-th variable by

$$z_{if} = \frac{r_{if} - 1}{M_f - 1}$$

  - compute the dissimilarity using methods for interval-scaled variables

Attributes of Mixed Type

- A database may contain all attribute types
  - Nominal, symmetric binary, asymmetric binary, numeric, ordinal
- One may use a weighted formula to combine their effects

$$d(i,j) = \frac{\sum_{f=1}^{p} \delta_{ij}^{(f)} d_{ij}^{(f)}}{\sum_{f=1}^{p} \delta_{ij}^{(f)}}$$

  - f is binary or nominal:

    $d_{ij}^{(f)} = 0$ if $x_{if} = x_{jf}$, or $d_{ij}^{(f)} = 1$ otherwise
  - f is numeric: use the normalized distance
  - f is ordinal
    - Compute ranks r_{if} and $z_{if} = \frac{r_{if} - 1}{M_f - 1}$
    - Treat z_{if} as interval-scaled

Cosine Similarity

- A **document** can be represented by thousands of attributes, each recording the *frequency* of a particular word (such as keywords) or phrase in the document.

Document	*team*	*coach*	*hockey*	*baseball*	*soccer*	*penalty*	*score*	*win*	*loss*	*season*
Document1	5	0	3	0	2	0	0	2	0	0
Document2	3	0	2	0	1	1	0	1	0	1
Document3	0	7	0	2	1	0	0	3	0	0
Document4	0	1	0	0	1	2	2	0	3	0

- Other vector objects: gene features in micro-arrays, …
- Applications: information retrieval, biologic taxonomy, gene feature mapping, ...
- Cosine measure: If d_1 and d_2 are two vectors (e.g., term-frequency vectors), then

$$\cos(d_1, d_2) = (d_1 \bullet d_2) / ||d_1|| \, ||d_2|| ,$$

where $\bullet$ indicates vector dot product, $||d||$: the length of vector d

Example: Cosine Similarity

- $\cos(d_1, d_2) = (d_1 \bullet d_2) / ||d_1|| \, ||d_2||$,
  where $\bullet$ indicates vector dot product, $||d||$: the length of vector d

- Ex: Find the **similarity** between documents 1 and 2.

$d_1 = (5, 0, 3, 0, 2, 0, 0, 2, 0, 0)$
$d_2 = (3, 0, 2, 0, 1, 1, 0, 1, 0, 1)$

$d_1 \bullet d_2 = 5*3+0*0+3*2+0*0+2*1+0*1+0*1+2*1+0*0+0*1 = 25$
$||d_1|| = (5*5+0*0+3*3+0*0+2*2+0*0+0*0+2*2+0*0+0*0)^{0.5} = (42)^{0.5} = 6.481$
$||d_2|| = (3*3+0*0+2*2+0*0+1*1+1*1+0*0+1*1+0*0+1*1)^{0.5} = (17)^{0.5} = 4.12$
$\cos(d_1, d_2) = 0.94$

Model Selection for kNN

- The number of neighbors k
  - Small k: overfitting (high variance)
  - Big k: bringing too many irrelevant points (high bias)
  - More discussions:

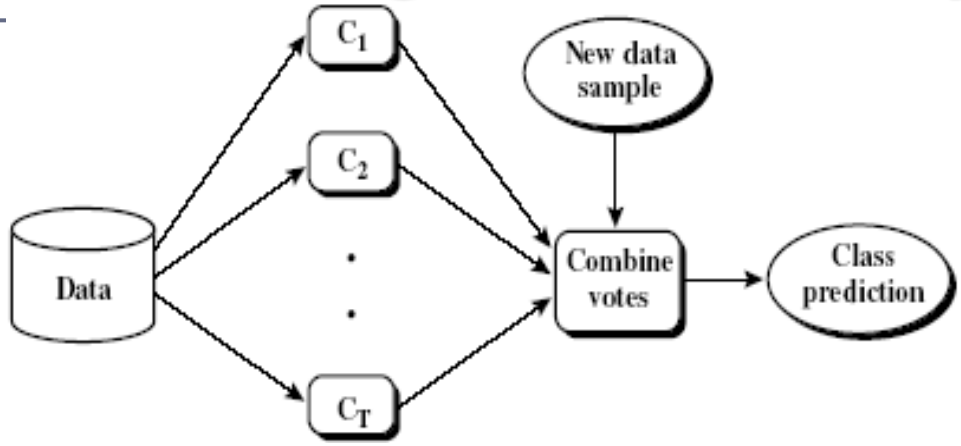
http://scott.fortmann-roe.com/docs/BiasVariance.html

