Machine Learning

Support Vector Machines SVM

Lesson 6

Data Classification problem

Training set:
$$D = \{(x_i, y_i), \dots, (x_N, y_N)\}$$

- $x_i: input data sample$ $y_i \in \{1, ..., K\}: class or label of input$
- Target: Construct function

$$f: X \to Y$$

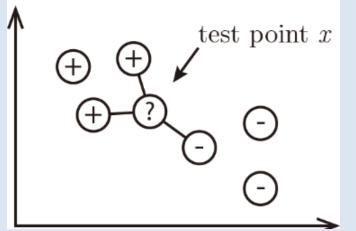
$$f(x_i) = y_i \quad \forall (x_i, y_i) \in D$$

Prediction of class for any unknown input

$$y^* = f(x^*)$$

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Nearest Neighbor classifier



- The simplest classification method
- Assumption: data belongs to the same category are neighbors
- **Classification rule:** Classify according to the neighbor(s)

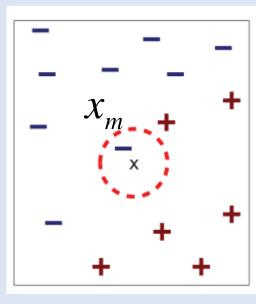
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Nearest Neighbor Classifier

Classification

 Find the nearest neighbor (according to a **distance function**)

$$x_m: \min_{n=1,\ldots,N} \left\{ dist(x^*, x_n) \right\}$$



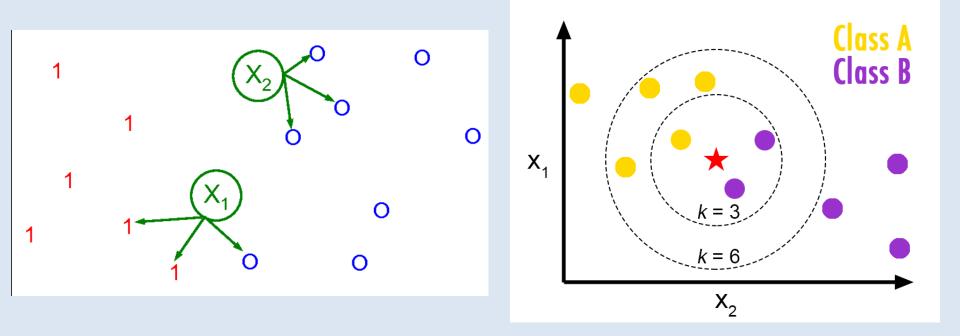
• Class of unknown x^* is similar to its neighbor

$$y^* = y_m$$

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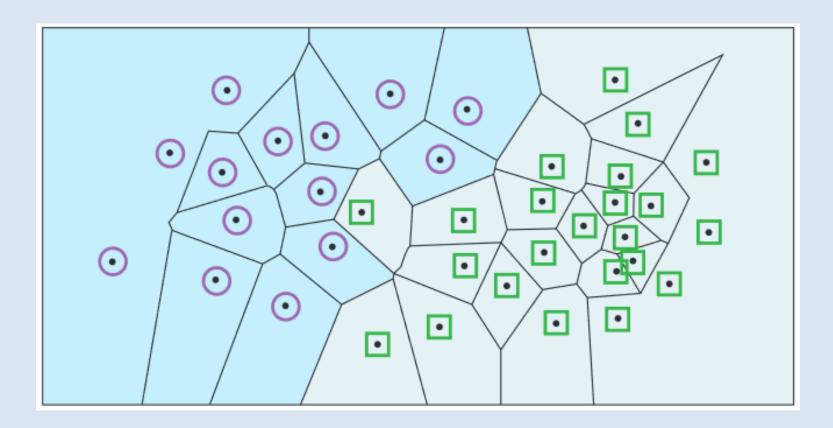
Extension to *k***-NN**

- Find k>1 neighbors
- Classify according to the class majority



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• Voronoi diagram



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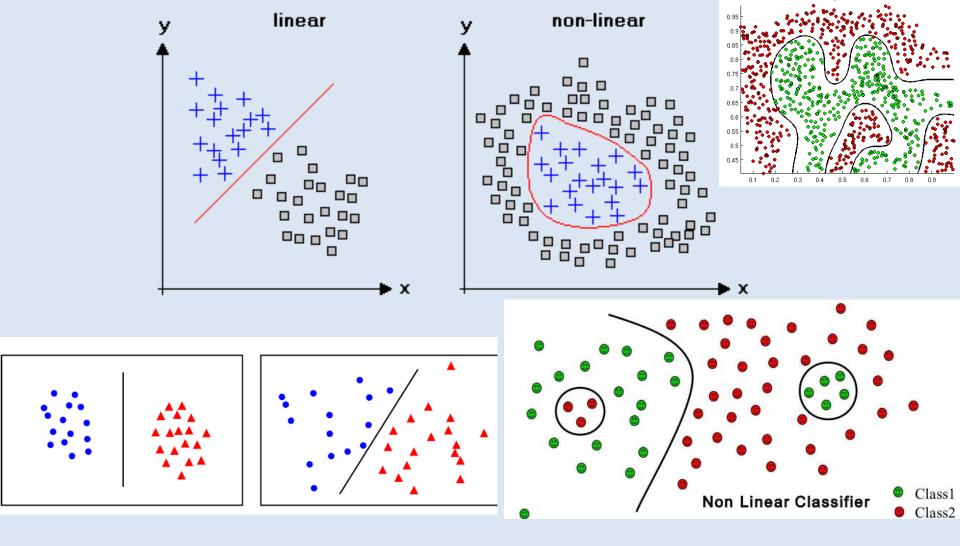
Linear Classifiers

- **K=2** classes Ω_1 , Ω_2
- Target: Construction of a hyperplane *f(x,w)* between data of 2 classes
- Decision boundaries:

if
$$f(x,w) \ge 0$$
 then $x \in \Omega_1$
else
if $f(x,w) < 0$ *then* $x \in \Omega_2$

• **w** are the unknown parameters

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linear classification

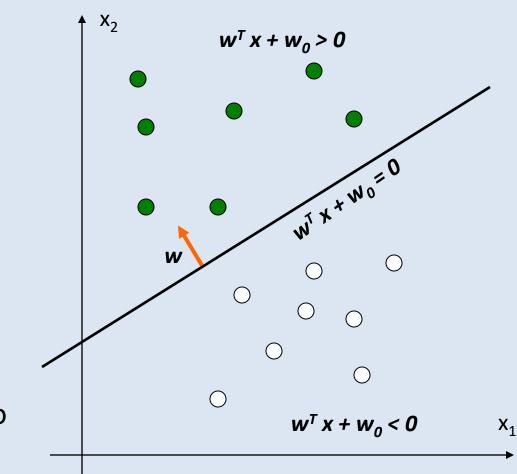
nonlinear classification

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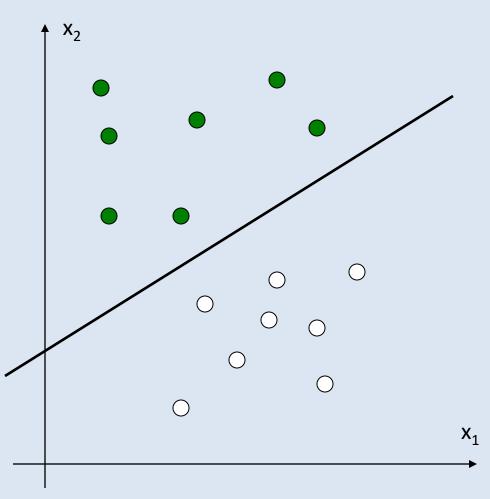
 $D = \{(x_i, y_i)\}_{i=1}^N$

