SVM learning

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R. BASILI
DIPARTIMENTO DI INGEGNERIA DELL'IMPRESA
UNIVERSITÀ DI ROMA "TOR VERGATA"
EMAIL: BASILI@INFO.UNIROMA2.IT

Summary

Perceptron Learning

Limitations of linear classifiers

Support Vector Machines

- Maximal margin classification
- Optimization with *hard* margin
- Optimization with *soft* margin

The roles of kernels in SVM-based learning

Linear Classifiers (1)

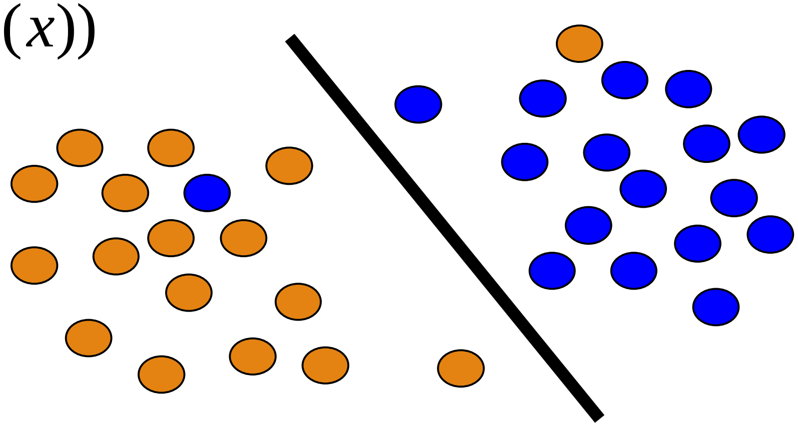
An hyperplane has equation :

$$f(\vec{x}) = \vec{x} \cdot \vec{w} + b, \quad \vec{x}, \vec{w} \in \Re^n, \; b \in \Re$$

$\vec{x}$ is the vector of the instance to be classified
$\vec{w}$ is the hyperplane gradient

Classification function:

$$h(x) = \mathrm{sign}(f(x))$$



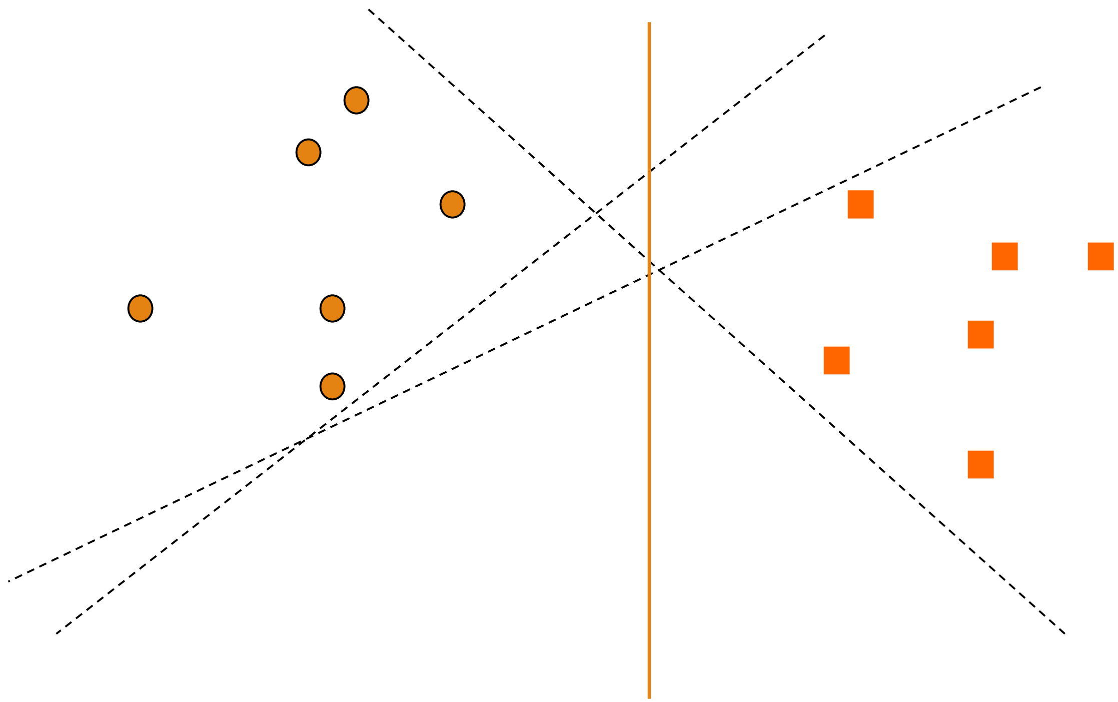
Linear Classifiers (2)

Computationally simple.

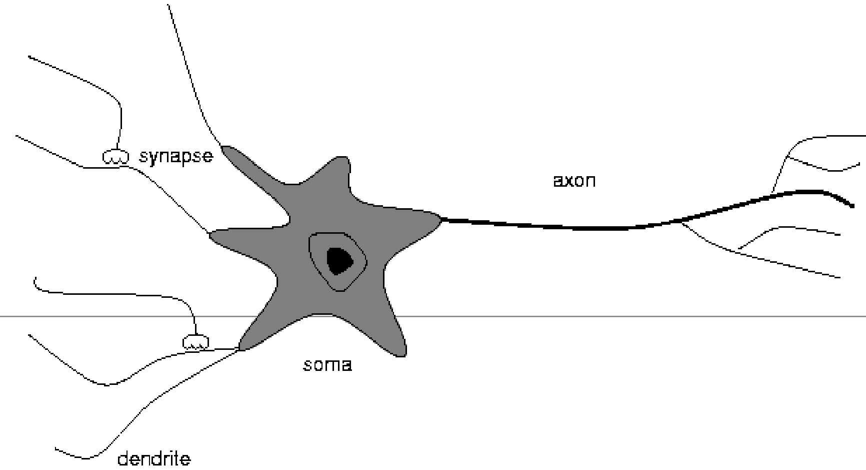
Basic idea: select an hypothesis that makes no mistake over training-set.

The separating function is equivalent to a neural net with just one neuron (perceptron)

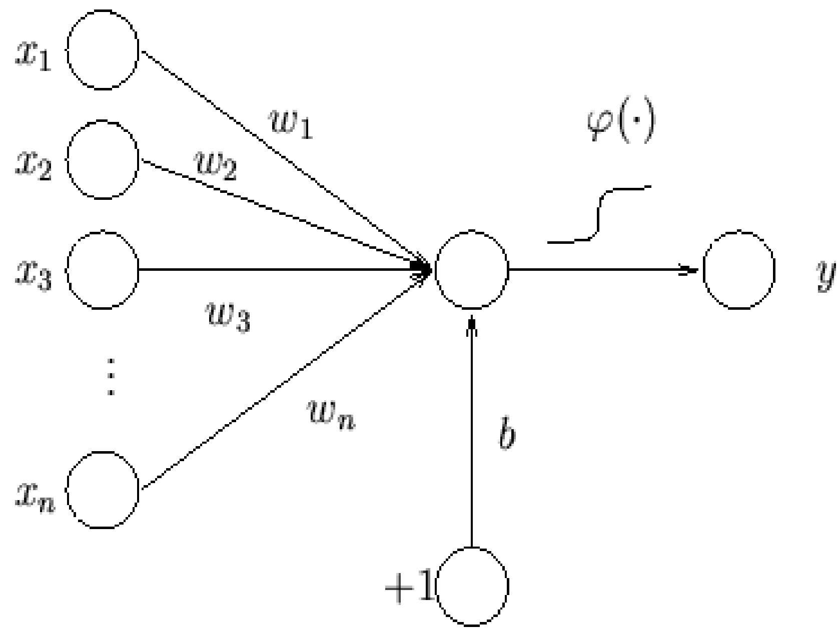
Which hyperplane?



Perceptron



$$\varphi(\vec{x}) = \operatorname{sgn}\left(\sum_{i=1..n} w_i \times x_i + b\right)$$



Notation

The functional margin of an example $(\vec{x}_i, y_i)$

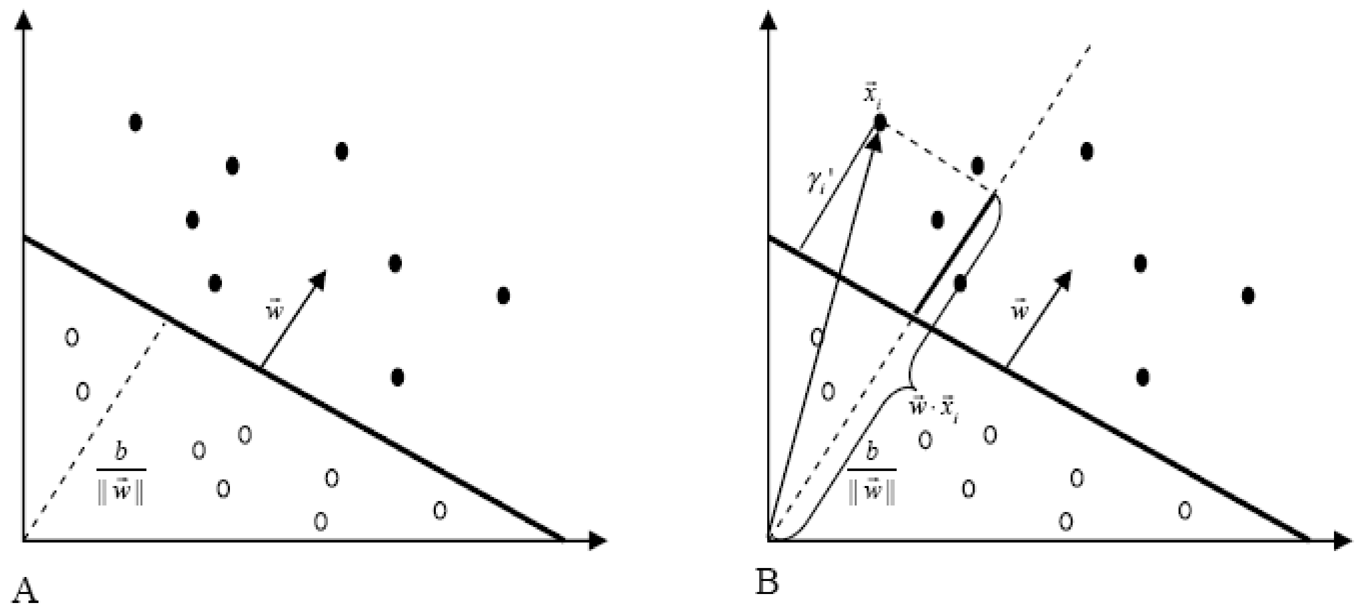
with respect to an hyerplane is:

$$\gamma_i = y_i(\vec{w} \cdot \vec{x}_i + b)$$

The distribution of functional margins of an hyperplane $(\vec{w}, b)$ with respect to a training set *S* is the distribution of margins of the examples in *S*.

