Métodos de kernel

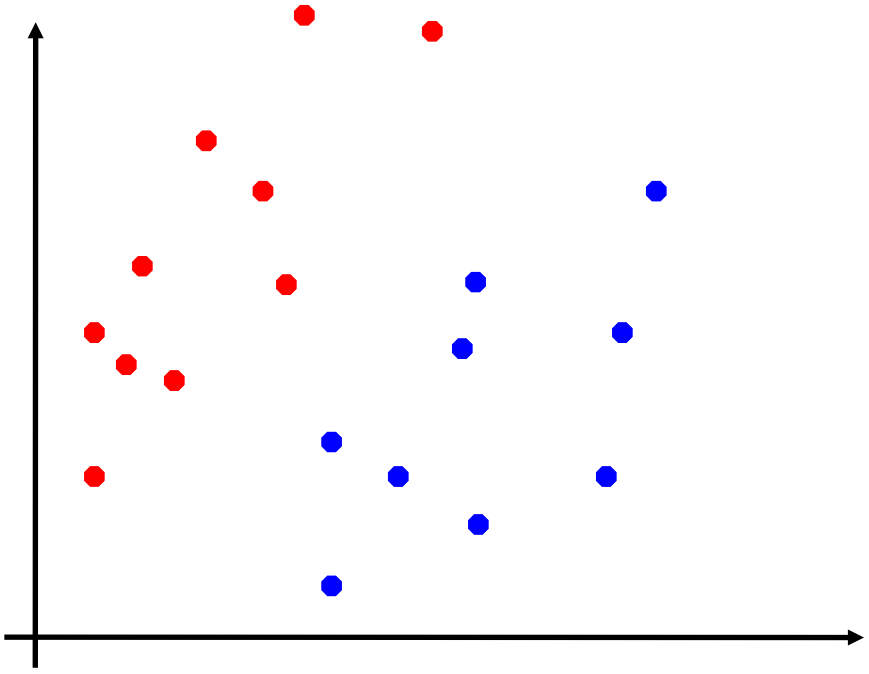
Resumen

- SVM - motivación
- SVM no separable
- Kernels
- Otros problemas
- Ejemplos

Muchas slides de Ronald Collopert

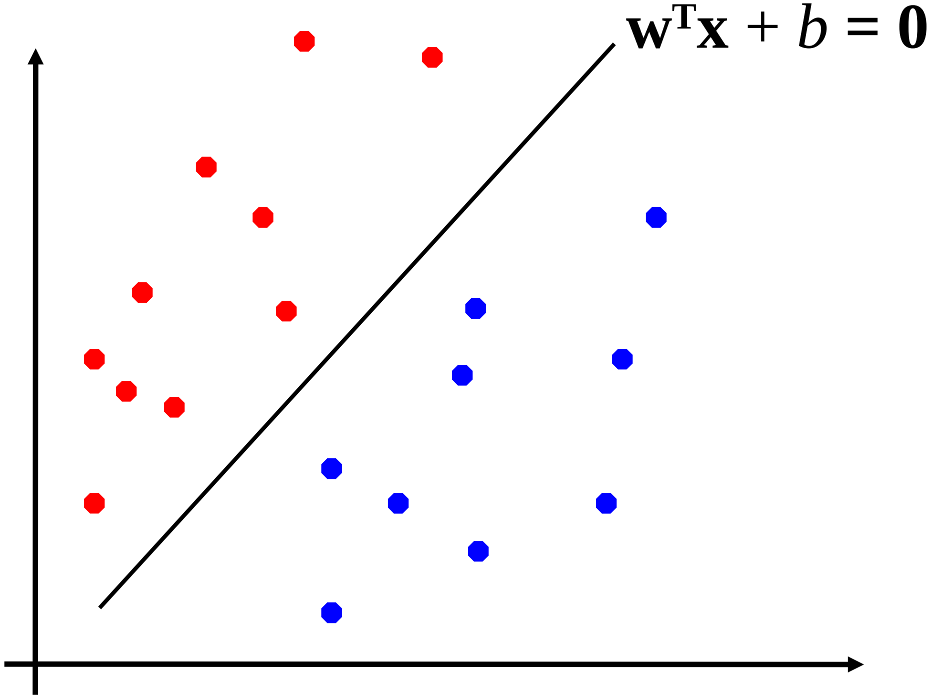
Back to Perceptron

Old method, linear solution



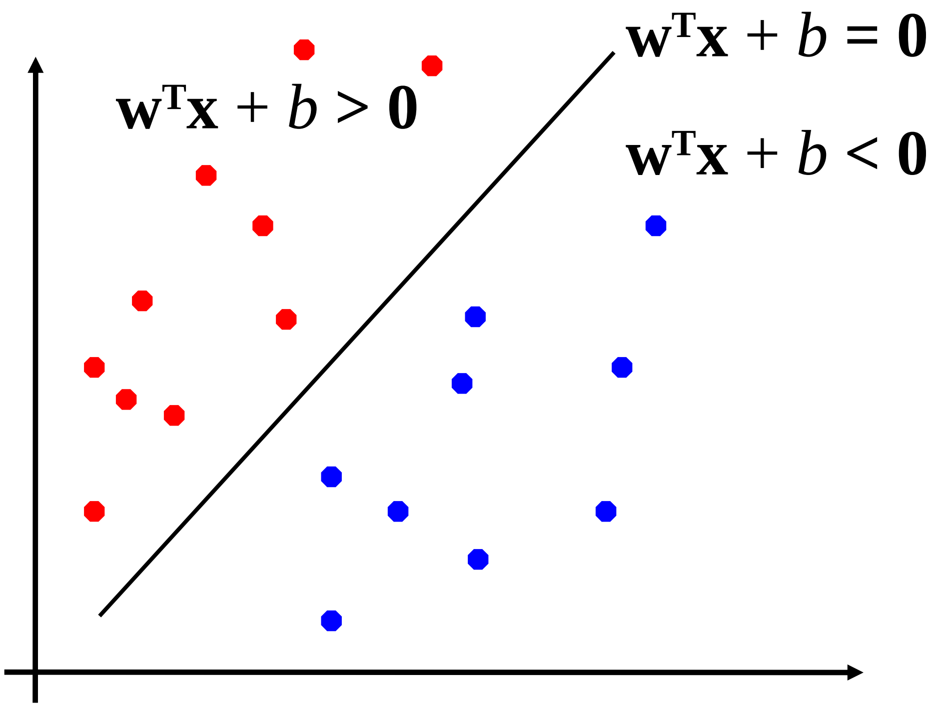
Back to Perceptron

Old method, linear solution



