Chapter 9. Advanced Classification: SVM

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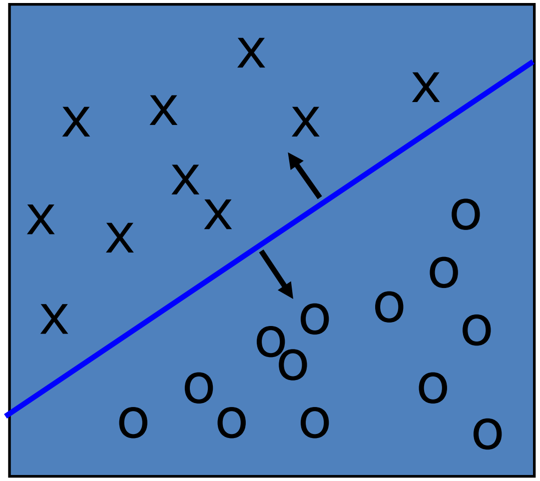
Introduction to Data Mining

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

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

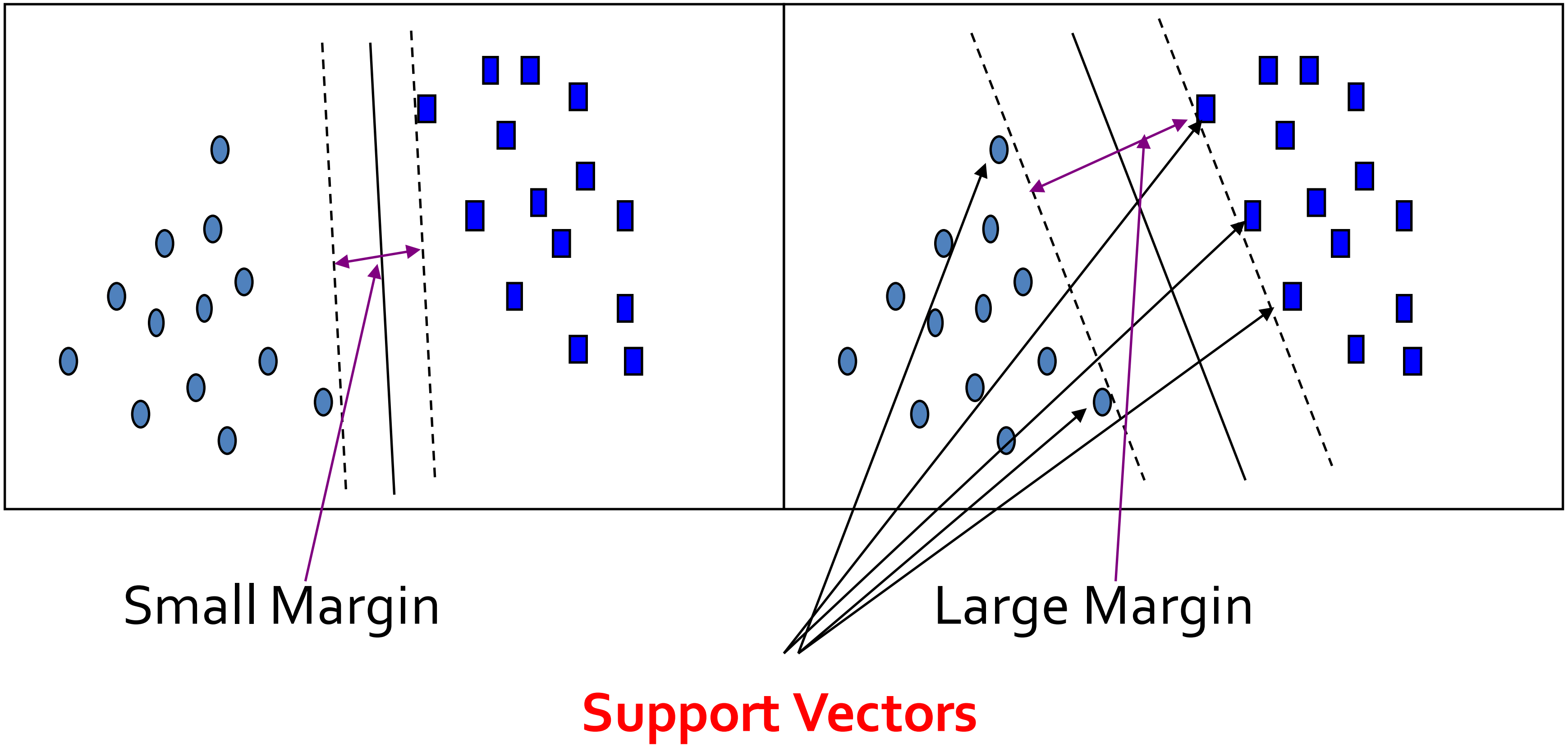
SVM: Support Vector Machines

