SVM: Máquina de Vectores Soporte

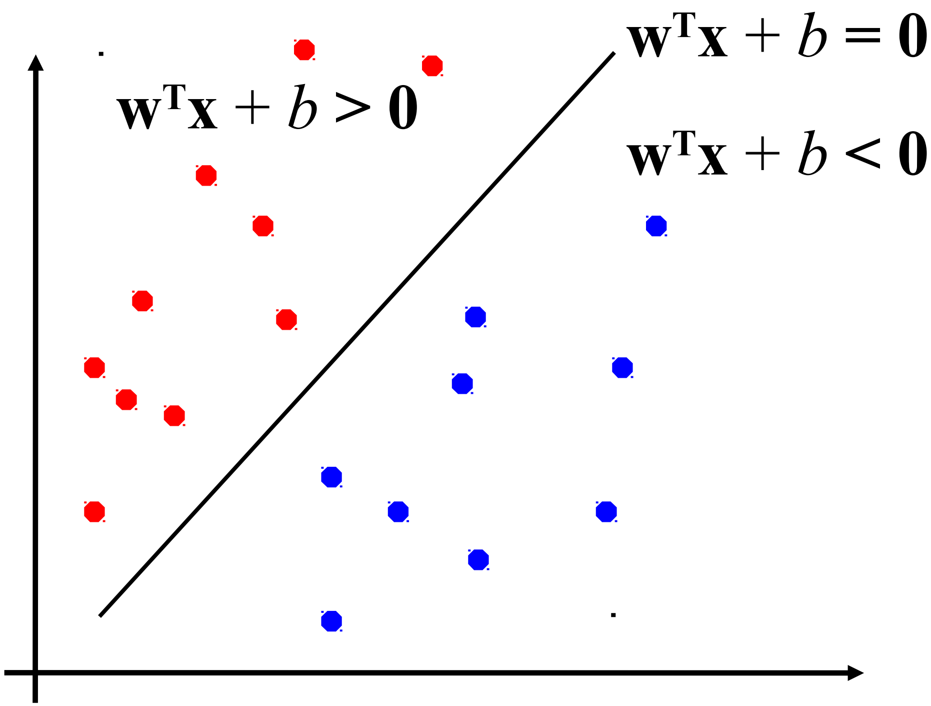
Resumen

- SVM - motivación
- SVM - formulación
- Kernels

Muchas slides de Ronald Collopert

Back to Perceptron

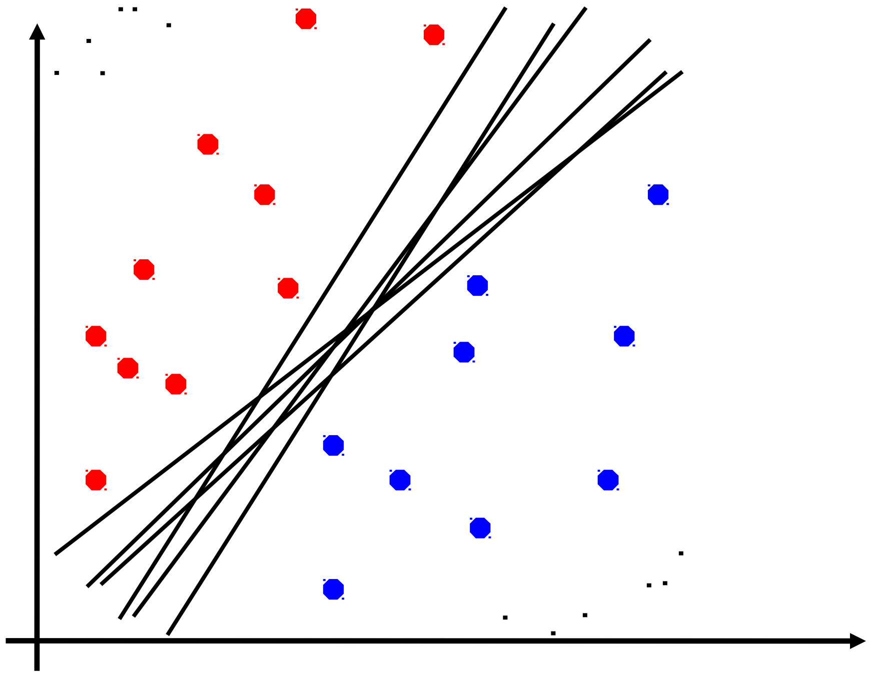
Old method, linear solution



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

Linear Separators

Which of the linear separators is optimal?

