Università degli Studi di Milano

Master Degree in Computer Science

Information Management course

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Data Mining:
Concepts and Techniques

(3rd ed.)

— Chapter 8, 9 —

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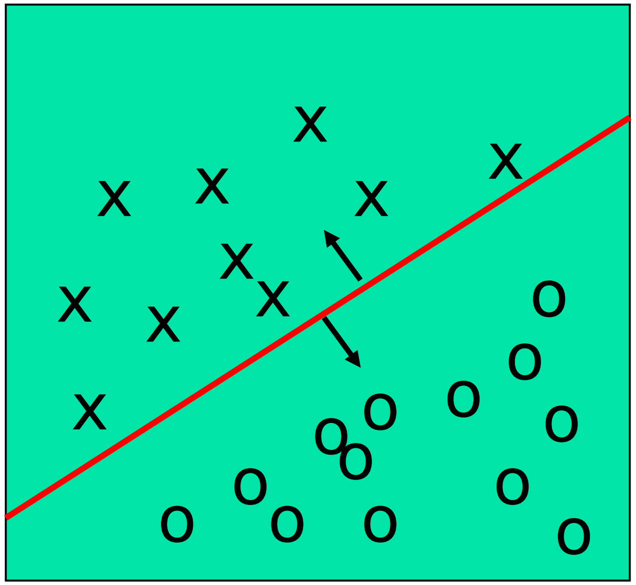
Classification methods

- Classification: Basic Concepts
- Decision Tree Induction
- Bayes Classification Methods
- Support Vector Machines
- Model Evaluation and Selection
- *Rule-Based Classification*
- *Techniques to Improve Classification Accuracy: Ensemble Methods*

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: $X \rightarrow Y$
- 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



Perceptron: finding a separating hyperplane

Hyperplane: $wx = b$

- Mathematical model:

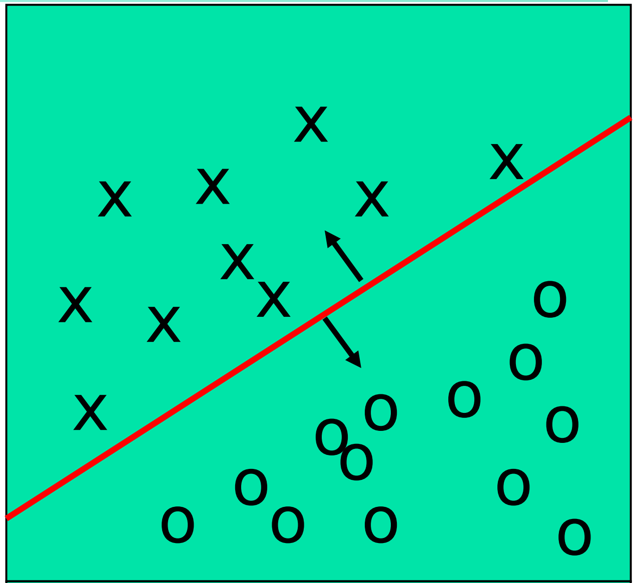
  find w

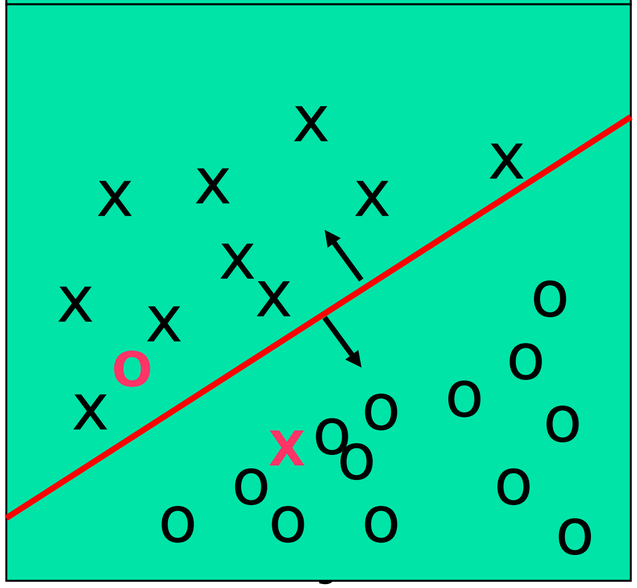
  s.t. $wx_k - b >= 0$ (forall k: $y_k = 1$)
  $wx_k - b < 0$ (forall k: $y_k = -1$)
  $|| w || = 1$