- A relatively new classification method for both <u>linear and nonlinear</u> data
- 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

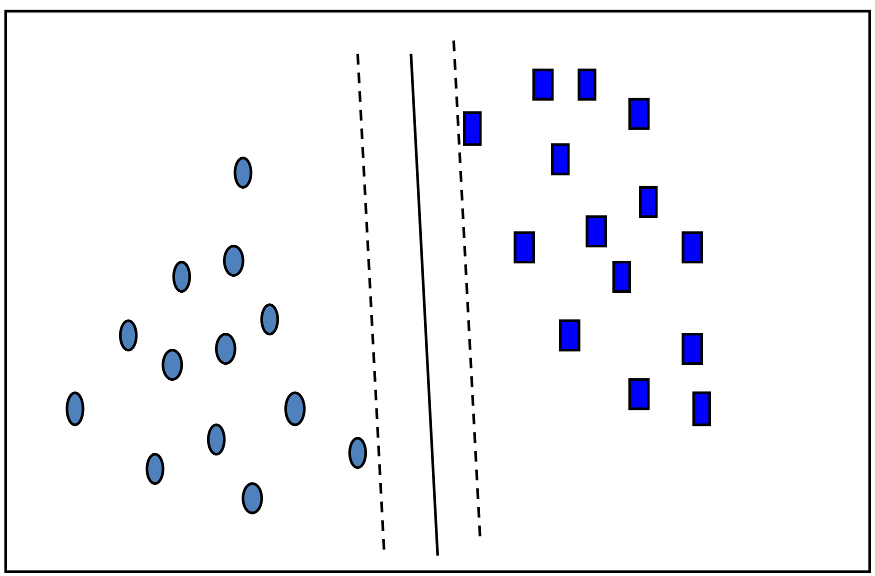


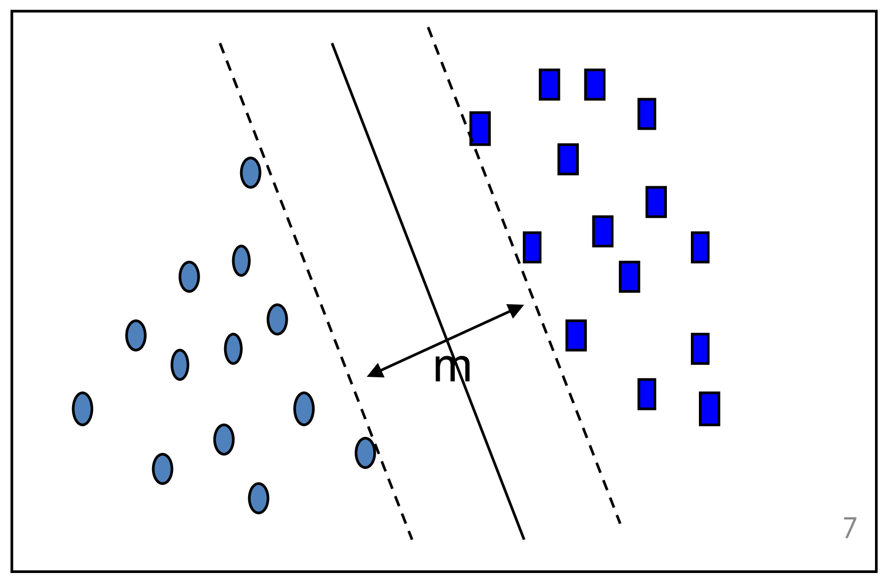
SVM: When Data Is Linearly Separable

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 separating hyperplane can be written as

