

Support Vector Machine

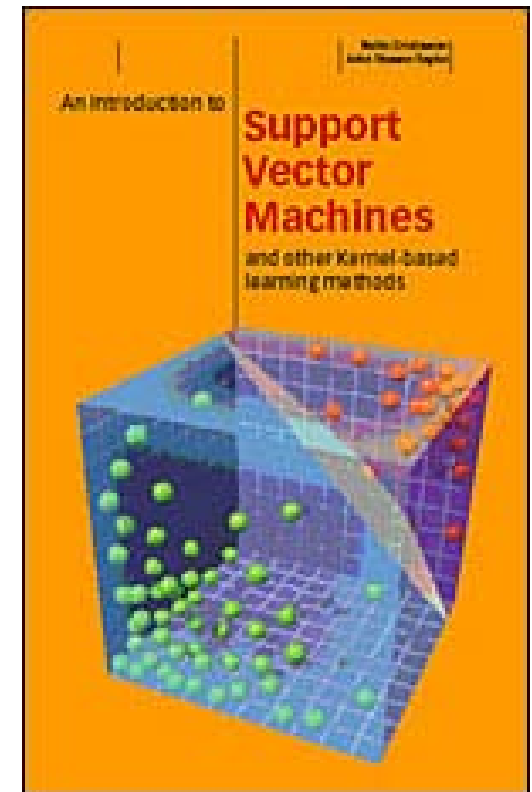
Definition

- ‘Support Vector Machine is a system for efficiently training **linear learning machines** in **kernel-induced feature spaces**, while respecting the insights of **generalisation** theory and exploiting **optimisation** theory.’

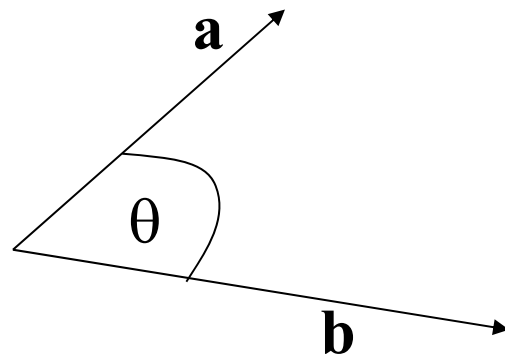
- **AN INTRODUCTION TO SUPPORT VECTOR MACHINES** (and other kernel-based learning methods)

N. Cristianini and J. Shawe-Taylor
Cambridge University Press
2000 ISBN: 0 521 78019 5

- Kernel Methods for Pattern Analysis
John Shawe-Taylor & Nello Cristianini
Cambridge University Press, 2004



The Scalar Product



$$\mathbf{a} \cdot \mathbf{b} = |\mathbf{a}| |\mathbf{b}| \cos \theta$$

The scalar or dot product is, in some sense, a measure of **Similarity**

Decision Function for binary classification

$$f(x) \in \mathbf{R}$$

$$f(x_i) \geq 0 \Rightarrow y_i = 1$$

$$f(x_i) < 0 \Rightarrow y_i = -1$$

Support Vector Machines

- SVMs pick **best** separating hyperplane according to some criterion
 - e.g. maximum margin
- Training process is an **optimisation**
- Training set is effectively reduced to a relatively small number of **support vectors**

Feature Spaces

- We may separate data by mapping to a higher-dimensional feature space
 - The feature space may even have an infinite number of dimensions!
- We need not **explicitly** construct the new feature space

Kernels

- We may use Kernel functions to **implicitly** map to a new feature space
- Kernel fn:

$$K(\mathbf{x}_1, \mathbf{x}_2) \in \mathbf{R}$$

- Kernel must be equivalent to an **inner product** in some feature space

Example Kernels

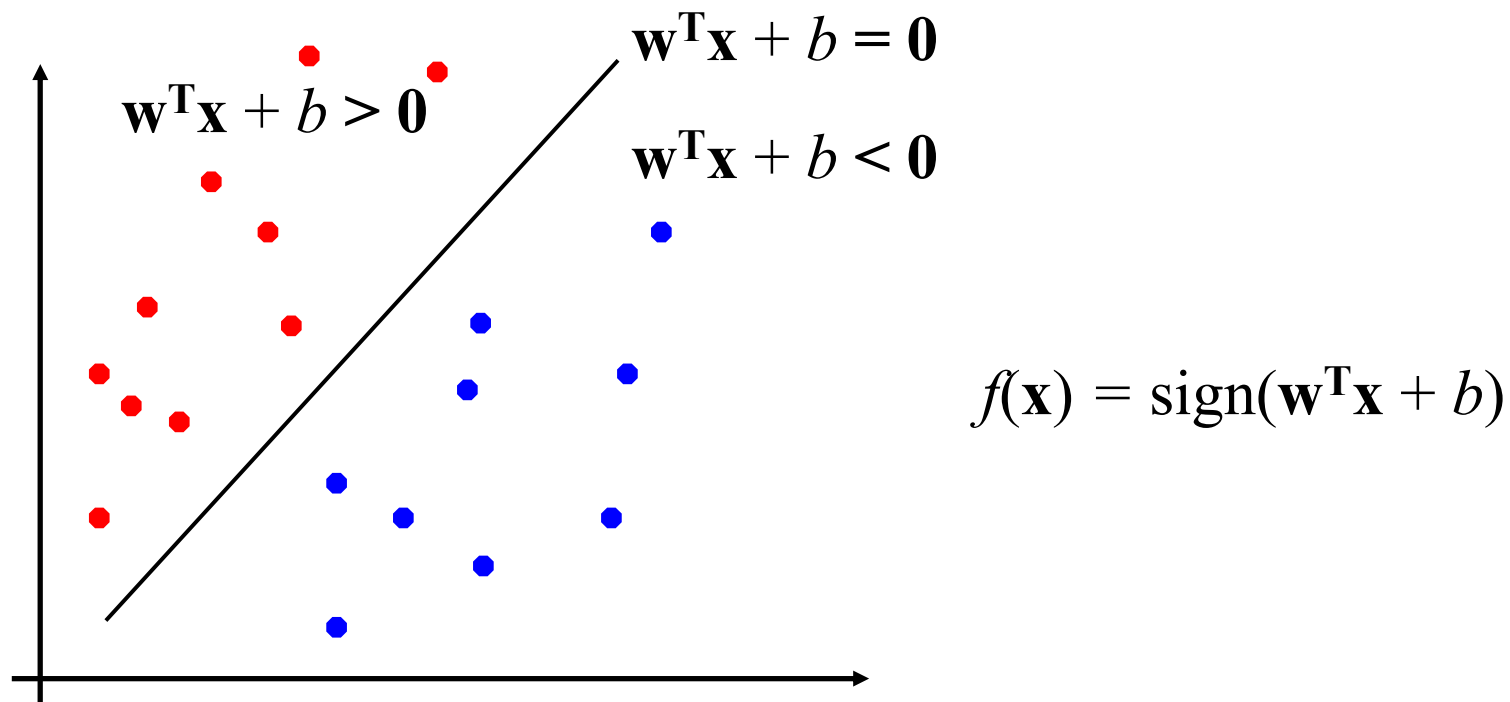
Linear: $\langle \mathbf{x} \cdot \mathbf{z} \rangle$

Polynomial: $P(\langle \mathbf{x} \cdot \mathbf{z} \rangle)$

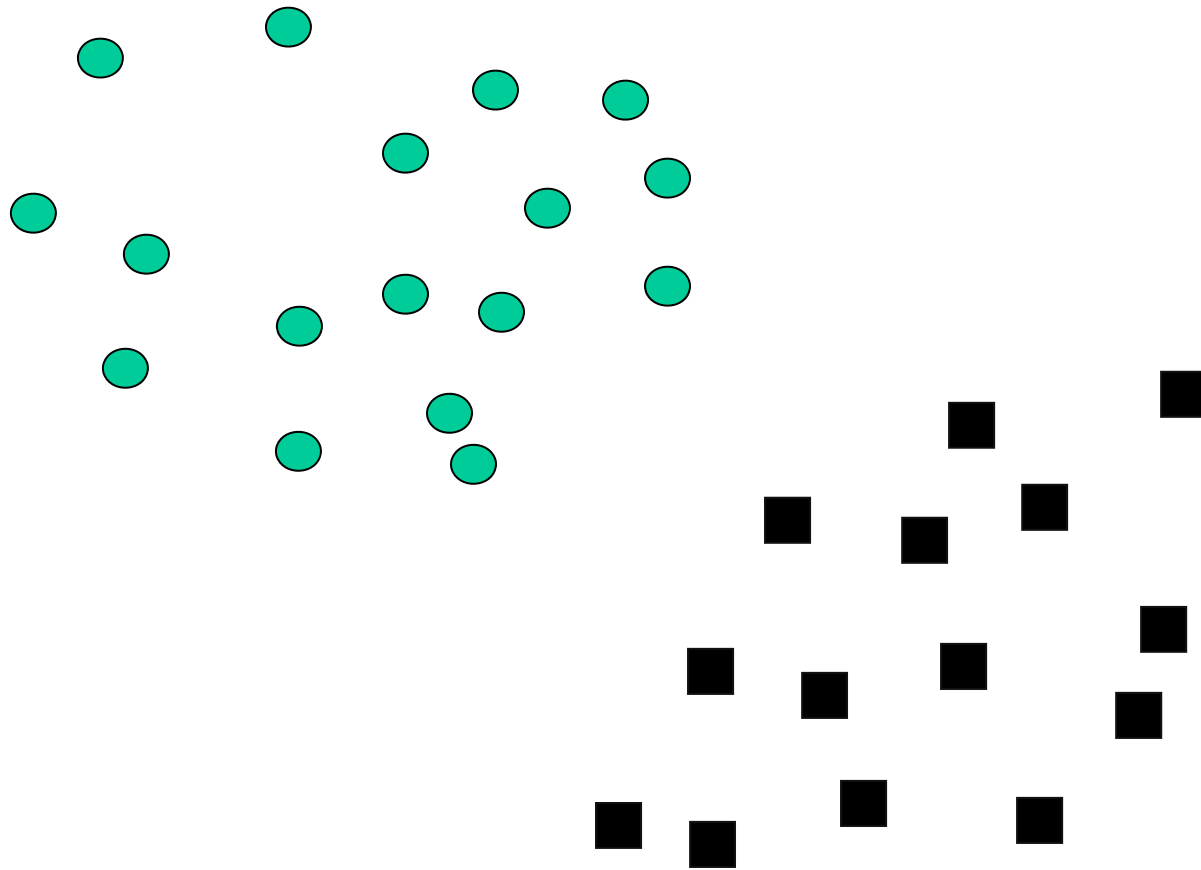
Gaussian: $\exp\left(-\|\mathbf{x} - \mathbf{z}\|^2 / \sigma^2\right)$