- The distance function

Matrix Data: Classification: Part 3

- SVM (Support Vector Machine)
- kNN (k Nearest Neighbor)
- Other Issues 
- Summary

Ensemble Methods: Increasing the Accuracy



- Ensemble methods
  - Use a combination of models to increase accuracy
  - Combine a series of k learned models, M_1, M_2, ..., M_k, with the aim of creating an improved model M^*
- Popular ensemble methods
  - Bagging: averaging the prediction over a collection of classifiers
  - Boosting: weighted vote with a collection of classifiers

Bagging: Boostrap Aggregation

- Analogy: Diagnosis based on multiple doctors' majority vote
- Training
  - Given a set D of *d* tuples, at each iteration *i*, a training set D_i of *d* tuples is sampled with replacement from D (i.e., bootstrap)
  - A classifier model M_i is learned for each training set D_i
- Classification: classify an unknown sample **X**
  - Each classifier M_i returns its class prediction
  - The bagged classifier M^* counts the votes and assigns the class with the most votes to **X**
- Prediction: can be applied to the prediction of continuous values by taking the average value of each prediction for a given test tuple

Performance of Bagging

- Accuracy
  - Often significantly better than a single classifier derived from D
  - For noise data: not considerably worse, more robust
  - Proved improved accuracy in prediction
- Example
  - Suppose we have 5 completely independent classifiers…
  - If accuracy is 70% for each
    - The final prediction is correct, if at least 3 classifiers make the correct prediction
      - 3 are correct: $\binom{5}{3} \times (.7^3)(.3^2)$
      - 4 are correct: $\binom{5}{4} \times (.7^4)(.3^1)$
      - 5 are correct: $\binom{5}{5} \times (.7^5)(.3^0)$
    - In all, 10 (.7^3)(.3^2)+5(.7^4)(.3)+(.7^5)
    - **83.7% majority vote accuracy**
  - 101 Such classifiers
    - **99.9% majority vote accuracy**

Boosting

- Analogy: Consult several doctors, based on a combination of weighted diagnoses—weight assigned based on the previous diagnosis accuracy
- How boosting works?
  - **Weights** are assigned to each training tuple
  - A series of k classifiers is iteratively learned
  - After a classifier M_t is learned, the weights are updated to allow the subsequent classifier, M_{t+1}, to **pay more attention to the training tuples that were misclassified** by M_t
  - The final **M* combines the votes** of each individual classifier, where the weight of each classifier's vote is a function of its accuracy
- Boosting algorithm can be extended for numeric prediction
- Comparing with bagging: Boosting tends to have greater accuracy, but it also risks overfitting the model to misclassified data

Adaboost (Freund and Schapire, 1997)

- Given a set of *d* class-labeled tuples, ($\mathbf{X_1}$, y_1), …, ($\mathbf{X_d}$, y_d)
- Initially, all the weights of tuples are set the same (1/d)
- Generate k classifiers in k rounds. At round t,
  - Tuples from D are sampled (with replacement) to form a training set D_t of the same size based on its weight
  - A classification model M_t is derived from D_t
  - If a tuple is misclassified, its weight is increased, o.w. it is decreased
    - $w_{t+1,j} \propto w_{t,j} \times \exp(-\alpha_t)$ if j is correctly classified
    - $w_{t+1,j} \propto w_{t,j} \times \exp(\alpha_t)$ if j is incorrectly classified