- *f(x)* linear function:
 - $f(x) = w^T x + w_0$
- Define a separating hyperplane between two classes



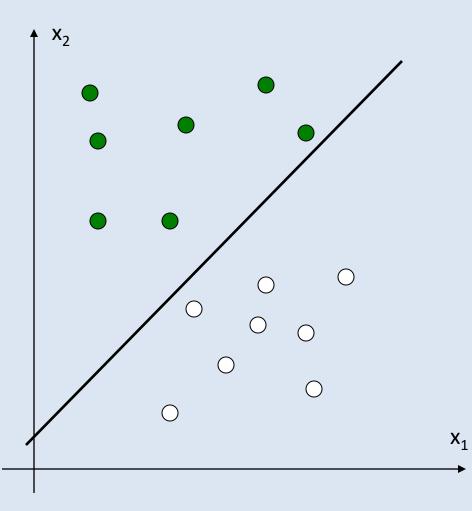
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Which is the **optimum hyperplane** that separates better two classes?



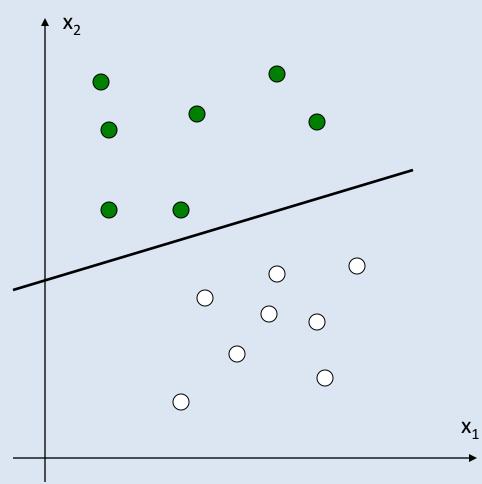
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Which is the **optimum hyperplane** that separates better two classes?



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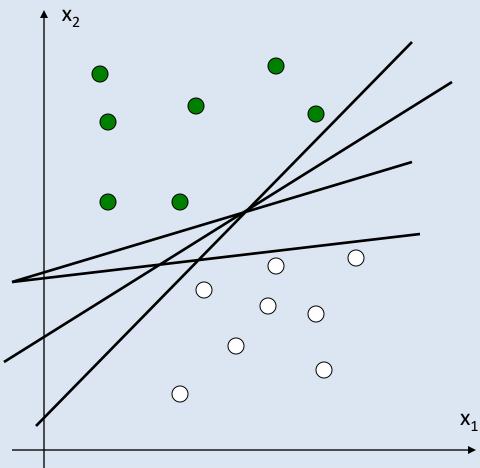
Which is the **optimum hyperplane** that separates better two classes?



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Which is the **optimum hyperplane** that separates better two classes?

Infinite number of solutions!

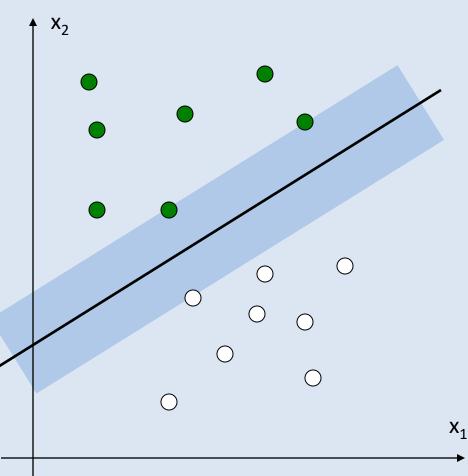


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Solution: Marginal Maximization

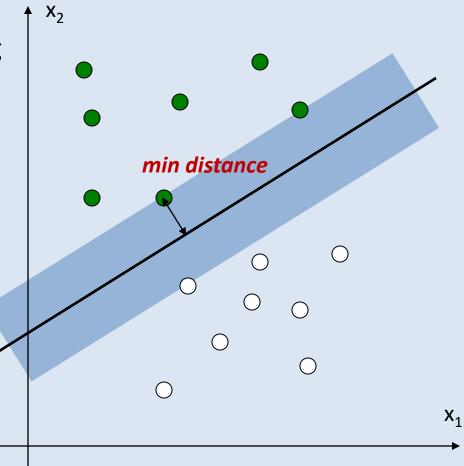
[Boser, Guyon, Vapnik '92], [Cortes & Vapnik '95]

The optimal separating hyperplane is the one that gives the maximum margin width



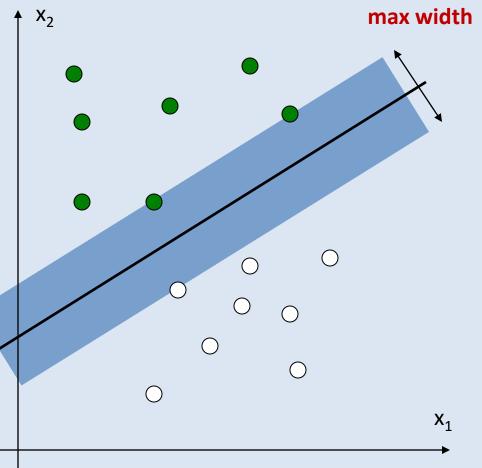
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 Definition 1: Margin is the minimum distance of N training samples to the hyperplane

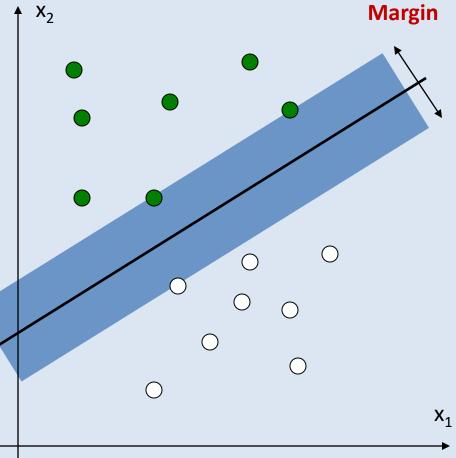


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- Definition 1: Margin is the minimum distance of N training samples to the hyperplane
- Definition 2: Margin is the maximum width of boundary around the separating hyperplane without covering any sample



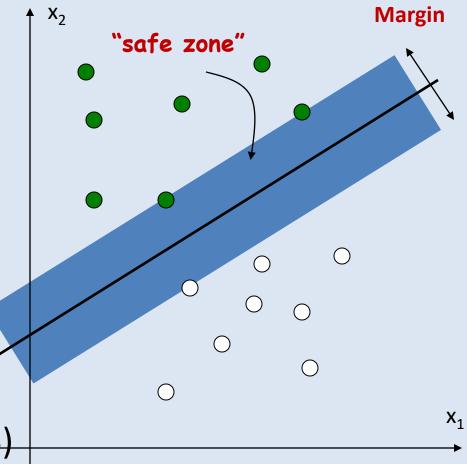
- Definition 1: Margin is the minimum distance of N training samples to the hyperplane
- Definition 2: Margin is the maximum width of boundary around the separating hyperplane without covering any sample



Why is the optimum solution?