Perceptron Revisited: Linear Separators

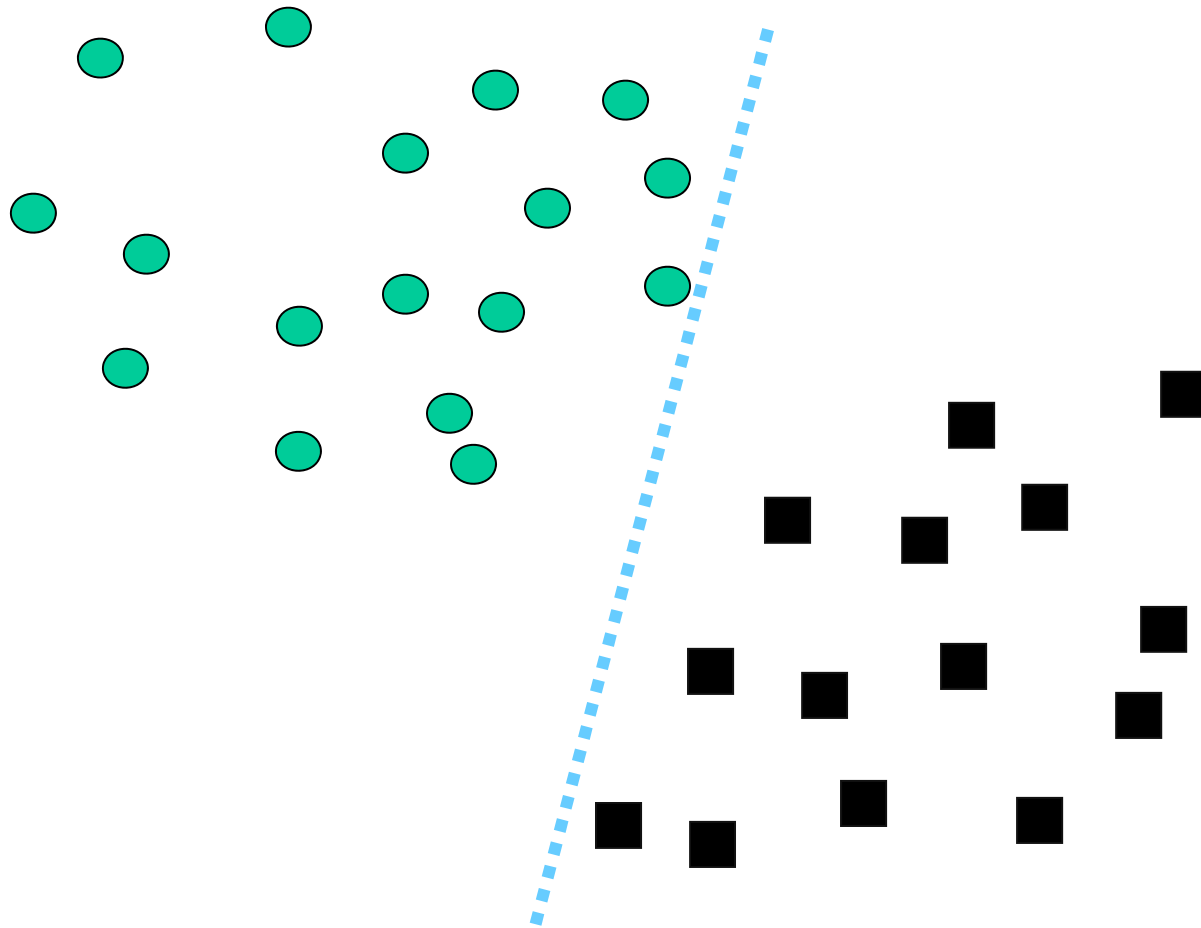
- Binary classification can be viewed as the task of separating classes in feature space:



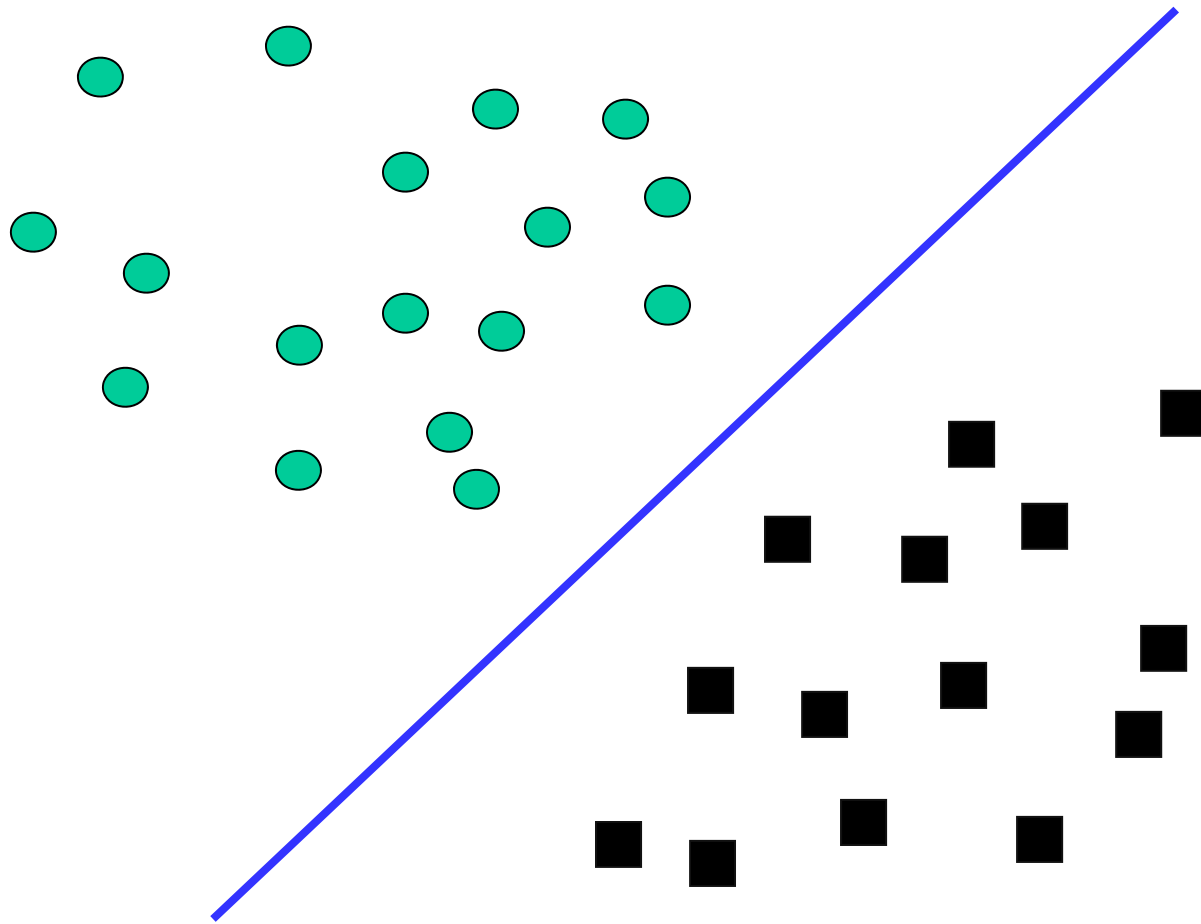
Which of the linear separators is optimal?



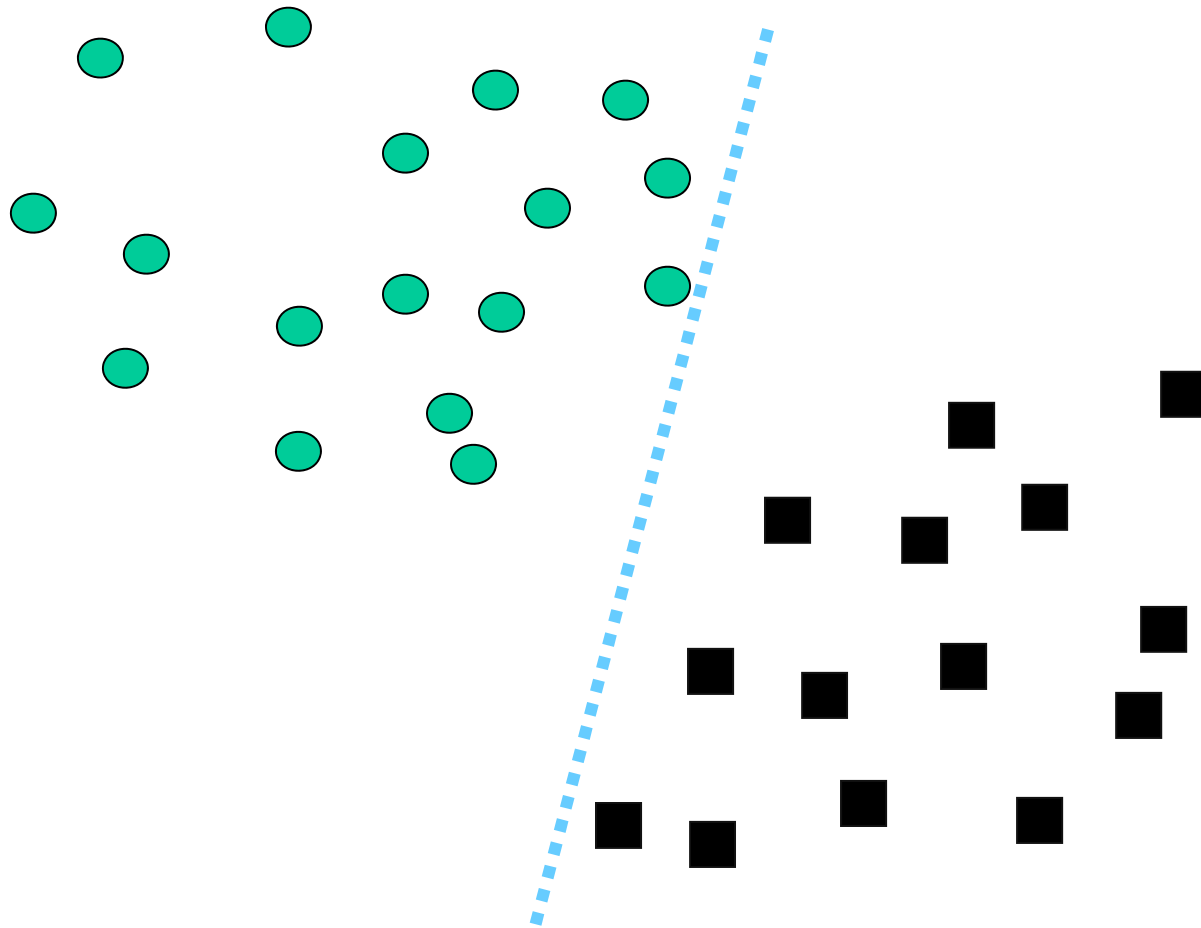
Best Linear Separator?