The functional margin of an hyperplane $(\vec{w}, b)$ with respect to *S* is the minimum margin of the distribution

Geometric Margin



Inner product and cosine distance

From

$$\cos(\vec{x},\vec{w}) = \frac{\vec{x}\cdot\vec{w}}{\|\vec{x}\|\cdot\|\vec{w}\|}$$

It follows that:

$$\|\vec{x}\|\cos(\vec{x},\vec{w}) = \frac{\vec{x}\cdot\vec{w}}{\|\vec{w}\|} = \vec{x}\cdot\frac{\vec{w}}{\|\vec{w}\|}$$

Norm of $\vec{x}$ times $\vec{x}$ cosine $\vec{w}$, i.e. the projection of $\vec{x}$ onto $\vec{w}$

Notations (2)

By normalizing the hyperplan equation, i.e. $\left(\frac{\vec{w}}{\|\vec{w}\|}, \frac{b}{\|\vec{w}\|}\right)$

we get the geometrical margin

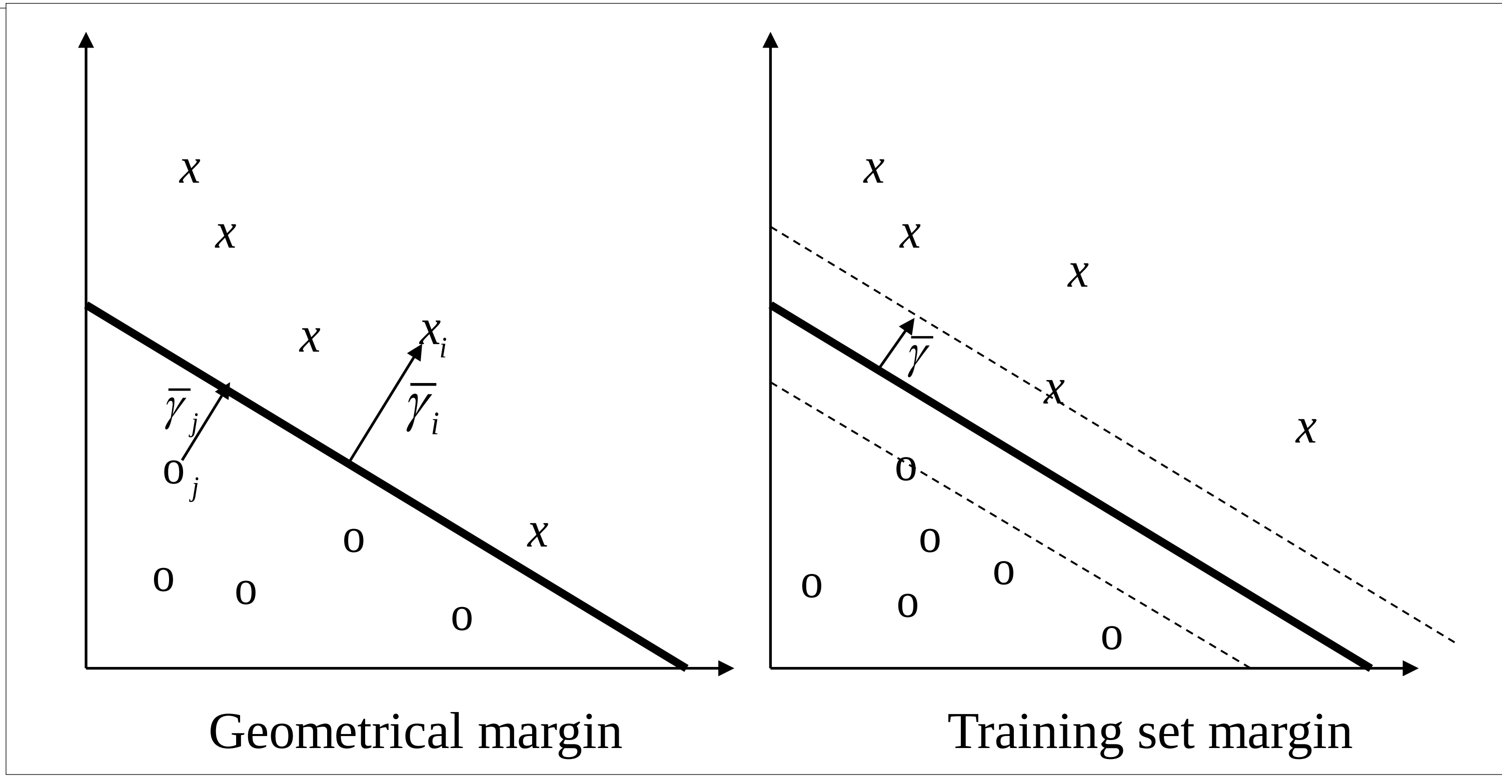
$$\gamma_i = y_i(\vec{w} \cdot \vec{x}_i + b)$$

The geometrical margin corresponds to the distance of points in S from the hyperplane.

For example in $\Re^2$

$$d(P, r) = \frac{|ax_0 + by_0 + c|}{\sqrt{a^2 + b^2}}$$

Geometric margin vs. data points in the training set

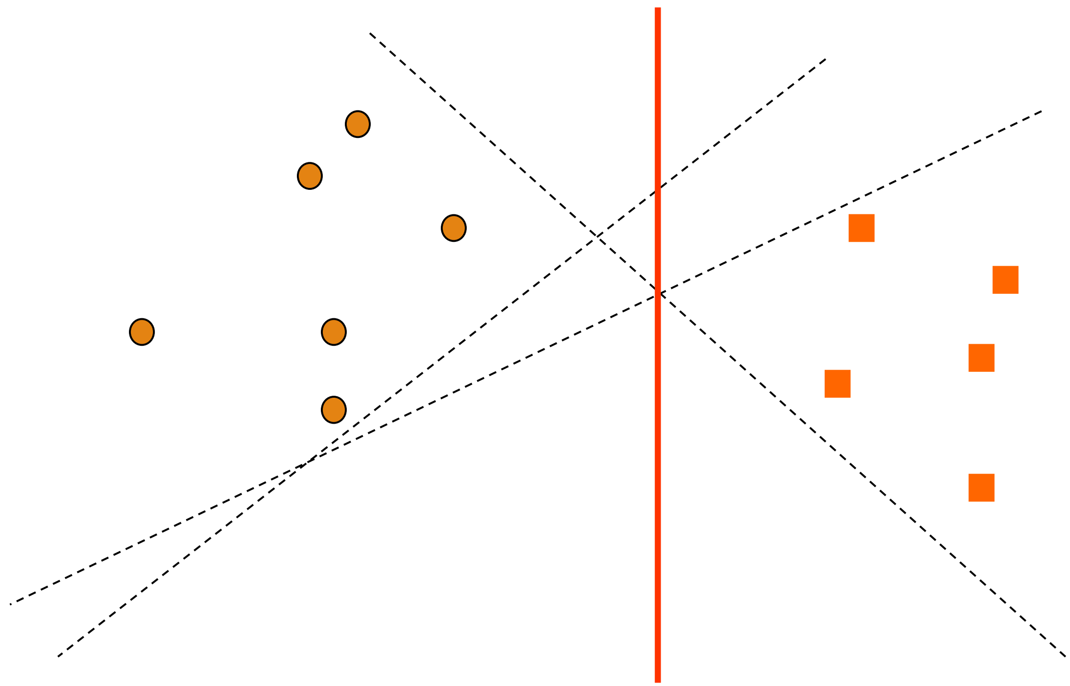


Notations (3)

The margin of the training set S is the maximal geometric margin among every hyperplane.