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

where **W**={w_1, w_2, …, w_n} is a weight vector and b a scalar (bias)

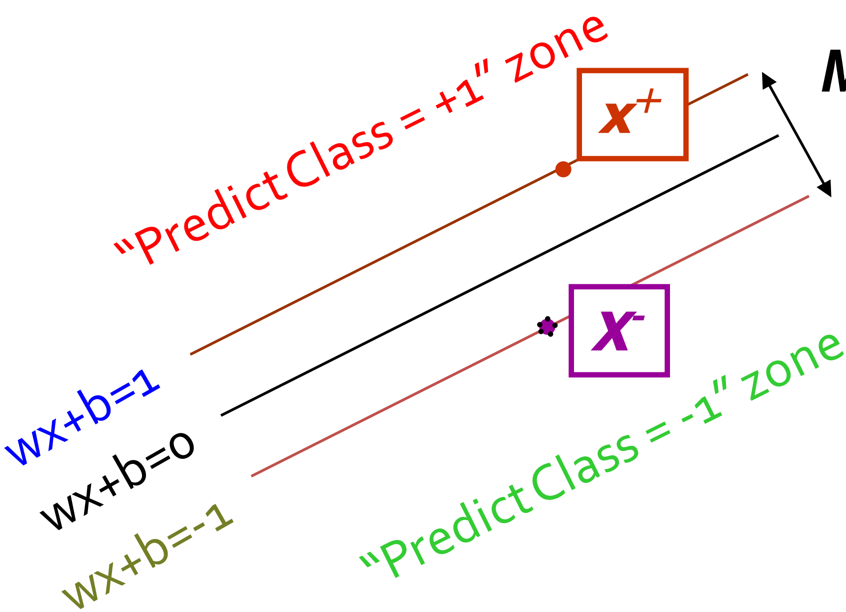
- For 2-D it can be written as: $w_0 + w_1 x_1 + w_2 x_2 = 0$
- The hyperplane defining the sides of the margin:

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

$$H_2: w_0 + w_1 x_1 + w_2 x_2 \leq -1 \text{ for } y_i = -1$$

- 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

Optimization: Maximize Margin Width



M=Margin Width

H_1: $wx_i + b \geq 1$ for $y_i = +1$

H_2: $wx_i + b \leq -1$ for $y_i = -1$

$\rightarrow$ $y_i\,(wx_i + b) \geq 1$ for all i

$$\max \quad M = \frac{(x^+ - x^-)\cdot w}{|w|} = \frac{2}{|w|}$$

$$\text{same as min} \quad \frac{1}{2} w^t w$$

What we know:

- $\boldsymbol{w} \,.\, \boldsymbol{x}^+ + b = +1$
- $\boldsymbol{w} \,.\, \boldsymbol{x}^- + b = -1$
- $\boldsymbol{w} \,.\, (\boldsymbol{x}^+ - \boldsymbol{x}^-) = 2$

Quadratic optimization problem:

$$\min \; \Phi(w) = \frac{1}{2} w^t w$$

$$\text{s.t.} \quad y_i(wx_i + b) \geq 1 \text{ for all i}$$

Solving the Optimization Problem

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

Primal	Dual
Find **w** and b such that $\Phi(\mathbf{w}) = \frac{1}{2}\mathbf{w}^T\mathbf{w}$ is minimized; and for all $\{(\mathbf{x_i}, y_i)\}$: $y_i(\mathbf{w}^T\mathbf{x_i} + b) \geq 1$	Find $\alpha_1 \ldots \alpha_N$ such that $\mathbf{Q}(\boldsymbol{\alpha}) = \sum\alpha_i - \frac{1}{2}\sum\sum\alpha_i\alpha_j y_i y_j \mathbf{x_i}^T\mathbf{x_j}$ is maximized and (1) $\sum\alpha_i y_i = 0$ (2) $\alpha_i \geq 0$ for all α_i