- Mathematical model:

  minimize $\sum_{i=1}^{m} d_k$

  s.t. $wx_k - b + d_k >= 0_k$ (forall k: $y_k = 1$)
  $wx_k - b - d_k < 0$ (forall k: $y_k = -1$)
  $|| w || = 1$





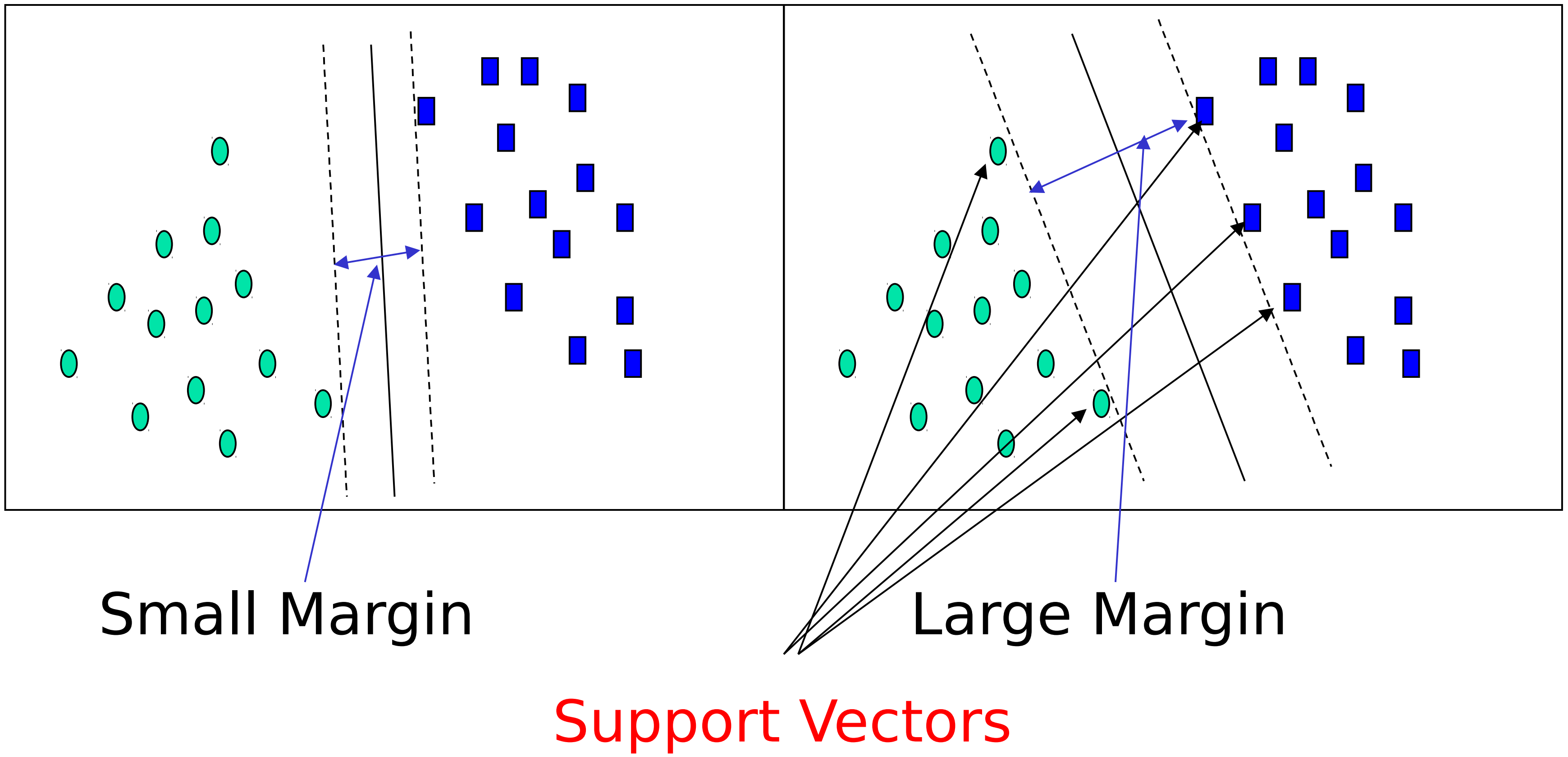
SVM—Support Vector Machines

- A classification method for both linear and nonlinear data
- Use a nonlinear mapping to map the original training data into a higher dimensional space
- In the new space, search for the linear optimal separating **hyperplane** (i.e. a “decision boundary”)
- Speedup by using **support vectors** (“essential” training tuples) and **margins** (defined by the support vectors)
- Theoretically, with an appropriate mapping to a sufficiently high dimensional space, data from two classes can always be separated by a hyperplane