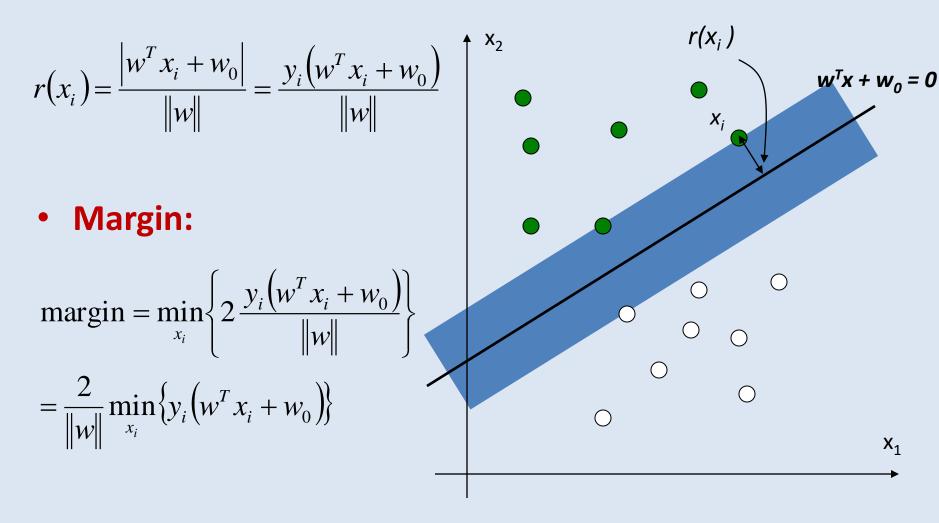
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- Solution: Find the hyperplane that maximizes the margin between two classes.
- ✓ This will minimize the risk of classifier's decision.
- ✓ Also, it will increase the generalization of classifier (Vapnick, 1963)



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Distance of any point x_i



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Marginal Maximization Problem

$$\left\{\hat{w}, \hat{w}_{0}\right\}: \max_{w, w_{0}} \left\{\frac{2}{\|w\|} \min_{x_{i}} \left\{y_{i} \left(w^{T} x_{i} + w_{0}\right)\right\}\right\}$$

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Marginal Maximization Problem

$$\left\{ \hat{w}, \hat{w}_0 \right\} : \max_{w, w_0} \left\{ \frac{2}{\|w\|} \min_{x_i} \left\{ y_i \left(w^T x_i + w_0 \right) \right\} \right\}$$

• **Solution: Use a** scaling factor k:

$$k \min_{x_i} \{ y_i (w^T x_i + w_0) \} = 1$$

Marginal Maximization Problem

$$\left\{ \hat{w}, \hat{w}_0 \right\} : \max_{w, w_0} \left\{ \frac{2}{\|w\|} \min_{x_i} \left\{ y_i \left(w^T x_i + w_0 \right) \right\} \right\}$$

• **Solution: Use a** scaling factor k:

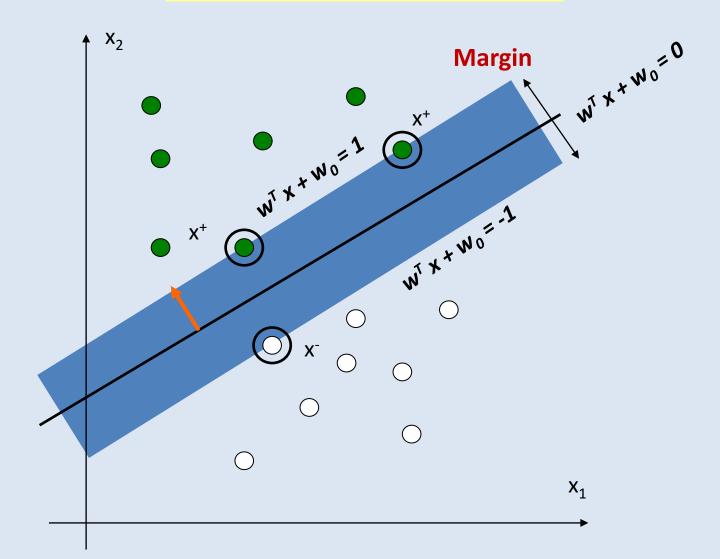
$$k \min_{x_i} \{ y_i (w^T x_i + w_0) \} = 1$$

• Thus margin becomes:

$$\frac{2}{\|w\|} \min_{x_i} \left\{ y_i \left(w^T x_i + w_0 \right) \right\} = \frac{2}{\|w\|}$$

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• Therefore: $\forall x_i \in D: y_i (w^T x_i + w_0) \ge 1$



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The objective function

We need to optimize $\|w\|^{-1}$ which is the same as **minimizing** $\|w\|^2$ subject to the **margin requirements**

$$\{\hat{w}, \hat{w}_{0}\}: \max_{w, w_{0}} \left\{ \frac{2}{\|w\|} \right\} \quad \text{s.t.} \quad y_{i} \left(w^{T} x_{i} + w_{0}\right) \ge 1 \quad \forall i$$

$$\{\hat{w}, \hat{w}_{0}\}: \min_{w, w_{0}} \left\{ \frac{1}{2} \|w\|^{2} \right\} \quad \text{s.t.} \quad y_{i} \left(w^{T} x_{i} + w_{0}\right) \ge 1 \quad \forall i$$

Quadratic Optimization Problem: minimize a quadratic function subject to a set of linear inequality constraints

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SVM Training Methodology

Training is formulated as an optimization problem
 Dual problem reduces computational complexity
 Kernel trick is used to reduce computation

Determination of the model parameters corresponds to a convex optimization problem.