LinearSVMs

- The classifier is a separating hyperplane.
- Most “important” training points are support vectors; they define the hyperplane.
- Quadratic optimization algorithms can identify which training points 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 dot products:

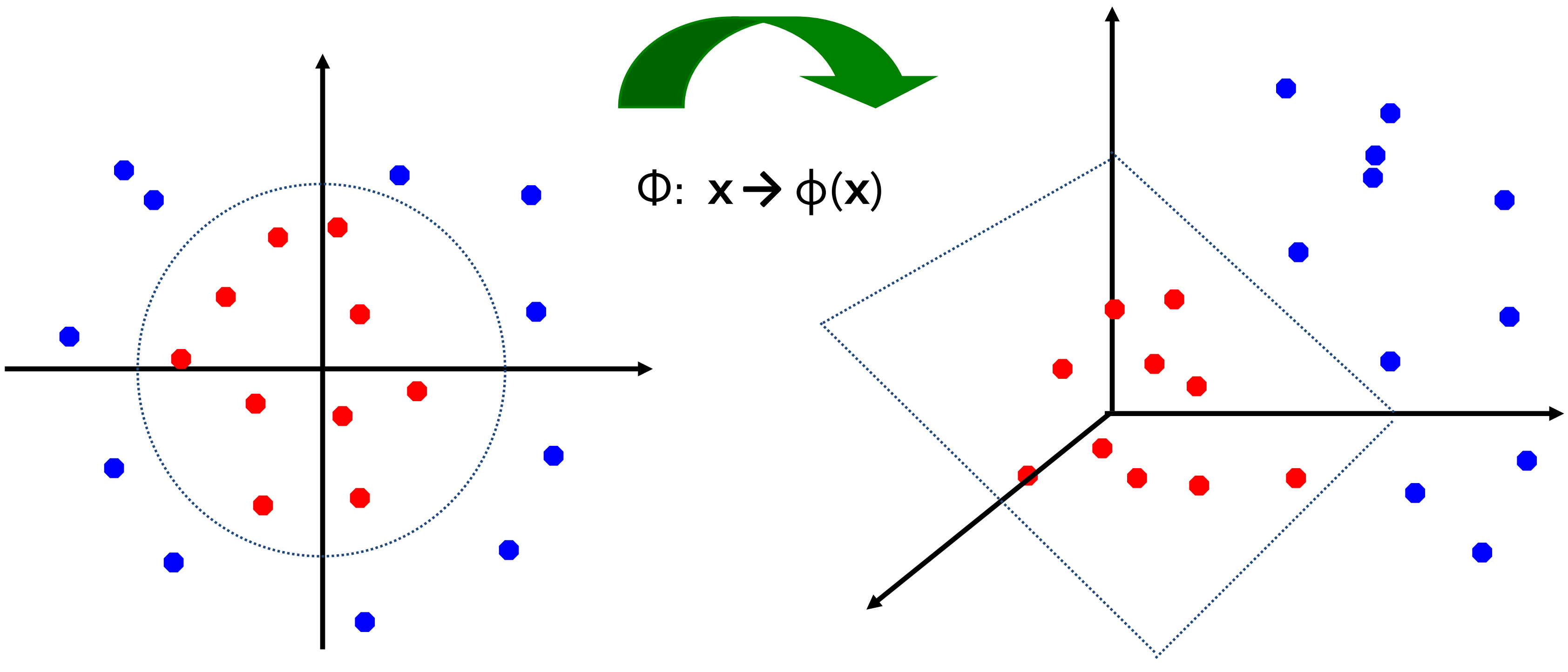
> Find $\alpha_1 \ldots \alpha_N$ such that
> $Q(\alpha) = \Sigma\alpha_i - \frac{1}{2}\Sigma\Sigma\alpha_i\alpha_j y_i y_j x_i^T x_j$ is maximized and
> (1) $\Sigma\alpha_i y_i = 0$
> (2) $0 \le \alpha_i \le C$ for all α_i