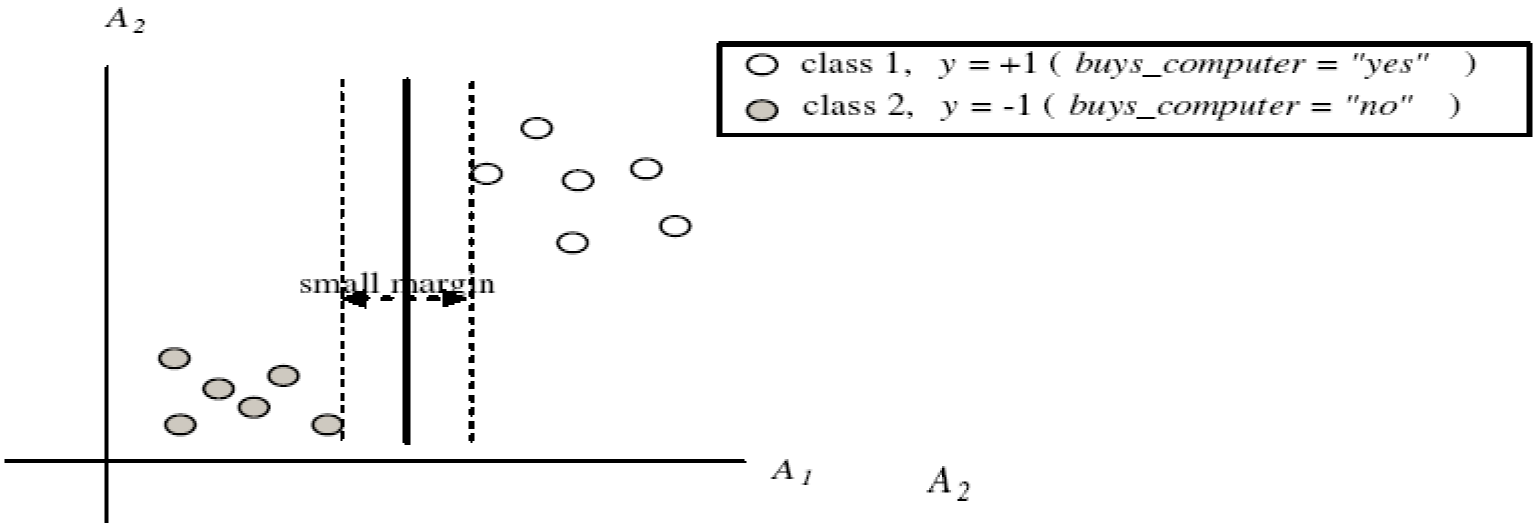
SVM—History and Applications

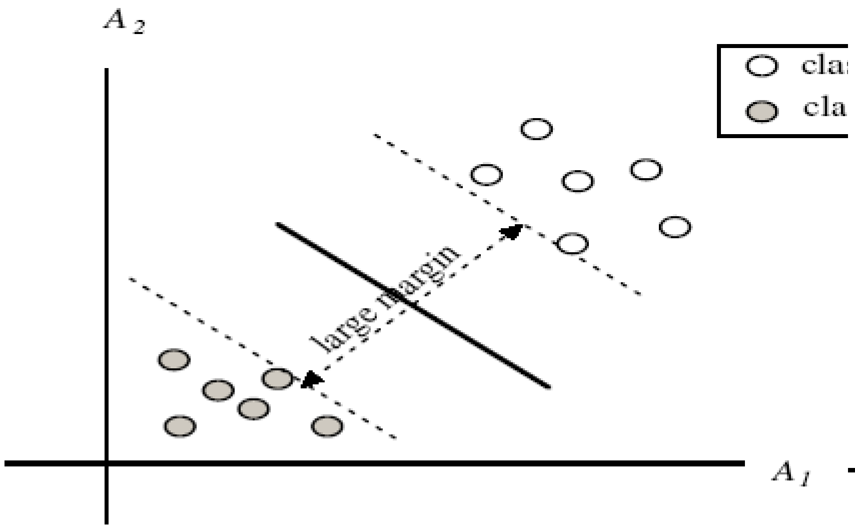
- Vapnik and colleagues (1992)—groundwork from Vapnik & Chervonenkis' statistical learning theory in 1960s
- Features: training can be slow but accuracy is high owing to their ability to model complex nonlinear decision boundaries (margin maximization)
- Used for: classification and numeric prediction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

