Support Vector Machine (SVM)

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PhD seminar: February 29, 2024

Introduction

SVM in the case of two classes $\{-1, +1\}$: find a function $f : \mathcal{X} \to \mathrm{R}$ which will be used to discriminate classes: $f(x) > 0$ will correspond to class $+1$ and $f(x) < 0$ to class -1.
We train the method on a training set $\{(x_i, y_i)\}_{i=1,..,n}$ where $x_i \in \mathcal{X} = \mathrm{R}^d$ and $y_i \in \{+1, -1\}$.

Summary

1. SVM with rigid margin
   - Theory
   - Programming

2. Generalization of the method
   - SVM with flexible margin
   - Non-linear case

3. Separation into several classes
   - Theory
   - Application

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Linearly separable data

Here we suppose that the data are linearly separable, and only two classes. That means there is a hyperplane H separating our data in two classes.

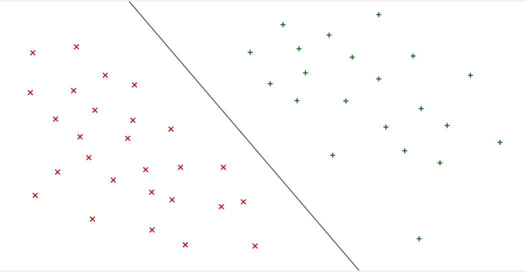

Figure: Two classes and a separator

Primal problem

H has equation $\langle w, x\rangle + b = 0$. The function f is therefore

$$f(x) = \mathrm{sign}(\langle w, x\rangle + b)$$

Question : How to choose w and b? We introduce the Margin such as the distance off the hyperplane H to the closest point :

$$\text{Margin} = \min_{x \in \mathcal{X}} d(x, H)$$

Our goal will be to maximize the margin. We first note that only few points of $\mathcal{X}$ have importance for the calculus of the margin ($= \min_{x \in \mathcal{X}} d(x, H)$) : we call them **support vector**.

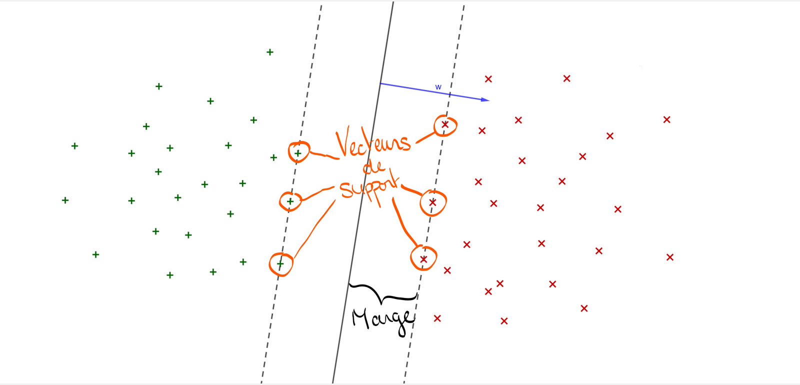

Figure: Support vector

We denote those support vectors by x_s, the margin is now given by:

$$\text{Margin} = d(x_s, H) = \frac{|\langle w, x_s \rangle + b|}{\|w\|}$$

where the chosen norm is the Euclidean norm on $\mathbb{R}^d$.
Note: w and b are not unique, since kw and kb are also solutions for any real k. To ensure uniqueness, we also impose the normalization condition: $|\langle w, x_s \rangle + b| = 1$ for support vectors x_s.
Finally,

$$\text{Margin} = \frac{1}{\|w\|}.$$

This brings us back to the mathematical problem of maximization of the margin. But we prefer write this problem as a minimization problem as follow :

$$\begin{cases} \min\limits_{w \in \mathrm{R}^d, b \in \mathrm{R}} \frac{1}{2} \|w\|^2 \\ y_i(\langle w, x_i \rangle + b) \geq 1, i = 1, ..., n \end{cases} \qquad \text{(Pb primal)}$$