Solution is straightforward (local solution is the global optimum)

□ Makes use of Lagrange multipliers

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Joseph-Louis Lagrange (1736-1813)

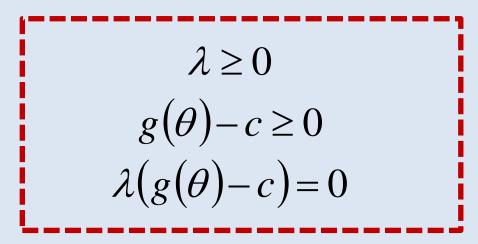
Optimization problem with linear inequality constraints

$$\min_{\theta} \{ f(\theta) \} \text{ s.t. } g(\theta) \ge c \Longrightarrow g(\theta) - c \ge 0$$

Lagrange function:

$$L(\theta,\lambda) = f(\theta) - \lambda(g(\theta) - c)$$

✓ Karush-Khun-Tucker (KKT) conditions:



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Solving the Optimization Problem

• Minimization Problem:

$$\{\hat{w}, \hat{w}_0\}: \min_{w, w_0} \{\frac{1}{2} \|w\|^2\}$$
 s.t. $y_i (w^T x_i + w_0) \ge 1 \quad \forall i$

• Lagrange function:

$$L(w, w_0, a) = \frac{1}{2} \|w\|^2 - \sum_{i=1}^N a_i (y_i (w^T x_i + w_0) - 1)$$

KKT conditions $\begin{cases} \forall i & a_i \ge 0\\ y_i \left(w^T x_i + w_0 \right) - 1 \ge 0\\ a_i \left(y_i \left(w^T x_i + w_0 \right) - 1 \right) = 0 \end{cases}$

a_i Lagrange multipliers

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Dual Optimization Problem

minimize
$$L(w, w_0, a) = \frac{1}{2} \|w\|^2 - \sum_{i=1}^N a_i (y_i (w^T x_i + w_0) - 1)$$

$$\frac{\partial L}{\partial w} = 0 \Longrightarrow \hat{w} = \sum_{i=1}^{N} a_i y_i x_i$$

$$\frac{\partial L}{\partial w_0} = 0 \Longrightarrow \sum_{i=1}^N a_i y_i = 0$$

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Prime problem minimize
$$L(w, w_0, a) = \frac{1}{2} ||w||^2 - \sum_{i=1}^N a_i (y_i (w^T x_i + w_0) - 1)$$

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Prime problem minimize
$$L(w, w_0, a) = \frac{1}{2} ||w||^2 - \sum_{i=1}^N a_i (y_i (w^T x_i + w_0) - 1)$$

$$\sum_{i=1}^N a_i y_i = 0 \qquad \hat{w} = \sum_{i=1}^N a_i y_i x_i$$

Dual problem

(maximize)
$$L_D(a) = \sum_{i=1}^N a_i - \frac{1}{2} \sum_{i=1}^N \sum_{j=1}^N a_i a_j y_i y_j x_i^T x_j$$

s.t. $a_i \ge 0$, $\sum_{i=1}^N a_i y_i = 0$

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Important Remarks

 The Prime problem has d+1 unknown parameters that must be tuned. These are the linear coefficients {w, w₀}, where d is the data dimension.

The **Dual problem** has **N unknown** parameters which are the Lagrange multipliers { **a**_i **i=1,..., N**}, where N is the number of training samples.



This is valuable and convenient for multi-dimensional data, where *d>>N*, since the dual search space is significantly lower in comparison with the prime search space.

2. The decision rule for choosing the class of an unknown sample *x* becomes:

$$\begin{aligned} f(x) &= w^T x + w_0 \\ \hat{w} &= \sum_{i=1}^N a_i y_i x_i \end{aligned} \Rightarrow f(x) = \sum_{i=1}^N a_i y_i x_i^T x + w_0 \end{aligned}$$

which is a **linear combination of dot products** of xwith all training samples x_i , where each one has a unique weight equal to the Langrange multiplier a_i .

3. According to the KKT conditions we have:

$$a_{i} \ge 0$$

$$y_{i}(w^{T}x_{i} + w_{0}) - 1 \ge 0$$

$$a_{i}(y_{i}(w^{T}x_{i} + w_{0}) - 1) = 0$$

$$\begin{cases} a_{i} = 0 \text{ and } y_{i}(w^{T}x_{i} + w_{0}) > 1 \\ y_{i}(w^{T}x_{i} + w_{0}) - 1 = 0 \text{ and } a_{i} > 0 \end{cases}$$

Thus:

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3. According to the KKT conditions we have:

Thus:

$$a_{i} \geq 0$$

$$y_{i}(w^{T}x_{i} + w_{0}) - 1 \geq 0$$

$$a_{i}(y_{i}(w^{T}x_{i} + w_{0}) - 1) = 0$$
Training samples of D
with zero weight outside
the margin
$$y_{i}(w^{T}x_{i} + w_{0}) - 1 = 0$$

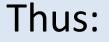
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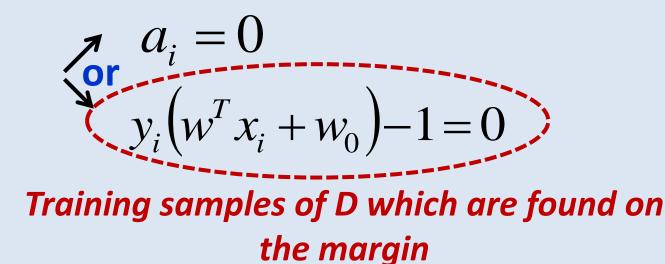
3. According to the KKT conditions we have:

$$a_{i} \ge 0$$

$$y_{i} \left(w^{T} x_{i} + w_{0} \right) - 1 \ge 0$$

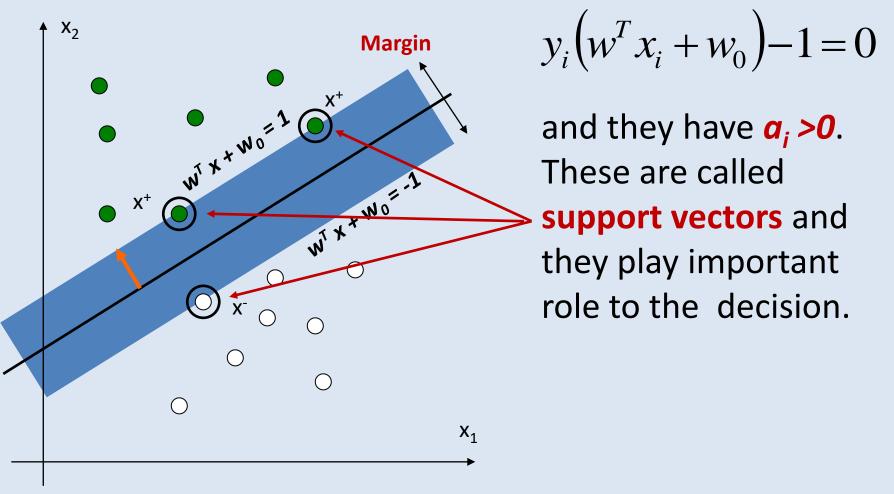
$$a_{i} \left(y_{i} \left(w^{T} x_{i} + w_{0} \right) - 1 \right) = 0$$