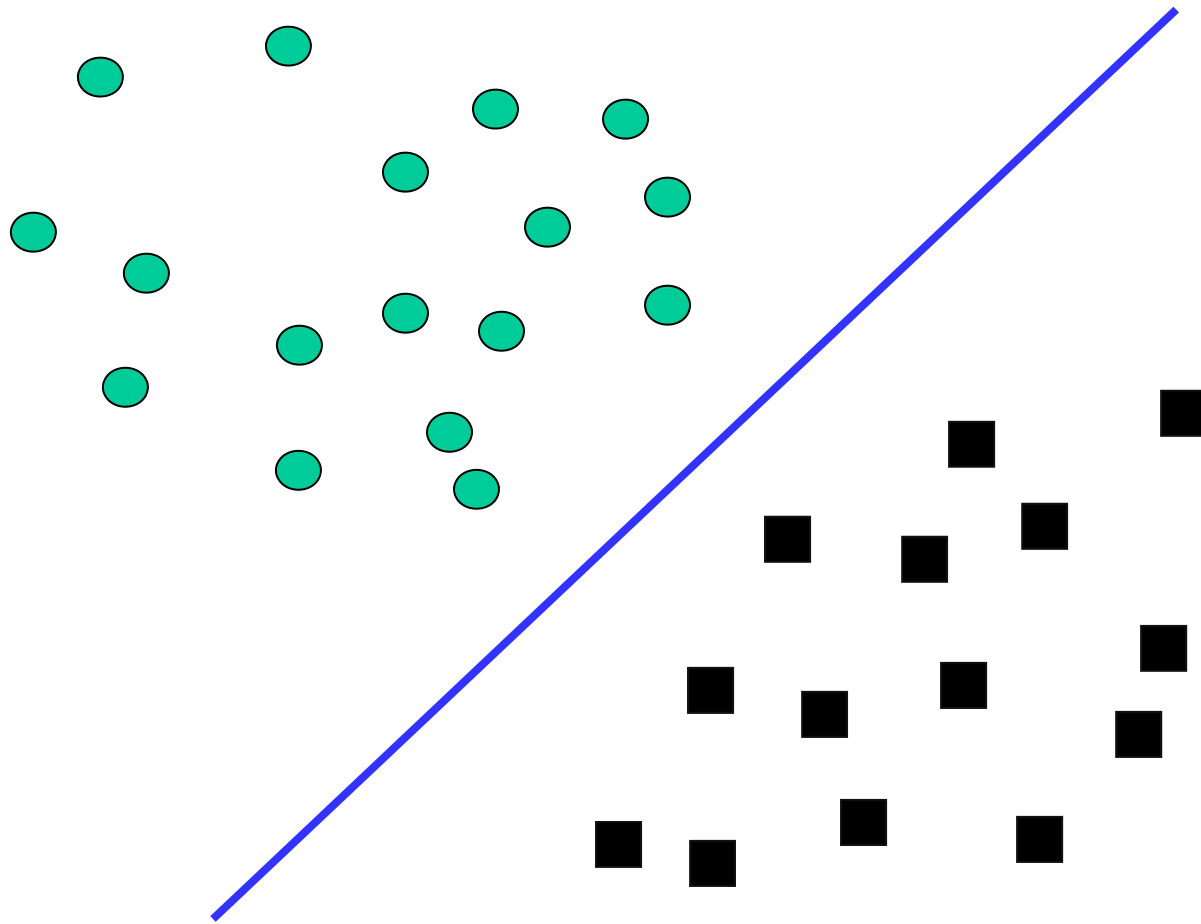
Best Linear Separator?



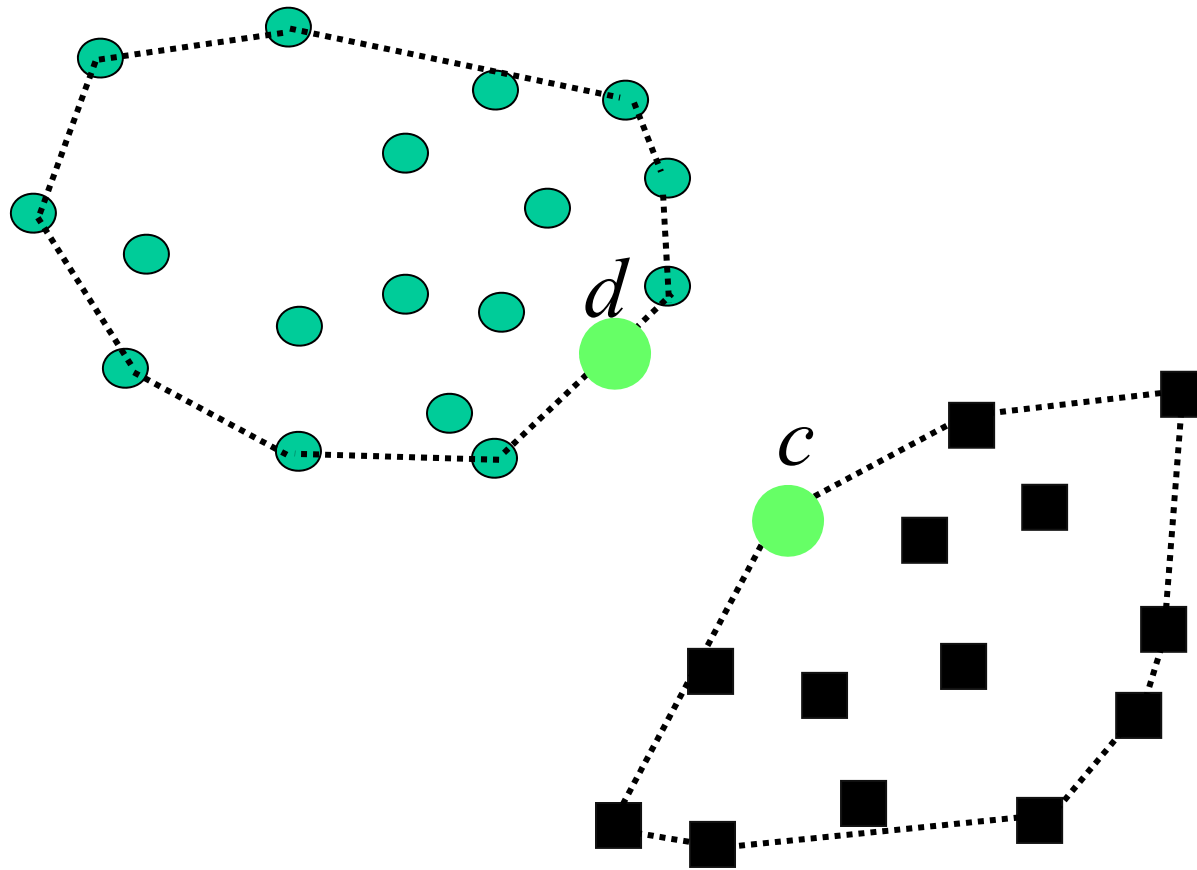
Best Linear Separator?



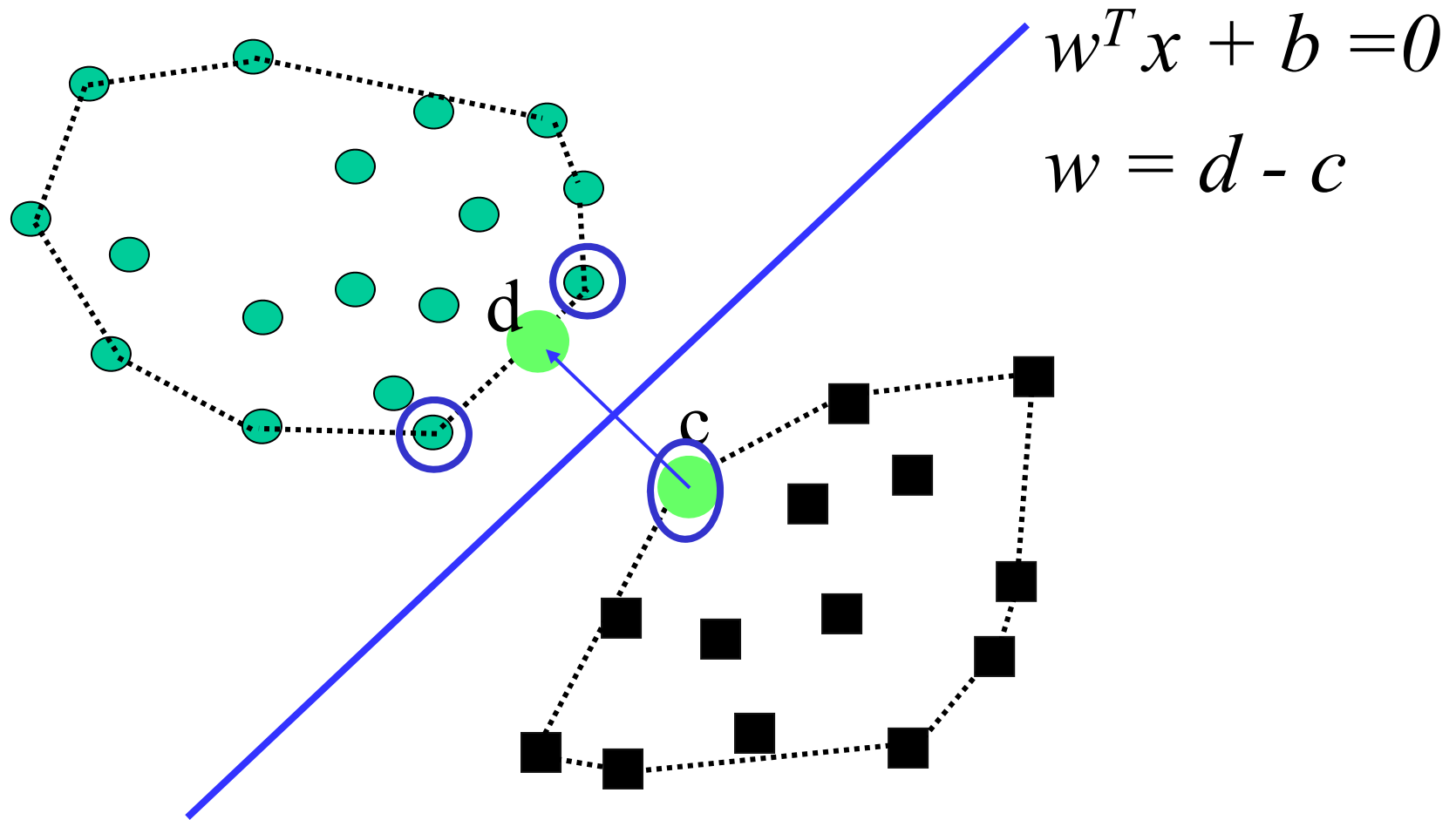
Best Linear Separator?