The hyperplane that corresponds to this (maximal) margin is called ***maximal margin hyperplane***

Maximal margin vs other margins



Perceptron: on-line algorithm

$\vec{w}_0 \leftarrow \vec{0}; b_0 \leftarrow 0; k \leftarrow 0; R \leftarrow \max_{1 \le i \le l} \| \vec{x}_i \|$

Repeat

for i = 1 to ℓ

if $y_i(\vec{w}_k \cdot \vec{x}_i + b_k) \le 0$ then

Classification Error

$$\boxed{\begin{aligned} \vec{w}_{k+1} &= \vec{w}_k + \eta y_i \vec{x}_i \\ b_{k+1} &= b_k + \eta y_i R^2 \end{aligned}}$$

adjustments

k = k + 1

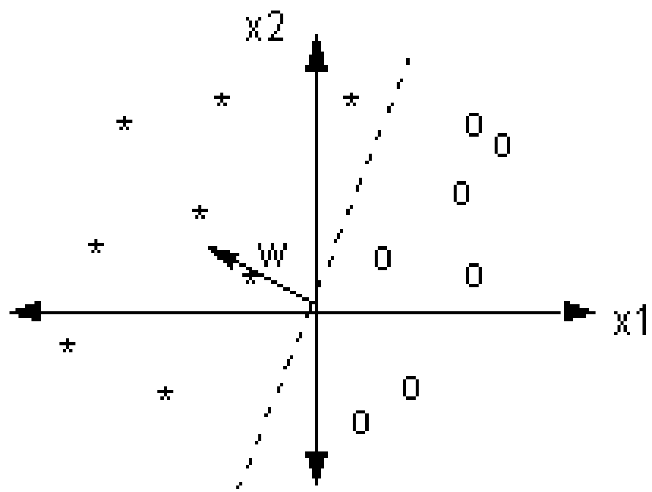
endif

endfor

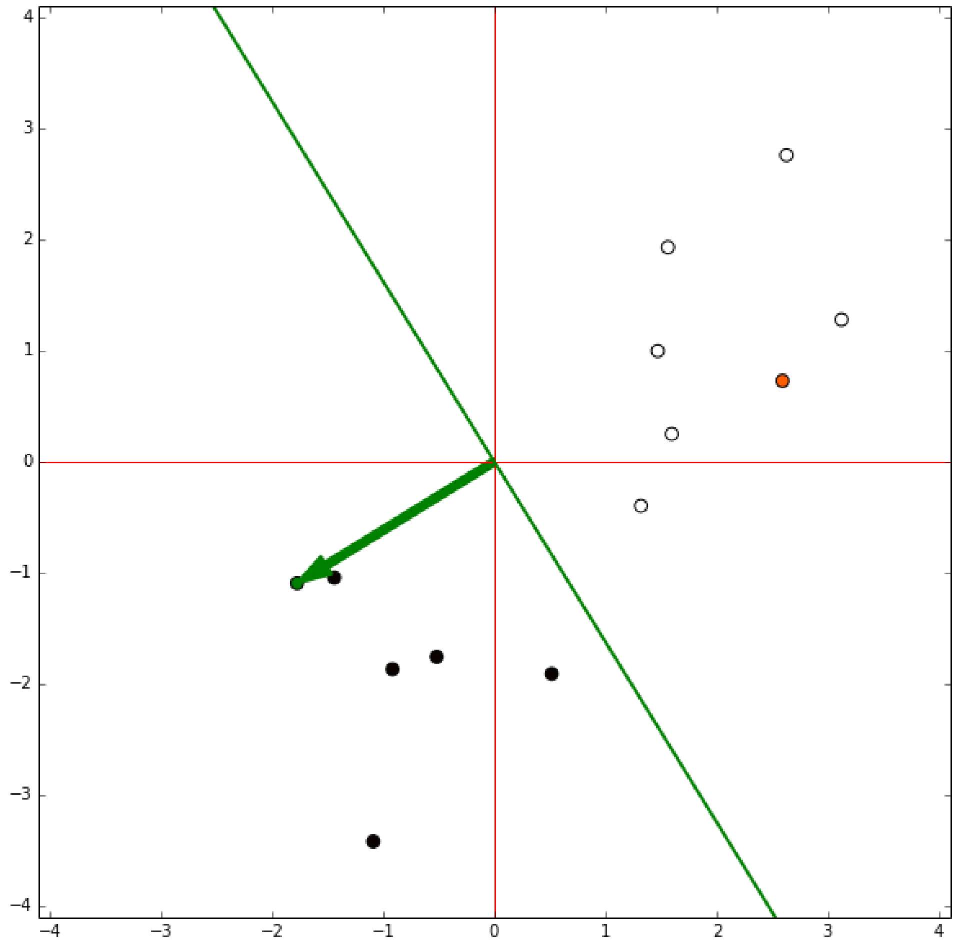
until no error is found

return k, $(\vec{w}_k, b_k)$

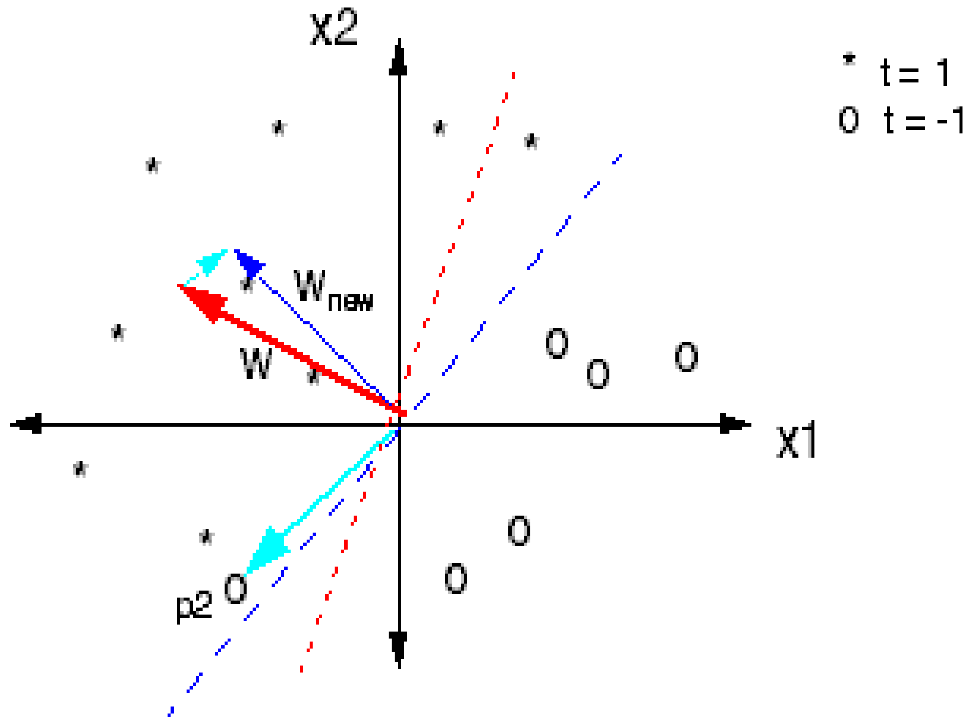
The mechanics of the perceptron



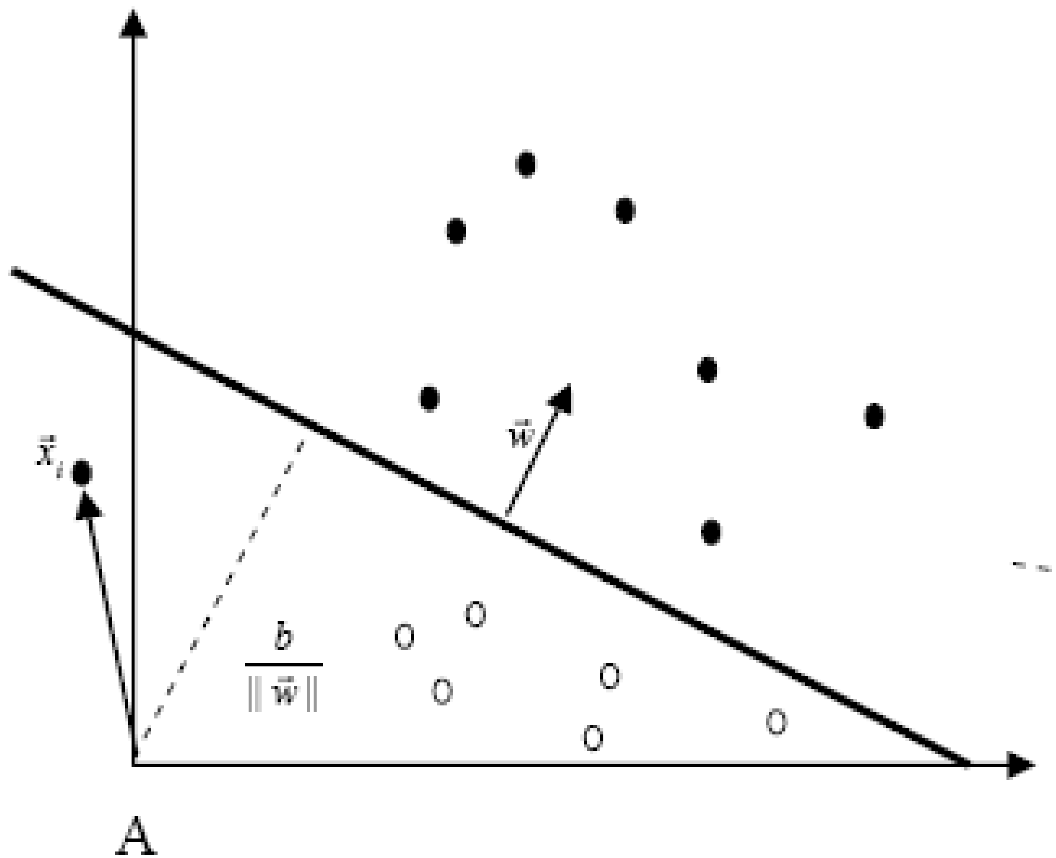
The mechanics of Perceptron: *on-line learning*