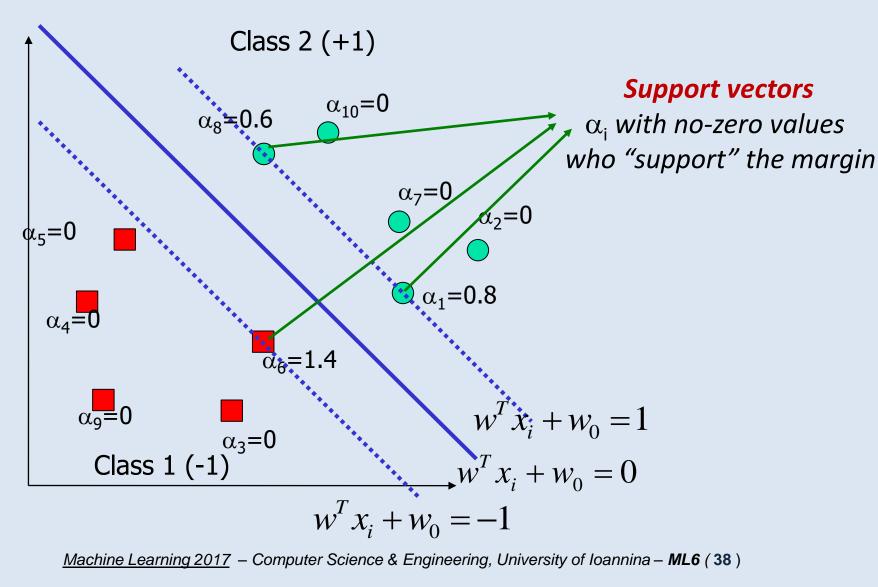


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- All training samples outside the margin have a_i=0 and they do not play any significant role to the decision.
- Training samples over the margin hold:

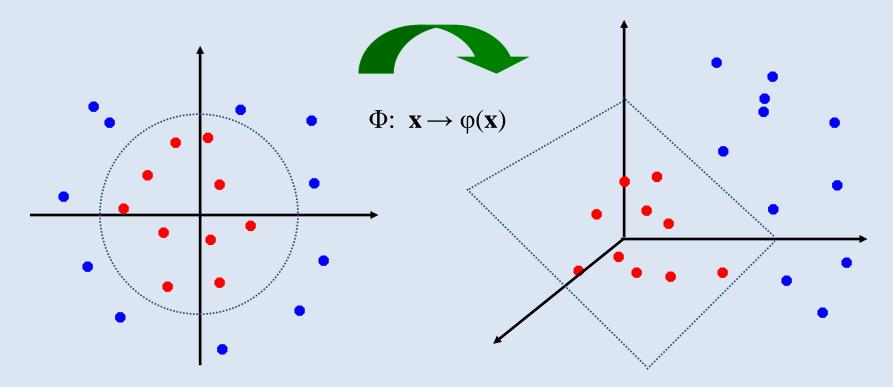


An example



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4. Kernel trick: Use a particular representation φ(x)
Idea: The original feature space is transformed into a (usually) larger feature space which increases the likelihood of being linear separable.



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• In the new space all dot products become:

$$x_i^T x_j \rightarrow \phi(x_i)^T \phi(x_j) \equiv K(x_i, x_j)$$

which is called kernel function and specifies similarity

• The new decision rule can be written as:

$$f(x) = \sum_{i=1}^{N} a_i y_i x_i^T x + w_0 \quad \to \quad f(x) = \sum_{i=1}^{N} a_i y_i \phi(x_i)^T \phi(x) + w_0$$
$$f(x) = \sum_{i=1}^{N} a_i y_i K(x_i, x) + w_0$$

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Examples of kernel functions

- Linear Kernel
- Polynomial Kernel
- Gaussian ή RBF Kernel
- Cosine

• Sigmoid

$$K(x_{i}, x_{j}) = x_{i}^{T} x_{j}$$

$$K(x_{i}, x_{j}) = (x_{i}^{T} x_{j} + 1)^{p}$$

$$K(x_{i}, x_{j}) = e^{-\frac{\|x_{i} - x_{j}\|^{2}}{2o^{2}}}$$

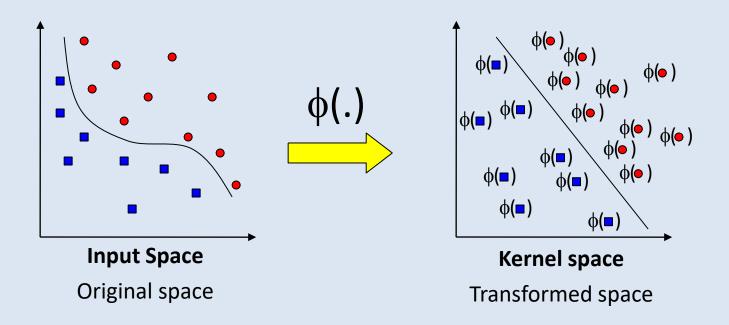
$$K(x_{i}, x_{j}) = \frac{x_{i}^{T} x_{j}}{\|x_{i}\|^{2} \|x_{j}\|^{2}}$$

$$K(x_{i}, x_{j}) = \frac{1}{1 + e^{-(\beta_{1} x_{i}^{T} x_{j})}}$$

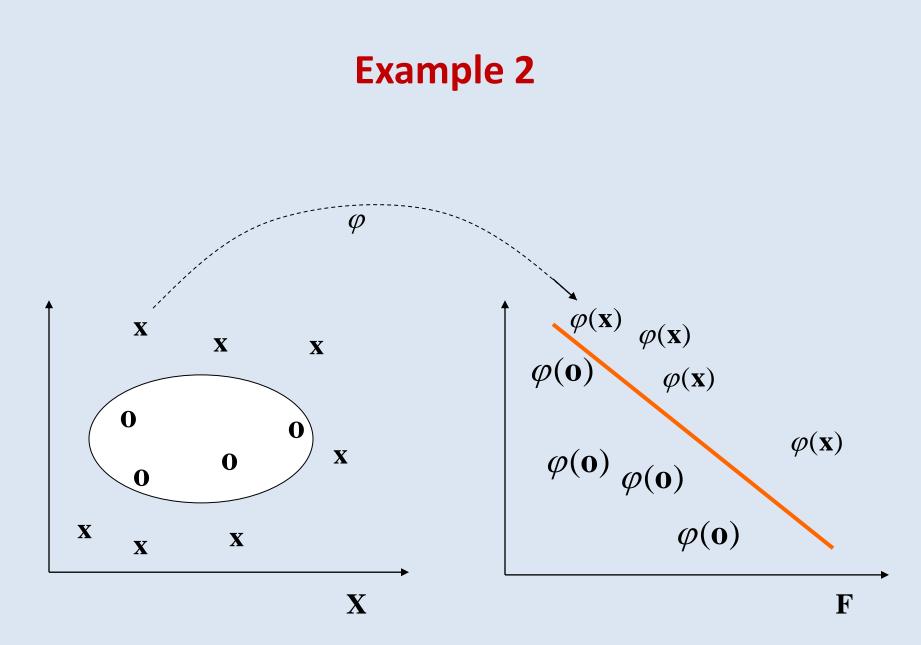
 $_i + \beta_0$

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Example 1: Construct a linear feature space using $\phi(x)$