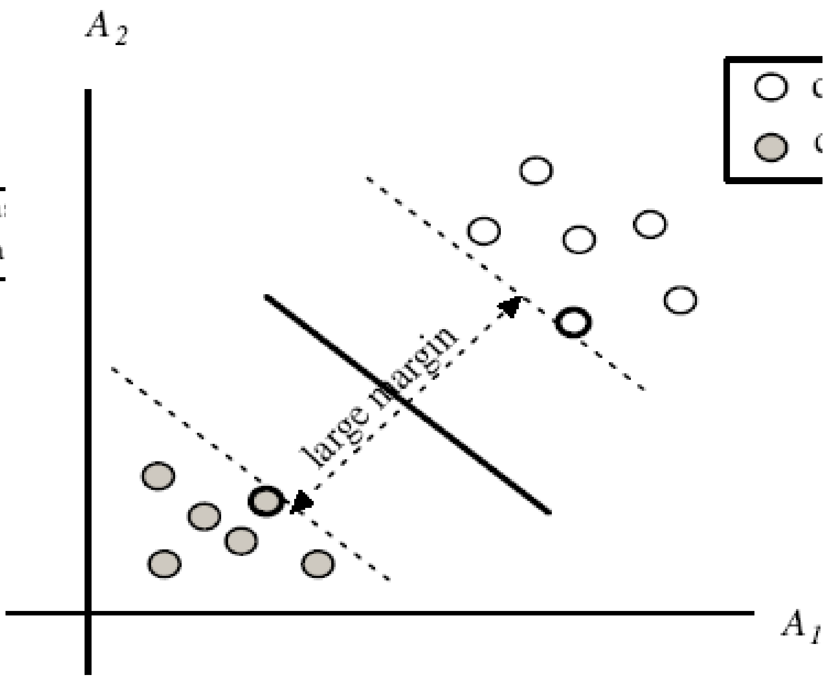
SVM—General Philosophy



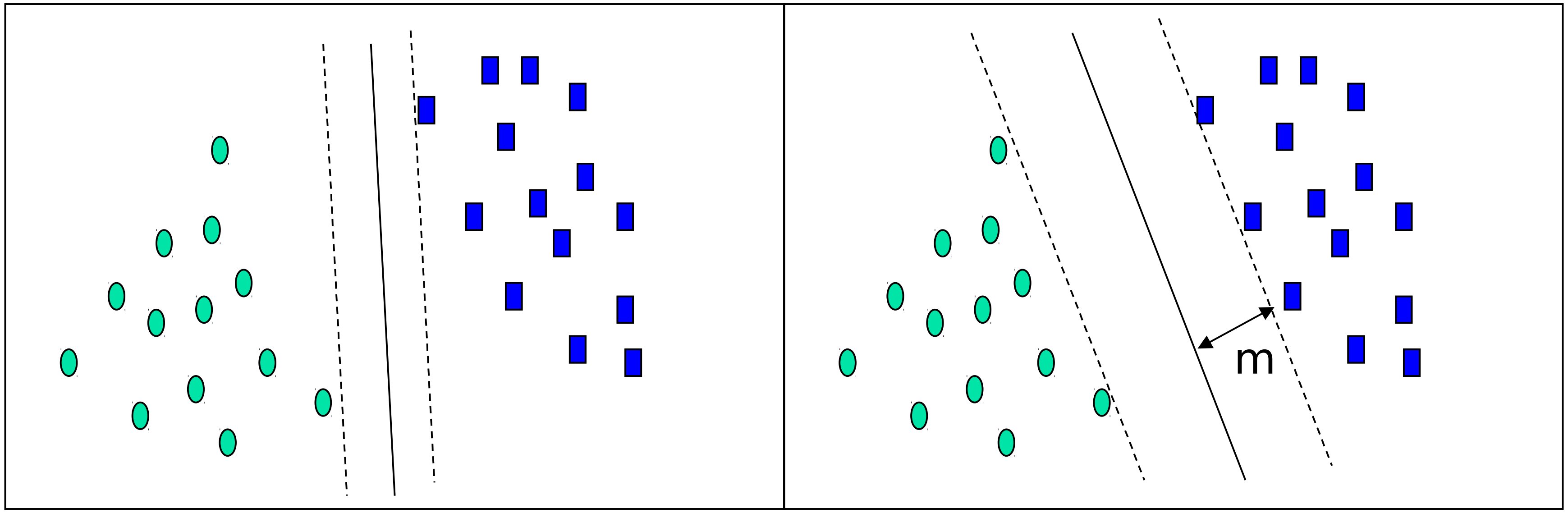
SVM—Margins and Support Vectors


A₂
class 1, y = +1 (buys_computer = "yes")
class 2, y = -1 (buys_computer = "no")
small margin
A₁





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 (<u>hyperplanes</u>) separating the two classes but we want to <u>find the best one</u> (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 hyperplane: **wx** = b

where **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 – A QP model

A hyperplane: **wx** = b

where **w** ={w$_1$, w$_2$, …, w$_n$} is a weight vector and b a scalar (bias)

- Separating margin: $D=\frac{2}{\|w\|}$ $\|w\|=\sqrt{\sum_{i=1}^{n}(w_i)^2}$
- Find an optimal hyperplane (linearly separable):

$$\min \frac{1}{2}\|w\|^2$$
$$s.t.\ y_k(w\,x_k-b)\geqslant 1\ \forall\, k=1\ldots m$$

- Find an optimal hyperplane (general):

$$\min \frac{1}{2}\|w\|^2+C\sum_{k=1}^{m} d_k$$
$$s.t.\ y_k(w\,x_k-b)+d_k\geqslant 1\ \forall\, k=1\ldots m$$
$$d_k\geqslant 0\ \forall\, k=1\ldots m$$

SVM – A QP model

- Find an optimal hyperplane (general):

$$min \frac{1}{2}\|w\|^2 + C\sum_{k=1}^{m} d_k$$
$$s.t.\ y_k(w x_k - b) + d_k \geqslant 1\ \forall k = 1 \ldots m$$
$$d_k \geqslant 0\ \forall k = 1 \ldots m$$

- Langrangean (dual) function:

$$L = min \frac{1}{2}\|w\|^2 + C\sum_{k=1}^{m} d_k - \sum_{k=1}^{m} \alpha_k (y_k(w x_k - b) + d_k - 1) - \sum_{k=1}^{m} \mu_k d_k$$