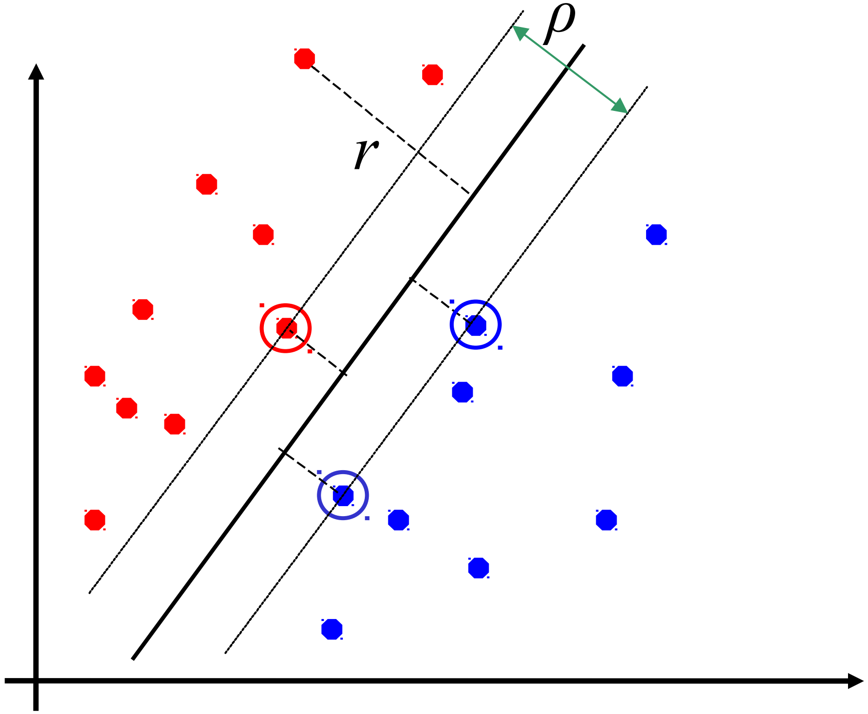


Classification Margin

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***.

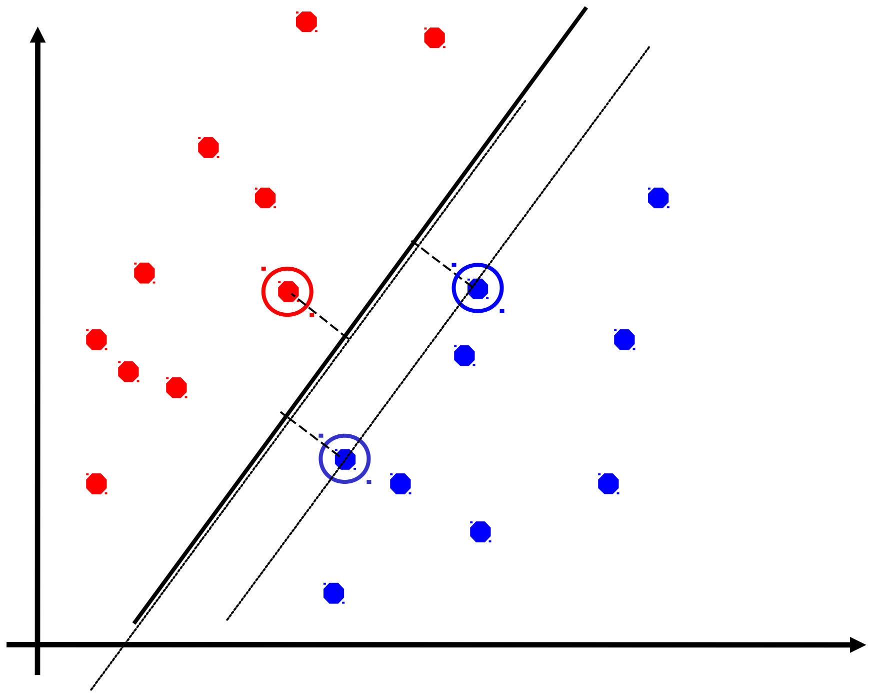
Margin ρ of the separator is the distance between support vectors.