Back to Perceptron

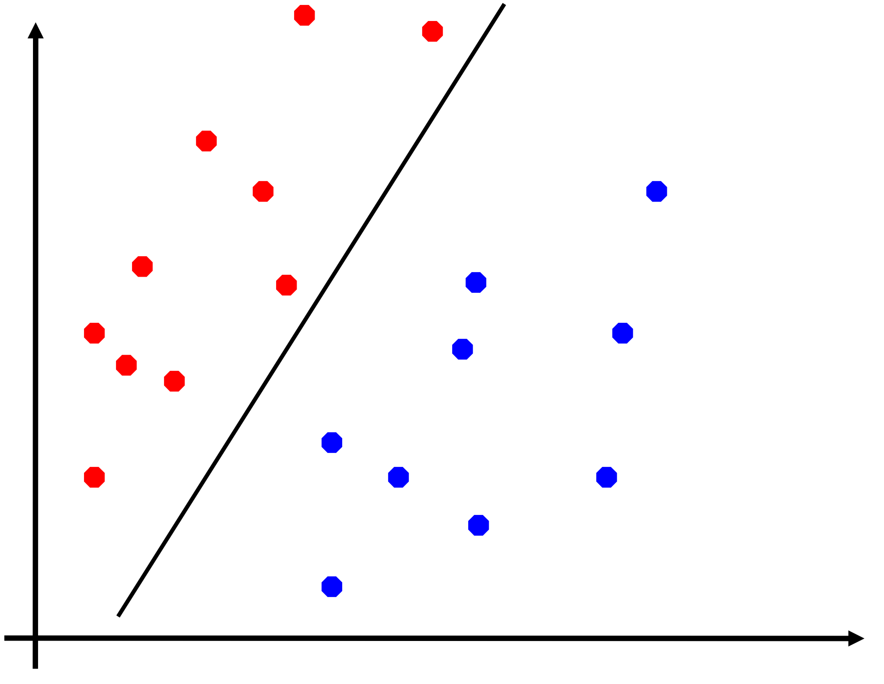
Old method, linear solution



$$f(\mathbf{x}) = \text{sign}(\mathbf{w}^T\mathbf{x} + b)$$

Linear Separators

Which of the linear separators is optimal?



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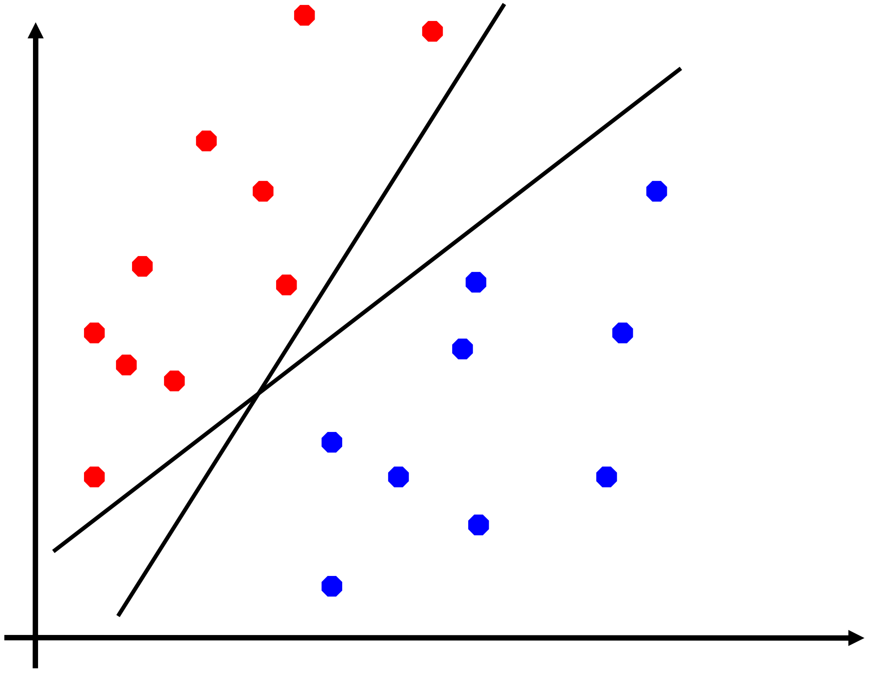
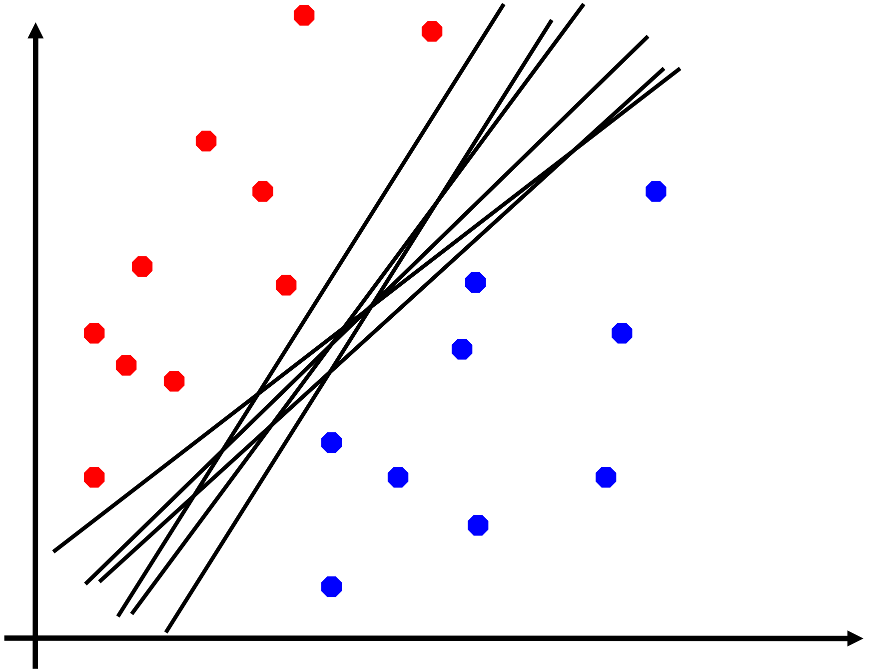