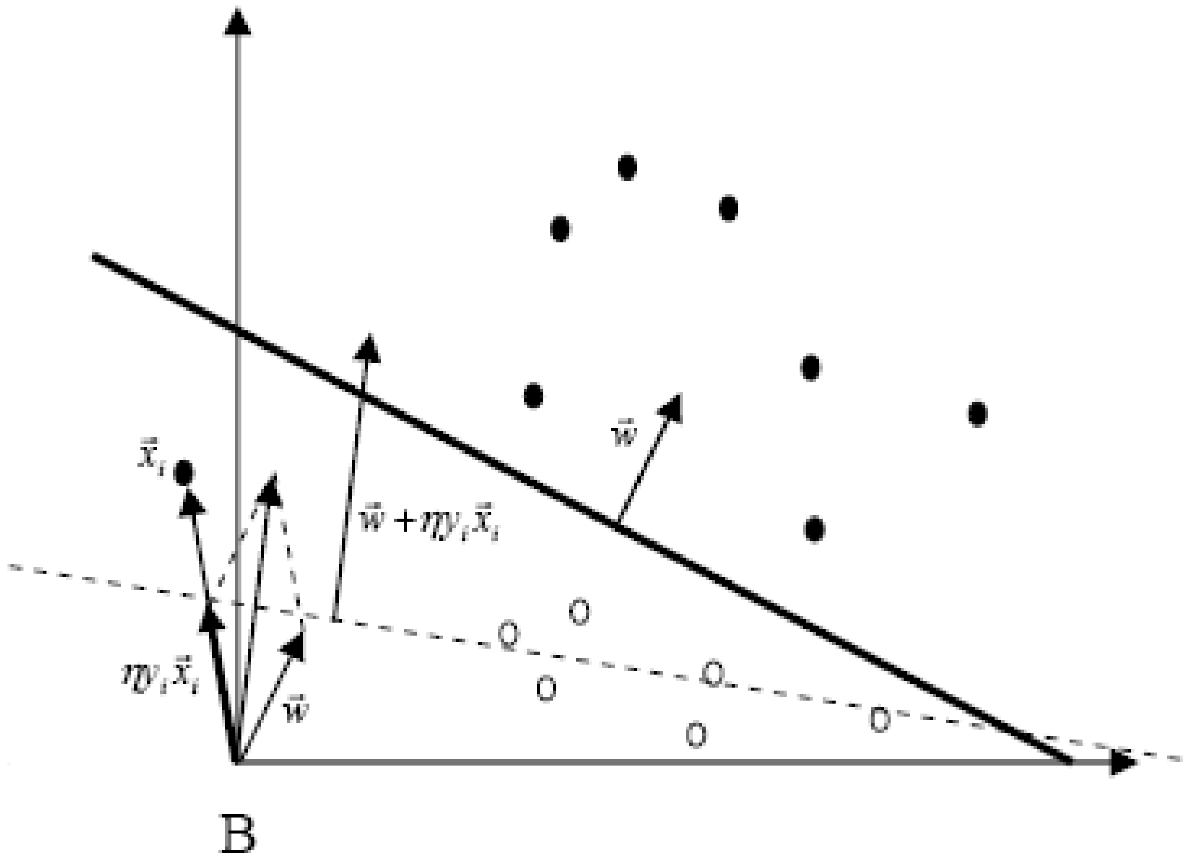
The adjusted hyperplane



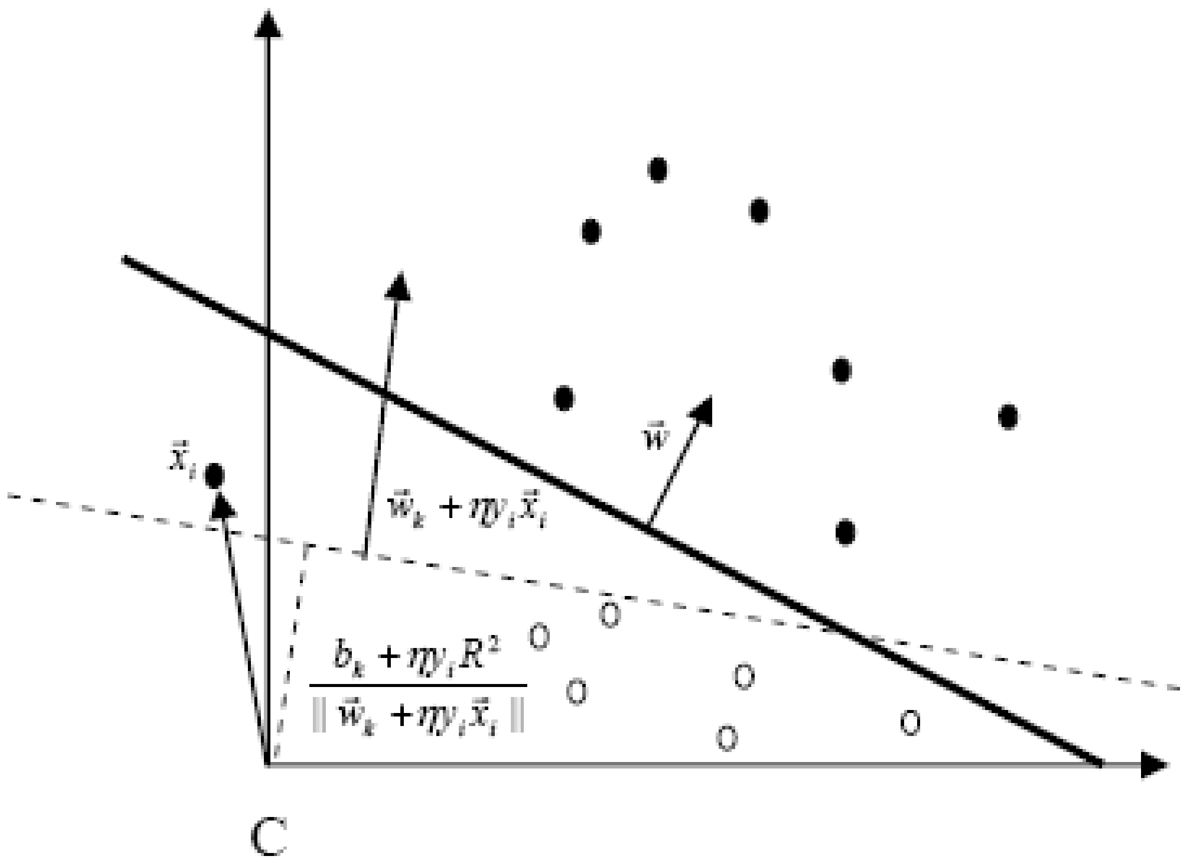
Perceptron: the management of an individual instance *x*



Adjusting the (hyper)plane directions



Adjusting the distance from the origins



Novikoff theorem

Given a non-trival training-set S $(|S|=m>>0)$ and:

$$R = \max_{1 \le i \le l} \| x_i \| .$$

If a vector $\mathbf{w}^*, \| \mathbf{w}^* \| = 1$, exists such that:

$$y_i(\langle \mathbf{w}^*, \mathbf{x}_i \rangle + b^*) \ge \gamma \qquad i = 1, \ldots, m,$$

with $\gamma > 0$, then the maximal number of errors made by the perceptron is :

$$t^* = \left(\frac{2R}{\gamma} \right)^2 ,$$

Consequences

The theorem states that whatever is the length of the geometrical margin, if data instances are linearly separable, then the perceptron is able to find the separating hyperplane in a finite number of steps.

This number is inversely proportional to the square of the margin.

This bound is invariant to the scale of individual *patterns*.

The learning rate is not critical but only affects the rate of convergence.

Duality

The decision function of linear classifiers can be written as follows:

$$h(x) = \operatorname{sgn}(\vec{w} \cdot \vec{x} + b) = \operatorname{sgn}\Big(\sum_{j=1...m} \alpha_j y_j \vec{x}_j \cdot \vec{x} + b\Big) =$$

$$\operatorname{sgn}\Big(\big(\sum_{i=1...m} \alpha_j y_j \vec{x}_j \cdot \vec{x}\big) + b\Big)$$

as well the adjustment function

$$\text{if} \;\; y_i\Big(\sum_{j=1...m} \alpha_j y_j \vec{x}_j \cdot \vec{x}_i + b\Big) \leq 0 \qquad \text{then} \;\; \alpha_i = \alpha_i + \eta$$

The learning rate η impacts only in the re-scaling of the hyperplanes, and does not influence the algorithm ($\eta = 1$.)

$\Longrightarrow$ Training data only appear in the scalar products!!

First property of SVMs

DUALITY is the first property of Support Vector Machines

The SVMs are learning machines of the kind:

$$f(x) = \mathrm{sgn}(\vec{w} \cdot \vec{x} + b) = \mathrm{sgn}\Big(\sum_{j=1\ldots m} \alpha_j y_j \vec{x}_j \cdot \vec{x} + b\Big)$$

It must be noted that (input, i.e. training & testing instances) data only appear in the scalar product

The matrix $G = \left(\left\langle \mathbf{x}_i \cdot \mathbf{x}_j \right\rangle\right)_{i,j=1}^{l}$ is called Gram matrix of the incoming distribution

Limitations of linear classifiers

- Problems in dealing with non linearly separale data
- Treatment of Noisy Data
- Data must be in real-value vector formalism, i.e. a underlying metric space topology is required