$$\alpha_t : weight\ for classifier\ t\ , the\ higher\ the\ better$$

AdaBoost

- Error rate: err($\mathbf{X}_j$) is the misclassification error of tuple $\mathbf{X}_j$. Classifier M_t error rate ($\epsilon_t = \text{error}(M_t)$) is the sum of the weights of the misclassified tuples:

$$error(M_t) = \sum_{j}^{d} w_{tj} \times err(\mathbf{X}_{tj})$$

- The weight of classifier M_t's vote is

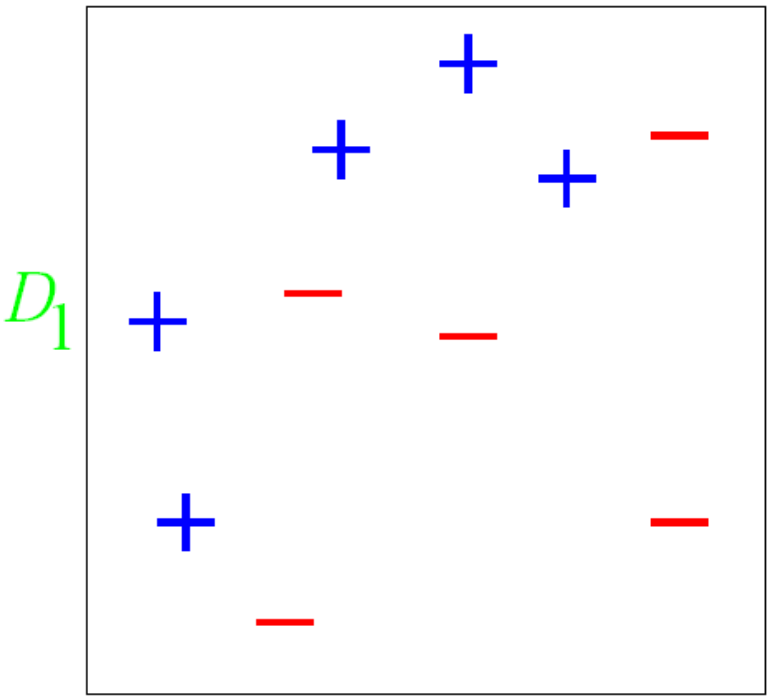
$$\alpha_t = \frac{1}{2} \ln \frac{1 - error(M_t)}{error(M_t)}$$

- Final classifier M*

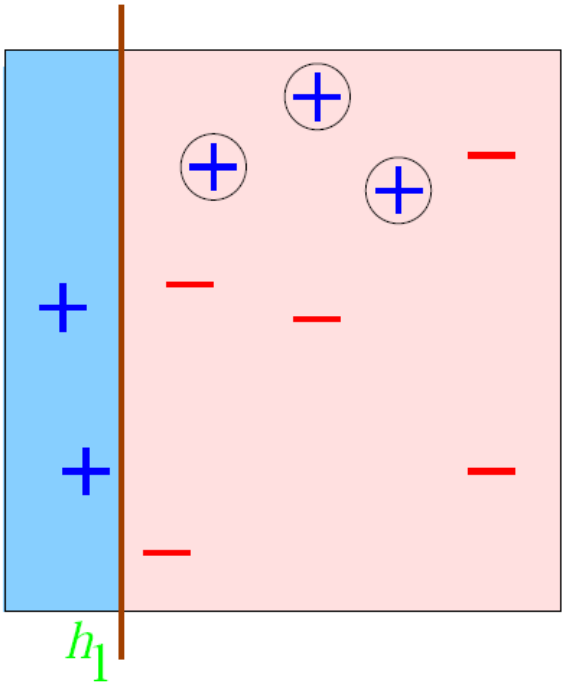
$$M^*(x) = sign(\sum_{t} \alpha_t M_t(x))$$

AdaBoost Example

- **From "A Tutorial on Boosting"**
  - By Yoav Freund and Rob Schapire
- Note they use h_t to represent classifier instead of M_t