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- 5. Estimate the constant term w_0
- Set of support vectors $S = \{x_i : y_i(w^T \phi(x_i) + w_0) = 1\}$
- Substituting

we take:

$$\hat{w} = \sum_{i=1}^{N} a_{j} y_{j} \phi(x_{j})$$
$$y_{i} \left(\sum_{x_{j} \in S} a_{j} y_{j} \phi(x_{j})^{T} \phi(x_{i}) + w_{0} \right) = 1 \quad \forall x_{i} \in S$$

Summing all:

$$\sum_{x_i \in S} y_i \left(\sum_{x_j \in S} a_j y_j K(x_j, x_i) + w_0 \right) = N_s = |S|$$
size of S

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Applications

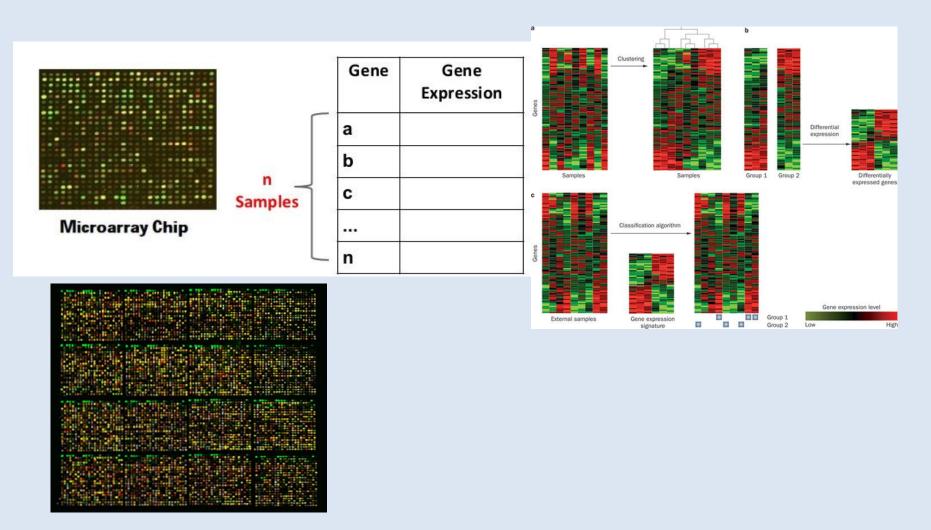
- Bioinformatics
- Text categorization mining



- Handwritten character recognition
- Computer Vision
- Time series analysis
- •

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• Bioinformatics – gene expression data



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• Text categorization – mining

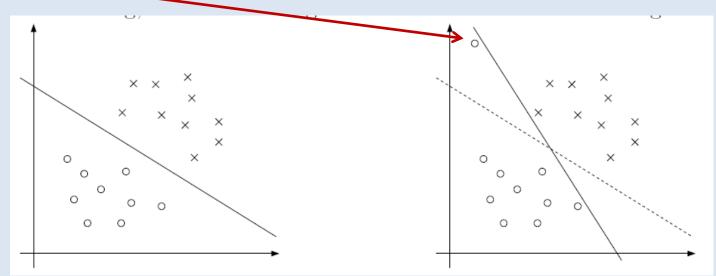


Bag of words (lexicon)

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Nonlinear SVM The non-separable case

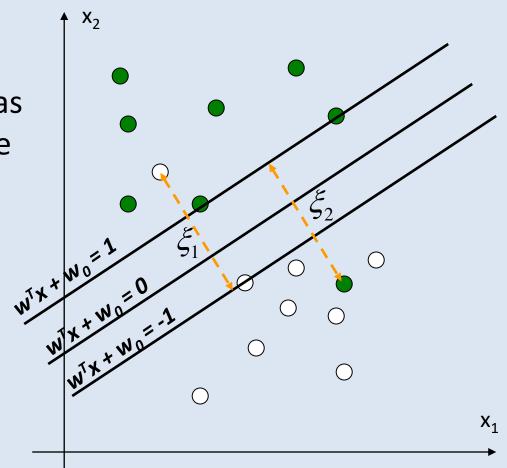
- ✓ Mapping data to a high dimensional space, via $\phi(x)$, increase the likelihood the data be separable.
- ✓ However, this cannot be guaranteed.
- Also, separating hyperplane might be susceptible to outliers.



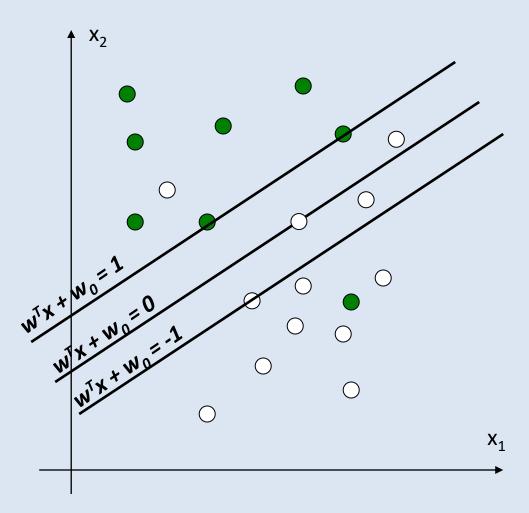
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Nonlinear SVM The non-separable case

- Need to make the algorithm work for nonlinearly separable cases, as well as to be less sensitive to outliers.
- Introduction of auxiliary variables \$\xi_i\$ which allow errors, i.e. samples being in erroneous side of margin.



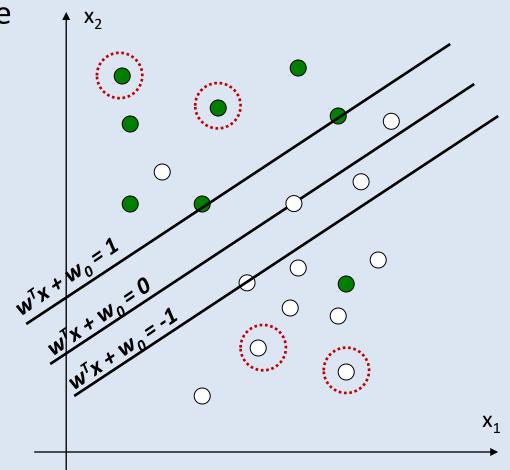
For any sample
$$x_i : \frac{\xi_i}{\xi_i} = |y_i - f(x_i)|$$



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For any sample
$$x_i : \frac{\xi_i}{\xi_i} = |y_i - f(x_i)|$$

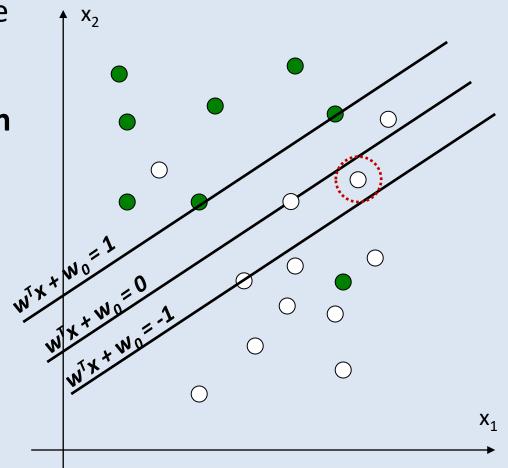
If x_i found in the right side (no error), then $\xi_i = 0$.