- Derivatives:

$$\frac{\partial L}{\partial w} = w - \sum_{k=1}^{m} \alpha_k y_k x_k$$
$$\frac{\partial L}{\partial b} = \sum_{k=1}^{m} \alpha_k y_k$$
$$\frac{\partial L}{\partial d_k} = C - \alpha_k - \mu_k$$

SVM – A QP model

- Langrangean (dual) function:

$$L = \min \frac{1}{2}\|w\|^2 + C\sum_{k=1}^{m} d_k - \sum_{k=1}^{m} \alpha_k \left(y_k (w x_k - b) + d_k - 1 \right) - \sum_{k=1}^{m} \mu_k d_k$$

- Optimality conditions:

$$\frac{\partial L}{\partial w} = w - \sum_{k=1}^{m} \alpha_k y_k x_k = 0$$

$$\frac{\partial L}{\partial b} = \sum_{k=1}^{m} \alpha_k y_k = 0$$

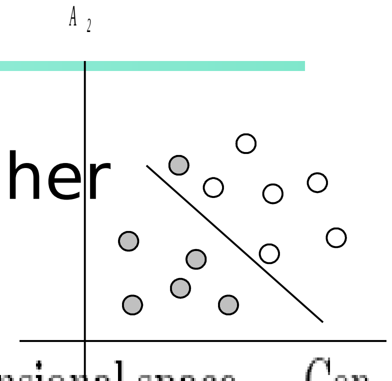
$$\frac{\partial L}{\partial d_k} = C - \alpha_k - \mu_k = 0$$

- Dual problem: … (blackboard discussion)
- Interpretation of KKT conditions: … (blackboard discussion)

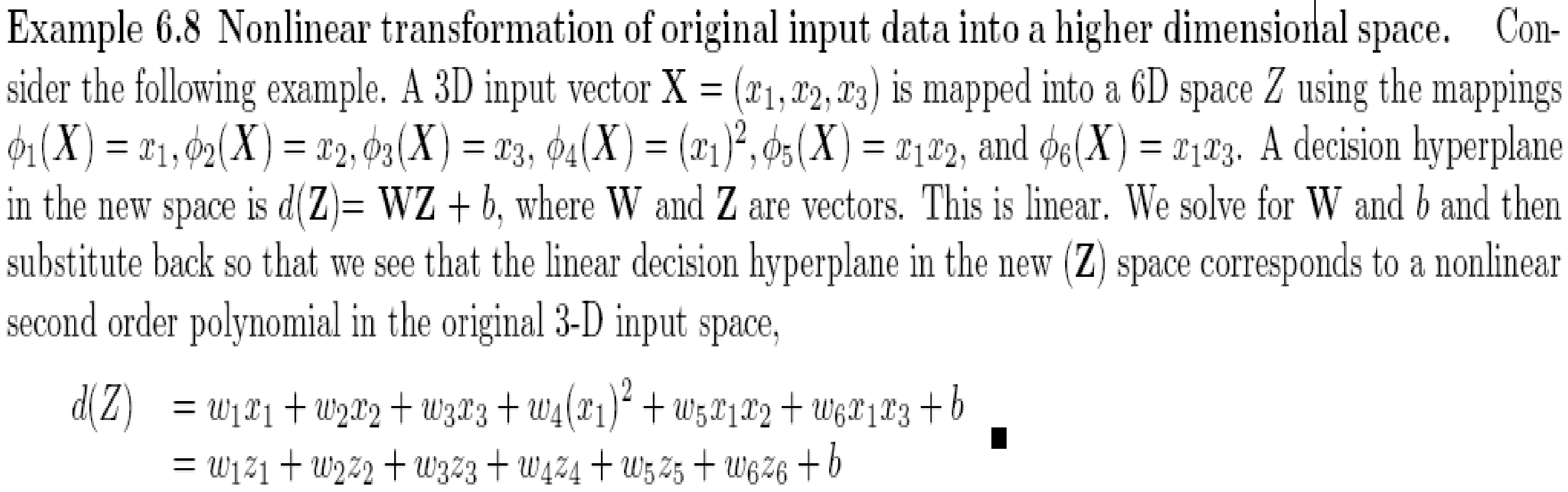
Why Is SVM Effective on High Dimensional Data?