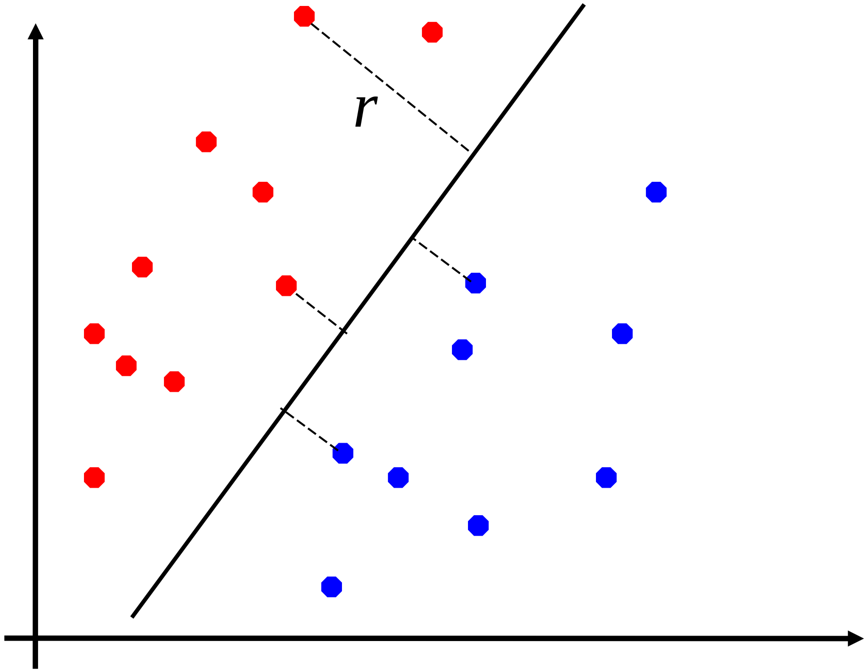
Linear Separators

Which of the linear separators is optimal?



Classification Margin

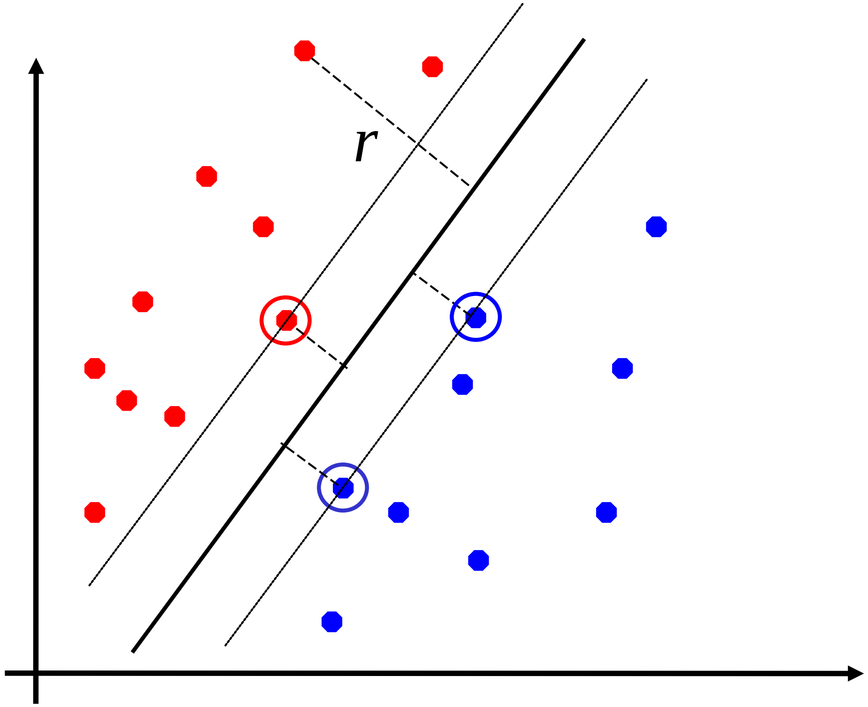
Distance from example $\mathbf{x}_i$ to the separator is $r = \dfrac{w^T x_i + b}{\|w\|}$



Classification Margin

Distance from example $\mathbf{x}_i$ to the separator is $r = \frac{w^T x_i + b}{\|w\|}$

Examples closest to the hyperplane are ***support vectors***.