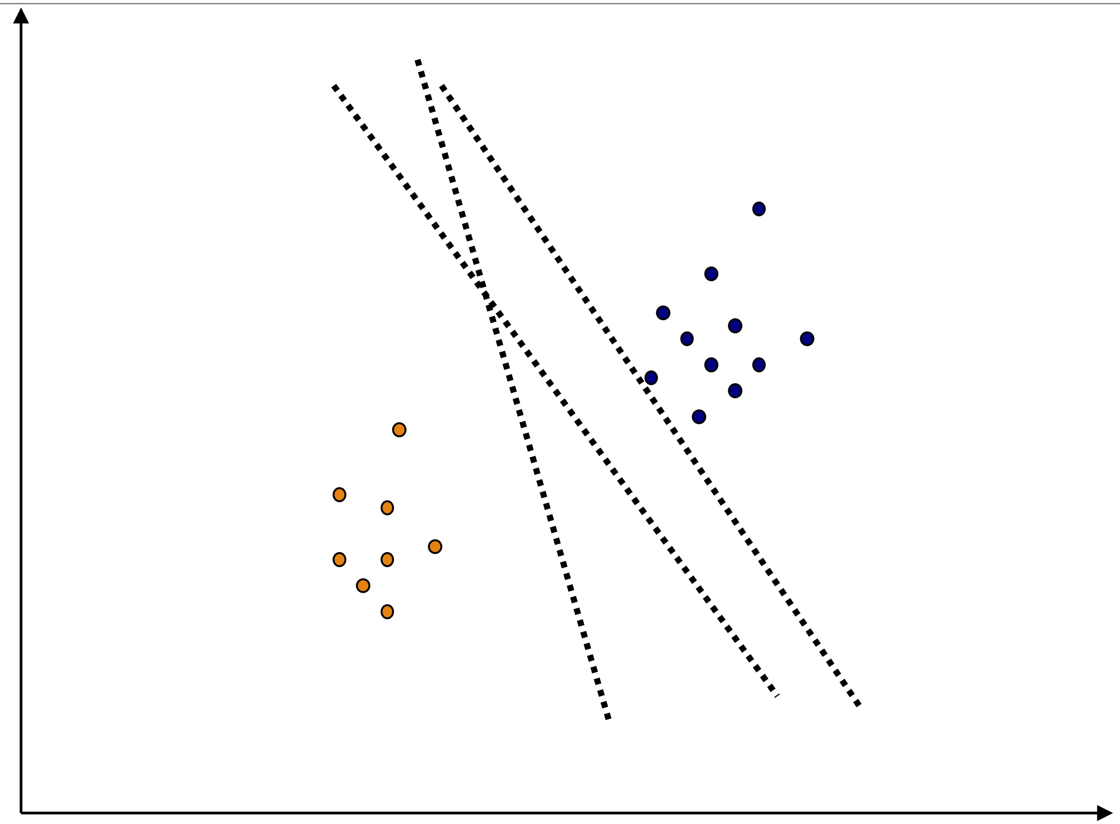
Solutions

Artificial Neural Networks (ANN) approach: augment the number of neurons, and organize them into layers $\Rightarrow$ multilayer neural neworks $\Rightarrow$ Learning through the Back-propagation algorithm (Rumelhart & McLelland, 91).

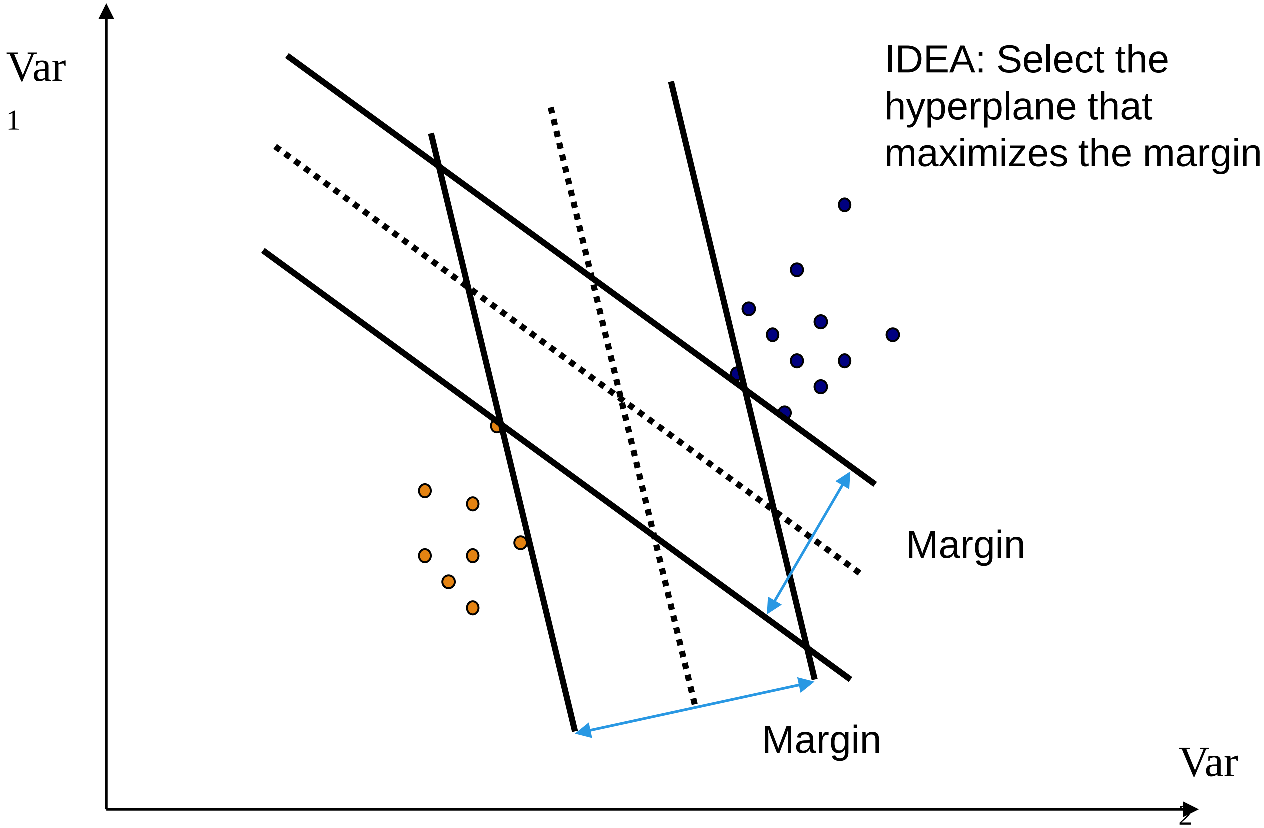
SVMs approach: Extend the representation by exploiting kernel functions (i.e. non linear often task dependent functions described by the Gram matrix).

- In this way the learning algorithms are decoupled from the application domain, that can be coded esclusively through task-specific kernel functions.
  - The feature modeling does not necessarily have to produce real-valued vectors but can be derived from intrinsic properties of the training objects
  - Complex data structures, e.g. sequences, trees, graphs or PCA-like decompositions (e.g. LSA), can be managed by individual kernels

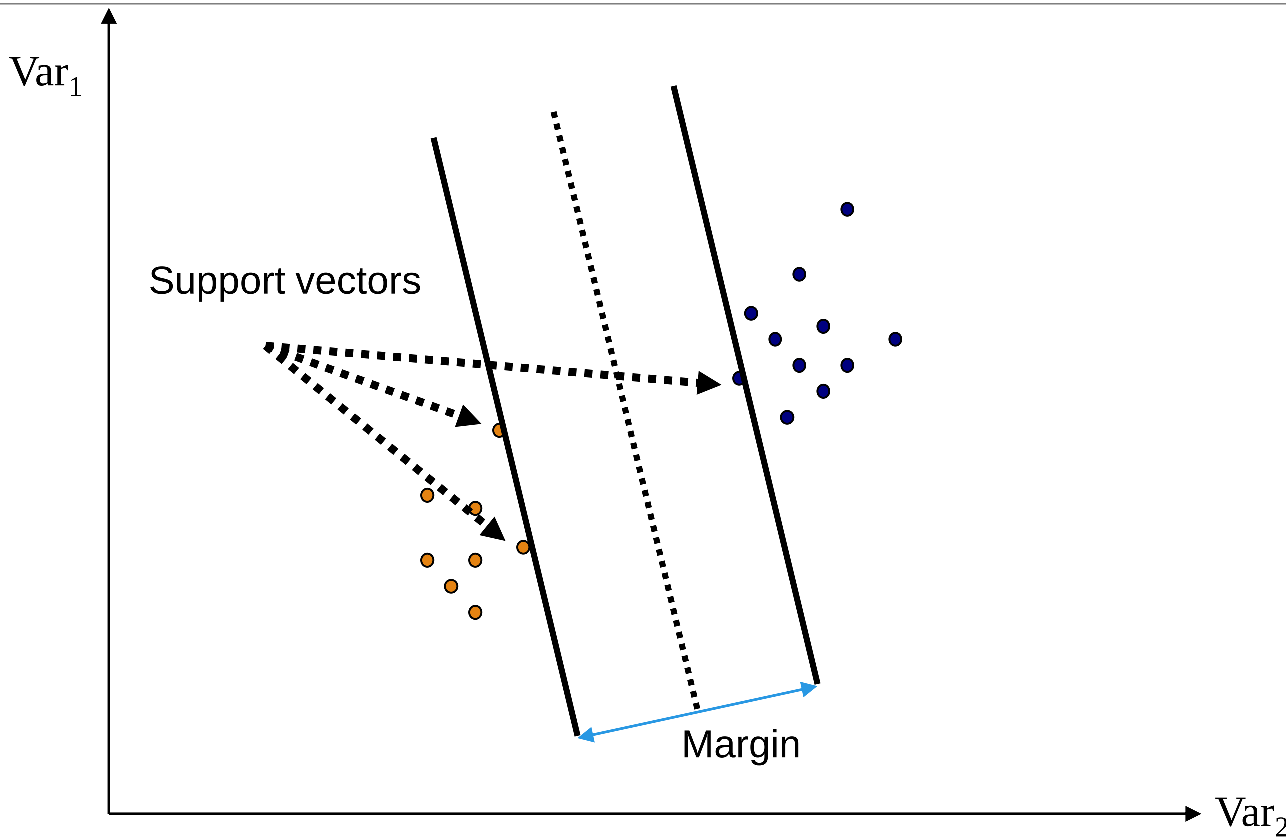
Which hyperplane?