- 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

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 $\phi_1(X) = x_1, \phi_2(X) = x_2, \phi_3(X) = x_3$, $\phi_4(X) = (x_1)^2, \phi_5(X) = x_1x_2$, and $\phi_6(X) = x_1x_3$. 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,

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

- Search for a linear separating hyperplane in the new space

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($\mathbf{X}_i$, $\mathbf{X}_j$) = Φ($\mathbf{X}_i$) Φ($\mathbf{X}_j$)
- Typical Kernel Functions

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

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

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

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

“geometric” Classifiers

- Advantages
  - Prediction accuracy is generally high
    - As compared to Bayesian methods – in general
  - Robust, works when training examples contain errors
  - Fast evaluation of the learned target function
    - Bayesian networks are normally slow
- Weaknesses
  - 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 vs. Neural Network

- **SVM**
  - Deterministic algorithm
  - Nice generalization properties
  - Hard to learn – learned in batch mode using quadratic programming techniques
  - Using kernels can learn very complex functions

- **Neural Network**
  - Nondeterministic algorithm
  - Generalizes well but doesn’t have strong mathematical foundation
  - Can easily be learned in incremental fashion
  - To learn complex functions—use multilayer perceptron (nontrivial)

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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Model Evaluation and Selection

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

Classifier Evaluation Metrics: Confusion Matrix

Confusion Matrix:

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

Example of Confusion Matrix:

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

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

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

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

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

  Accuracy = (TP + TN)/All
- **Error rate:** *1 – accuracy*, or

  Error rate = (FP + FN)/All

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

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

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

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

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

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

  - Perfect score is 1.0
- Inverse relationship between precision & recall
- ***F* measure (*F*$_1$ or *F*-score)**: harmonic mean of precision and recall,

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

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

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

Classifier Evaluation Metrics: Example

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

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

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

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

Evaluating Classifier Accuracy: Holdout & Cross-Validation Methods

- **Holdout method**
  - Given data is randomly partitioned into two independent sets
    - Training set (e.g., 2/3) for model construction
    - Test set (e.g., 1/3) for accuracy estimation
  - Random sampling: a variation of holdout
    - Repeat holdout k times
    - Accuracy = avg. of the accuracies obtained

- **Cross-validation** (*k*-fold, where k = 10 is most popular)
  - Randomly partition the data into *k mutually exclusive* subsets, each approximately equal size
  - At *i*-th iteration, use D_i as test set and others as training set
  - Leave-one-out: *k* -fold with *k* = # of tuples (small sized data)
  - Stratified cross-validation: folds are clustered so that class dist. in each class is approx. the same as that in the initial data

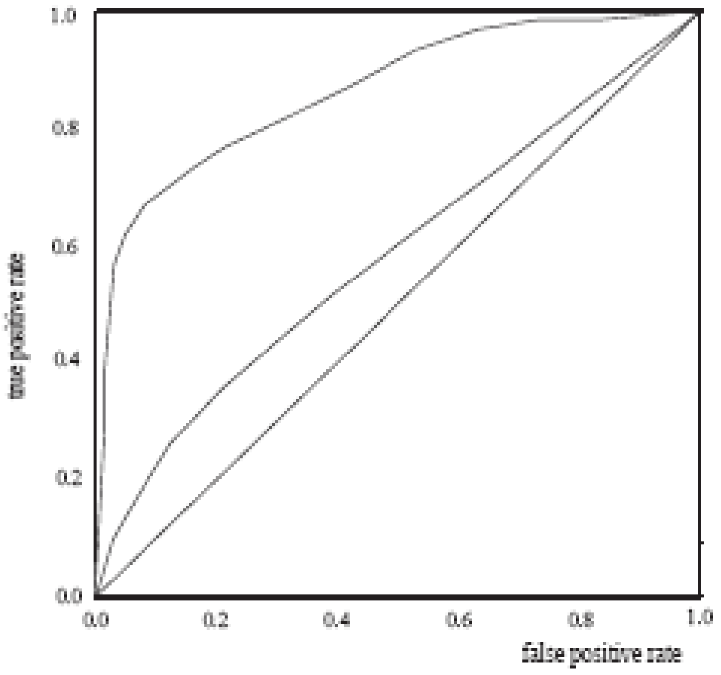
Evaluating Classifier Accuracy: Bootstrap