Lagrangian

We introduce the Lagrangian of this minimization problem

$$\begin{array}{ccccc} \mathcal{L} & : & \mathrm{R}^d \times \mathrm{R} \times \mathrm{R}_+^n & \to & \mathrm{R} \\ & & (w, b, \alpha) & \mapsto & \frac{1}{2}\|w\|^2 - \sum_{i=1}^{n} \alpha_i [y_i(\langle w, x_i \rangle + b) - 1] \end{array}$$

Saddle point of the Lagrangian

A saddle point of this Lagrangian is $(w^*, b^*, \alpha^*) \in \mathrm{R}^d \times \mathrm{R} \times \mathrm{R}_+^n$ such as for all (w, b, α), we have
$\mathcal{L}(w^*, b^*, \alpha) \leq \mathcal{L}(w^*, b^*, \alpha^*) \leq \mathcal{L}(w, b, \alpha^*)$.

Thanks to Kuhn-Tucker theorem, we need to find a saddle point of the Lagrangian, and this point satisfies the primal problem. So first we need to minimize $\mathcal{L}$ over (w, b) :

$$\begin{cases} \nabla_w \mathcal{L}(w^*, b^*, \alpha^*) & = & 0 \\ \dfrac{\partial \mathcal{L}}{\partial b}(w^*, b^*, \alpha^*) & = & 0. \end{cases}$$

which leads to :

$$\begin{cases} \displaystyle\sum_{k=1}^{n} \alpha_k^* y_k x_k & = & w^* \\ \displaystyle\sum_{k=1}^{n} \alpha_k^* y_k & = & 0. \end{cases} \tag{1}$$

Re-injecting these expressions into the formula of the Lagrangian, for $\mathcal{L}(w, b, \alpha)$, we thus define the function $\theta(\alpha) = \mathcal{L}(w^*, b^*, \alpha)$:

$$\theta(\alpha) = \sum_{k=1}^{n} \alpha_k - \frac{1}{2} \sum_{i,j=1}^{n} \alpha_i \alpha_j y_i y_j \langle x_i, x_j \rangle.$$

We now have to maximize this function, so the problem is now write :

$$\begin{cases} \max\limits_{\alpha \in \mathrm{R}^n} \theta(\alpha) \\ \sum\limits_{k=1}^{n} \alpha_k y_k = 0 \\ \alpha_k \geq 0 \text{ for all } 1 \leq k \leq n. \end{cases}$$

To recover w^* with the formula $\sum_{k=1}^{n} \alpha_k^* y_k x_k = w^*$, so we need to have α^*. To find α^*, we solve the minimization problem :

$$\begin{cases} \min\limits_{\alpha \in \mathrm{R}^n} -\theta(\alpha) = \min\limits_{\alpha \in \mathrm{R}^n} \left(-\sum_{k=1}^{n} \alpha_k + \frac{1}{2} \sum_{i,j=1}^{n} \alpha_i \alpha_j y_i y_j \langle x_i, x_j \rangle \right) \\ \sum_{k=1}^{n} \alpha_k y_k = 0 \\ \alpha_k \geq 0 \text{ for all } 1 \leq k \leq n. \end{cases} \tag{Pb dual}$$

And we find b^* with : $y_s(\langle w^*, x_s \rangle + b^*) = 1$. To be sure we have a support vector, we have to chose x_s such as α_s be maximal.