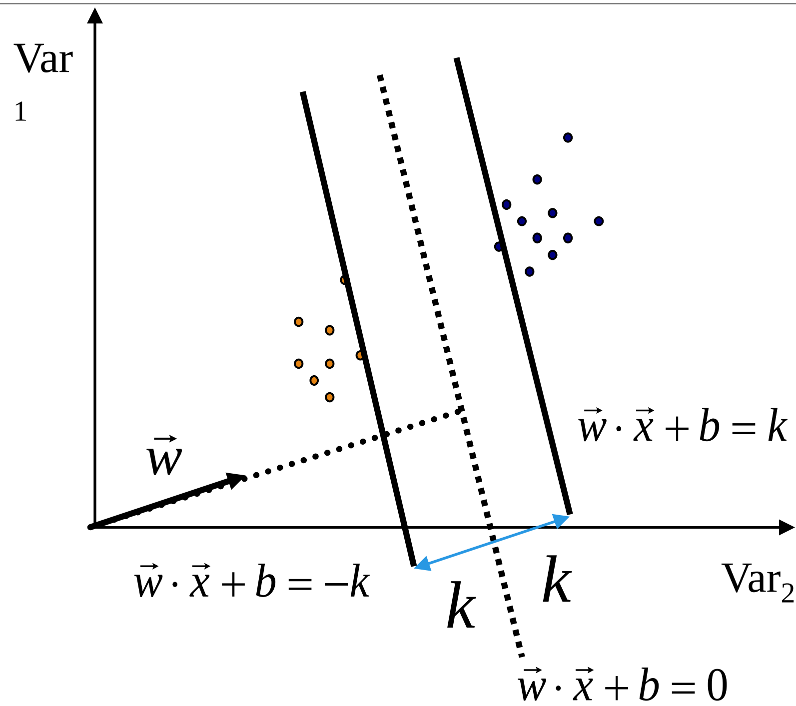
Maximum Margin Hyperplanes



Support Vectors



How to get the maximum margin?



The geometric margin is:

$$\frac{2|k|}{\|w\|}$$

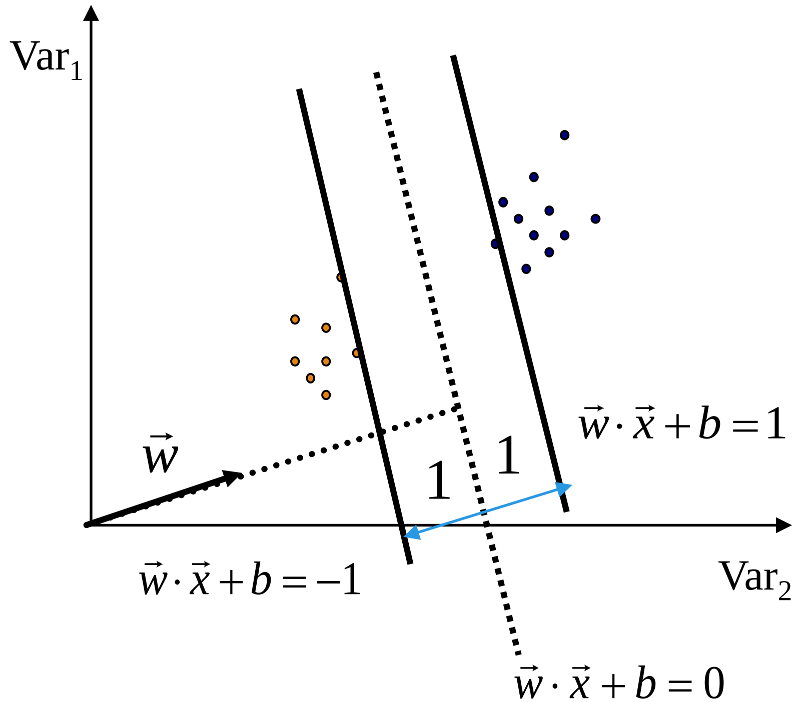
Optimization problem

$$MAX \ \frac{2|k|}{\|\vec{w}\|}$$

$$\vec{w} \cdot \vec{x} + b \geq +k, \ \text{if } \vec{x} \text{ is a positive ex.}$$

$$\vec{w} \cdot \vec{x} + b \leq -k, \ \text{se } \vec{x} \text{ is a negativ ex.}$$

Scaling the hyperplane …



There is a scale for which *k=1*.

The optimization problem becomes:

$$\max \frac{2}{\|\vec{w}\|}$$

$$\vec{w}\cdot\vec{x}+b \geq +1, \text{ if } \vec{x} \text{ is positive}$$

$$\vec{w}\cdot\vec{x}+b \leq -1, \text{ if } \vec{x} \text{ is negative}$$

The optimization problem

The optimal hyperplane satyisfies:

- Minimize $\tau(\vec{w}) = \frac{1}{2}\|\vec{w}\|^2$
- Under: $y_i\,((\vec{w} \cdot \vec{x}_i) + b) \geq 1 \quad i = 1, \ldots, m$

The dual problem is simpler

Definition of the Lagrangian

Def. 2.24 *Let $f(\vec{w})$, $h_i(\vec{w})$ and $g_i(\vec{w})$ be the objective function, the equality constraints and the inequality constraints (i.e. $\geq$) of an optimization problem, and let $L(\vec{w}, \vec{\alpha}, \vec{\beta})$ be its Lagrangian, defined as follows:*

$$L(\vec{w}, \vec{\alpha}, \vec{\beta}) = f(\vec{w}) - \sum_{i=1}^{m} \alpha_i g_i(\vec{w}) - \sum_{i=1}^{l} \beta_i h_i(\vec{w})$$

$$f(\vec{w}) = \tau(\vec{w}) = \frac{1}{2}\|\vec{w}\|^2$$

$$y_i((\vec{w} \cdot \vec{x}_i) + b) \geq 1, \quad i = 1, \ldots, l$$

$\vec{\beta}$ are not used as no equality constrant is needed in the primal equation

Dual optimization problem

The ***Lagrangian dual problem*** *of the above primal problem is*

$$maximize \quad \theta(\vec{\alpha}, \vec{\beta})$$

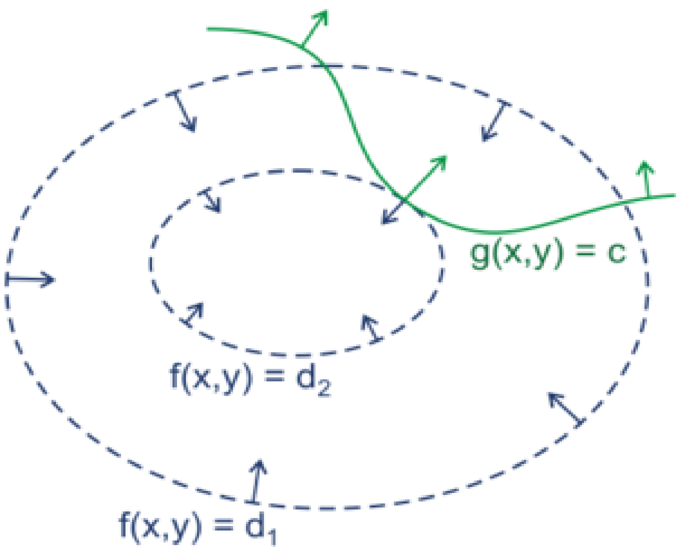
$$subject\ \ to \quad \vec{\alpha} \geq \vec{0}$$

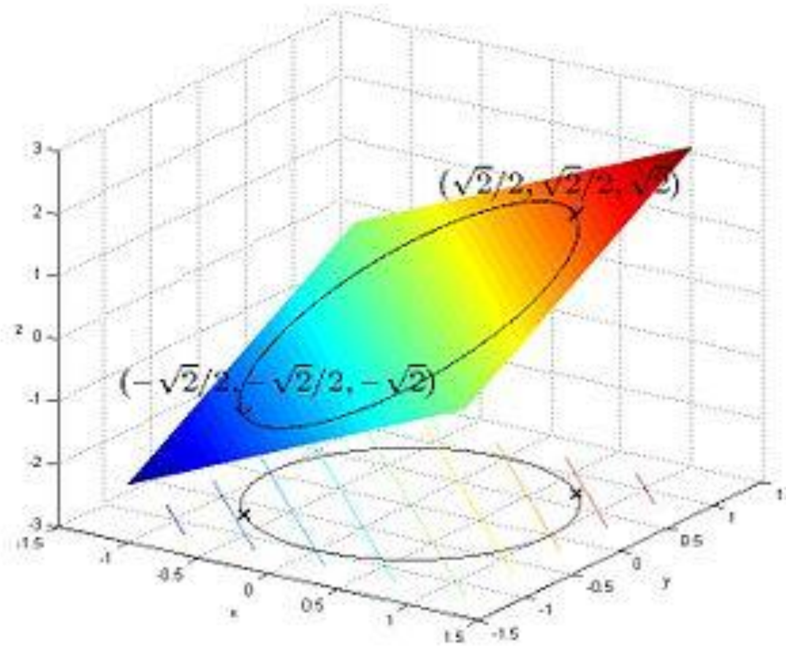
where $\theta(\vec{\alpha}, \vec{\beta}) = inf_{w \in W} \;\; L(\vec{w}, \vec{\alpha}, \vec{\beta})$

Notice that the multipliers $\vec{\beta}$ are not used in the dual optimization problem as no equality constrant is imposed in the primal form

Graphically:

Two examples of constrained optmization (with equalities)





$$f(x,y) = x^2 + y^2$$
$$g(x,y) = c$$

$$f(x,y) = x + y$$
$$g(x,y) = x^2 + y^2 - 1$$

Dual Optimization problem

The **Lagrangian dual problem** *of the above primal problem is*

$$maximize \quad \theta(\vec{\alpha}, \vec{\beta})$$

$$subject \ \ to \quad \vec{\alpha} \geq \vec{0}$$

$$where \ \theta(\vec{\alpha}, \vec{\beta}) = inf_{w \in W} \quad L(\vec{w}, \vec{\alpha}, \vec{\beta})$$

Notice that the multipliers $\vec{\beta}$ are not used in the targeted optimization as no equality constrant is imposed

Transforming into the dual

The Lagrangian corresponding to our problem becomes:

$$L(\vec{w}, b, \vec{\alpha}) = \frac{1}{2}\vec{w} \cdot \vec{w} - \sum_{i=1}^{m} \alpha_i [y_i(\vec{w} \cdot \vec{x}_i + b) - 1]$$