- **Bootstrap**
  - Works well with small data sets
  - Samples the given training tuples uniformly *with replacement*
    - i.e., each time a tuple is selected, it is equally likely to be selected again and re-added to the training set
- Several bootstrap methods, and a common one is **.632 boostrap**
  - A data set with *d* tuples is sampled *d* times, with replacement, resulting in a training set of *d* samples. The data tuples that did not make it into the training set end up forming the test set. About 63.2% of the original data end up in the bootstrap, and the remaining 36.8% form the test set (since $(1 – 1/d)^d \approx e^{-1} = 0.368$)
  - Repeat the sampling procedure *k* times, overall accuracy of the model:

$$Acc(M) = \frac{1}{k}\sum_{i=1}^{k}(0.632 \times Acc(M_i)_{test\_set} + 0.368 \times Acc(M_i)_{train\_set})$$

Model Selection: ROC Curves

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



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

Issues Affecting Model Selection

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

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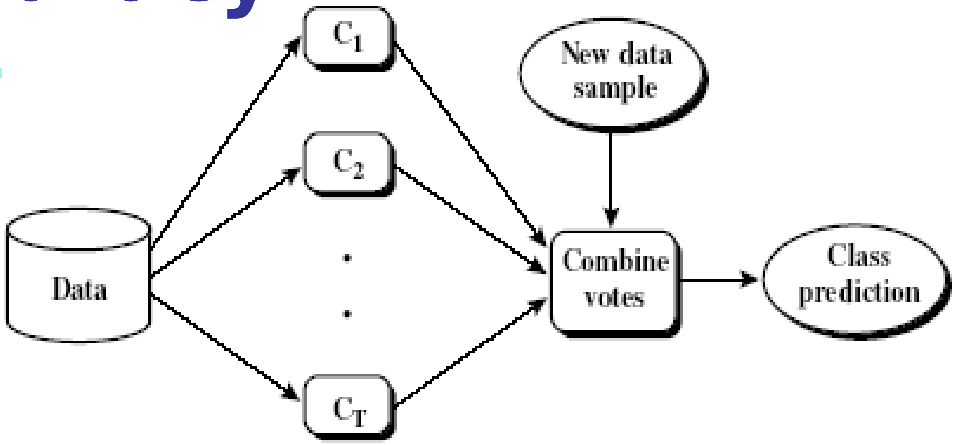
Ensemble Methods: Increasing the Accuracy



- 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
  - Ensemble: combining a set of heterogeneous 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
- Accuracy
  - Often significantly better than a single classifier derived from D
  - For noise data: not considerably worse, more robust
  - Proved improved accuracy in prediction

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_i is learned, the weights are updated to allow the subsequent classifier, M_{i+1}, to **pay more attention to the training tuples that were misclassified** by M_i
  - 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 i,
  - Tuples from D are sampled (with replacement) to form a training set D_i of the same size
  - Each tuple's chance of being selected is based on its weight
  - A classification model M_i is derived from D_i
  - Its error rate is calculated using D_i as a test set
  - If a tuple is misclassified, its weight is increased, o.w. it is decreased
- Error rate: err($\mathbf{X_j}$) is the misclassification error of tuple $\mathbf{X_j}$. Classifier M_i error rate is the sum of the weights of the misclassified tuples:

$$error(M_i) = \sum_j^d w_j \times err(X_j)$$

- The weight of classifier M_i's vote is $\log \frac{1-error(M_i)}{error(M_i)}$

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