We have to resolve this optimization problem. It is a minimization problem with constraints

$$\begin{cases} \min\limits_{w \in \mathrm{R}^d, b \in \mathrm{R}} \frac{1}{2} \|w\|^2 \\ y_i(\langle w, x_i \rangle + b) \geq 1, i = 1, ..., n \end{cases} \qquad \text{(Pb primal)}$$

We use the penalisation method. We introduce $\epsilon > 0$ and call the penalized function $\tilde{J}$ as follow :

$$\tilde{J}(w, b) = \frac{1}{2} \|w\|^2 + \frac{1}{\epsilon} \frac{1}{n} \|c(w, b)_+\|_1 \qquad (2)$$

where $c_i(w, b)_+ = \max(1 - y_i(\langle w, x_i \rangle + b) \; ; \; 0)$

$$\begin{cases} \min\limits_{\alpha \in \mathbb{R}^n} \langle \alpha, \frac{1}{2} G\alpha - U \rangle \\ \sum\limits_{k=1}^{n} \alpha_k y_k = 0 \\ \alpha_k \geq 0 \text{ for all } 1 \leq k \leq n. \end{cases}, \qquad \text{(Pb dual)}$$

where $G = (\langle x_i y_i, x_j y_j \rangle)_{i,j}$ and $U = (1, ..., 1)^T$. We will use an optimal (or constant) step gradient algorithm for the quadratic function $\alpha \mapsto \langle \alpha, \frac{1}{2} G\alpha - U \rangle$, coupled with a projection onto $\mathbb{R}^n_+$ and $\text{Vect}(y)^\perp$ to take constraints into account.

Warning : The matrix G is not necessarily positive definite and therefore our function is not necessarily convex!

Convexification

Tikhonov's regularization method : We introduce $\nu > 0$ and define the function F :

$$F(\alpha) = \langle \alpha, \frac{1}{2}(G + \nu I_n)\alpha - U \rangle$$

We therefore have :

$$\nabla F(\alpha) = (G + \nu I_n)\alpha - U$$

We choose ν so that $G + \nu I_n$ is symmetrical positive definite.

Method : Gradient algorithm on the quadratic function F coupled with a projection on $\mathrm{Vect}(y)^{\perp}$ and on R_{+}^{n}.
If we denote ρ^k the descent step, the method at iteration k is written :

$$\alpha^{k+1} = \alpha^k - \rho^k \nabla F(\alpha^k)$$

Then for projection:
$\lambda^k := \alpha^k - \langle \alpha^k, \frac{y}{\|y\|} \rangle \frac{y}{\|y\|}$
$\alpha_i^k = \max(0, \lambda_i^k)$

Choice of ρ^k :

- fixed-step gradient method $\rho^k = \rho$ fixed.
- optimal step gradient method.

Property

Let $Q(x) = \frac{1}{2}\langle Ax, x\rangle - \langle b, x\rangle$ be a quadratic function where $A \in \mathcal{S}n^{++}(\mathrm{R})$ and $b \in \mathrm{R}^n$, then the optimal step at iteration k, denoted ρ_o^k is given by

$$\rho_o^k = \frac{\|Ax_k - b\|^2}{\langle A(Ax_k - b), Ax_k - b\rangle} \tag{3}$$

For our quadratic function, we have the optimal step given by :

$$\rho^k = \frac{\|d^k\|^2}{\langle d^k, (G + \nu I_n)d^k\rangle}$$

where $d^k = (G + \nu I_n)\alpha^k - U$

Model comparison

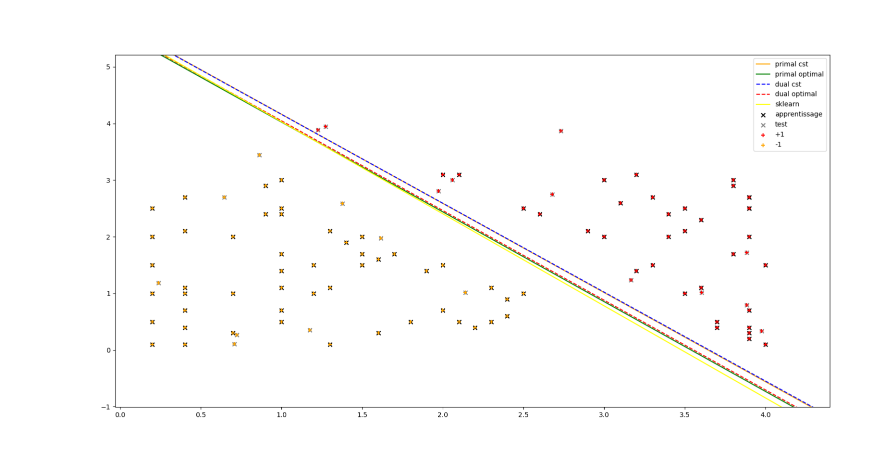

Figure: Different results compare with sklearn: optimal step are the best.