Find Closest Points in Convex Hulls

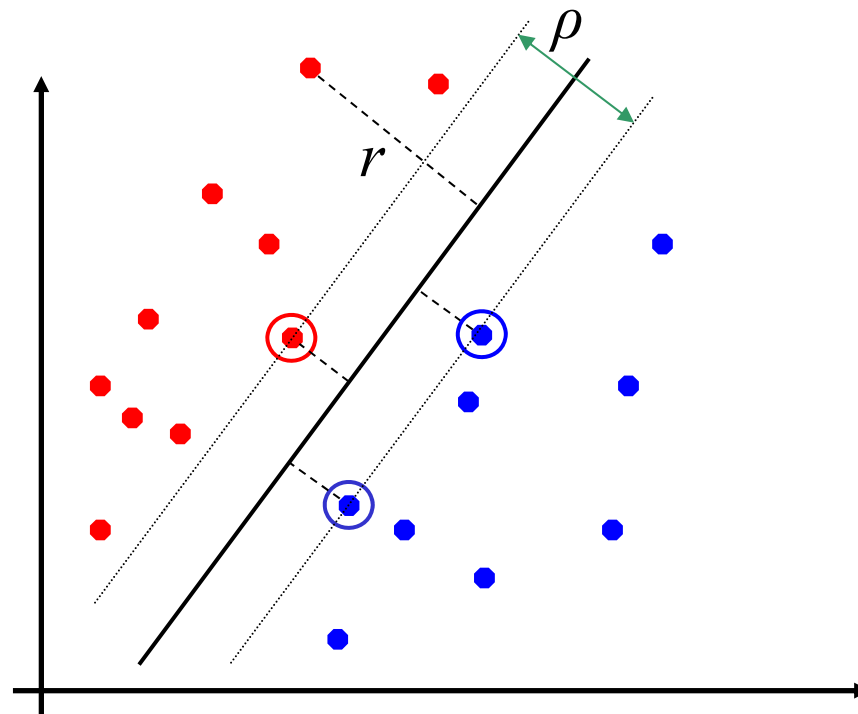


Plane Bisect Closest Points



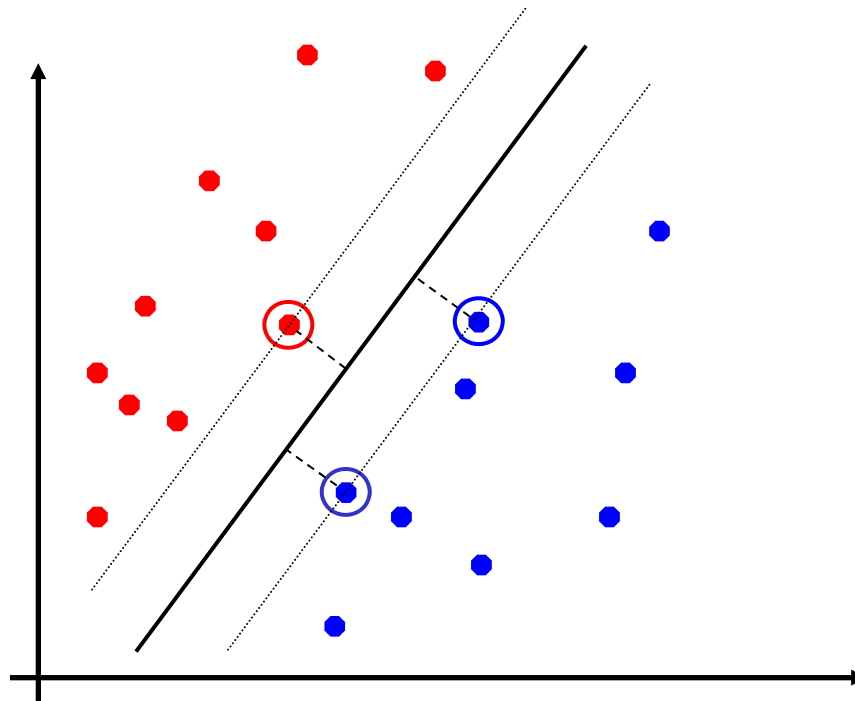
Classification Margin

- Distance from example data to the separator is $r = \frac{\mathbf{w}^T \mathbf{x} + b}{\|\mathbf{w}\|}$
- Data closest to the hyperplane are *support vectors*.
- *Margin* ρ of the separator is the width of separation between classes.



Maximum Margin Classification

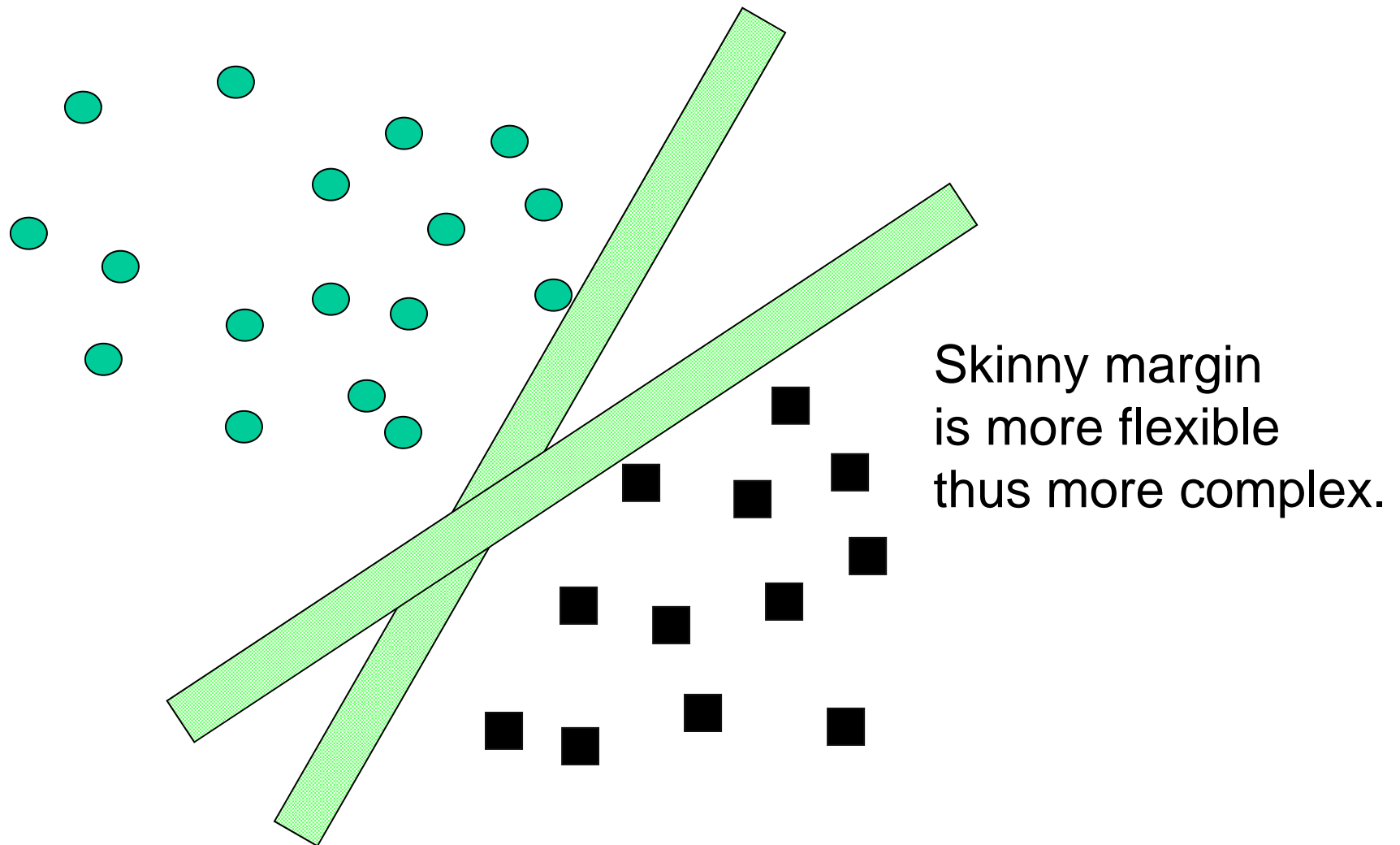
- Maximizing the margin is good according to intuition and theory.
- Implies that only support vectors are important; other training examples are ignorable.