In order to solve the dual problem we compute

$$\theta(\vec{\alpha}, \vec{\beta}) = inf_{w \in W} \; L(\vec{w}, \vec{\alpha}, \vec{\beta})$$

and then imposing derivatives to 0, wrt $\vec{w}$

Transforming into the dual (cont.)

$$L(\vec{w}, b, \vec{\alpha}) = \frac{1}{2}\vec{w}\cdot\vec{w} - \sum_{i=1}^{m} \alpha_i[y_i(\vec{w}\cdot\vec{x}_i + b) - 1]$$

Imposing derivatives = 0 wrt $\vec{w}$

$$\frac{\partial L(\vec{w}, b, \vec{\alpha})}{\partial \vec{w}} = \vec{w} - \sum_{i=1}^{m} y_i \alpha_i \vec{x}_i = \vec{0} \quad \Rightarrow \quad \vec{w} = \sum_{i=1}^{m} y_i \alpha_i \vec{x}_i$$

and wrt *b*

$$\frac{\partial L(\vec{w}, b, \vec{\alpha})}{\partial b} = \sum_{i=1}^{m} y_i \alpha_i = 0$$

Transforming into the dual (cont.)

$$\vec{w} = \sum_{i=1}^{m} y_i \alpha_i \vec{x}_i \qquad \frac{\partial L(\vec{w}, b, \vec{\alpha})}{\partial b} = \sum_{i=1}^{m} y_i \alpha_i = 0$$

… by substituting into the objective function

$$\begin{aligned} L(\vec{w}, b, \vec{\alpha}) &= \frac{1}{2}\vec{w} \cdot \vec{w} - \sum_{i=1}^{m} \alpha_i [y_i(\vec{w} \cdot \vec{x}_i + b) - 1] = \\ &= \frac{1}{2} \sum_{i,j=1}^{m} y_i y_j \alpha_i \alpha_j \vec{x}_i \cdot \vec{x}_j - \sum_{i,j=1}^{m} y_i y_j \alpha_i \alpha_j \vec{x}_i \cdot \vec{x}_j + \sum_{i=1}^{m} \alpha_i \\ &= \sum_{i=1}^{m} \alpha_i - \frac{1}{2} \sum_{i,j=1}^{m} y_i y_j \alpha_i \alpha_j \vec{x}_i \cdot \vec{x}_j \end{aligned}$$

Dual Optimization problem

$$maximize \quad \sum_{i=1}^{m} \alpha_i - \frac{1}{2} \sum_{i,j=1}^{m} y_i y_j \alpha_i \alpha_j \vec{x_i} \cdot \vec{x_j}$$

$$subject\ \ to \quad \alpha_i \geq 0, \quad i = 1, .., m$$

$$\sum_{i=1}^{m} y_i \alpha_i = 0$$

- The formulation depends on the set of variables $\underline{\alpha}$ and not from $\underline{w}$ and b
- It has a simpler form
- It makes explicit the individual contributions (α_i) of (a selected set of) examples (x_i)

Khun-Tucker Theorem

Necessary (and sufficent) conditions for the existence of the optimal solution are the following:

$$\frac{\partial L(\vec{w}^*, \vec{\alpha}^*, \vec{\beta}^*)}{\partial \vec{w}} = \vec{0}$$

$$\frac{\partial L(\vec{w}^*, \vec{\alpha}^*, \vec{\beta}^*)}{\partial \vec{\beta}} = \vec{0}$$

$$\boxed{\alpha_i^* g_i(\vec{w}^*) = 0, \quad i = 1, .., m}$$

$$g_i(\vec{w}^*) \leq 0, \quad i = 1, .., m$$

$$\alpha_i^* \geq 0, \quad i = 1, .., m$$

$$\vec{w} = \sum_{i=1}^{m} y_i \alpha_i \vec{x}_i$$

$$\sum_{i=1}^{m} y_i \alpha_i = 0$$

Karush-Kuhn-Tucker constraint

Some consequences

Lagrange constraints: $\sum_{i=1}^{m} a_i y_i = 0 \qquad \vec{w} = \sum_{i=1}^{m} \alpha_i y_i \vec{x}_i$

Karush-Kuhn-Tucker constraints

$$\alpha_i \cdot [y_i(\vec{x}_i \cdot \vec{w} + b) - 1] = 0, \qquad i = 1, \ldots, m$$

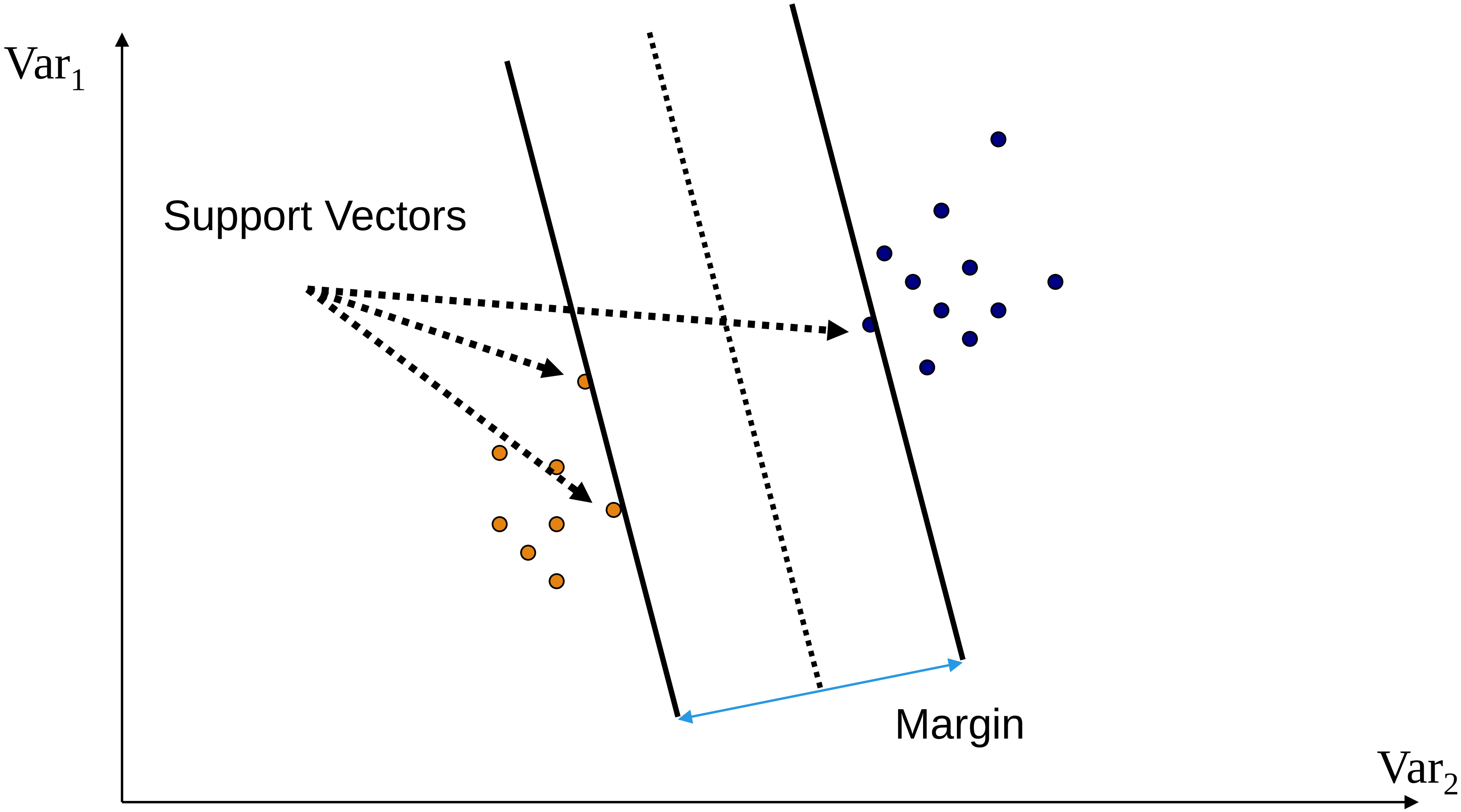
The support vector are $\vec{x}_i$ having not null α_i i.e. such that $y_i(\vec{x}_i \cdot \vec{w} + b) = -1$

They lie on the frontier

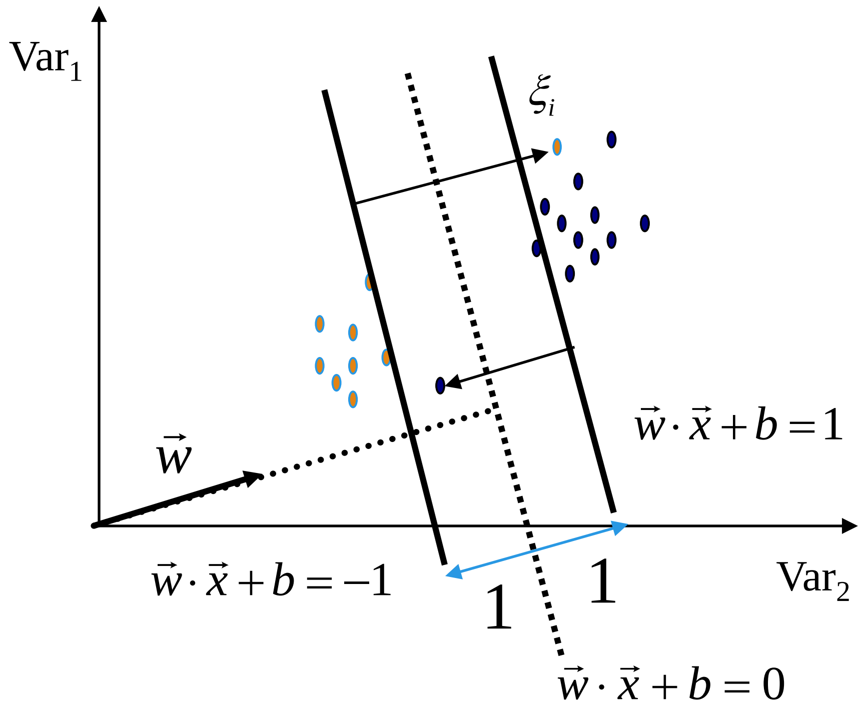
b is derived through the following formula