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For any sample
$$x_i : \frac{\xi_i}{\xi_i} = |y_i - f(x_i)|$$

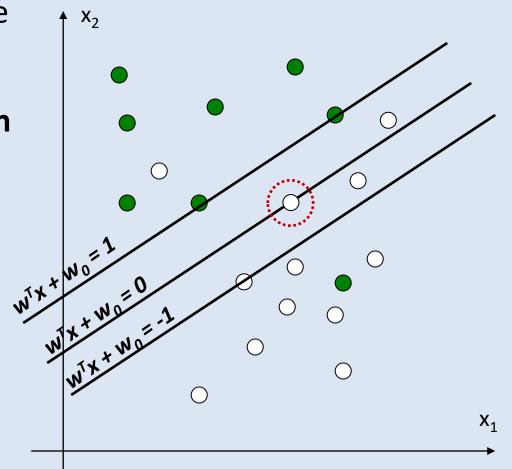
- If x_i found in the right side
 (no error), then ξ_i = 0.
- If found inside the margin but in the right side ξ_i < 1



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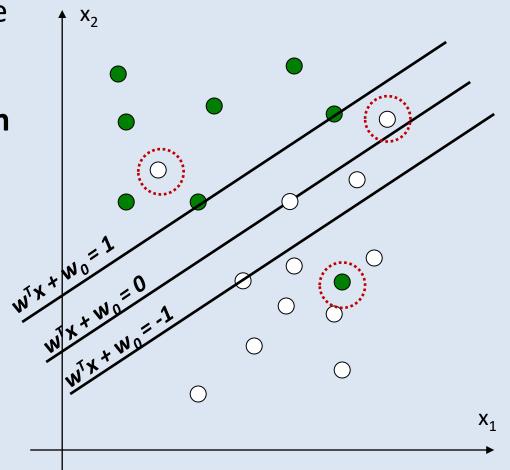
For any sample
$$x_i : \frac{\xi_i}{\xi_i} = |y_i - f(x_i)|$$

- If x_i found in the right side
 (no error), then ξ_i = 0.
- If found inside the margin but in the right side ξ_i < 1
- If found exactly in the hyperplane where $w^T x + w_0 = 0$ then $\xi_i = 1$



For any sample
$$x_i : \frac{\xi_i}{\xi_i} = |y_i - f(x_i)|$$

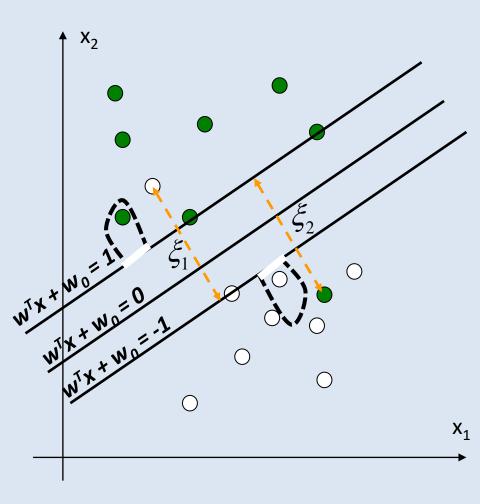
- If x_i found in the right side
 (no error), then ξ_i = 0.
- If found inside the margin but in the right side ξ_i < 1
- If found exactly in the hyperplane where $w^T x + w_0 = 0$ then $\xi_i = 1$
- If it is wrong classified then ξ_i > 1



 We allow margin be less than 1

$$\forall i \quad y_i \left(w^T x_i + w_0 \right) \ge 1 - \xi_i$$

 ξ_i plays to role of error tolerance for every sample
 x_i and sets up the local margin which allows
 margin to enter the space of other class.



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Nonlinear SVM

Objective function:

•
$$\sum_{i=1}^{N} \xi_i$$
 is the total error tolerance of training set

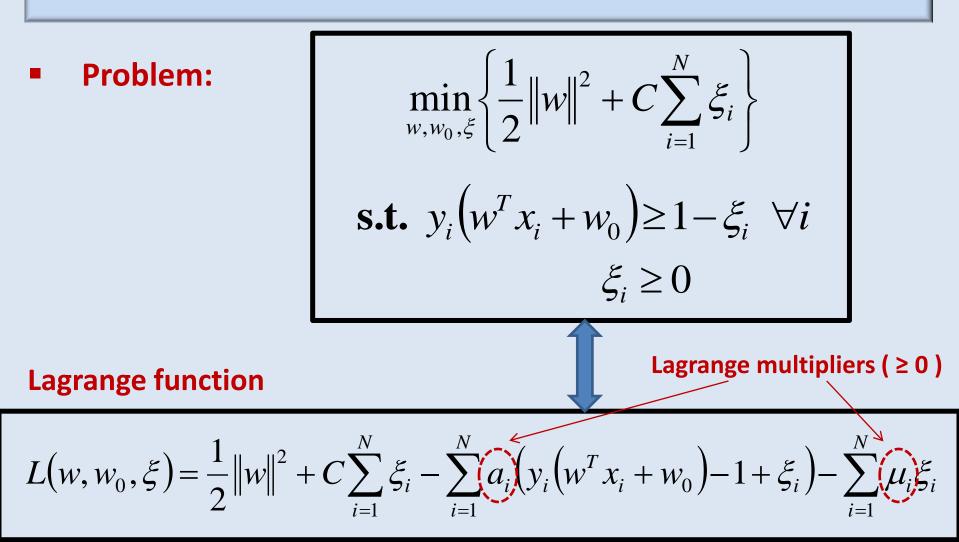
Problem:

$$\min_{w,w_0,\xi} \left\{ \frac{1}{2} \|w\|^2 + C \sum_{i=1}^N \xi_i \right\}$$

s.t. $y_i \left(w^T x_i + w_0 \right) \ge 1 - \xi_i \quad \forall i$
 $\xi_i \ge 0$

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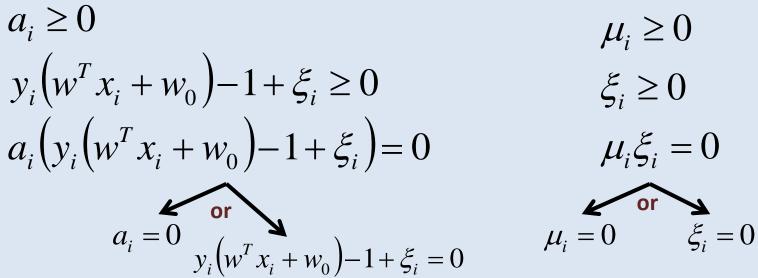




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minimize
$$L(w, w_0, \xi) = \frac{1}{2} \|w\|^2 + C \sum_{i=1}^N \xi_i - \sum_{i=1}^N a_i (y_i (w^T x_i + w_0) - 1 + \xi_i) - \sum_{i=1}^N \mu_i \xi_i$$