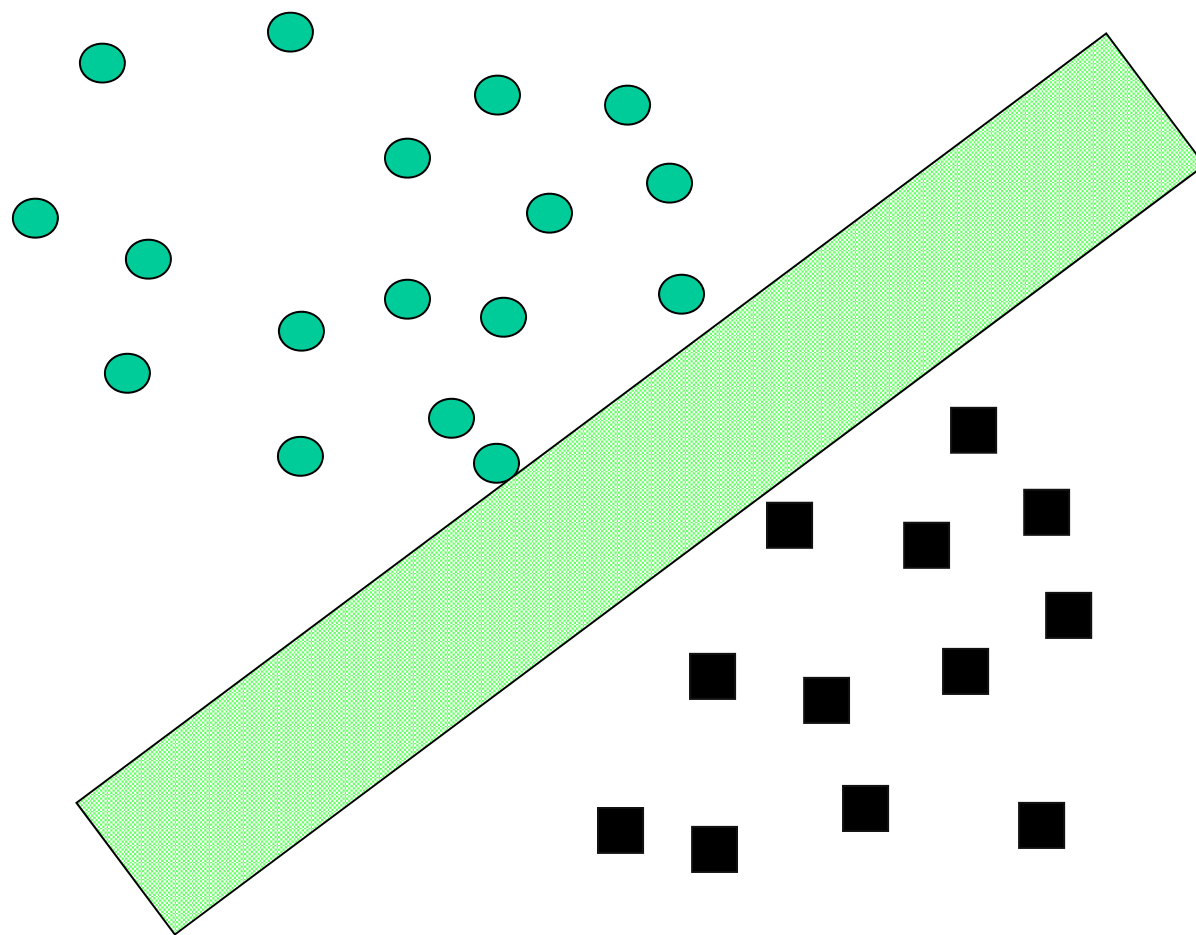
Statistical Learning Theory

- Misclassification error and the function complexity bound generalization error.
- Maximizing margins minimizes complexity.
- “Eliminates” **overfitting**.
- Solution depends only on *Support Vectors* not number of attributes.

Margins and Complexity



Margins and Complexity



Fat margin
is less complex.

Linear SVM Mathematically

- Assuming all data is at distance larger than 1 from the hyperplane, the following two constraints follow for a training set $\{(\mathbf{x}_i, y_i)\}$

$$\mathbf{w}^T \mathbf{x}_i + b \geq 1 \quad \text{if } y_i = 1$$

$$\mathbf{w}^T \mathbf{x}_i + b \leq -1 \quad \text{if } y_i = -1$$

- For support vectors, the inequality becomes an equality; then, since each example's distance from the

- hyperplane is $r = \frac{\mathbf{w}^T \mathbf{x} + b}{\|\mathbf{w}\|}$ the margin is: $\rho = \frac{2}{\|\mathbf{w}\|}$

Linear SVMs Mathematically (cont.)

- Then we can formulate the *quadratic optimization problem*:

Find \mathbf{w} and b such that

$$\rho = \frac{2}{\|\mathbf{w}\|} \quad \text{is maximized and for all } \{(\mathbf{x}_i, y_i)\}$$
$$\mathbf{w}^T \mathbf{x}_i + b \geq 1 \text{ if } y_i = 1; \quad \mathbf{w}^T \mathbf{x}_i + b \leq -1 \text{ if } y_i = -1$$

A better formulation:

Find \mathbf{w} and b such that

$$\Phi(\mathbf{w}) = \frac{1}{2} \mathbf{w}^T \mathbf{w} \quad \text{is minimized and for all } \{(\mathbf{x}_i, y_i)\}$$
$$y_i (\mathbf{w}^T \mathbf{x}_i + b) \geq 1$$

Solving the Optimization Problem

Find \mathbf{w} and b such that

$$\Phi(\mathbf{w}) = \frac{1}{2} \mathbf{w}^T \mathbf{w} \text{ is minimized and for all } \{(\mathbf{x}_i, y_i)\}$$
$$y_i (\mathbf{w}^T \mathbf{x}_i + b) \geq 1$$

- 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:

Find $\alpha_1 \dots \alpha_N$ such that

$$\mathbf{Q}(\boldsymbol{\alpha}) = \sum \alpha_i - \frac{1}{2} \sum \sum \alpha_i \alpha_j y_i y_j \mathbf{x}_i^T \mathbf{x}_j \text{ is maximized and}$$

$$(1) \sum \alpha_i y_i = 0$$

$$(2) \alpha_i \geq 0 \text{ for all } \alpha_i$$

The Optimization Problem Solution

- The solution has the form:

$$\mathbf{w} = \sum \alpha_i y_i \mathbf{x}_i \quad b = y_k - \mathbf{w}^T \mathbf{x}_k \text{ for any } \mathbf{x}_k \text{ such that } \alpha_k \neq 0$$

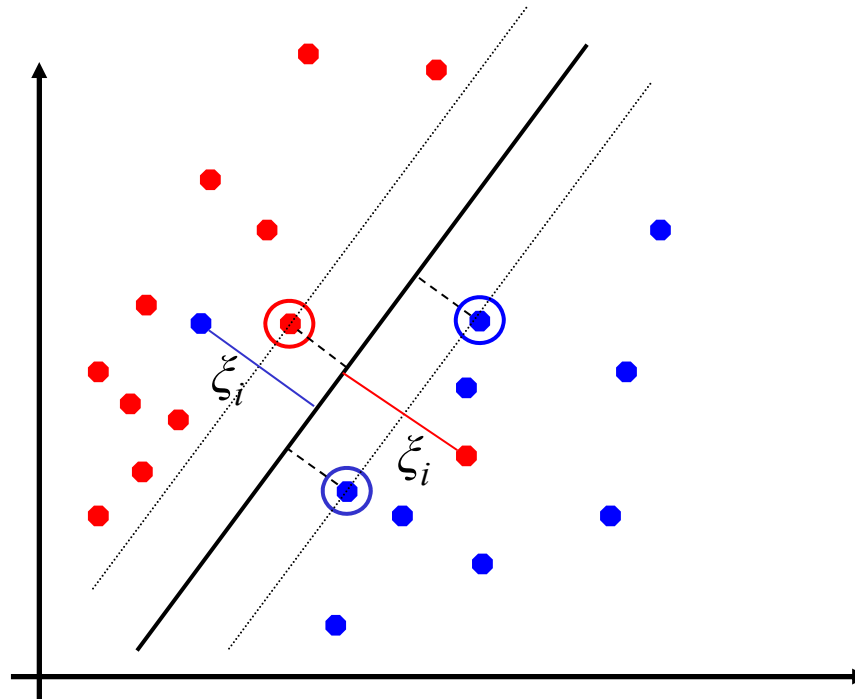
- Each non-zero α_i indicates that corresponding \mathbf{x}_i is a support vector.
- Then the classifying function will have the form:

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

- Notice that it relies on an *inner product* between the test point \mathbf{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 training points!

Soft Margin Classification

- What if the training set is not linearly separable?
- *Slack variables* ξ_i can be added to allow misclassification of difficult or noisy examples.



Soft Margin Classification Mathematically

- The old formulation:

Find \mathbf{w} and b such that

$$\Phi(\mathbf{w}) = \frac{1}{2} \mathbf{w}^T \mathbf{w} \text{ is minimized and for all } \{(\mathbf{x}_i, y_i)\} \\ y_i (\mathbf{w}^T \mathbf{x}_i + b) \geq 1$$

- The new formulation incorporating slack variables:

Find \mathbf{w} and b such that

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

- Parameter C can be viewed as a way to control overfitting.

Soft Margin Classification – Solution

- The **dual problem** for soft margin classification:

Find $\alpha_1 \dots \alpha_N$ such that

$Q(\boldsymbol{\alpha}) = \sum \alpha_i - \frac{1}{2} \sum \sum \alpha_i \alpha_j y_i y_j \mathbf{x}_i^T \mathbf{x}_j$ is maximized and

(1) $\sum \alpha_i y_i = 0$

(2) $0 \leq \alpha_i \leq C$ 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:

$$\mathbf{w} = \sum \alpha_i y_i \mathbf{x}_i$$

$$b = y_k (1 - \xi_k) - \mathbf{w}^T \mathbf{x}_k \text{ where } k = \underset{k}{\operatorname{argmax}} \alpha_k$$

But neither \mathbf{w} nor b are needed explicitly for classification!