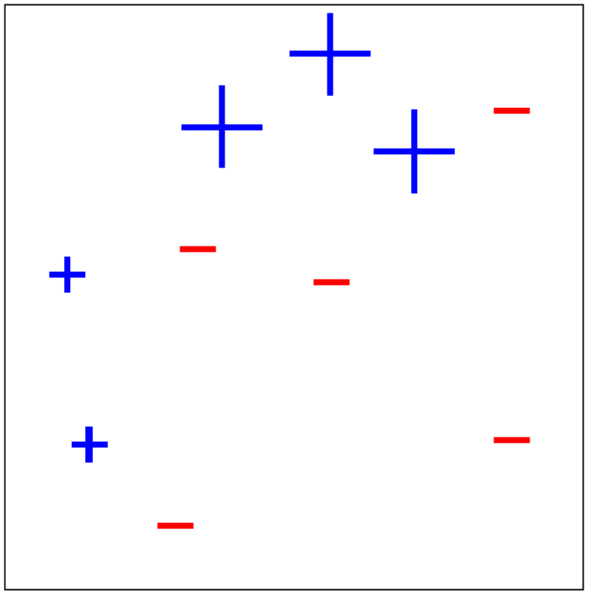


Round 1

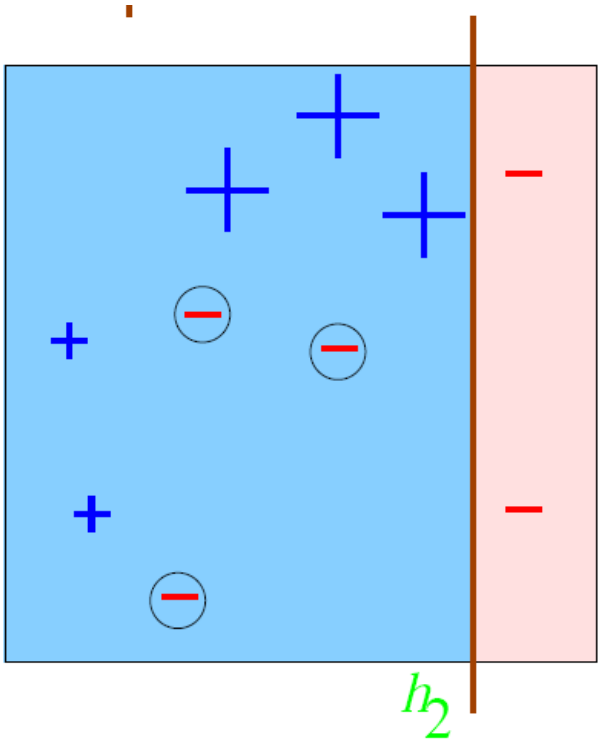


$\varepsilon_1 = 0.30$

$\alpha_1 = 0.42$

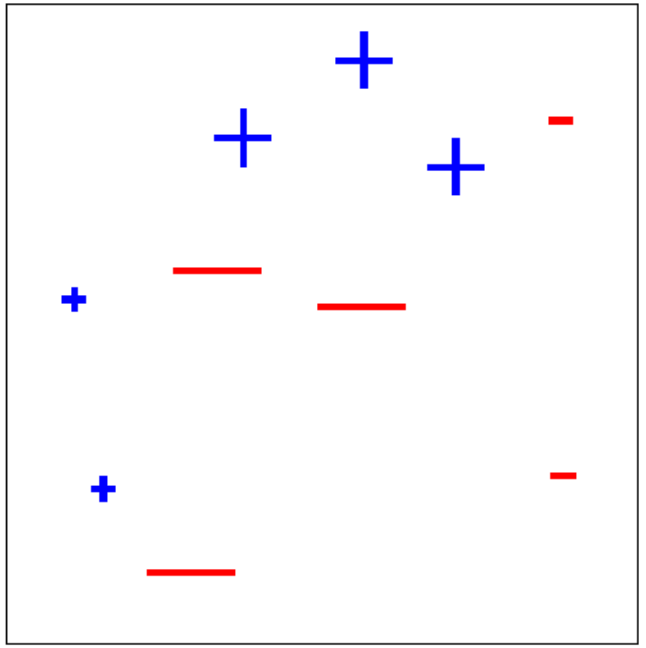


Round 2

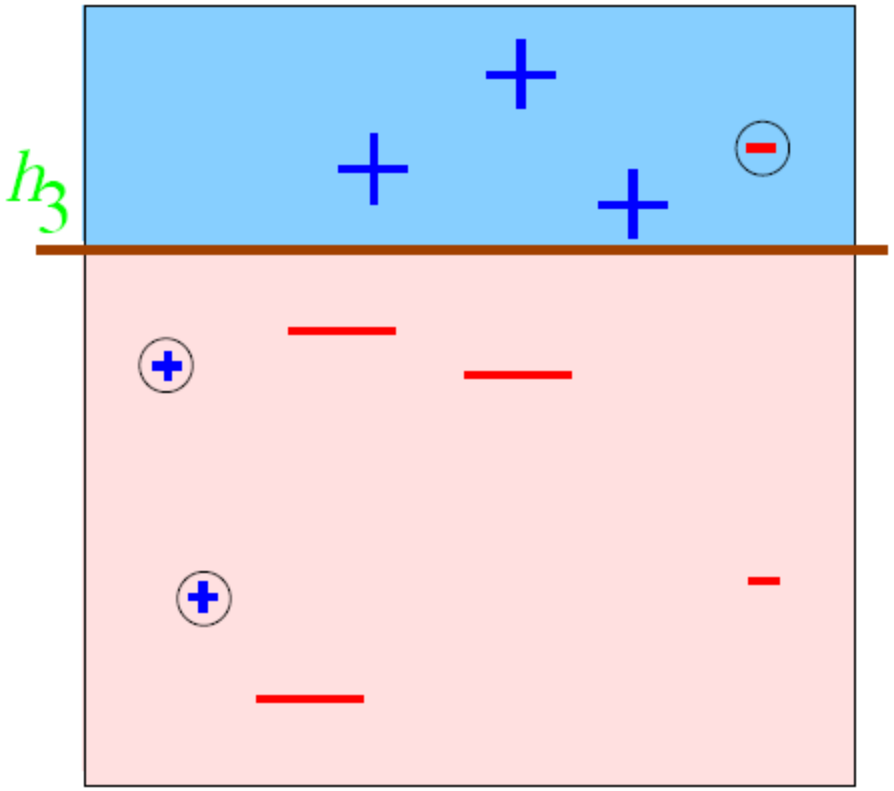


$\varepsilon_2 = 0.21$

$\alpha_2 = 0.65$



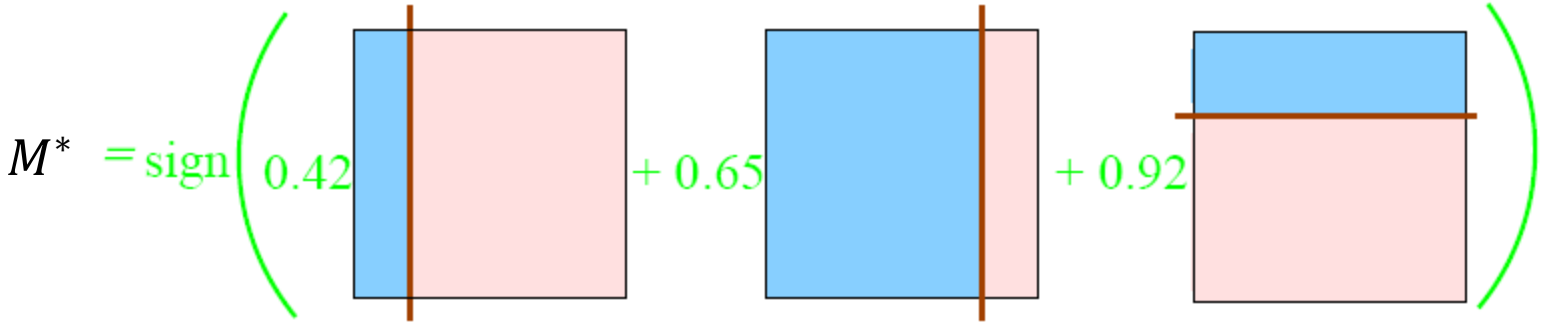
Round 3

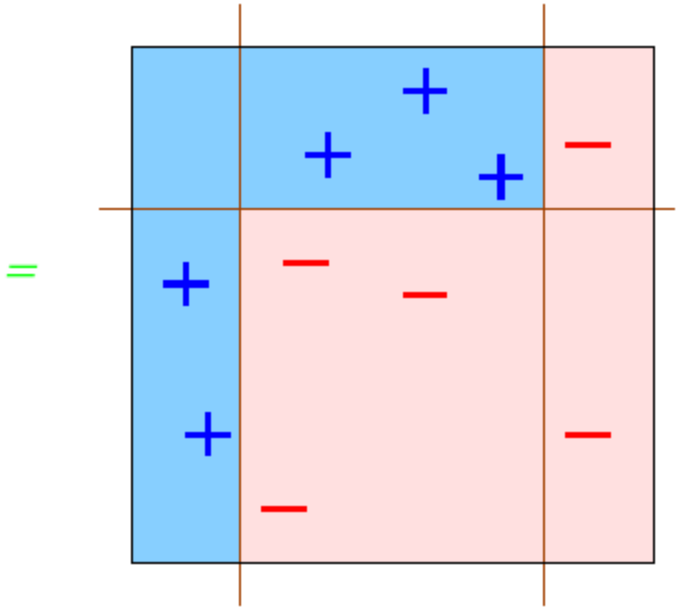


$\varepsilon_3 = 0.14$

$\alpha_3 = 0.92$

Final Model





Random Forest (Breiman 2001)

- Random Forest:
  - Each classifier in the ensemble is a *decision tree* classifier and is generated using a random selection of attributes at each node to determine the split
  - During classification, each tree votes and the most popular class is returned