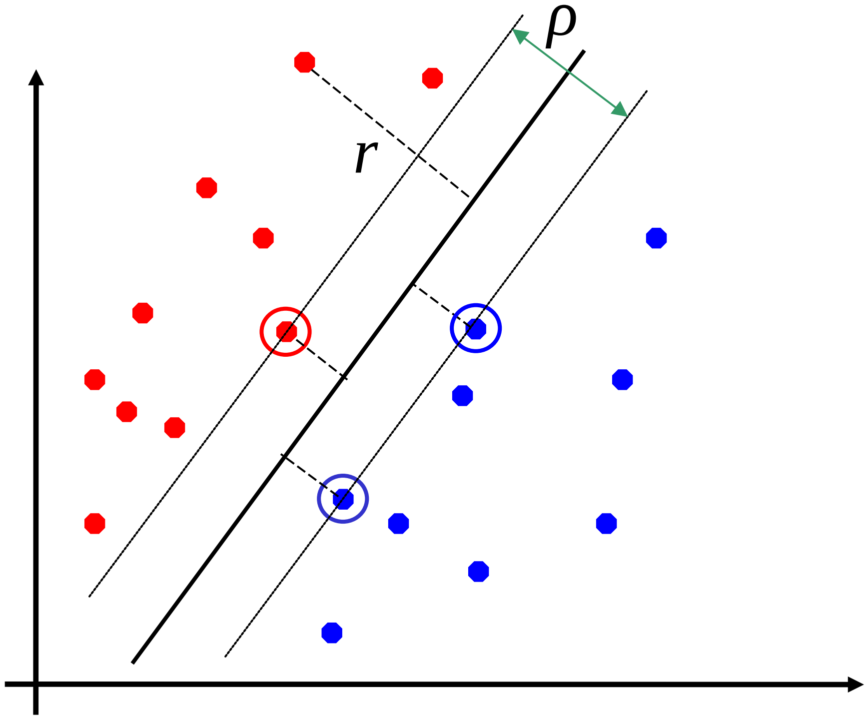


Classification Margin

Distance from example $\mathbf{x}_i$ to the separator is $r = \frac{w^T x_i + b}{\|w\|}$

Examples closest to the hyperplane are ***support vectors***.

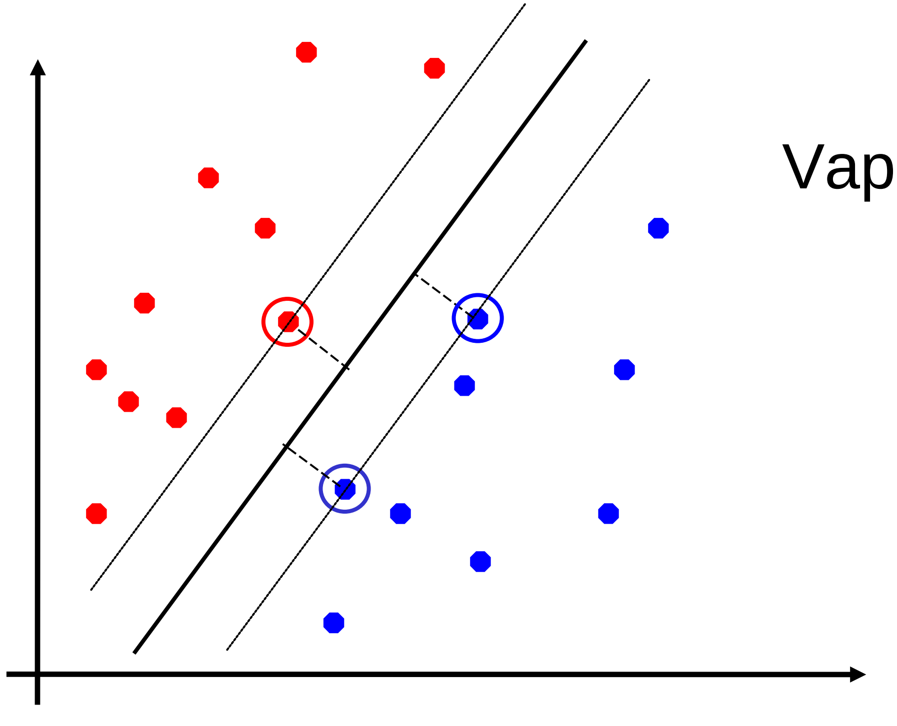
Margin ρ of the separator is the distance between support vectors.



Maximum Margin Classification

Maximizing the margin is good according to intuition and learning theory.

Implies that only support vectors matter; other training examples are ignorable.



Vapnik: Et< Ea + f(VC/m)

SVM formulation

- Training set:

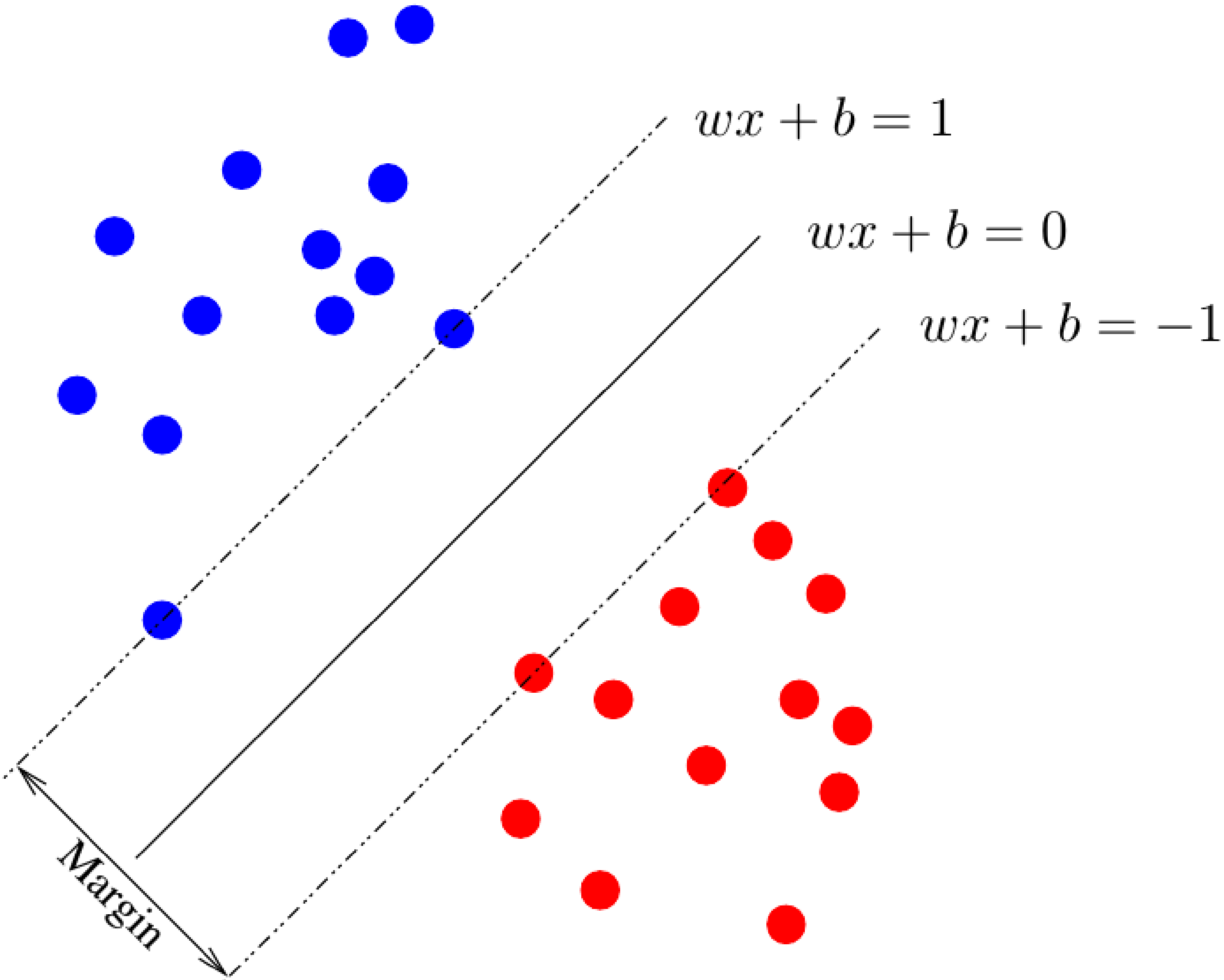
$$(x_t, y_t)_{t=1\dots T} \in \mathbb{R}^d \times \{-1, 1\}$$

- We would like to find *one* hyperplane

$$wx + b = 0 \quad (w \in \mathbb{R}^d,\ b \in \mathbb{R})$$

which separates the two classes and maximizes the margin.

SVM formulation



SVM formulation

- Margin to *maximize*:

$$\mathrm{dist}(wx + b = 1,\ wx + b = -1) = \frac{2}{\|w\|}$$

- We would like to minimize:

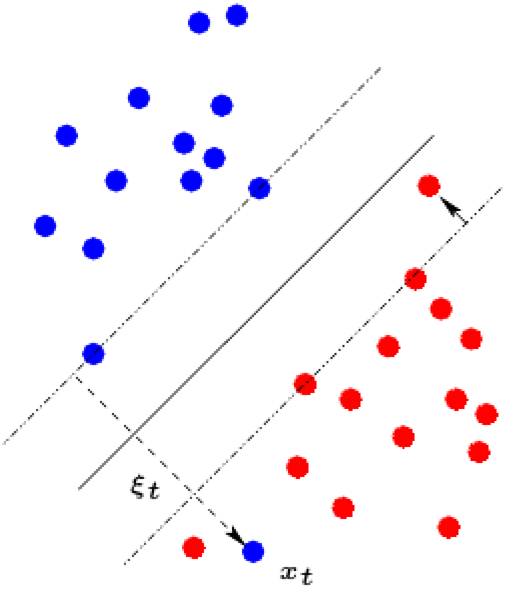
$$J(w,\ b) = \frac{\|w\|^2}{2}$$

Under the constraints:

$$y_t(wx_t + b) \geq 1 \quad \forall t$$

SVM formulation

This minimization problem does not have any solution if the two classes are not separable.



SVM formulation

- Relax the constraints: use a soft margin instead of a hard margin.
- We would like to minimize:

$$J(w, b, \xi) = \frac{\|w\|^2}{2} + C \sum_{t=1}^{T} \xi_t$$

Under the constraints:

$$y_t(wx_t + b) \geq 1 - \xi_t \quad \forall t$$

$$\xi_t \geq 0 \quad \forall t$$

SVM formulation

- We want to find u such that:

$$J(u) = \inf_{v \in U} J(v)$$

$$u \in U = \{v \in \mathbb{R}^n \;:\; \varphi_i(v) \leq 0 \quad \forall i\}$$

- Introduce the Lagrangian:

$$L(v,\, \mu) = J(v) + \sum_i \mu_i \, \varphi_i(v) \qquad (\mu_i \geq 0)$$

SVM formulation

- Theorem: If (u, λ) is a saddle point of the Lagrangian L, then (u, λ) is a solution of the constrained minimization problem.

- (u, λ) is a saddle point of the function L if u is a minimum for the function $v \mapsto L(v, \lambda)$ and λ is a maximum for the function $\mu \mapsto L(u, \mu)$.