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

Theoretical Justification for Maximum Margins

- Vapnik has proved the following:

The class of optimal linear separators has VC dimension h bounded from above as

$$h \leq \min \left\{ \left\lceil \frac{D^2}{\rho^2} \right\rceil, m_0 \right\} + 1$$

where ρ is the margin, D is the diameter of the smallest sphere that can enclose all of the training examples, and m_0 is the dimensionality.

- Intuitively, this implies that regardless of dimensionality m_0 we can minimize the VC dimension by maximizing the margin ρ .
- Thus, complexity of the classifier is kept small regardless of dimensionality.

VC维

- VC维（Vapnik-Chervonenkis Dimension）的概念是为了研究学习过程一致收敛的速度和推广性，由统计学理论定义的有关函数集学习性能的一个重要指标。
- 传统定义是：对一个指示函数集，如果存在 H 个样本能够被函数集中的函数按所有可能的 2^H 种形式分开，则称函数集能够把 H 个样本打散；函数集的VC维就是它能打散的最大样本数目 H 。若对任意数目的样本都有函数能将它们打散，则函数集的VC维是无穷大，有界实函数的VC维可以通过用一定的阈值将它转化成指示函数来定义。
- VC维反映了函数集的学习能力，VC维越大则学习机器越复杂（容量越大），遗憾的是，目前尚没有通用的关于任意函数集VC维计算的理论，只对一些特殊的函数集知道其VC维。例如在 N 维空间中线性分类器和线性实函数的VC维是 $N+1$ 。

Linear SVMs: Overview

- 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 \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 $\alpha_1 \dots \alpha_N$ such that

$Q(\boldsymbol{\alpha}) = \sum \alpha_i - \frac{1}{2} \sum \sum \alpha_i \alpha_j y_i y_j \mathbf{x}_i^T \mathbf{x}_j$ is maximized and

(1) $\sum \alpha_i y_i = 0$

(2) $0 \leq \alpha_i \leq C$ for all α_i

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

Linear SVM for Non-linearly Separable Problems

No kernel

- What if the problem is not linearly separable?
 - Introduce slack variables
 - Need to minimize:

$$L(w) = \frac{\|\vec{w}\|^2}{2} + C \left(\sum_{i=1}^N \xi_i \right)$$

Measures prediction error

Parameter

Inverse size of margin
between hyperplanes

Slack variable

- Subject to ($i=1, \dots, N$):

$$\begin{cases} (1) & y_i * (\vec{w} \bullet \vec{x}_i + b) \geq 1 - \xi_i \\ (2) & 0 \leq \xi_i \end{cases}$$

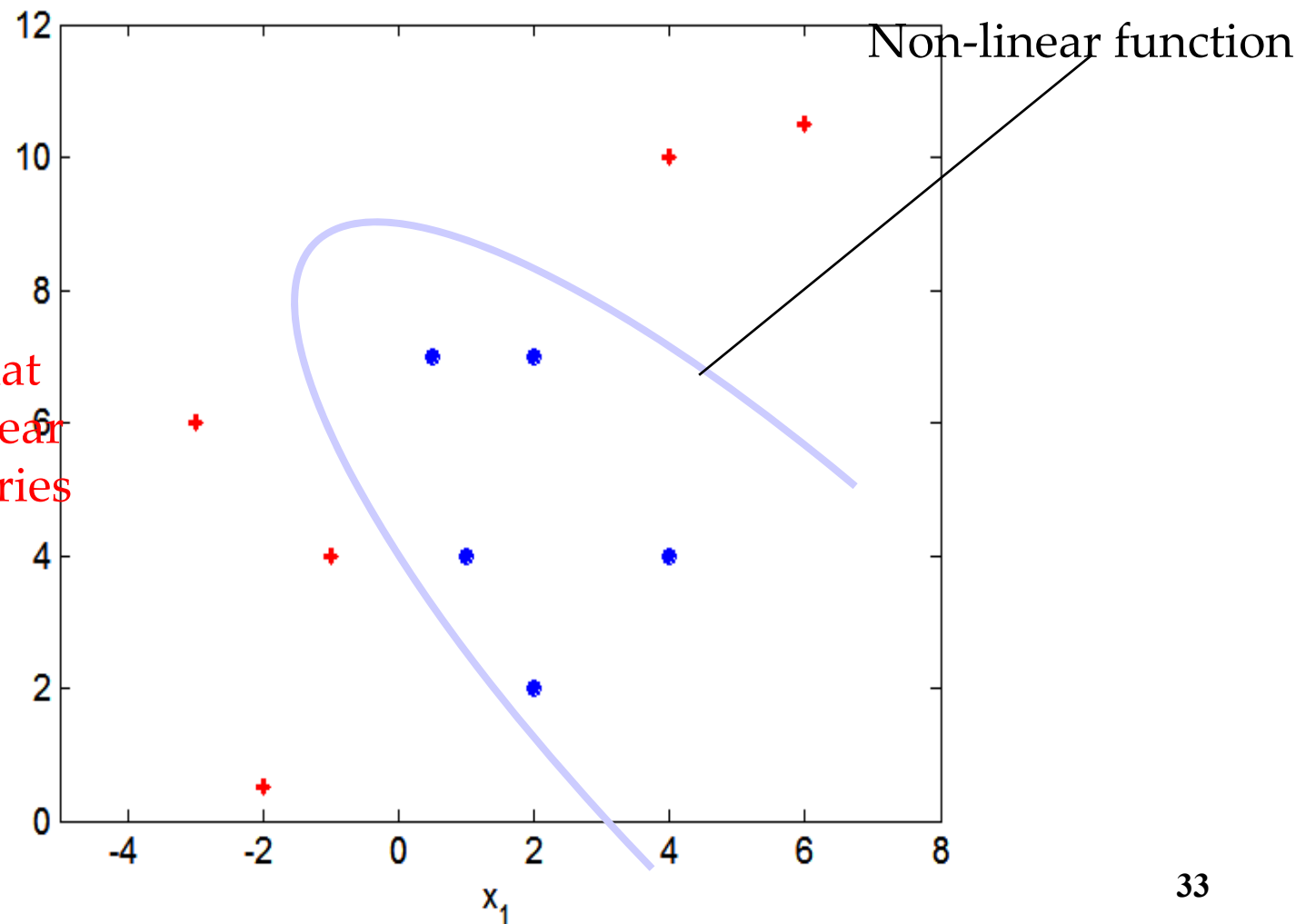
allows constraint violation
to a certain degree

- C is chosen using a validation set trying to keep the margins wide while keeping the training error low.

Nonlinear Support Vector Machines

- What if decision boundary is not linear?

Alternative 1:
Use technique that
Employs non-linear
decision boundaries

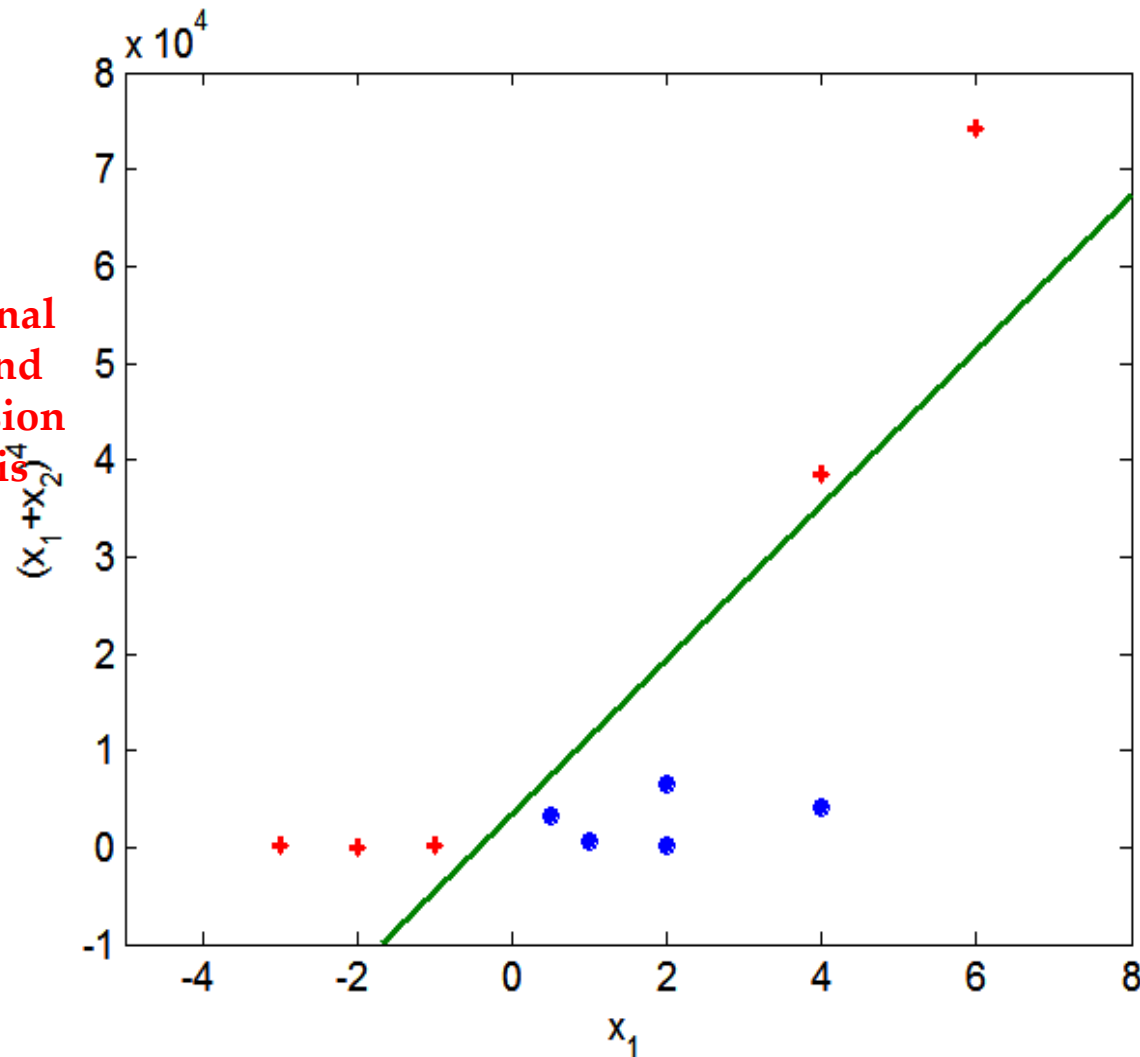


Nonlinear Support Vector Machines

1. Transform data into higher dimensional space
2. Find the best hyperplane using the methods introduced earlier

Alternative 2:

Transform into a higher dimensional attribute space and find linear decision boundaries in this space



Nonlinear Support Vector Machines

1. Choose a non-linear function ϕ to transform into a different, usually higher dimensional, attribute space
2. Minimize

$$L(w) = \frac{\|\vec{w}\|^2}{2}$$

- but subjected to the following N constraints:

$$\left\{ \begin{array}{l} y_i(\vec{w} \bullet \phi(\vec{x}_i) + b) \geq 1 \quad i = 1, \dots, N \end{array} \right.$$

Find a good hyperplane
in the transformed space

Remark: The Soft Margin SVM can be generalized similarly.