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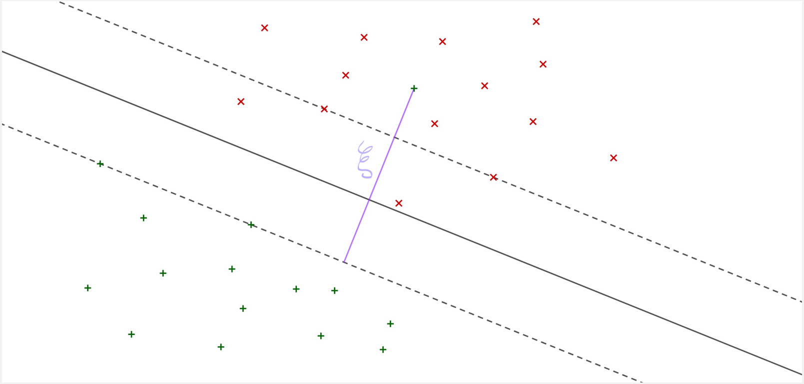
Data cannot be strictly separated

We add constraint release variables $\xi_i = \max(0, 1 - y_i(\langle w, x_i \rangle + b))$ for each constraint, called the hinge loss.



Optimization problem

Our primal problem become:

$$\begin{cases} \min\limits_{w \in \mathbb{R}^d, b \in \mathbb{R}} \frac{1}{2} \|w\|^2 + C \sum\limits_i \xi_i \\ y_i(\langle w, x_i \rangle + b) \geq 1 - \xi_i, \ i = 1, ..., n \\ \xi_i \geq 0, \ i = 1, ..., n \end{cases} \tag{4}$$

(where $C > 0$ is a balancing variable)

No-linear case

In many cases we can't find a linear separator. But SVM can deal with that with the kernel tricks.

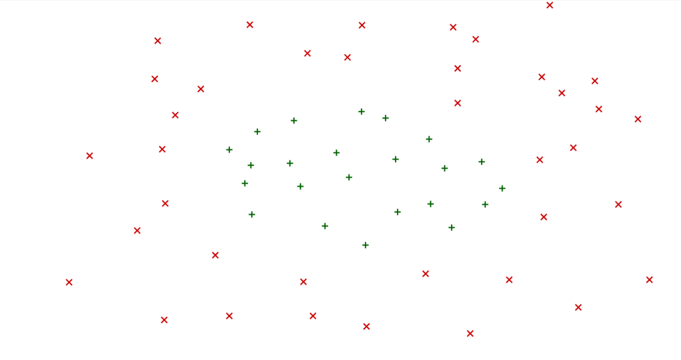


Figure: No linear separation

Principle: We solve the SVM problem in a feature space $\mathcal{H}$ where data are linearly separable. $\mathcal{H}$ is an Hilbert space with the scalar product $\langle . \, , . \rangle_{\mathcal{H}}$. We introduce the representative function $\phi : \mathcal{X} \to \mathcal{H}$. We have to solve the following dual problem

$$\begin{cases} \min_{\alpha \in \mathrm{R}^n} \left(-\sum_{k=1}^{n} \alpha_k + \frac{1}{2} \sum_{i,j=1}^{n} \alpha_i \alpha_j y_i y_j \langle \phi(x_i), \phi(x_j) \rangle_{\mathcal{H}} \right) \\ \sum_{k=1}^{n} \alpha_k y_k = 0 \\ \alpha_k \geq 0 \text{ for all } 1 \leq k \leq n. \end{cases} \qquad \text{(Pb dual)}$$

Kernel Trick

Warning ! The scalar product $\langle \phi(x_i), \phi(x_j) \rangle_{\mathcal{H}}$ can be time-consuming, both computationally and memory-intensive to evaluate.