SVM formulation

- Our Lagrangian:

$$L(w, b, \xi, \alpha, \mu) = J(w, b, \xi) + \sum_t \alpha_t[1 - \xi_t - y_t(wx_t + b)] - \sum_t \mu_t \xi_t$$

$$= \frac{\|w\|^2}{2} + C\sum_{t=1}^{T} \xi_t + \sum_t \alpha_t[1 - \xi_t - y_t(wx_t + b)] - \sum_t \mu_t \xi_t$$

$$(\alpha_t \geq 0 \quad \text{and} \quad \mu_t \geq 0)$$

- Look for (w, b, ξ) minimum of L:

$$\frac{\partial L}{\partial w} = 0 \quad \Leftrightarrow \quad w = \sum_t \alpha_t y_t \, x_t$$

$$\frac{\partial L}{\partial b} = 0 \quad \Leftrightarrow \quad \sum_t \alpha_t y_t = 0$$

$$\frac{\partial L}{\partial \xi} = 0 \quad \Leftrightarrow \quad C - \alpha_t - \mu_t = 0$$

SVM formulation

- Insert in the Lagrangian:

$$L = \sum_t \alpha_t - \frac{1}{2} \sum_{s,t} \alpha_s \alpha_t y_s y_t \, x_s x_t$$

$$0 \le \alpha_t \le C$$

$$\sum_t \alpha_t y_t = 0$$

$$w = \sum_t \alpha_t y_t \, x_t$$

- Look for $(\alpha, \, \mu)$ maximum of L:

$$\begin{aligned} \alpha_t [1 - \xi_t - y_t (w x_t + b)] &= 0 \\ \mu_t \xi_t &= 0 \end{aligned}$$

SVM formulation

- Finaly, we "just" have to minimize

$$\alpha \mapsto \frac{1}{2}\alpha^{\mathbf{T}} Q \alpha - \alpha^{\mathbf{T}} 1$$

where

$$Q_{ij} = y_i y_j \, x_i x_j$$

Under the constraints

$$0 \le \alpha_t \le C \quad \text{and} \quad \sum_t \alpha_t y_t = 0$$

- Then we obtain w and b with

$$w = \sum_t \alpha_t y_t \, x_t$$

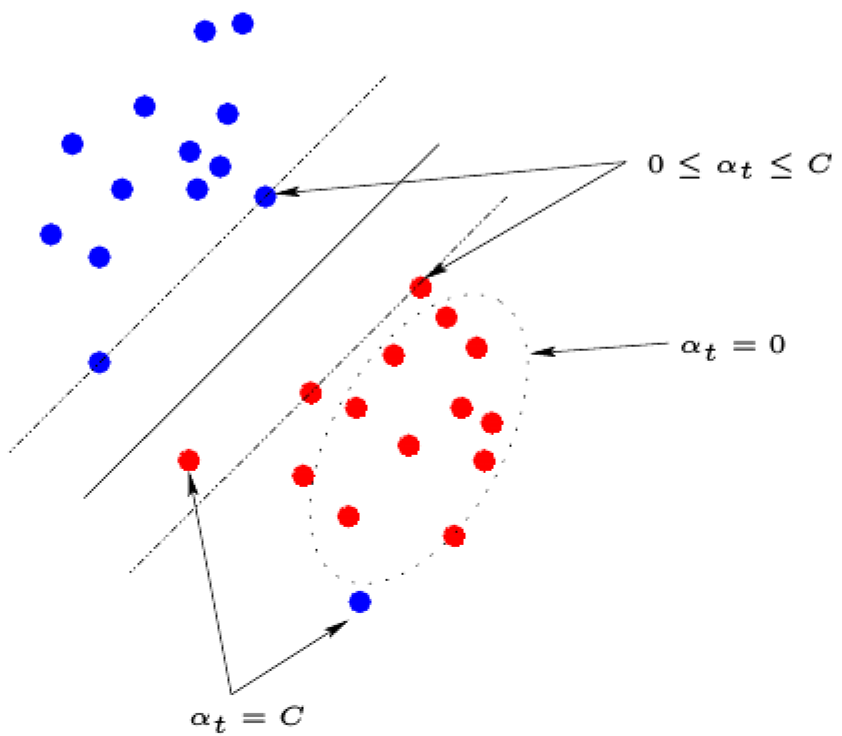
$$\alpha_t [1 - \xi_t - y_t(w x_t + b)] = 0$$

SVM formulation - end

- Note that the decision function could be rewritten as:

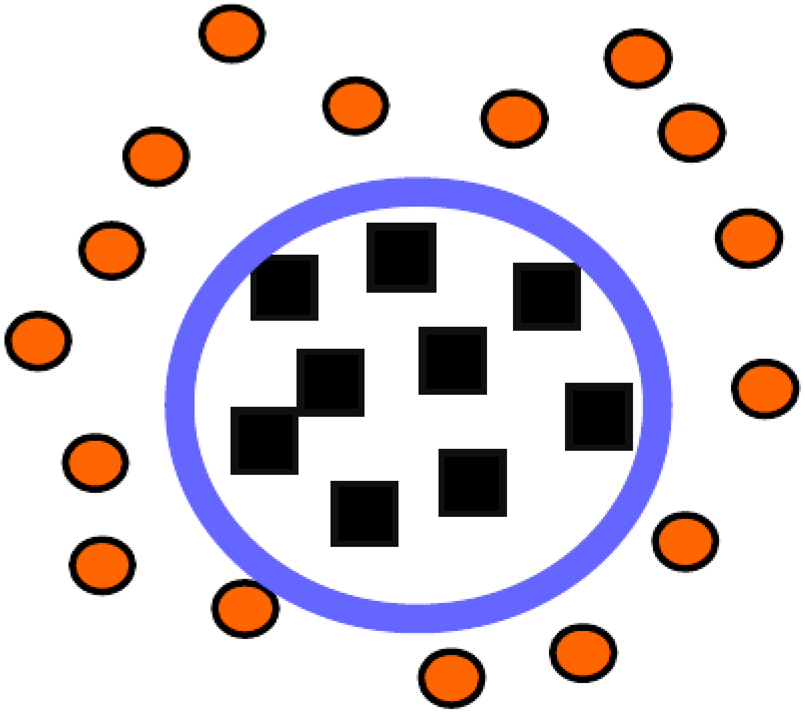
$$x \mapsto \sum_t \alpha_t y_t \, x_t x + b$$

- Training examples x_t with $\alpha_t \neq 0$ are support vectors.