KKT conditions



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minimize
$$L(w, w_0, \xi) = \frac{1}{2} \|w\|^2 + C \sum_{i=1}^N \xi_i - \sum_{i=1}^N a_i (y_i (w^T x_i + w_0) - 1 + \xi_i) - \sum_{i=1}^N \mu_i \xi_i$$

Partial derivatives

$$\frac{\partial L}{\partial w} = 0 \Longrightarrow \hat{w} = \sum_{i=1}^{N} a_i y_i x_i$$
$$\frac{\partial L}{\partial w_0} = 0 \Longrightarrow \sum_{i=1}^{N} a_i y_i = 0$$
$$\frac{\partial L}{\partial \xi_i} = 0 \Longrightarrow a_i = C - \mu_i$$

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minimize
$$L(w, w_0, \xi) = \frac{1}{2} ||w||^2 + C \sum_{i=1}^N \xi_i - \sum_{i=1}^N a_i (y_i (w^T x_i + w_0) - 1 + \xi_i) - \sum_{i=1}^N \mu_i \xi_i$$

Dual form of the problem
maximize $L_D(a) = \sum_{i=1}^N a_i - \frac{1}{2} \sum_{i=1}^N \sum_{j=1}^N a_i a_j y_i y_j x_i^T x_j$
s.t. $0 \le a_i \le C$, $\sum_{i=1}^N a_i y_i = 0$

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maximize
$$L_D(a) = \sum_{i=1}^N a_i - \frac{1}{2} \sum_{i=1}^N \sum_{j=1}^N a_i a_j y_i y_j x_i^T x_j$$

s.t. $0 \le a_i \le C$, $\sum_{i=1}^N a_i y_i = 0$

If *a_i* > 0 then *x_i* are support vectors:

$$y_i (w^T x_i + w_0) - 1 + \xi_i = 0$$

• If $a_i < C$ then $\mu_i > 0$ and $\xi_i = 0$. It holds: $y_i \left(w^T x_i + w_0 \right) - 1 = 0$

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maximize
$$L_D(a) = \sum_{i=1}^N a_i - \frac{1}{2} \sum_{i=1}^N \sum_{j=1}^N a_i a_j y_i y_j x_i^T x_j$$

s.t. $0 \le a_i \le C$, $\sum_{i=1}^N a_i y_i = 0$

- If $a_i = C$ then $\mu_i = 0$ and $\xi_i > 0$. Sample x_i is inside the margin
 - If $\xi_i \leq 1$ then x_i is **right classified**,
 - If $\xi_i > 1$ then x_i is wrong classified

maximize
$$L_D(a) = \sum_{i=1}^N a_i - \frac{1}{2} \sum_{i=1}^N \sum_{j=1}^N a_i a_j y_i y_j x_i^T x_j$$

s.t. $0 \le a_i \le C$, $\sum_{i=1}^N a_i y_i = 0$

- If $a_i = C$ then $\mu_i = 0$ and $\xi_i > 0$. Sample x_i is inside the margin
 - If $\xi \le 1$ then x_i is **right classified**,
 - If $\xi_i > 1$ then x_i is wrong classified

The SMO algorithm

J. Platt, Fast Training of Support Vector Machines using Sequential Minimal Optimization, MIT Press (1998).

- Sequential Minimal Optimization (SMO)
- Solving the dual problem

maximize
$$L_D(a) = \sum_{i=1}^N a_i - \frac{1}{2} \sum_{i=1}^N \sum_{j=1}^N a_i a_j y_i y_j x_i^T x_j$$

s.t. $0 \le a_i \le C$, $\sum_{i=1}^N a_i y_i = 0$

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SMO algorithmic structure

- SMO breaks this problem into a series of smallest possible sub-problems, which are then solved sequentially.
- The smallest problem involves **two such multipliers :**

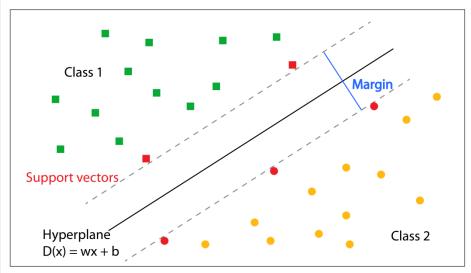
$$0 \le a_1, a_2 \le C$$
 and $a_1y_1 + a_2y_2 = -\sum_{i=3}^N a_iy_i = \zeta$

• This reduced problem can be solved analytically:

$$a_{1} = y_{1}(\zeta - a_{2}y_{2}) \qquad \hat{a}_{2} : \max_{a_{2}} \left\{ L_{D}(a) \right\}_{a_{1} = y_{1}(\zeta - a_{2}y_{2})}$$
$$a_{2}^{(new)} = \begin{cases} C & \text{if } \hat{a}_{2} > C \\ \hat{a}_{2} & \text{if } 0 \le \hat{a}_{2} \le C \\ 0 & \text{if } \hat{a}_{2} < 0 \end{cases} \qquad \hat{a}_{1} = y_{1}(\zeta - \hat{a}_{2}y_{2})$$

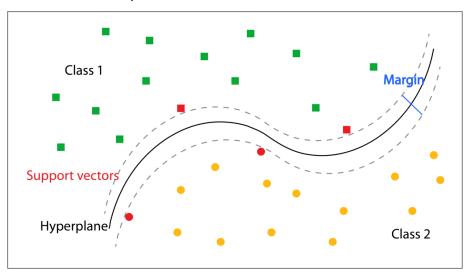
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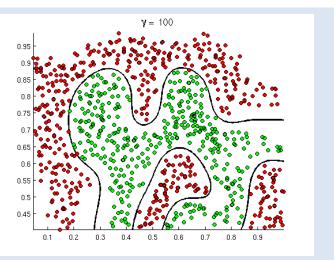
Examples of non-linear svm classification

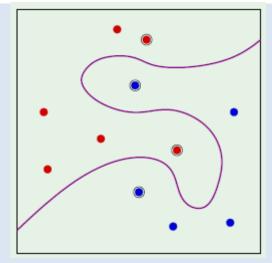


A. Linear separation

B. Non-linear separation







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Multi-class Classification Working with more than 2 classes

Two general schemes

> one vs. all classifiers

Pairwise Classifiers

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One vs. All Classifiers

- One classifier for every class j = 1, ..., K
- Samples of examined class are positive (label +1), while rest samples from all other K-1 classes are negative examples with label -1.
- Training the K different classifiers and construct functions:

$$f_j(x) = \varphi \left(w_{j0} + \sum_{i=1}^d w_{ji} x_i \right)$$

 Decision rule: Classify an unknown sample x to the class with the maximum function value:

$$c(x) = \underset{j=1,\dots,K}{\operatorname{arg\,max}} f_j(x)$$

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Pairwise Classifiers

- One classifier for every pair of classes (j, k)
- Training the K*(K-1) classifiers and construct separating functions for every pair:

$$f_{jk}(x) = \varphi \left(w_0^{(j,k)} + \sum_{j=1}^d w_j^{(j,k)} x_j \right)$$

- **Decision rule:** Classify an unknown sample x to the class with the most votes among all classifiers.
- In case of equivalence use the functions' values for taking the decision.