Example: Polynomial Kernel Function

Polynomial Kernel Function:

$$\Phi(x_1, x_2) = (x_1^2, x_2^2, \sqrt{2} * x_1, \sqrt{2} * x_2, 1)$$

$$K(u, v) = \Phi(u) \bullet \Phi(v) = (u \bullet v + 1)^2$$

A Support Vector Machine with polynomial kernel function classifies a new example z as follows:

$$\text{sign}((\sum \lambda_i y_i * \Phi(x_i) \bullet \Phi(z)) + b) =$$

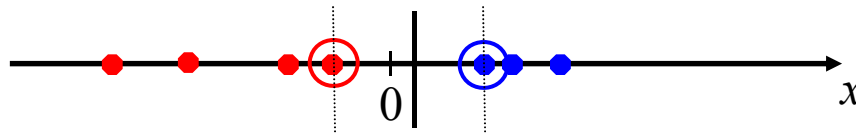
$$\text{sign}((\sum \lambda_i y_i * (x_i \bullet z + 1)^2) + b)$$

Remark: λ_i and b are determined using the methods for linear SVMs that were discussed earlier

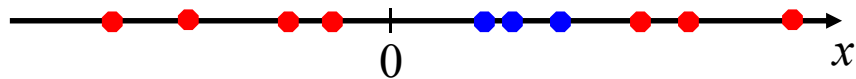
Kernel function trick: perform computations in the original space, although we solve an optimization problem in the transformed space \rightarrow more efficient.

Non-linear SVMs

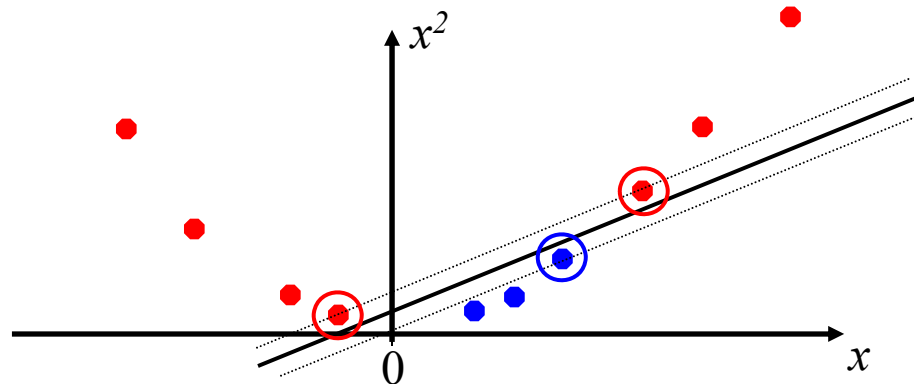
- Datasets that are linearly separable with some noise work out great:



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



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



Nonlinear Classification

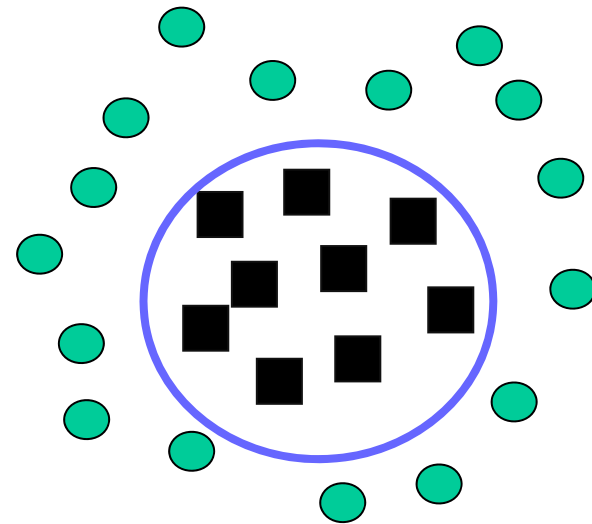
$$x = [a, b]$$

$$x \square w = w_1 a + w_2 b$$

↓

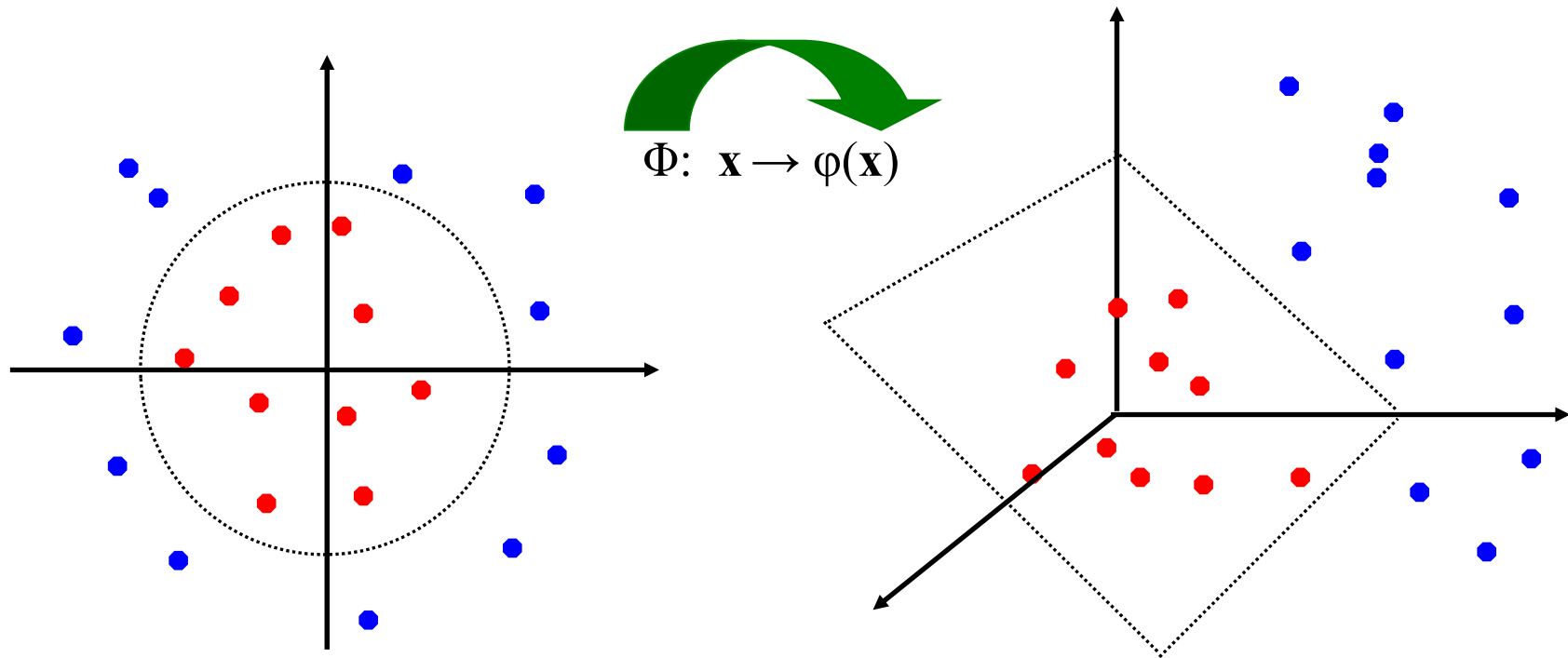
$$\theta(x) = [a, b, ab, a^2, b^2]$$

$$\theta(x) \square w = w_1 a + w_2 b + w_3 ab + w_4 a^2 + w_5 b^2$$



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 inner product between vectors $K(\mathbf{x}_i, \mathbf{x}_j) = \mathbf{x}_i^T \mathbf{x}_j$
- If every datapoint is mapped into high-dimensional space via some transformation $\Phi: \mathbf{x} \rightarrow \phi(\mathbf{x})$, the inner product becomes:

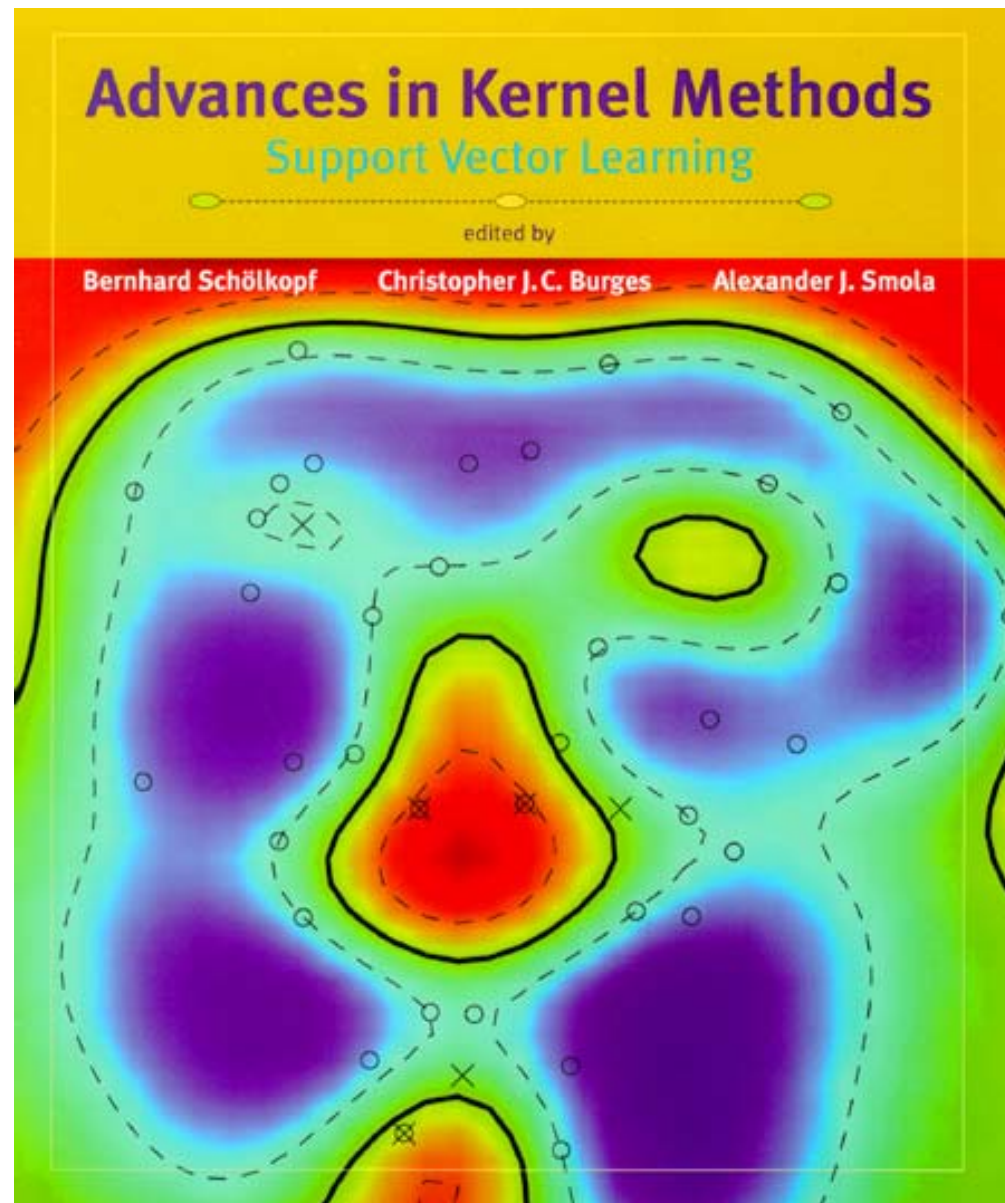
$$K(\mathbf{x}_i, \mathbf{x}_j) = \phi(\mathbf{x}_i)^T \phi(\mathbf{x}_j)$$

- A *kernel function* is some function that corresponds to an inner product into some 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 $K(\mathbf{x}_i, \mathbf{x}_j) = \phi(\mathbf{x}_i)^T \phi(\mathbf{x}_j)$:

$$\begin{aligned} K(\mathbf{x}_i, \mathbf{x}_j) &= (1 + \mathbf{x}_i^T \mathbf{x}_j)^2 = 1 + x_{i1}^2 x_{j1}^2 + 2 x_{i1} x_{j1} x_{i2} x_{j2} + x_{i2}^2 x_{j2}^2 + 2 x_{i1} x_{j1} + 2 x_{i2} x_{j2} = \\ &= [1 \ x_{i1}^2 \ \sqrt{2} x_{i1} x_{i2} \ x_{i2}^2 \ \sqrt{2} x_{i1} \ \sqrt{2} x_{i2}]^T [1 \ x_{j1}^2 \ \sqrt{2} x_{j1} x_{j2} \ x_{j2}^2 \ \sqrt{2} x_{j1} \ \sqrt{2} x_{j2}] = \\ &= \phi(\mathbf{x}_i)^T \phi(\mathbf{x}_j), \quad \text{where } \phi(\mathbf{x}) = [1 \ x_1^2 \ \sqrt{2} x_1 x_2 \ x_2^2 \ \sqrt{2} x_1 \ \sqrt{2} x_2] \end{aligned}$$



Positive Definite Matrices

A square matrix A is *positive definite* if $x^T A x > 0$ for all nonzero column vectors x .

It is *negative definite* if $x^T A x < 0$ for all nonzero x .

It is *positive semi-definite* if $x^T A x \geq 0$.

And *negative semi-definite* if $x^T A x \leq 0$ for all x .

What Functions are Kernels?

- For some functions $K(\mathbf{x}_i, \mathbf{x}_j)$ checking that $K(\mathbf{x}_i, \mathbf{x}_j) = \phi(\mathbf{x}_i)^T \phi(\mathbf{x}_j)$ 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:

$K =$

$K(\mathbf{x}_1, \mathbf{x}_1)$	$K(\mathbf{x}_1, \mathbf{x}_2)$	$K(\mathbf{x}_1, \mathbf{x}_3)$...	$K(\mathbf{x}_1, \mathbf{x}_N)$
$K(\mathbf{x}_2, \mathbf{x}_1)$	$K(\mathbf{x}_2, \mathbf{x}_2)$	$K(\mathbf{x}_2, \mathbf{x}_3)$		$K(\mathbf{x}_2, \mathbf{x}_N)$
...
$K(\mathbf{x}_N, \mathbf{x}_1)$	$K(\mathbf{x}_N, \mathbf{x}_2)$	$K(\mathbf{x}_N, \mathbf{x}_3)$...	$K(\mathbf{x}_N, \mathbf{x}_N)$

Examples of Kernel Functions

- Linear: $K(\mathbf{x}_i, \mathbf{x}_j) = \mathbf{x}_i^T \mathbf{x}_j$
- Polynomial of power p : $K(\mathbf{x}_i, \mathbf{x}_j) = (1 + \mathbf{x}_i^T \mathbf{x}_j)^p$
- Gaussian (radial-basis function network): $K(\mathbf{x}_i, \mathbf{x}_j) = e^{-\frac{\|\mathbf{x}_i - \mathbf{x}_j\|^2}{2\sigma^2}}$
- Two-layer perceptron: $K(\mathbf{x}_i, \mathbf{x}_j) = \tanh(\beta_0 \mathbf{x}_i^T \mathbf{x}_j + \beta_1)$

Non-linear SVMs Mathematically

- Dual problem formulation:

Find $\alpha_1 \dots \alpha_N$ such that

$Q(\boldsymbol{\alpha}) = \sum \alpha_i - \frac{1}{2} \sum \sum \alpha_i \alpha_j y_i y_j K(\mathbf{x}_i, \mathbf{x}_j)$ is maximized and

(1) $\sum \alpha_i y_i = 0$

(2) $\alpha_i \geq 0$ for all α_i

- The solution is:

$$f(\mathbf{x}) = \sum \alpha_i y_i K(\mathbf{x}_i, \mathbf{x}_j) + b$$

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

SVM applications

- SVMs were originally proposed by Boser, Guyon and Vapnik in 1992 and gained increasing popularity in late 1990s.
- SVMs are currently among the best performers for a number of classification tasks ranging from text to genomic data.
- SVM techniques have been extended to a number of tasks such as regression [Vapnik *et al.* '97], principal component analysis [Schölkopf *et al.* '99], etc.
- Most popular optimization algorithms for SVMs are SMO [Platt '99] and SVM^{light} [Joachims' 99], both use *decomposition* to hill-climb over a subset of α_i 's at a time.
- Tuning SVMs remains a black art: selecting a specific kernel and parameters is usually done in a try-and-see manner.

SVM Extensions

- Regression
- Variable Selection
- Boosting
- Density Estimation
- Unsupervised Learning
 - Novelty/Outlier Detection
 - Feature Detection
 - Clustering

Many Applications

- Speech Recognition
- Data Base Marketing
- Quark Flavors in High Energy Physics
- Dynamic Object Recognition
- Knock Detection in Engines
- Protein Sequence Problem
- Text Categorization
- Breast Cancer Diagnosis
- Cancer Tissue classification
- Translation initiation site recognition in DNA
- Protein fold recognition

Support Vector Machine Resources

- **SVM Application List**
<http://www.clopinet.com/isabelle/Projects/SVM/applist.html>
- **Kernel machines**
<http://www.kernel-machines.org/>
- **Pattern Classification and Machine Learning**
<http://clopinet.com/isabelle/#projects>
- **R a GUI language for statistical computing and graphics**
<http://www.r-project.org/>
- **Kernel Methods for Pattern Analysis – 2004**
<http://www.kernel-methods.net/>
- **An Introduction to Support Vector Machines**
(and other kernel-based learning methods)
<http://www.support-vector.net/>
- **Kristin P. Bennett web page**
<http://www.rpi.edu/~bennek>
- **Isabelle Guyon's home page**
<http://clopinet.com/isabelle>

Support Vector Machine References

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Summary Support Vector Machines

- Support vector machines learn hyperplanes that separate two classes maximizing the *margin between them (the empty space between the instances of the two classes)*.
- Support vector machines introduce slack variables—in the case that classes are not linear separable—trying to maximize margins while keeping the training error low.
- The most popular versions of SVMs use non-linear kernel functions and map the attribute space into a higher dimensional space to facilitate finding “good” linear decision boundaries in the modified space.
- Support vector machines find “margin optimal” hyperplanes by solving a convex quadratic optimization problem. However, this optimization process is quite slow and support vector machines tend to fail if the number of examples goes beyond 500/5000/50000...
- In general, support vector machines accomplish quite high accuracies, if compared to other techniques.
- In the last 10 years, support vector machines have been generalized for other tasks such as regression, PCA, outlier detection,...

Kernels—What can they do for you?

- Some machine learning/statistical problems only depend on the dot-product of the objects in the dataset $O=\{x_1,\dots,x_n\}$ and not on other characteristics of the objects in the dataset; in other words, those techniques only depend on the gram matrix of O which stores $x_1 \bullet x_1, x_1 \bullet x_2, \dots, x_n \bullet x_n$ (http://en.wikipedia.org/wiki/Gramian_matrix).
- These techniques can be generalized by mapping the dataset into a higher dimensional space as long as the non-linear mapping ϕ can be kernelized; that is, a kernel function K can be found such that:

$$K(u,v) = \phi(u) \bullet \phi(v)$$

In this case the results are computed in the mapped space based on $K(x_1,x_1), K(x_1,x_2), \dots, K(x_n,x_n)$ which is called the kernel trick: http://en.wikipedia.org/wiki/Kernel_trick

- Kernels have been successfully used to generalize PCA, K-means, support vector machines, and many other techniques, allowing them to use non-linear coordinate systems, more complex decision boundaries, or more complex cluster boundaries.