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
- If all other training examples are removed and the training is repeated, the same separating hyperplane would be found

Non-linear SVMs: Feature Spaces

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



The "Kernel Trick"

- The classifier relies on dot product between vectors $K(x_i,x_j)=x_i^Tx_j$
- If every data point is mapped into high-dimensional space via some transformation Φ: $x \rightarrow \phi(x)$, the dot product becomes:

$$K(x_i,x_j)= \phi(x_i)^T\phi(x_j)$$

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

2-dimensional vectors $x=[x_1\ \ x_2]$; let $K(x_i,x_j)=(1 + x_i^Tx_j)^2$,

Need to show that $K(x_i,x_j)= \phi(x_i)^T\phi(x_j)$:

$$K(x_i,x_j)=(1 + x_i^Tx_j)^2,$$

$$= 1+ x_{i1}^2x_{j1}^2 + 2\, x_{i1}x_{j1}\, x_{i2}x_{j2}+ x_{i2}^2x_{j2}^2 + 2x_{i1}x_{j1} + 2x_{i2}x_{j2}$$

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

$$= \phi(x_i)^T\phi(x_j), \quad \text{where } \phi(x) = [1\ \ x_1^2\ \ \sqrt{2}\, x_1x_2\ \ x_2^2\ \ \sqrt{2}x_1\ \ \sqrt{2}x_2]$$

What Functions are Kernels?

- For some functions $K(x_i,x_j)$ checking that

  $K(x_i,x_j)= \phi(x_i)^T\phi(x_j)$ can be cumbersome.
- Mercer's theorem:

  Every semi-positive definite symmetric function is a kernel
- Semi-positive definite symmetric functions correspond to a semi-positive definite symmetric Gram matrix:

K=

$K(\mathbf{x_1},\mathbf{x_1})$	$K(\mathbf{x_1},\mathbf{x_2})$	$K(\mathbf{x_1},\mathbf{x_3})$	…	$K(\mathbf{x_1},\mathbf{x_N})$
$K(\mathbf{x_2},\mathbf{x_1})$	$K(\mathbf{x_2},\mathbf{x_2})$	$K(\mathbf{x_2},\mathbf{x_3})$		$K(\mathbf{x_2},\mathbf{x_N})$
…	…	…	…	…
$K(\mathbf{x_N},\mathbf{x_1})$	$K(\mathbf{x_N},\mathbf{x_2})$	$K(\mathbf{x_N},\mathbf{x_3})$	…	$K(\mathbf{x_N},\mathbf{x_N})$

Kernel Functions for Nonlinear Classification

- Instead of computing the dot product on the transformed data, it is mathematically 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

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

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

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

Non-linear SVMs: Optimization

- Dual problem formulation:

> Find $\alpha_1 \ldots \alpha_N$ such that
> $Q(\alpha) = \Sigma\alpha_i - \frac{1}{2}\Sigma\Sigma\alpha_i\alpha_j y_i y_j K(x_i, x_j)$ is maximized and
> (1) $\Sigma\alpha_i y_i = 0$
> (2) $\alpha_i \geq 0$ for all α_i

- The solution is:

$$f(x) = \Sigma\alpha_i y_i K(x_i, x_j) + b$$

- Optimization techniques for finding α_i's remain the same!

SVM Applications

- SVM has been used successfully in many real-world problems
  - Text (and hypertext) categorization
  - Image classification
  - Bioinformatics (Protein classification, Cancer classification)
  - Hand-written character recognition

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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