- Two Methods to construct Random Forest:
  - Forest-RI (*random input selection*): Randomly select, at each node, F attributes as candidates for the split at the node. The CART methodology is used to grow the trees to maximum size
  - Forest-RC (*random linear combinations*): Creates new attributes (or features) that are a linear combination of the existing attributes (reduces the correlation between individual classifiers)
- Comparable in accuracy to Adaboost, but more robust to errors and outliers
- Insensitive to the number of attributes selected for consideration at each split, and faster than bagging or boosting

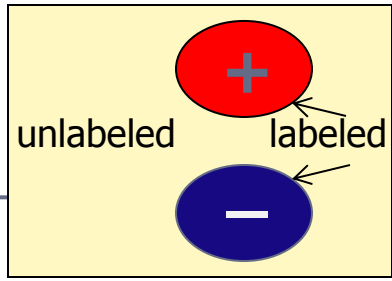
Classification of Class-Imbalanced Data Sets

- Class-imbalance problem: Rare positive example but numerous negative ones, e.g., medical diagnosis, fraud, oil-spill, fault, etc.
- Traditional methods assume a balanced distribution of classes and equal error costs: not suitable for class-imbalanced data
- Typical methods for imbalance data in 2-class classification:
  - **Oversampling:** re-sampling of data from positive class
  - **Under-sampling:** randomly eliminate tuples from negative class
  - **Threshold-moving:** moves the decision threshold, t, so that the rare class tuples are easier to classify, and hence, less chance of costly false negative errors
  - Ensemble techniques: Ensemble multiple classifiers introduced above
- Still difficult for class imbalance problem on multiclass tasks