We call the **kernel function** $k : \mathcal{X} \times \mathcal{X} \to \mathrm{R}$ such that there exists a representation function ϕ and a representation space $\mathcal{H}$ such that $k(x, x') = \langle \phi(x), \phi(x') \rangle_{\mathcal{H}}\ \forall (x, x') \in \mathcal{X}$.

Kernel trick

So the dual problem become :

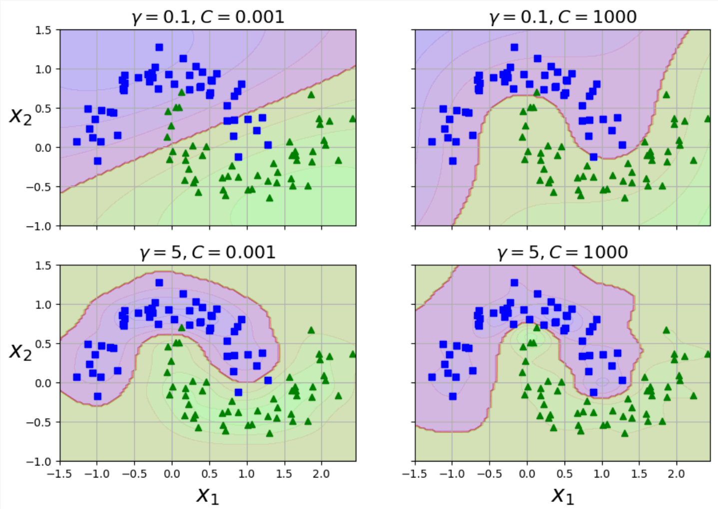
$$\begin{cases} \min_{\alpha \in R^n} \left(- \sum_{k=1}^{n} \alpha_k + \frac{1}{2} \sum_{i,j=1}^{n} \alpha_i \alpha_j y_i y_j k(x_i, x_j) \right) \\ \sum_{k=1}^{n} \alpha_k y_k = 0 \\ \alpha_k \geq 0 \text{ for all } 1 \leq k \leq n. \end{cases} \qquad \text{(Pb dual)}$$

Example of classic kernel :

1. Polynomial kernel : $k(x, x') = (\langle x, x' \rangle + c)^p$.
2. Radial basis function (RBF) : $k(x, x') = \exp \frac{\|x - x'\|^2}{2\sigma^2}$.

Example of RBF kernel

With the kernel $k(x, x') = \exp(\gamma \|x - x'\|^2)$ and flexible margin :



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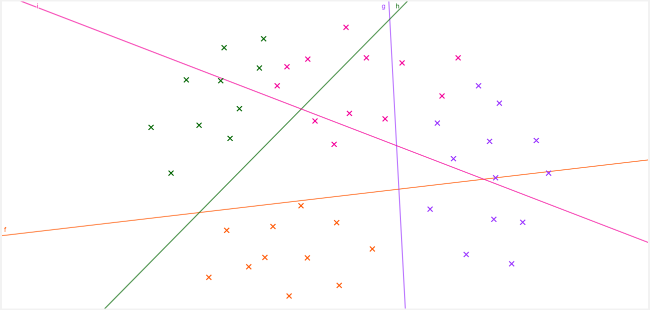
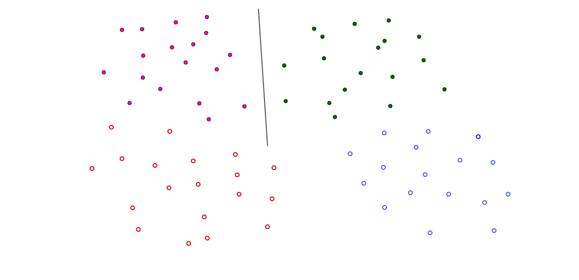
OVR (One Versus Rest)

This involves creating a function for each k classes, which separates the elements of that class from all other elements. We call g_k the function linked to the following class k : $g_k(x) = \langle w_k, x \rangle + b_k$. The class of a point will be given by $\tilde{k} = \arg\min_k g_k(x)$.