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/ρ)

where f is a monotonically increasing function and VC is a complexity measure

SVM formulation

- Training set:

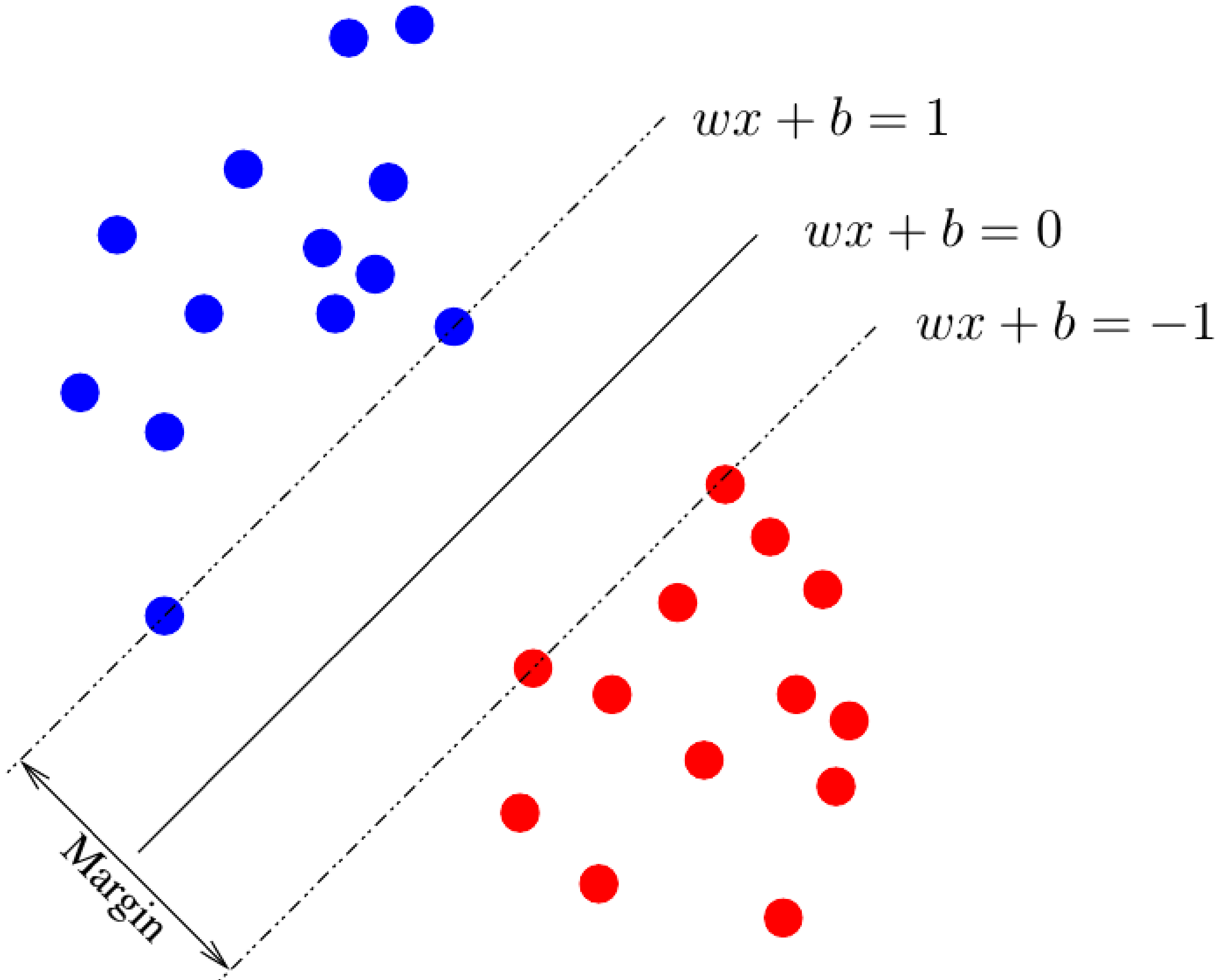
$$(x_t, y_t)_{t=1\ldots T} \in \mathbb{R}^d \times \{-1, 1\}$$