Multiclass Classification

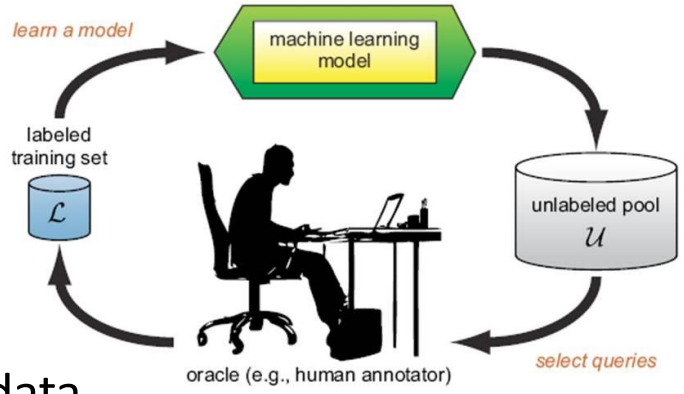
- Classification involving more than two classes (i.e., > 2 Classes)
- Method 1. **One-vs.-all** (OVA): Learn a classifier one at a time
  - Given m classes, train m classifiers: one for each class
  - Classifier j: treat tuples in class j as *positive* & all others as *negative*
  - To classify a tuple **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

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

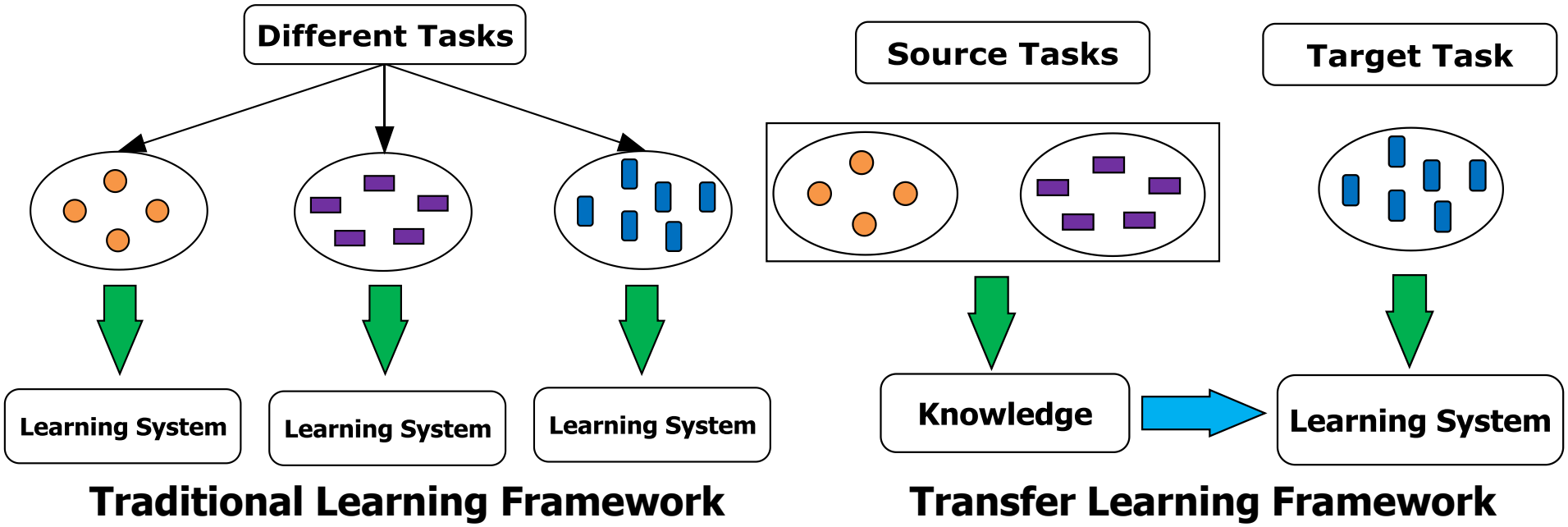
Active Learning



- 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

Matrix Data: Classification: Part 3

- SVM (Support Vector Machine)
- kNN (k Nearest Neighbor)
- Other Issues
- Summary 

- Support Vector Machine
  - Support vectors; Maximum marginal hyperplane; Linear separable; Linear inseparable; Kernel tricks
- Instance-Based Learning
  - Lazy learning vs. eager learning; K-nearest neighbor algorithm; Similarity / dissimilarity measures
- Other Topics
  - Ensemble; Class imbalanced data; multi-class classification; semi-supervised learning; active learning; transfer learning