$$b^* = -\frac{\vec{w}^* \cdot \vec{x}^+ + \vec{w}^* \cdot \vec{x}^-}{2}$$

Support Vectors



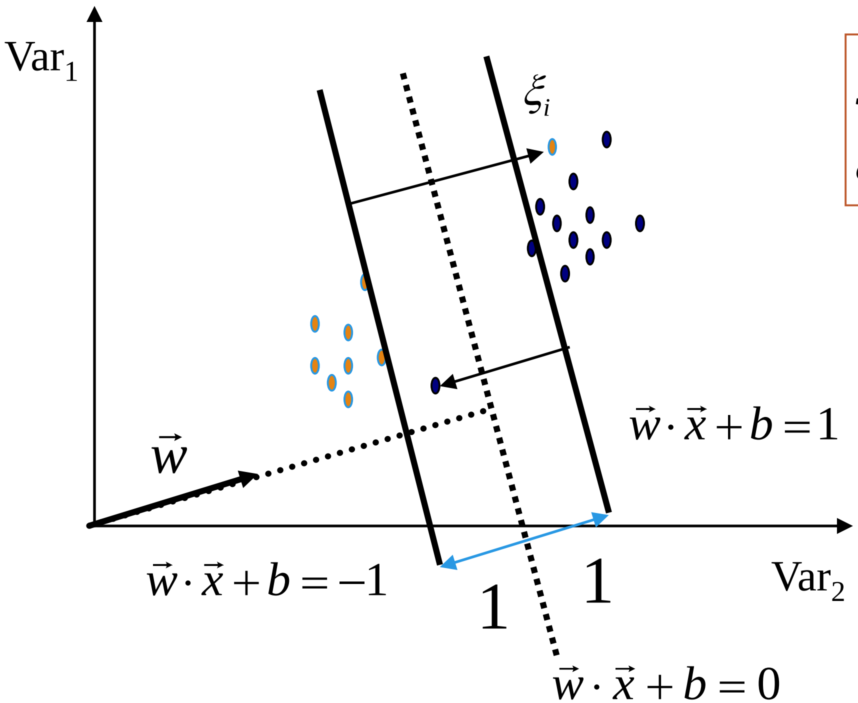
Non linearly separable training data



Slack variables ξ_i are introduced

Mistakes are allowed and the optimization function is penalized

Soft Margin SVMs



New constraints:

$$\boxed{\begin{array}{l} y_i(\vec{w}\cdot\vec{x}_i+b)\geq 1-\xi_i \quad \forall \vec{x}_i \\ \xi_i \geq 0 \end{array}}$$

Objective function:

$$\boxed{\min \frac{1}{2}\|\vec{w}\|^2 + C\sum_i \xi_i}$$

C is the *trade-off* between margin and errors

Converting in the dual form

$$\begin{cases} min \quad ||\vec{w}|| + C\sum_{i=1}^{m} \xi_i^2 \\ y_i(\vec{w} \cdot \vec{x_i} + b) \geq 1 - \xi_i, \quad \forall i = 1, .., m \\ \xi_i \geq 0, \quad i = 1, .., m \end{cases}$$

$$L(\vec{w}, b, \vec{\xi}, \vec{\alpha}) = \frac{1}{2}\vec{w} \cdot \vec{w} + \frac{C}{2}\sum_{i=1}^{m} \xi_i^2 - \sum_{i=1}^{m} \alpha_i [y_i(\vec{w} \cdot \vec{x_i} + b) - 1]$$

deriving wrt $\vec{w}, \vec{\xi}$ and b

Partial derivatives

$$\frac{\partial L(\vec{w}, b, \vec{\xi}, \vec{\alpha})}{\partial \vec{w}} = \vec{w} - \sum_{i=1}^{m} y_i \alpha_i \vec{x}_i = \vec{0} \quad \Rightarrow \quad \vec{w} = \sum_{i=1}^{m} y_i \alpha_i \vec{x}_i$$

$$\frac{\partial L(\vec{w}, b, \vec{\xi}, \vec{\alpha})}{\partial \vec{\xi}} = C\vec{\xi} - \vec{\alpha} = \vec{0}$$

$$\frac{\partial L(\vec{w}, b, \vec{\xi}, \vec{\alpha})}{\partial b} = \sum_{i=1}^{m} y_i \alpha_i = 0$$

Substitution in the objective function

$$= \sum_{i=1}^{m} \alpha_i - \frac{1}{2} \sum_{i,j=1}^{m} y_i y_j \alpha_i \alpha_j \vec{x_i} \cdot \vec{x_j} + \frac{1}{2C} \vec{\alpha} \cdot \vec{\alpha} - \frac{1}{C} \vec{\alpha} \cdot \vec{\alpha} =$$

$$= \sum_{i=1}^{m} \alpha_i - \frac{1}{2} \sum_{i,j=1}^{m} y_i y_j \alpha_i \alpha_j \vec{x_i} \cdot \vec{x_j} - \frac{1}{2C} \vec{\alpha} \cdot \vec{\alpha} =$$

$$= \sum_{i=1}^{m} \alpha_i - \frac{1}{2} \sum_{i,j=1}^{m} y_i y_j \alpha_i \alpha_j \left(\vec{x_i} \cdot \vec{x_j} + \frac{1}{C} \delta_{ij} \right),$$

δ_{ij} of Kronecker

Dual optimization problem
(the final form)

$$\sum_{i=1}^{m} \alpha_i - \frac{1}{2} \sum_{i,j=1}^{m} y_i y_j \alpha_i \alpha_j \left(\vec{x_i} \cdot \vec{x_j} + \frac{1}{C} \delta_{ij} \right)$$

$$\alpha_i \geq 0, \quad \forall i = 1, .., m$$

$$\textstyle\sum_{i=1}^{m} y_i \alpha_i = 0$$

Soft Margin Support Vector Machines

$$\min \frac{1}{2}\|\vec{w}\|^2 + C\sum_i \xi_i \qquad \begin{array}{l} y_i(\vec{w}\cdot\vec{x}_i + b) \geq 1-\xi_i \quad \forall \vec{x}_i \\ \xi_i \geq 0 \end{array}$$

The algorithm tries to keep ξ_i =0 and then maximizes the margin.

The algorithm minimizes the sums of distances from the hyperplane and not the number of errors (as it corresponds to an NP-complete problem)

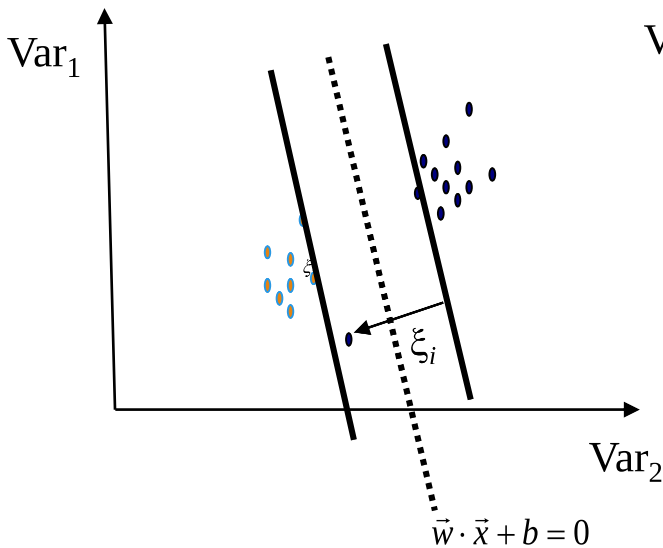
If $C \to \infty$, the solution tends to conform to the hard margin solution

ATT.!!!: if $C = 0$ then $\|\vec{w}\|=0$. Infact it is always possible to satisfy:

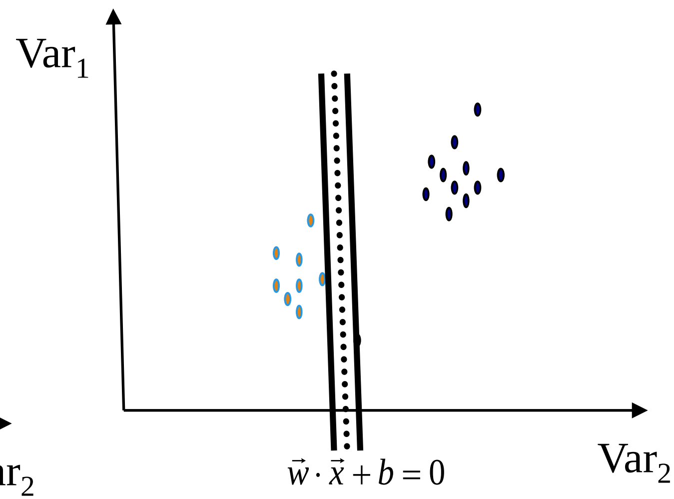
$$y_i b \geq 1-\xi_i \quad \forall \vec{x}_i$$

If *C* grows, it tends to limit the number of tolerated errors. Infinite settings for C provide the number of errors to be 0, exactly as in the *hard-margin* formulation.

Robustness: *Soft* vs *Hard Margin* SVMs



Soft Margin SVM



Hard Margin SVM

Soft vs Hard Margin SVMs

A Soft-Margin SVM has always a solution

A *Soft-Margin* SVM is more robust wrt *odd* training examples

- *Insufficient Representation (e.g. Limited Vocabularies)*
- *High ambiguity of (linguistic) features*

An *Hard-Margin* SVM requires no parameter

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