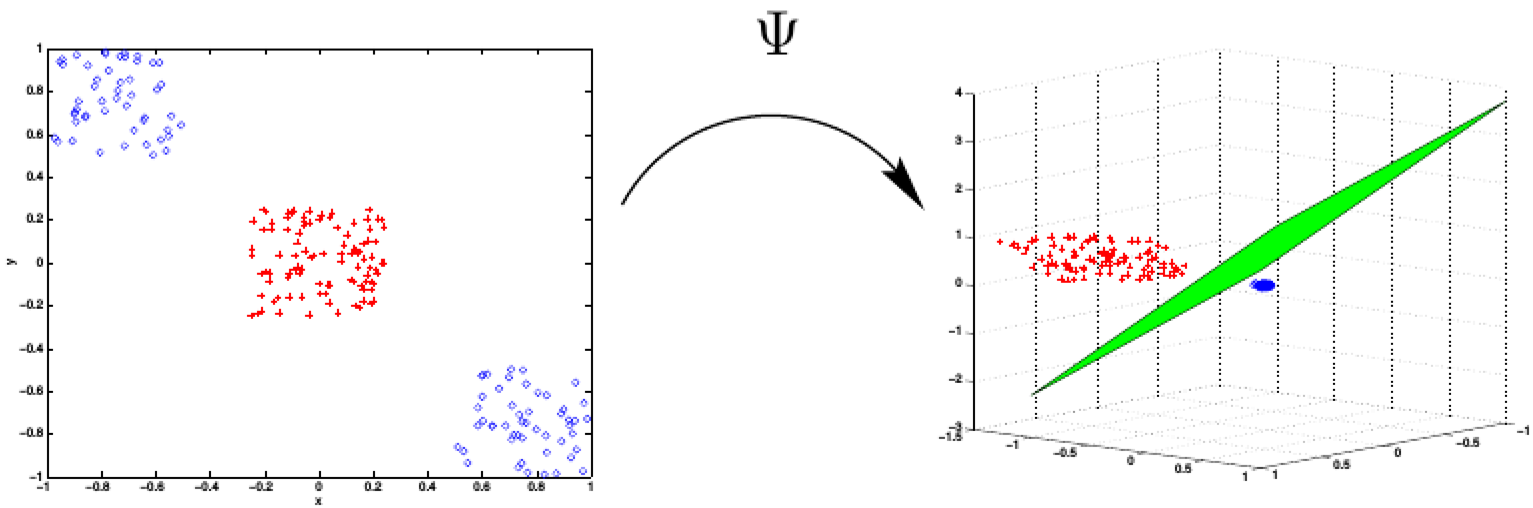
Kernels

What about this problem?



Kernels

- Project the data into a higher dimensional space: it should be easier to separate the two classes.
- Given a function $\Psi : \mathbb{R}^d \rightarrow F$, work with $\Psi(x_t)$ instead of working with x_t.



Kernels

- Note that we have only dot products $\Psi(x_s)\Psi(x_t)$ to compute.
- Unfortunately, it could be expensive in a high dimensional space.
- Use instead a kernel: a function $(x, z) \mapsto k(x, z)$ which represents a dot product in a "hidden" feature space.

$$k(x, z) = \Psi(x)\Psi(z)$$

- Example: instead of

$$\Psi(x) = \begin{pmatrix} x_1^2 \\ \sqrt{2}x_1x_2 \\ x_2^2 \end{pmatrix}$$

use

$$k(x, z) = (xz)^2$$

Kernels

- Polynomial:

$$k(x,\, z) = (u\, xz + v)^p \quad (u \in \mathbb{R},\ v \in \mathbb{R},\ p \in \mathbb{N}_+^*)$$

- Gaussian:

$$k(x,\, z) = \exp\left(-\frac{\|x - z\|^2}{2\sigma^2}\right) \quad (\sigma \in \mathbb{R}_+^*)$$

- ⚠ The function

$$k(x,\, z) = \tanh(u\, xz + v)$$

is not a kernel!

Kernels

- Any symmetric positive-definite kernel f(u,v) is a dot product in some space. Not matter what is the space.
- Kernel algebra → linear combinations of kernels are kernels
- Open door: kernels for non-vectorial objects

Using SVMs

- Choose a kernel $k()$.
- Minimize

$$\alpha \;\mapsto\; \frac{1}{2}\alpha^{\mathbf{T}} Q \alpha - \alpha^{\mathbf{T}} 1$$

where

$$Q_{ij} = y_i y_j \, k(x_i, x_j)$$

Under the constraints

$$0 \;\leq\; \alpha_t \;\leq\; C \quad \text{and} \quad \sum_t \alpha_t y_t = 0$$

- For $0 < \alpha_t < C$, compute b using

$$1 - y_t \left[\sum_s \alpha_s y_s \, k(x_s, x_t) + b \right] \;=\; 0$$

Using SVMs

- The decision function will be

$$x \;\mapsto\; \operatorname{sign}\left(\sum_t \alpha_t y_t \, k(x_t, x) + b\right)$$

Summary

- SVMs maximize the margin (*in the feature space*)
- Use the soft margin trick
- Project the data into a higher dimensional space for non-linear relations
- Kernels simplify the computation
- A Lagrangian method leads to a "nice" quadratic minimization problem under constraints.

In practice

- In order to tune the capacity, the kernel is the most important parameter to choose.
  - Polynomial kernel: increasing the degree will increase the capacity.
  - Gaussian kernel: increasing σ will decrease the capacity.
- Tune C, the trade-off between the margin and the errors.
  - For non-noisy data sets, C usually has not much influence.
  - Carefully choose C for noisy data sets: small values usually give better results.