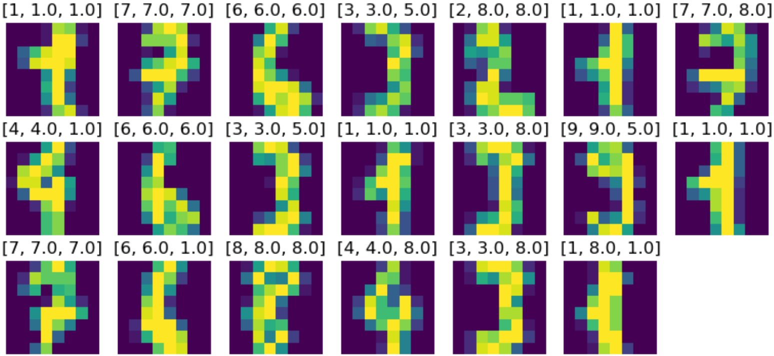
OVO (One Versus One)

This involves creating a classifying function for each class, separates it from every other class. In this way, the classes are tested two by two. If we have n classes, we will build $n(n-1)/2$ classifying functions. We then make a majority vote.



Handwriting recognition

Her we take 80 learning data and 20 test data :



legend : [reference,OVR,OVO]

Proportion OVO

For 20 test data

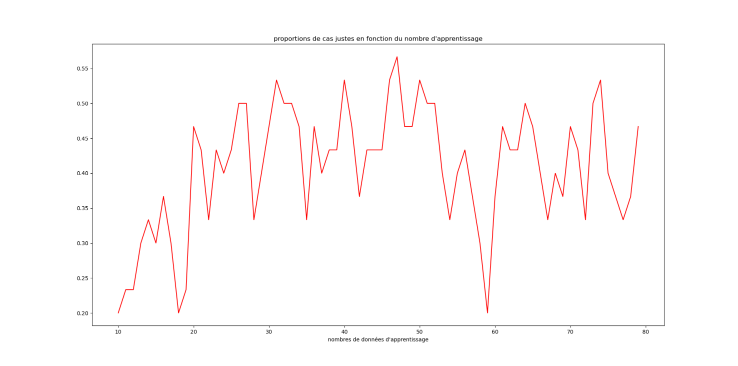
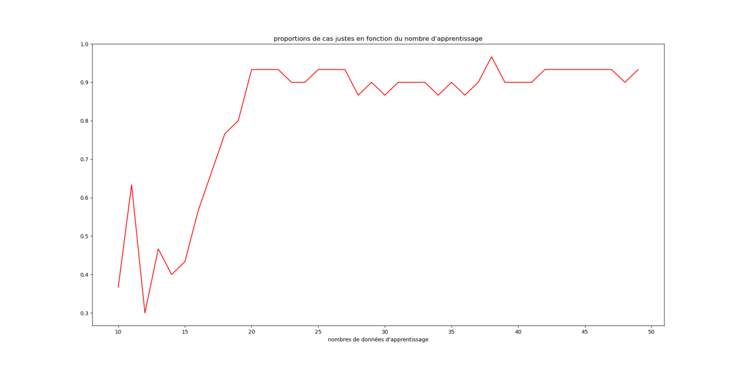


Figure: Percentage of correct estimation by number of learning data

Proportion OVR

For 20 test data



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Conclusion

The SVM method can be used to find the class of an object, provided we have enough training data and find the right kernel to use.

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Thanks for your attention