- 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:

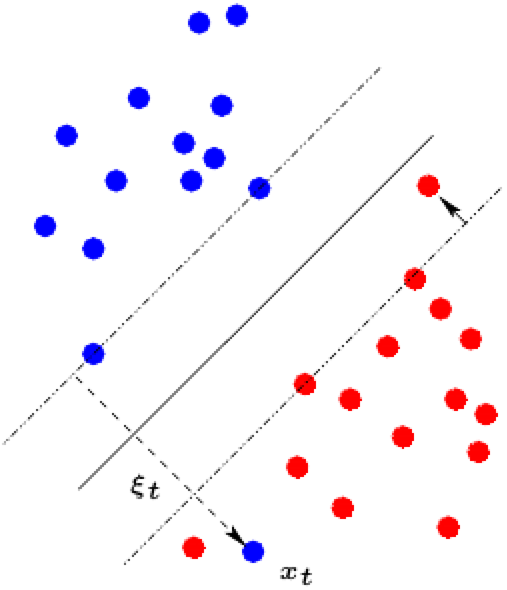
$$J(w,\ b) = \frac{\|w\|^2}{2}$$

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 (α, μ) 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

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

- Then we obtain w and b with

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

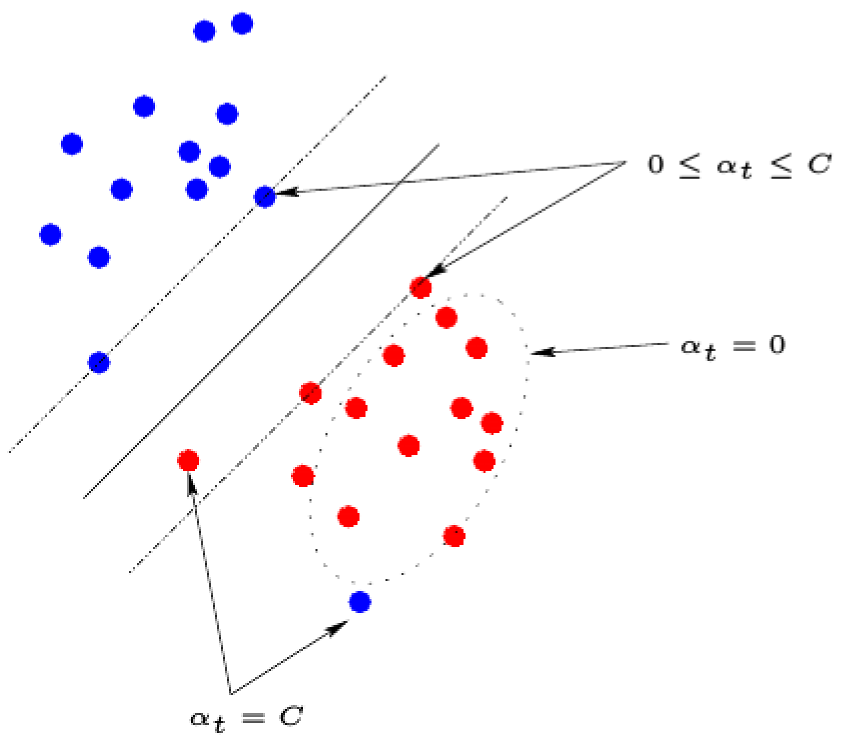
$$\alpha_t [1 - \xi_t - y_t (w x_t + b)] = 0$$

SVM formulation - end

- Note that the decision function could be rewritten as:

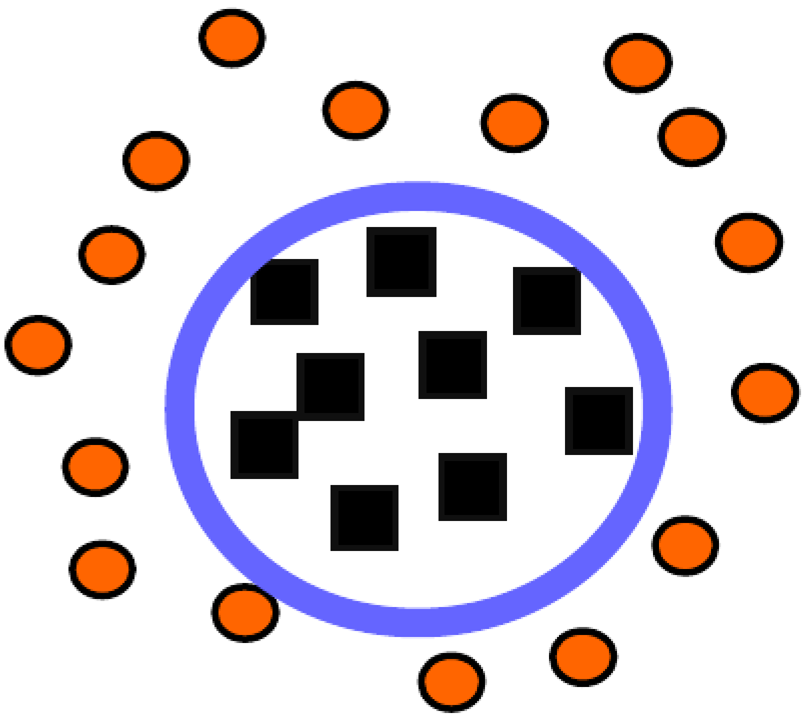
$$x \mapsto \sum_t \alpha_t y_t \, x_t x + b$$

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



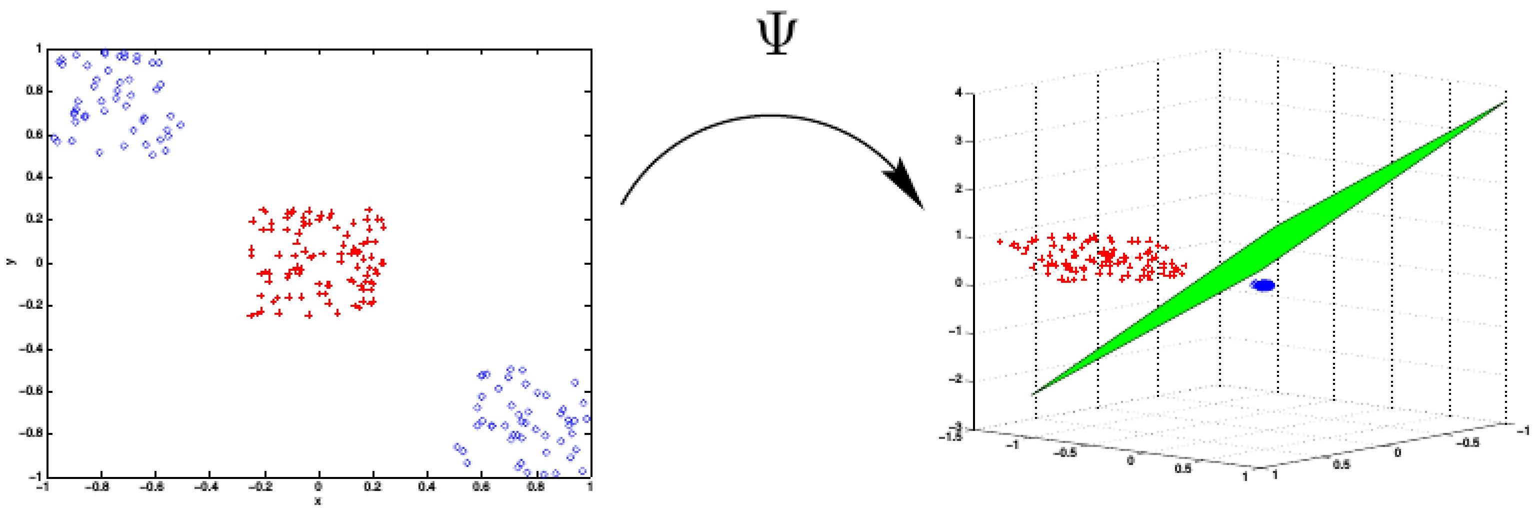
Kernels

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

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

In practice

- Parameter C controls the solution. Must be carefully selected using validation or K-folds
- When using a kernel, the same should be done for its parameters (all combinations!)

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-...

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.