Otros problemas con kernels

Other methods

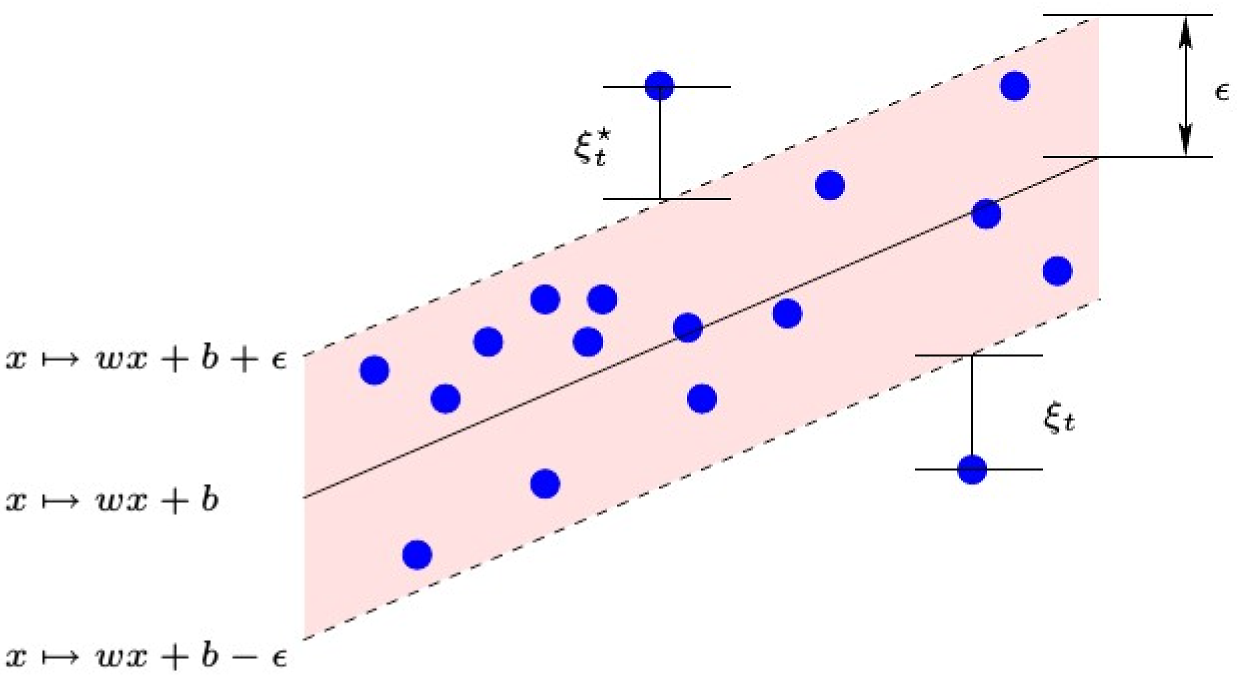
- Any Machine Learning method that only depends on inner products of the data can use kernels
- Lots of methods: kernel-pca, kernel regression, kernel-...

Multiclass classification

- Use ensembles: OVA, OVO. Ovo is more efficient
- There are some direct multiclass SVM formulations, not better than OVO.
- Lots of papers, diverse results

Regression

- We are looking for an hyperplane $x \mapsto wx + b$ such that...



Regression

- We would like to minimize
$$\frac{1}{2}\|w\|^2 + C\sum_t |wx_t + b - y_t|_\epsilon$$
where
$$|u|_\epsilon = \max(0, |u| - \epsilon)$$
- "Epsilon insensitive loss": we "ignore" errors lower than ϵ.
- Equivalent to minimize
$$\frac{1}{2}\|w\|^2 + C\sum_t (\xi_t + \xi_t^\star)$$
under the constraints
$$(wx_t + b) - y_t \leq \epsilon + \xi_t$$
$$y_t - (wx_t + b) \leq \epsilon + \xi_t^\star$$
$$\xi_t,\ \xi_t^\star \geq 0$$

Regression

- Non-linear regression via kernels
- A new parameter to set: the tube

Novelty detection

- Classical: use a density function, points below a threshold are outliers
- Two kernel versions

Novelty detection

- Tax & Duin: Find the minimal hypersphere that contains all the data, points outside are outliers

$$\min_{R,z,a} \quad R^2 + \frac{1}{m\nu}\sum_{i=1}^{m} z_i$$

$$s.t. \quad (x_i - a)^T (x_i - a) \le R^2 + z_i$$

$$z_i \ge 0 \quad i = 1,..,m$$

$$\longrightarrow$$

$$\min_{\alpha} \quad -\sum_{i=1}^{m} \alpha_i K(x_i, x_i) + \sum_{i,j=1}^{m} \alpha_i \alpha_j K(x_i, x_j)$$

$$s.t. \quad \sum_{i=1}^{m} \alpha_i = 1$$

$$\frac{1}{m\nu} \ge \alpha_i \ge 0 \quad i = 1,..,m$$

Outlier: $K(v,v) - 2\sum_{i=1}^{m} \alpha_i K(v, x_i) + \sum_{i,j=1}^{m} \alpha_i \alpha_j K(x_i, x_j) - R^2 \ge 0$

Novelty detection

- Scholkopf et al.: Only for Gaussian Kernel, find the hyperplane with max distance to the origin that left all points in one side.

$$\min_{\alpha} \quad \sum_{i,j=1}^{m} \alpha_i \alpha_j K(x_i, x_j)$$

$$s.t. \quad \sum_{i=1}^{m} \alpha_i = 1$$

$$\frac{1}{m\nu} \geq \alpha_i \geq 0 \quad i = 1,..,m$$

Outlier:

$$f(z) = sign\left(\sum_{j=1}^{m} \alpha_j K(x_j, v) - b \right)$$

Code

- Some examples in classification (R code)